



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2018 – 10:46 PM EST

PDB ID : 3IKM
Title : Crystal structure of human mitochondrial DNA polymerase holoenzyme
Authors : Lee, Y.-S.; Kennedy, W.D.; Yin, Y.W.
Deposited on : 2009-08-06
Resolution : 3.24 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

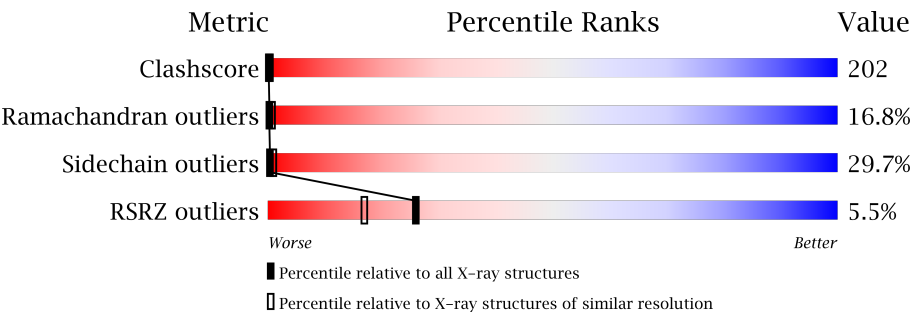
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 112137 | 1383 (3.28-3.20) |
| Ramachandran outliers | 110173 | 1358 (3.28-3.20) |
| Sidechain outliers | 110143 | 1357 (3.28-3.20) |
| RSRZ outliers | 101464 | 1252 (3.28-3.20) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 1172 | <div><div>5%</div><div>5%45%34%9%7%</div></div> |
| 1 | D | 1172 | <div><div>4%</div><div>5%43%34%11%7%</div></div> |
| 2 | B | 427 | <div><div>7%</div><div>11%50%17%5%17%</div></div> |
| 2 | C | 427 | <div><div>4%</div><div>6%54%25%8%7%</div></div> |
| 2 | E | 427 | <div><div>7%</div><div>6%55%19%.17%</div></div> |
| 2 | F | 427 | <div><div>5%</div><div>5%54%25%8%7%</div></div> |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29480 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 polymerase subunit gamma-1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 1093 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8681 | 5505 | 1537 | 1589 | 50 | | | |
| 1 | D | 1094 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8695 | 5515 | 1540 | 1590 | 50 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 354 | ASN | - | SEE REMARK 999 | UNP P54098 |
| A | 355 | SER | - | SEE REMARK 999 | UNP P54098 |
| D | 354 | ASN | - | SEE REMARK 999 | UNP P54098 |
| D | 354A | SER | - | SEE REMARK 999 | UNP P54098 |

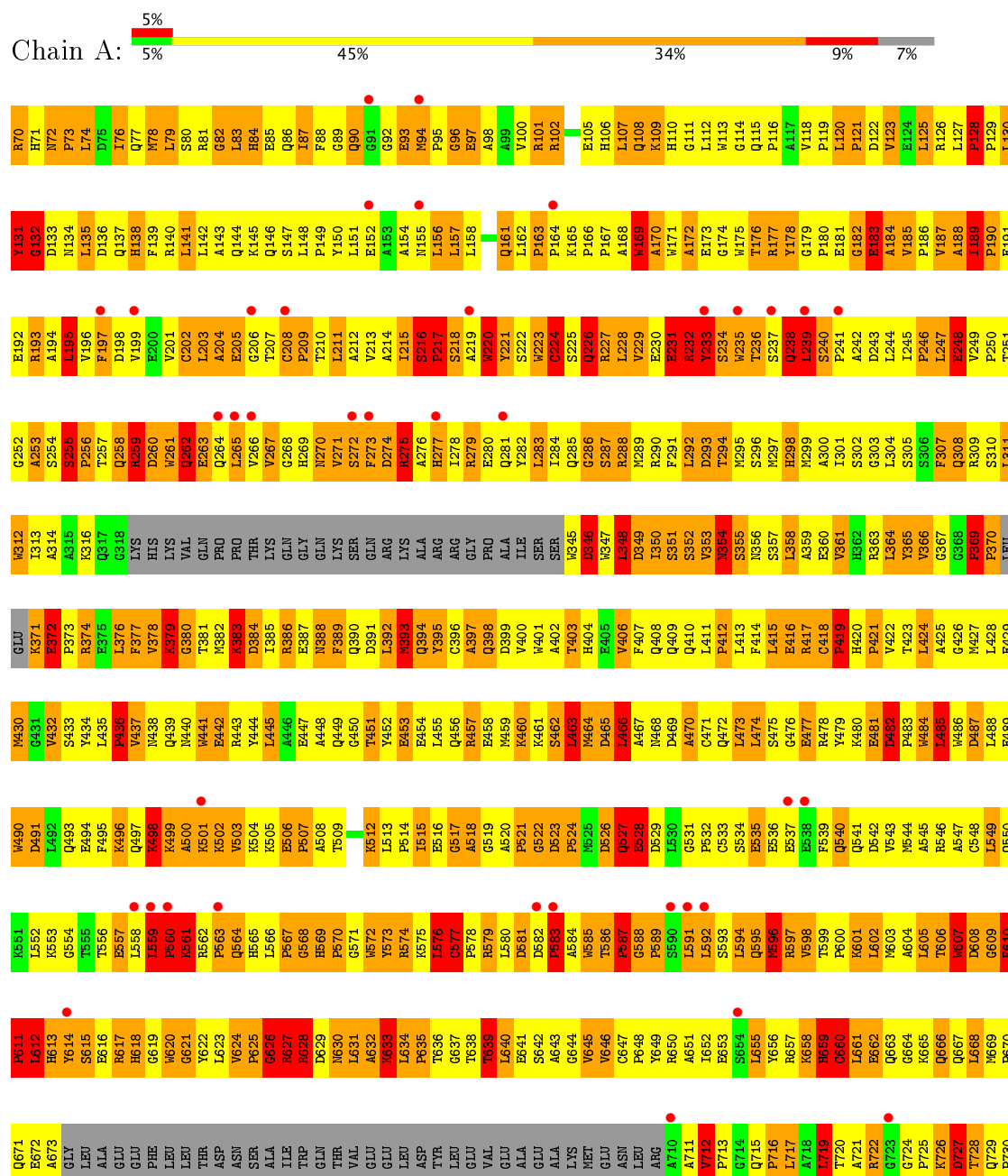
- Molecule 2 is a protein called DNA polymerase subunit gamma-2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 355 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2871 | 1840 | 504 | 511 | 16 | | | |
| 2 | C | 396 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3181 | 2031 | 563 | 571 | 16 | | | |
| 2 | E | 355 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2871 | 1840 | 504 | 511 | 16 | | | |
| 2 | F | 396 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3181 | 2031 | 563 | 571 | 16 | | | |

3 Residue-property plots

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

- Molecule 1: DNA polymerase subunit gamma-1



| | | | | | | |
|-------|-------|-------|------|------|------|------|
| A1033 | A1034 | A1093 | C913 | R852 | A791 | S731 |
| R1034 | R1035 | T1094 | T914 | R853 | L792 | Y732 |
| K1035 | K1036 | S1095 | A915 | R854 | L793 | Y733 |
| S1036 | S1037 | R1096 | F916 | R855 | L794 | H734 |
| M1037 | M1038 | V1097 | G917 | E856 | N795 | G735 |
| M1038 | M1039 | V1098 | G918 | E857 | N796 | G736 |
| K1039 | K1040 | M1099 | R919 | T858 | P857 | N736 |
| K1040 | K1041 | V1100 | T920 | T859 | G737 | G737 |
| M1041 | M1042 | V1101 | L921 | R860 | P738 | P738 |
| E1042 | E1043 | Q1102 | Q922 | L861 | Y739 | Y739 |
| M1043 | M1044 | S1103 | Q923 | A862 | F800 | D741 |
| V1044 | V1045 | Q984 | R924 | S863 | V742 | V742 |
| A1045 | A1046 | R985 | R925 | R864 | D743 | D743 |
| E1046 | E1047 | Y986 | S926 | A865 | I744 | I744 |
| R1047 | R1048 | A887 | R927 | R866 | P745 | P745 |
| V1108 | V1109 | K988 | G928 | R867 | G746 | G746 |
| L1109 | L1110 | T989 | T929 | D868 | R807 | N748 |
| K1110 | K1111 | K990 | D930 | R869 | N748 | N748 |
| G1111 | G1112 | G991 | L931 | V870 | F749 | F749 |
| M1112 | M1113 | L992 | H932 | G871 | F750 | F750 |
| L1113 | L1114 | R993 | S933 | S872 | K811 | K751 |
| V1114 | V1115 | Y994 | K934 | E873 | M812 | L752 |
| A1115 | A1116 | S1055 | T935 | L874 | M813 | P753 |
| M1116 | M1117 | R996 | A936 | K875 | H814 | H754 |
| K1117 | K1118 | M1057 | T937 | A876 | K815 | K755 |
| F1058 | F1059 | S998 | T938 | M877 | L816 | D756 |
| M1059 | M1060 | E1000 | G940 | V878 | R817 | G757 |
| K1060 | K1061 | E1001 | V941 | K879 | R818 | M758 |
| L1061 | L1062 | G1002 | S942 | P881 | L821 | S759 |
| S1063 | S1064 | M1003 | R943 | P882 | P822 | N761 |
| M1064 | M1065 | V1004 | E944 | G883 | R823 | V762 |
| A1065 | A1066 | R1006 | H945 | T885 | A824 | G763 |
| S1067 | S1068 | E1007 | K947 | L886 | R825 | S764 |
| D1068 | D1069 | L1008 | F948 | M827 | I826 | P766 |
| I1069 | I1070 | M1009 | F949 | H828 | R827 | F766 |
| P1070 | P1071 | L1010 | N950 | P829 | A767 | A767 |
| R1071 | R1072 | V1011 | Y951 | D890 | K768 | K768 |
| P1073 | P1074 | D1013 | G952 | V891 | D769 | D769 |
| V1074 | V1075 | R1014 | R953 | D892 | F770 | F770 |
| LEU | LEU | T1015 | Y955 | S893 | L771 | L771 |
| GLY | GLY | E1016 | G956 | Q894 | P772 | P772 |
| CYS | CYS | G1017 | A957 | E895 | K773 | K773 |
| CYS | CYS | R1018 | G958 | L896 | M774 | M774 |
| ILE | ILE | V1019 | Q959 | I897 | E775 | E775 |
| SER | SER | P1200 | P960 | A899 | D776 | D776 |
| ARG | ARG | S1201 | F961 | A900 | T778 | T778 |
| ALA | ALA | L1022 | A962 | V901 | L779 | L779 |
| LEU | LEU | Q1023 | E963 | I902 | Q780 | Q780 |
| GLU | GLU | D1024 | R964 | G903 | A781 | A781 |
| PRO | PRO | L1025 | L965 | D904 | G842 | G842 |
| SER | SER | R1026 | L966 | A905 | Q843 | Q843 |
| ALA | ALA | V1027 | N967 | H906 | V844 | V844 |
| VAL | VAL | K1027 | Q967 | F907 | G845 | G845 |
| GLN | GLN | Q1028 | F969 | A908 | T846 | T846 |
| E1090 | E1091 | Q1029 | N970 | G909 | S786 | S786 |
| E1091 | E1092 | E1030 | H971 | R910 | S787 | S787 |
| E1092 | E1093 | T1032 | R972 | T851 | T850 | T850 |
| F1092 | F1093 | F1092 | G912 | T851 | P789 | P789 |
| F1092 | F1093 | F1092 | G912 | T851 | T850 | T850 |

• Molecule 1: DNA polymerase subunit gamma-1

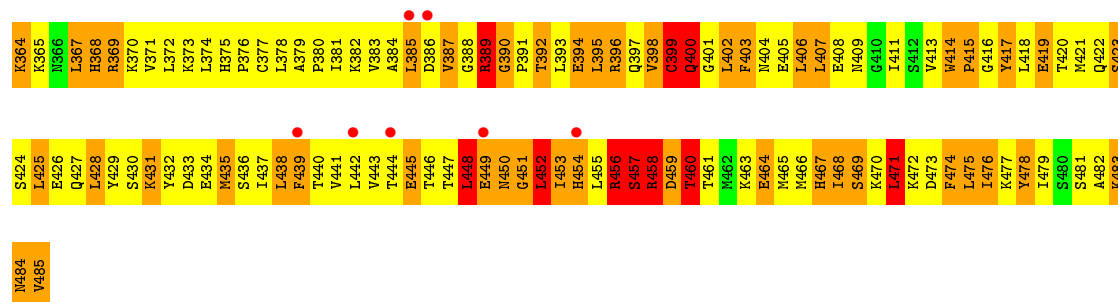


| | | | | | | |
|------|------|-------|-------|------|------|-------|
| R70 | H71 | P1213 | P1214 | R153 | Q154 | P1213 |
| H72 | P73 | A1217 | A1218 | R155 | R156 | Q1214 |
| L74 | L75 | D1219 | D1220 | T156 | T157 | T158 |
| D75 | T76 | T1221 | T1222 | L158 | L159 | L160 |
| Q77 | Q78 | L1223 | L1224 | R161 | R162 | R163 |
| L79 | S80 | T1225 | T1226 | M163 | M164 | M165 |
| R81 | R82 | E1227 | E1228 | F166 | F167 | F168 |
| G83 | G84 | K1229 | K1230 | Y166 | Y167 | Y168 |
| L85 | L86 | L1231 | L1232 | K167 | K168 | K169 |
| R88 | R89 | E1233 | E1234 | L168 | L169 | L170 |
| G90 | G91 | K1235 | K1236 | L171 | L172 | L173 |
| P93 | P94 | P1237 | P1238 | L174 | L175 | L176 |
| P95 | P96 | P1239 | P1240 | L177 | L178 | L179 |
| G96 | G97 | G98 | G99 | F179 | F180 | F181 |
| A98 | A99 | A100 | A101 | K180 | K181 | K182 |
| V100 | V101 | V102 | V103 | L181 | L182 | L183 |
| R102 | R103 | R104 | R105 | L184 | L185 | L186 |
| E105 | E106 | E107 | E108 | L187 | L188 | L189 |
| H106 | H107 | H108 | H109 | L190 | L191 | L192 |
| L107 | L108 | L109 | L110 | K191 | K192 | K193 |
| Q108 | Q109 | Q110 | Q111 | L193 | L194 | L195 |
| H110 | H111 | H112 | H113 | T194 | T195 | T196 |
| G111 | G112 | G113 | G114 | D196 | D197 | D198 |
| L112 | L113 | L114 | L115 | C197 | C198 | C199 |
| H113 | H114 | H115 | H116 | R198 | R199 | R200 |
| G114 | G115 | G116 | G117 | T199 | T200 | T201 |
| T202 | T203 | T204 | T205 | P200 | P201 | P202 |
| L120 | L121 | L122 | L123 | S201 | S202 | S203 |
| D124 | D125 | D126 | D127 | E202 | E203 | E204 |
| R126 | R127 | R128 | R129 | K204 | K205 | K206 |
| L127 | L128 | L129 | L130 | L206 | L207 | L208 |
| P128 | P129 | P130 | P131 | M208 | M209 | M210 |
| E130 | E131 | E132 | E133 | R209 | R210 | R211 |
| G132 | G133 | G134 | G135 | F210 | F211 | F212 |
| E183 | E184 | E185 | E186 | L212 | L213 | L214 |
| P186 | P187 | P188 | P189 | T214 | T215 | T216 |
| S237 | S238 | S239 | S240 | K216 | K217 | K218 |
| Q238 | Q239 | Q240 | Q241 | L218 | L219 | L220 |
| L242 | L243 | L244 | L245 | R219 | R220 | R221 |
| D243 | D244 | D245 | D246 | E221 | E222 | E223 |
| R247 | R248 | R249 | R250 | K223 | K224 | K225 |
| L249 | L250 | L251 | L252 | S225 | S226 | S227 |
| P249 | P250 | P251 | P252 | Q226 | Q227 | Q228 |
| E249 | E250 | E251 | E252 | R227 | R228 | R229 |
| S253 | S254 | S255 | S256 | A228 | A229 | A230 |
| T257 | T258 | T259 | T260 | L228 | L229 | L230 |
| E260 | E261 | E262 | E263 | E230 | E231 | E232 |
| R263 | R264 | R265 | R266 | Q231 | Q232 | Q233 |
| L267 | L268 | L269 | L270 | L232 | L233 | L234 |
| T270 | T271 | T272 | T273 | T234 | T235 | T236 |
| S272 | S273 | S274 | S275 | E236 | E237 | E238 |
| F273 | F274 | F275 | F276 | R237 | R238 | R239 |
| D274 | D275 | D276 | D277 | Q238 | Q239 | Q240 |
| G275 | G276 | G277 | G278 | L239 | L240 | L241 |
| A276 | A277 | A278 | A279 | S240 | S241 | S242 |
| E277 | E278 | E279 | E280 | P241 | P242 | P243 |
| R279 | R280 | R281 | R282 | E243 | E244 | E245 |
| E280 | E281 | E282 | E283 | R244 | R245 | R246 |
| A281 | A282 | A283 | A284 | L246 | L247 | L248 |
| ILE | ILE | ILE | ILE | T247 | T248 | T249 |
| ALA | ALA | ALA | ALA | K248 | K249 | K250 |
| SER | SER | SER | SER | P249 | P250 | P251 |
| W346 | W347 | W348 | W349 | E250 | E251 | E252 |
| D346 | D347 | D348 | D349 | S251 | S252 | S253 |
| L348 | L349 | L350 | L351 | Q252 | Q253 | Q254 |
| S351 | S352 | S353 | S354 | L253 | L254 | L255 |
| N354 | N355 | N356 | N357 | T254 | T255 | T256 |
| SER | SER | SER | SER | E255 | E256 | E257 |
| ASV | ASV | ASV | ASV | L356 | L357 | L358 |
| S355 | S356 | S357 | S358 | A357 | A358 | A359 |
| L356 | L357 | L358 | L359 | E358 | E359 | E360 |
| S359 | S360 | S361 | S362 | I301 | I302 | I303 |
| R361 | R362 | R363 | R364 | G303 | G304 | G305 |
| L362 | L363 | L364 | L365 | L304 | L305 | L306 |
| V363 | V364 | V365 | V366 | S305 | S306 | S307 |
| G365 | G366 | G367 | G368 | F307 | F308 | F309 |
| P367 | P368 | P369 | P370 | Q308 | Q309 | Q310 |
| E370 | E371 | E372 | E373 | S310 | S311 | S312 |
| L369 | L370 | L371 | L372 | T311 | T312 | T313 |
| E370 | E371 | E372 | E373 | P312 | P313 | P314 |

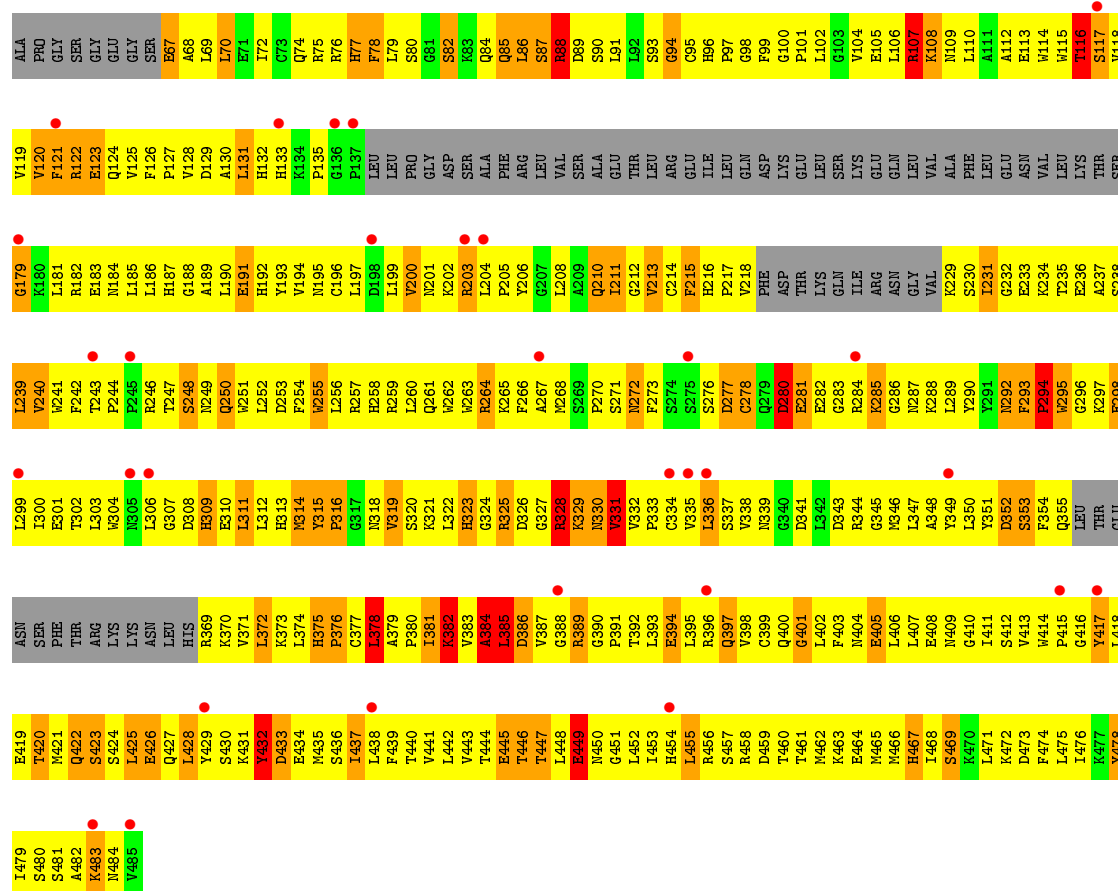
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|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|
| Q1214 | Q1154 | T1094 | R1034 | T974 | T914 | R853 | E793 | H733 | A673 | H613 | K553 | D491 | G431 | K371 |
| G1215 | I1155 | S1095 | K1035 | Q775 | A915 | A854 | I794 | H734 | GLY | Y614 | G554 | D492 | V432 | E372 |
| E1216 | T1156 | R1096 | S1036 | Q776 | F916 | V855 | K796 | G735 | LEU | S615 | T595 | Q493 | S433 | E373 |
| A1217 | N1157 | V1097 | Q1037 | R977 | G917 | E856 | K796 | N736 | ALA | R616 | T556 | Q494 | R434 | R374 |
| L1218 | L1158 | N1098 | K1038 | A978 | N918 | P857 | I798 | G737 | GLU | R617 | E557 | F495 | L435 | E375 |
| D1219 | L1159 | V1099 | K1039 | A979 | N919 | T858 | S799 | P738 | GLU | R618 | L558 | K496 | P436 | L376 |
| T1220 | T1160 | V1100 | K1040 | R980 | T920 | R859 | S799 | T739 | PRO | Q497 | L559 | Q497 | V437 | F377 |
| Y1221 | T1161 | V1101 | W1041 | R981 | L921 | L860 | F800 | N740 | LEU | W620 | P560 | K498 | Q438 | V378 |
| Q1222 | C1162 | E1042 | E1042 | A982 | G922 | S863 | W801 | D741 | LEU | W621 | P561 | K499 | Q439 | R379 |
| I1223 | S1103 | S1043 | V1043 | Q983 | G923 | N864 | N802 | V742 | THR | G621 | K499 | A500 | N440 | G380 |
| I1224 | F1164 | S1104 | V1044 | Q984 | G924 | N864 | N803 | D743 | ASP | K623 | P563 | K501 | N441 | T381 |
| E1225 | A1105 | A1045 | A1045 | N985 | G925 | A865 | H805 | I744 | ASN | A504 | D564 | K502 | E442 | K382 |
| Y1226 | V1106 | N986 | E1046 | N986 | G926 | R866 | H806 | P745 | SER | P625 | H565 | K503 | R443 | K383 |
| T1227 | K1167 | A987 | R1047 | A987 | A927 | P867 | K806 | G746 | ALA | G626 | L566 | K504 | Y444 | D384 |
| G1228 | L1168 | A1048 | A1048 | A988 | G928 | D868 | R807 | C747 | ILE | R627 | P567 | K505 | L445 | I385 |
| E1229 | G1169 | T989 | R989 | T989 | T929 | R869 | R808 | W748 | TRP | R628 | G568 | E506 | A446 | R386 |
| S1230 | K1170 | K1050 | K1050 | K990 | D930 | V870 | S809 | F749 | GLN | D629 | H569 | GLN | A447 | E387 |
| L1231 | G1051 | L1111 | G1051 | G991 | L931 | G871 | S810 | P750 | THR | N630 | P570 | T509 | A448 | N388 |
| D1232 | G1052 | L1112 | G1052 | L992 | H932 | S872 | Q811 | K751 | VAL | L631 | G571 | A510 | Q449 | F389 |
| L1233 | T1053 | R993 | E973 | R993 | S933 | E973 | H812 | L752 | GLU | R632 | H572 | S511 | Q450 | Q390 |
| V1234 | V1114 | N994 | L874 | R994 | G934 | K375 | H813 | P753 | GLU | R633 | H573 | K512 | T451 | D391 |
| S1235 | A1115 | S995 | K375 | R995 | T935 | A876 | H814 | H754 | LEU | L634 | H574 | L513 | T452 | L392 |
| Q1236 | M1116 | R996 | A876 | R996 | G936 | K376 | W815 | K755 | ASP | P635 | H575 | P514 | Y453 | K393 |
| I1237 | K1117 | N997 | N877 | N997 | T937 | N877 | L816 | D756 | TYR | T636 | L576 | I515 | E454 | D394 |
| G1238 | W1118 | S998 | V878 | S998 | T938 | V878 | P817 | G757 | LEU | G637 | C577 | E516 | L455 | K395 |
| F1239 | L1119 | D999 | Q879 | D999 | V938 | Q879 | R818 | N758 | GLU | T638 | P578 | G517 | Q456 | C396 |
| F1180 | K1060 | E1000 | A880 | E1000 | G940 | A880 | S819 | S759 | VAL | T639 | H579 | A518 | R457 | A397 |
| S1181 | L1061 | G1001 | P881 | G1001 | L941 | P881 | A820 | C760 | GLU | L640 | H580 | G519 | E458 | K398 |
| A1182 | E1062 | E1002 | P882 | E1002 | S942 | P882 | L821 | N761 | ALA | A520 | D582 | G520 | M459 | D399 |
| V1183 | S1063 | K1003 | G883 | K1003 | R943 | G883 | P822 | V762 | GLU | S642 | H583 | P521 | K460 | V400 |
| L1184 | I1064 | L1004 | V884 | L1004 | E944 | V884 | R823 | G763 | ALA | A643 | P583 | G522 | K461 | H401 |
| I1185 | A1065 | V1005 | T885 | V1005 | H945 | T885 | A824 | S764 | LVS | G644 | H584 | D623 | S462 | H402 |
| D1186 | T1066 | R1006 | R825 | R1006 | A946 | P765 | R825 | P765 | MET | V645 | H585 | P524 | L463 | T403 |
| G1127 | G1127 | E1007 | R827 | E1007 | K947 | F766 | I826 | F766 | GLU | V646 | H586 | M525 | M464 | H404 |
| R1128 | D1068 | L1008 | G888 | L1008 | L948 | R888 | R827 | A767 | LEU | P647 | P587 | D526 | D465 | E405 |
| L1189 | I1069 | N1009 | A889 | N1009 | F949 | A889 | H828 | K768 | LEU | P648 | G588 | Q527 | L466 | V406 |
| R1190 | P1070 | D890 | D890 | D890 | N950 | D890 | P829 | D769 | GLU | R649 | P589 | E528 | A467 | F407 |
| K1191 | R1071 | V881 | V881 | V881 | G951 | V881 | D830 | F770 | ATL | R650 | S590 | D529 | N468 | Q408 |
| E1192 | T1072 | G952 | D892 | G952 | G952 | D892 | H831 | L771 | ATL | A651 | L591 | G530 | D469 | Q409 |
| V1193 | D1012 | R953 | S893 | D1012 | R953 | S893 | D832 | P772 | V712 | L652 | L592 | P532 | A470 | Q410 |
| T1194 | R1014 | I954 | Q894 | R1014 | I954 | Q894 | E833 | K773 | G714 | S653 | L593 | P532 | C471 | L411 |
| M1195 | T1015 | V955 | E895 | T1015 | V955 | E895 | E834 | N774 | G715 | S654 | L594 | G533 | Q472 | P412 |
| D1196 | E1016 | G956 | L896 | E1016 | G956 | L896 | G835 | E775 | Q715 | L655 | D595 | G533 | L473 | L413 |
| C1197 | CYS | A957 | R897 | CYS | A957 | R897 | L836 | D776 | P716 | X656 | H596 | E536 | L474 | L414 |
| K1198 | CYS | G1017 | R898 | CYS | G1017 | R898 | H837 | G777 | L717 | R657 | R597 | E537 | S475 | L415 |
| T1199 | Y1139 | Q959 | A899 | Y1139 | Q959 | A899 | G838 | T778 | ATL | R658 | V598 | E538 | G476 | E416 |
| P1200 | L1140 | P960 | A900 | L1140 | P960 | A900 | H839 | L779 | LEU | H659 | T599 | F539 | E477 | R417 |
| S1201 | V1141 | F961 | V901 | S1201 | F961 | V901 | I840 | Q780 | T720 | C660 | P600 | Q540 | R478 | C418 |
| N1202 | ALA | A962 | L902 | N1202 | A962 | L902 | L841 | A781 | ATL | L661 | K601 | Q541 | Y479 | P419 |
| P1203 | LEU | E963 | G903 | P1203 | E963 | G903 | P842 | G782 | R722 | E662 | L602 | D542 | K480 | H420 |
| T1204 | GLU | R964 | D904 | T1204 | R964 | D904 | Q843 | P783 | G723 | Q663 | H603 | V543 | E481 | P421 |
| G1205 | PRO | L965 | A905 | G1205 | L965 | A905 | H844 | G784 | G724 | G664 | A604 | H544 | D482 | V422 |
| M1206 | SER | L966 | H906 | M1206 | L966 | H906 | V845 | G785 | P725 | K665 | L605 | A545 | P483 | T423 |
| E1207 | ALA | N967 | F907 | E1207 | N967 | F907 | T846 | A786 | K726 | Q666 | T606 | R546 | W484 | L424 |
| R1208 | VAL | Q968 | A908 | R1208 | Q968 | A908 | G847 | S787 | D728 | Q667 | H607 | A547 | L485 | A425 |
| C1209 | GLN | P969 | G909 | C1209 | P969 | G909 | G848 | S788 | T728 | L668 | D608 | C548 | W486 | A426 |
| A1150 | R1030 | N970 | N910 | A1150 | N970 | N910 | T849 | P789 | Q729 | M669 | D609 | L549 | D487 | M427 |
| G1211 | E1091 | H971 | H911 | G1211 | H971 | H911 | I850 | R790 | P730 | P670 | F610 | Q550 | L488 | L428 |
| I1212 | T1032 | R972 | G912 | I1212 | R972 | G912 | T851 | A791 | S731 | Q671 | P611 | Q551 | E489 | E429 |
| P1213 | L1153 | L973 | C913 | P1213 | L973 | C913 | R852 | L792 | Y732 | E672 | L612 | L552 | W490 | M430 |

- Molecule 2: DNA polymerase subunit gamma-2

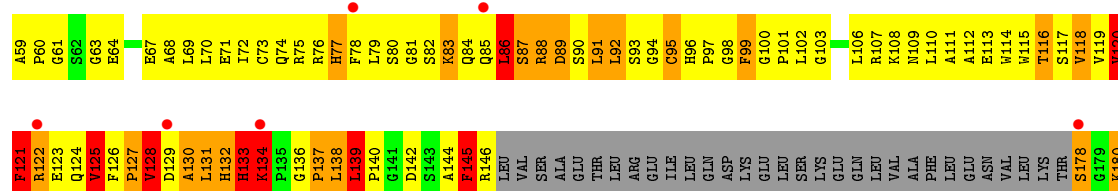




• Molecule 2: DNA polymerase subunit gamma-2



• Molecule 2: DNA polymerase subunit gamma-2



| | | | | | |
|------|----------------------|------|--|--|--|
| A452 | K483 M454 V485 | Q422 | R363 R364 R365 R366 R367 R368 R369 R370 R371 R372 R373 R374 R375 R376 R377 R378 R379 R380 R381 R382 R383 R384 R385 R386 R387 R388 R389 R390 R391 R392 R393 R394 R395 R396 R397 R398 R399 Q400 Q401 Q402 Q403 Q404 Q405 Q406 Q407 Q408 Q409 Q410 Q411 Q412 Q413 Q414 Q415 Q416 Q417 Q418 Q419 Q420 Q421 | E301 T302 L303 M304 N305 L306 G307 D308 S309 K310 E310 L311 L312 H313 M314 Y315 P316 G317 N318 Y319 S320 K321 L322 H323 G324 R325 D326 G327 R328 K329 N330 Y331 L332 H333 M334 Y335 L336 G337 D338 S339 K340 E341 L342 H343 M344 Y345 P346 G347 N348 Y349 L350 H351 M352 S353 P354 Q355 L356 T357 E358 N359 K360 | W241 T242 L243 M244 P245 R246 T247 S248 A249 Q250 W251 L252 D253 P254 W255 L256 R257 H258 L259 V260 W261 K262 L263 W264 R265 F266 G267 W268 S269 T270 Z271 G212 V213 G214 S274 S275 H216 T217 F218 F219 D220 T221 K222 Q223 L224 R225 W226 G227 H228 K229 Y290 S230 N292 S293 F294 W295 G296 T297 E298 N299 L230 W240 |
| | | S423 | | | |
| | | S424 | | | |
| | | L425 | | | |
| | | E426 | | | |
| | | Q427 | | | |
| | | L428 | | | |
| | | Y429 | | | |
| | | S430 | | | |
| | | K431 | | | |
| Y432 | | | | | |
| D433 | | | | | |
| E434 | | | | | |
| M435 | | | | | |
| S436 | | | | | |
| L437 | | | | | |
| L438 | | | | | |
| F439 | | | | | |
| T440 | | | | | |
| V441 | | | | | |
| L442 | | | | | |
| V443 | | | | | |
| T444 | | | | | |
| E445 | | | | | |
| T446 | | | | | |
| T447 | | | | | |
| L448 | | | | | |
| E449 | | | | | |
| M450 | | | | | |
| G451 | | | | | |
| L452 | | | | | |
| L453 | | | | | |
| H454 | | | | | |
| L455 | | | | | |
| R456 | | | | | |
| S457 | | | | | |
| R458 | | | | | |
| D459 | | | | | |
| T460 | | | | | |
| T461 | | | | | |
| M462 | | | | | |
| K463 | | | | | |
| E464 | | | | | |
| M465 | | | | | |
| M466 | | | | | |
| H467 | | | | | |
| T468 | | | | | |
| S469 | | | | | |
| K470 | | | | | |
| L471 | | | | | |
| K472 | | | | | |
| D473 | | | | | |
| F474 | | | | | |
| L475 | | | | | |
| T476 | | | | | |
| K477 | | | | | |
| Y478 | | | | | |
| L479 | | | | | |
| S480 | | | | | |
| S481 | | | | | |

4 Data and refinement statistics

| Property | Value | Source |
|---|--|------------------|
| Space group | P 32 | Depositor |
| Cell constants a, b, c, α , β , γ | 138.39Å 138.39Å 226.31Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 46.92 – 3.24 46.92 – 3.25 | Depositor EDS |
| % Data completeness (in resolution range) | 89.5 (46.92-3.24) 89.5 (46.92-3.25) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.12 (at 3.25Å) | Xtriage |
| Refinement program | CNS 1.2 | Depositor |
| R, R_{free} | 0.284 , 0.303 0.362 , (Not available) | Depositor DCC |
| R_{free} test set | No test flags present. | DCC |
| Wilson B-factor (Å ²) | 93.9 | Xtriage |
| Anisotropy | 0.065 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 64.7 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$ | Xtriage |
| Estimated twinning fraction | 0.008 for -h,-k,l 0.459 for h,-h-k,-l 0.009 for -k,-h,-l | Xtriage |
| F_o, F_c correlation | 0.83 | EDS |
| Total number of atoms | 29480 | wwPDB-VP |
| Average B, all atoms (Å ²) | 85.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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 ⓘ

5.1 Standard geometry ⓘ

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 | 0.72 | 10/8913 (0.1%) | 1.33 | 149/12100 (1.2%) |
| 1 | D | 0.81 | 18/8927 (0.2%) | 1.45 | 161/12118 (1.3%) |
| 2 | B | 0.60 | 2/2944 (0.1%) | 0.99 | 16/3981 (0.4%) |
| 2 | C | 0.68 | 0/3262 | 1.31 | 47/4411 (1.1%) |
| 2 | E | 0.67 | 6/2944 (0.2%) | 1.11 | 23/3981 (0.6%) |
| 2 | F | 0.64 | 0/3262 | 1.28 | 37/4411 (0.8%) |
| All | All | 0.72 | 36/30252 (0.1%) | 1.31 | 433/41002 (1.1%) |

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 | 4 |
| 1 | D | 1 | 3 |
| 2 | B | 0 | 1 |
| 2 | C | 0 | 1 |
| 2 | E | 1 | 2 |
| 2 | F | 0 | 1 |
| All | All | 2 | 12 |

All (36) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | D | 358 | GLU | CG-CD | 12.87 | 1.71 | 1.51 |
| 2 | E | 385 | LEU | CA-CB | -11.49 | 1.27 | 1.53 |
| 1 | D | 352 | SER | N-CA | 9.45 | 1.65 | 1.46 |
| 1 | A | 232 | ARG | N-CA | -8.85 | 1.28 | 1.46 |
| 2 | E | 382 | LYS | N-CA | -8.69 | 1.28 | 1.46 |
| 2 | B | 280 | ASP | C-O | -8.67 | 1.06 | 1.23 |
| 1 | D | 352 | SER | CA-C | 8.29 | 1.74 | 1.52 |
| 1 | D | 358 | GLU | CB-CG | -8.14 | 1.36 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1 | D | 249 | VAL | CB-CG1 | -7.88 | 1.36 | 1.52 |
| 1 | A | 232 | ARG | CA-CB | -7.53 | 1.37 | 1.53 |
| 1 | A | 216 | SER | CB-OG | -7.33 | 1.32 | 1.42 |
| 1 | D | 361 | ARG | CZ-NH1 | 7.17 | 1.42 | 1.33 |
| 1 | A | 232 | ARG | CB-CG | 7.12 | 1.71 | 1.52 |
| 1 | D | 280 | GLU | CG-CD | 7.10 | 1.62 | 1.51 |
| 1 | D | 359 | VAL | CB-CG2 | -6.86 | 1.38 | 1.52 |
| 1 | D | 358 | GLU | CD-OE1 | 6.86 | 1.33 | 1.25 |
| 1 | A | 870 | VAL | CB-CG1 | -6.53 | 1.39 | 1.52 |
| 1 | A | 231 | GLU | C-O | -6.29 | 1.11 | 1.23 |
| 1 | D | 280 | GLU | CB-CG | 6.28 | 1.64 | 1.52 |
| 1 | D | 915 | ALA | CA-CB | -6.13 | 1.39 | 1.52 |
| 1 | A | 1038 | TRP | CB-CG | 6.08 | 1.61 | 1.50 |
| 2 | E | 382 | LYS | CB-CG | -5.93 | 1.36 | 1.52 |
| 2 | E | 331 | VAL | CA-CB | 5.91 | 1.67 | 1.54 |
| 2 | E | 382 | LYS | CA-CB | 5.84 | 1.66 | 1.53 |
| 1 | A | 239 | LEU | CA-CB | -5.77 | 1.40 | 1.53 |
| 1 | D | 870 | VAL | CA-CB | -5.77 | 1.42 | 1.54 |
| 2 | B | 281 | GLU | CG-CD | 5.65 | 1.60 | 1.51 |
| 1 | D | 248 | GLU | N-CA | -5.54 | 1.35 | 1.46 |
| 2 | E | 381 | ILE | C-O | -5.51 | 1.12 | 1.23 |
| 1 | A | 229 | VAL | CA-CB | 5.42 | 1.66 | 1.54 |
| 1 | A | 229 | VAL | N-CA | 5.40 | 1.57 | 1.46 |
| 1 | D | 503 | VAL | CA-CB | 5.36 | 1.66 | 1.54 |
| 1 | D | 870 | VAL | CB-CG1 | -5.33 | 1.41 | 1.52 |
| 1 | D | 361 | ARG | CB-CG | 5.31 | 1.66 | 1.52 |
| 1 | D | 869 | ARG | CG-CD | -5.14 | 1.39 | 1.51 |
| 1 | D | 359 | VAL | C-O | 5.09 | 1.33 | 1.23 |

All (433) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 2 | E | 382 | LYS | N-CA-C | 16.56 | 155.72 | 111.00 |
| 2 | E | 385 | LEU | N-CA-C | 16.34 | 155.11 | 111.00 |
| 1 | D | 248 | GLU | CA-C-N | -14.80 | 84.64 | 117.20 |
| 2 | B | 280 | ASP | C-N-CA | 14.32 | 157.51 | 121.70 |
| 1 | A | 1212 | ILE | C-N-CD | -12.99 | 92.03 | 120.60 |
| 1 | D | 347 | TRP | N-CA-C | 12.67 | 145.20 | 111.00 |
| 1 | D | 171 | TRP | N-CA-C | -12.65 | 76.84 | 111.00 |
| 1 | D | 721 | ALA | N-CA-C | -12.53 | 77.17 | 111.00 |
| 1 | D | 810 | SER | N-CA-C | -12.41 | 77.49 | 111.00 |
| 1 | D | 559 | LEU | CA-CB-CG | 12.39 | 143.80 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | D | 1037 | GLN | N-CA-C | 11.88 | 143.06 | 111.00 |
| 1 | A | 379 | LYS | N-CA-C | -11.75 | 79.27 | 111.00 |
| 2 | E | 382 | LYS | N-CA-CB | -11.64 | 89.64 | 110.60 |
| 1 | D | 206 | GLY | N-CA-C | -11.61 | 84.07 | 113.10 |
| 2 | F | 319 | VAL | N-CA-C | -11.45 | 80.09 | 111.00 |
| 2 | E | 381 | ILE | CA-C-N | -11.32 | 92.29 | 117.20 |
| 1 | A | 239 | LEU | N-CA-C | 11.07 | 140.90 | 111.00 |
| 1 | D | 627 | ARG | N-CA-C | -11.03 | 81.21 | 111.00 |
| 1 | D | 358 | GLU | OE1-CD-OE2 | -11.03 | 110.07 | 123.30 |
| 1 | A | 1025 | LEU | CA-CB-CG | -11.00 | 90.01 | 115.30 |
| 1 | D | 352 | SER | O-C-N | -10.95 | 105.19 | 122.70 |
| 1 | D | 132 | GLY | N-CA-C | 10.77 | 140.03 | 113.10 |
| 2 | E | 384 | ALA | N-CA-C | 10.75 | 140.02 | 111.00 |
| 2 | C | 448 | LEU | CA-CB-CG | 10.65 | 139.80 | 115.30 |
| 1 | A | 238 | GLN | CA-CB-CG | 10.65 | 136.82 | 113.40 |
| 1 | A | 533 | CYS | N-CA-C | -10.62 | 82.31 | 111.00 |
| 1 | A | 609 | GLY | N-CA-C | -10.62 | 86.56 | 113.10 |
| 1 | D | 248 | GLU | O-C-N | 10.50 | 139.50 | 122.70 |
| 2 | F | 286 | GLY | N-CA-C | -10.46 | 86.95 | 113.10 |
| 1 | A | 274 | ASP | N-CA-C | -10.45 | 82.79 | 111.00 |
| 1 | D | 737 | GLY | N-CA-C | -10.43 | 87.03 | 113.10 |
| 1 | D | 1069 | ILE | C-N-CD | -10.22 | 98.12 | 120.60 |
| 2 | F | 208 | LEU | CA-CB-CG | -10.11 | 92.05 | 115.30 |
| 1 | D | 274 | ASP | N-CA-C | -10.05 | 83.85 | 111.00 |
| 2 | C | 460 | THR | N-CA-C | -9.87 | 84.35 | 111.00 |
| 2 | B | 340 | GLY | N-CA-C | -9.84 | 88.49 | 113.10 |
| 2 | C | 319 | VAL | N-CA-C | -9.72 | 84.77 | 111.00 |
| 1 | D | 351 | SER | N-CA-C | -9.71 | 84.80 | 111.00 |
| 1 | D | 736 | ASN | N-CA-C | 9.60 | 136.92 | 111.00 |
| 2 | E | 78 | PHE | N-CA-C | -9.54 | 85.25 | 111.00 |
| 2 | E | 385 | LEU | N-CA-CB | -9.49 | 91.41 | 110.40 |
| 1 | A | 1205 | GLY | N-CA-C | -9.49 | 89.37 | 113.10 |
| 1 | D | 1196 | ASP | N-CA-C | -9.49 | 85.38 | 111.00 |
| 2 | E | 381 | ILE | C-N-CA | 9.48 | 145.40 | 121.70 |
| 1 | D | 672 | GLU | N-CA-C | -9.47 | 85.44 | 111.00 |
| 1 | D | 786 | ALA | N-CA-C | -9.45 | 85.49 | 111.00 |
| 2 | F | 357 | THR | N-CA-C | -9.38 | 85.69 | 111.00 |
| 2 | C | 208 | LEU | CA-CB-CG | -9.27 | 93.97 | 115.30 |
| 1 | D | 167 | PRO | N-CA-C | -9.25 | 88.06 | 112.10 |
| 2 | F | 121 | PHE | N-CA-C | 9.14 | 135.67 | 111.00 |
| 2 | C | 450 | ASN | N-CA-C | -9.12 | 86.37 | 111.00 |
| 1 | A | 1010 | LEU | CA-CB-CG | -9.08 | 94.41 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2 | C | 303 | LEU | N-CA-C | 9.05 | 135.44 | 111.00 |
| 1 | D | 645 | VAL | N-CA-C | 8.99 | 135.27 | 111.00 |
| 1 | D | 115 | GLN | C-N-CD | -8.98 | 100.84 | 120.60 |
| 1 | D | 178 | TYR | N-CA-C | -8.97 | 86.78 | 111.00 |
| 2 | C | 342 | LEU | N-CA-C | -8.96 | 86.81 | 111.00 |
| 1 | D | 726 | LYS | N-CA-C | 8.91 | 135.05 | 111.00 |
| 2 | C | 454 | HIS | N-CA-C | -8.86 | 87.09 | 111.00 |
| 1 | A | 627 | ARG | N-CA-C | -8.85 | 87.11 | 111.00 |
| 1 | A | 523 | ASP | N-CA-C | -8.84 | 87.13 | 111.00 |
| 2 | C | 279 | GLN | N-CA-C | 8.80 | 134.76 | 111.00 |
| 1 | A | 238 | GLN | N-CA-C | 8.77 | 134.68 | 111.00 |
| 1 | D | 615 | SER | N-CA-C | -8.74 | 87.41 | 111.00 |
| 1 | D | 346 | ASP | C-N-CA | -8.71 | 99.93 | 121.70 |
| 2 | C | 399 | CYS | N-CA-C | -8.66 | 87.62 | 111.00 |
| 2 | F | 460 | THR | N-CA-C | -8.65 | 87.64 | 111.00 |
| 1 | A | 923 | GLY | N-CA-C | -8.51 | 91.83 | 113.10 |
| 1 | D | 787 | SER | N-CA-C | -8.48 | 88.11 | 111.00 |
| 1 | D | 879 | GLN | N-CA-C | 8.47 | 133.87 | 111.00 |
| 1 | A | 1044 | VAL | N-CA-C | -8.43 | 88.23 | 111.00 |
| 1 | A | 178 | TYR | N-CA-C | -8.39 | 88.35 | 111.00 |
| 2 | C | 452 | LEU | CA-CB-CG | 8.38 | 134.57 | 115.30 |
| 1 | A | 938 | THR | N-CA-C | -8.31 | 88.55 | 111.00 |
| 1 | A | 1212 | ILE | N-CA-C | 8.29 | 133.37 | 111.00 |
| 2 | F | 471 | LEU | CA-CB-CG | -8.28 | 96.27 | 115.30 |
| 2 | C | 390 | GLY | N-CA-C | 8.25 | 133.72 | 113.10 |
| 2 | C | 456 | ARG | N-CA-C | 8.24 | 133.26 | 111.00 |
| 1 | D | 360 | HIS | N-CA-C | -8.21 | 88.84 | 111.00 |
| 1 | D | 523 | ASP | N-CA-C | -8.20 | 88.85 | 111.00 |
| 1 | D | 279 | ARG | N-CA-C | 8.17 | 133.07 | 111.00 |
| 1 | D | 176 | THR | N-CA-C | 8.15 | 133.02 | 111.00 |
| 1 | D | 533 | CYS | N-CA-C | -8.15 | 88.98 | 111.00 |
| 1 | D | 1010 | LEU | CA-CB-CG | -8.15 | 96.55 | 115.30 |
| 2 | C | 357 | THR | N-CA-C | -8.15 | 89.00 | 111.00 |
| 2 | F | 320 | SER | N-CA-C | 8.15 | 133.00 | 111.00 |
| 1 | D | 1027 | LYS | N-CA-C | 8.12 | 132.91 | 111.00 |
| 1 | D | 735 | GLY | N-CA-C | 8.10 | 133.35 | 113.10 |
| 2 | F | 342 | LEU | N-CA-C | -8.09 | 89.16 | 111.00 |
| 1 | D | 1233 | LYS | N-CA-C | -8.08 | 89.19 | 111.00 |
| 1 | D | 576 | LEU | CA-CB-CG | 8.06 | 133.85 | 115.30 |
| 2 | F | 390 | GLY | N-CA-C | 8.02 | 133.14 | 113.10 |
| 1 | D | 606 | THR | N-CA-C | 7.99 | 132.57 | 111.00 |
| 1 | A | 79 | LEU | N-CA-C | -7.97 | 89.48 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | D | 1069 | ILE | N-CA-C | -7.95 | 89.53 | 111.00 |
| 2 | F | 279 | GLN | N-CA-C | 7.93 | 132.42 | 111.00 |
| 2 | F | 339 | ASN | N-CA-C | -7.89 | 89.69 | 111.00 |
| 1 | A | 615 | SER | N-CA-C | -7.88 | 89.72 | 111.00 |
| 1 | D | 243 | ASP | N-CA-C | -7.86 | 89.77 | 111.00 |
| 1 | D | 912 | GLY | N-CA-C | 7.78 | 132.54 | 113.10 |
| 1 | A | 915 | ALA | N-CA-C | -7.77 | 90.02 | 111.00 |
| 1 | A | 576 | LEU | CA-CB-CG | 7.76 | 133.16 | 115.30 |
| 1 | A | 188 | ALA | N-CA-C | 7.76 | 131.95 | 111.00 |
| 1 | A | 1127 | GLY | N-CA-C | 7.75 | 132.47 | 113.10 |
| 1 | A | 1210 | TYR | N-CA-C | 7.68 | 131.74 | 111.00 |
| 1 | D | 286 | GLY | N-CA-C | -7.66 | 93.94 | 113.10 |
| 2 | B | 286 | GLY | N-CA-C | -7.65 | 93.98 | 113.10 |
| 1 | A | 782 | GLY | N-CA-C | -7.63 | 94.01 | 113.10 |
| 1 | A | 204 | ALA | N-CA-C | -7.62 | 90.42 | 111.00 |
| 1 | D | 1038 | TRP | N-CA-C | 7.61 | 131.55 | 111.00 |
| 1 | A | 605 | LEU | N-CA-C | 7.61 | 131.53 | 111.00 |
| 1 | D | 232 | ARG | N-CA-C | 7.59 | 131.50 | 111.00 |
| 2 | F | 133 | HIS | N-CA-C | 7.58 | 131.47 | 111.00 |
| 1 | A | 537 | GLU | N-CA-C | 7.57 | 131.44 | 111.00 |
| 1 | D | 359 | VAL | CB-CA-C | -7.56 | 97.03 | 111.40 |
| 1 | A | 182 | GLY | N-CA-C | 7.55 | 131.98 | 113.10 |
| 1 | A | 238 | GLN | O-C-N | 7.53 | 134.75 | 122.70 |
| 1 | A | 741 | ASP | N-CA-C | -7.52 | 90.69 | 111.00 |
| 1 | A | 485 | LEU | CA-CB-CG | 7.49 | 132.53 | 115.30 |
| 1 | D | 249 | VAL | N-CA-C | 7.49 | 131.23 | 111.00 |
| 1 | A | 132 | GLY | N-CA-C | 7.48 | 131.81 | 113.10 |
| 1 | D | 922 | GLN | N-CA-C | 7.48 | 131.21 | 111.00 |
| 1 | A | 912 | GLY | N-CA-C | 7.46 | 131.76 | 113.10 |
| 1 | D | 177 | ARG | N-CA-C | 7.45 | 131.12 | 111.00 |
| 2 | C | 343 | ASP | N-CA-C | -7.45 | 90.89 | 111.00 |
| 1 | D | 869 | ARG | NE-CZ-NH1 | -7.45 | 116.58 | 120.30 |
| 1 | D | 1236 | GLN | N-CA-C | 7.42 | 131.05 | 111.00 |
| 2 | E | 381 | ILE | N-CA-C | -7.42 | 90.98 | 111.00 |
| 1 | D | 669 | MET | N-CA-C | -7.41 | 90.98 | 111.00 |
| 1 | D | 728 | THR | N-CA-C | -7.39 | 91.04 | 111.00 |
| 1 | A | 203 | LEU | CA-CB-CG | -7.37 | 98.34 | 115.30 |
| 1 | D | 180 | PRO | N-CA-C | -7.37 | 92.94 | 112.10 |
| 1 | D | 231 | GLU | N-CA-C | 7.37 | 130.90 | 111.00 |
| 1 | D | 1130 | CYS | N-CA-C | 7.33 | 130.79 | 111.00 |
| 1 | A | 872 | SER | N-CA-C | -7.33 | 91.21 | 111.00 |
| 2 | C | 459 | ASP | N-CA-C | 7.33 | 130.79 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 602 | LEU | N-CA-C | -7.32 | 91.24 | 111.00 |
| 1 | D | 566 | LEU | N-CA-C | -7.30 | 91.28 | 111.00 |
| 2 | E | 381 | ILE | O-C-N | 7.29 | 134.36 | 122.70 |
| 1 | D | 568 | GLY | N-CA-C | -7.28 | 94.89 | 113.10 |
| 2 | E | 433 | ASP | N-CA-C | -7.27 | 91.37 | 111.00 |
| 1 | A | 195 | LEU | CA-CB-CG | 7.26 | 132.01 | 115.30 |
| 1 | D | 644 | GLY | N-CA-C | -7.26 | 94.94 | 113.10 |
| 1 | D | 75 | ASP | N-CA-C | -7.26 | 91.39 | 111.00 |
| 1 | A | 735 | GLY | N-CA-C | 7.23 | 131.18 | 113.10 |
| 1 | A | 996 | ARG | N-CA-C | 7.19 | 130.42 | 111.00 |
| 2 | C | 204 | LEU | N-CA-C | 7.18 | 130.39 | 111.00 |
| 2 | F | 196 | CYS | CA-CB-SG | 7.18 | 126.92 | 114.00 |
| 2 | B | 281 | GLU | CA-C-N | -7.18 | 101.41 | 117.20 |
| 1 | A | 1207 | GLU | N-CA-C | -7.11 | 91.80 | 111.00 |
| 1 | A | 1208 | ARG | N-CA-C | -7.08 | 91.88 | 111.00 |
| 1 | D | 233 | TYR | N-CA-C | 7.07 | 130.10 | 111.00 |
| 2 | F | 127 | PRO | N-CA-C | -7.07 | 93.72 | 112.10 |
| 2 | B | 280 | ASP | CA-C-N | -7.05 | 101.69 | 117.20 |
| 1 | D | 1015 | THR | N-CA-C | 7.05 | 130.03 | 111.00 |
| 1 | D | 357 | ALA | C-N-CA | -7.05 | 104.08 | 121.70 |
| 1 | A | 1236 | GLN | N-CA-C | 7.01 | 129.93 | 111.00 |
| 2 | C | 471 | LEU | CA-CB-CG | -6.97 | 99.26 | 115.30 |
| 1 | D | 1237 | PRO | N-CA-C | 6.97 | 130.23 | 112.10 |
| 1 | D | 768 | LYS | N-CA-C | -6.97 | 92.18 | 111.00 |
| 2 | F | 343 | ASP | N-CA-C | -6.93 | 92.29 | 111.00 |
| 1 | A | 1211 | GLY | N-CA-C | -6.93 | 95.78 | 113.10 |
| 1 | D | 991 | GLY | N-CA-C | 6.92 | 130.41 | 113.10 |
| 1 | D | 891 | VAL | CA-CB-CG1 | -6.91 | 100.53 | 110.90 |
| 2 | C | 320 | SER | N-CA-C | 6.90 | 129.62 | 111.00 |
| 1 | A | 759 | SER | N-CA-C | 6.88 | 129.57 | 111.00 |
| 2 | F | 457 | SER | N-CA-C | 6.87 | 129.55 | 111.00 |
| 1 | D | 633 | LYS | N-CA-C | 6.86 | 129.53 | 111.00 |
| 1 | A | 122 | ASP | N-CA-C | 6.83 | 129.43 | 111.00 |
| 2 | C | 318 | ASN | N-CA-C | -6.82 | 92.60 | 111.00 |
| 1 | A | 1031 | GLU | N-CA-C | -6.81 | 92.62 | 111.00 |
| 1 | A | 258 | GLN | N-CA-C | -6.80 | 92.64 | 111.00 |
| 1 | D | 710 | ALA | N-CA-C | 6.79 | 129.35 | 111.00 |
| 1 | D | 846 | THR | N-CA-C | -6.79 | 92.68 | 111.00 |
| 2 | E | 384 | ALA | CA-C-N | -6.76 | 102.33 | 117.20 |
| 2 | F | 318 | ASN | N-CA-C | -6.76 | 92.75 | 111.00 |
| 2 | C | 286 | GLY | N-CA-C | -6.74 | 96.26 | 113.10 |
| 1 | D | 1180 | PHE | N-CA-C | 6.74 | 129.19 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | A | 259 | ARG | N-CA-C | 6.73 | 129.18 | 111.00 |
| 1 | A | 1232 | GLU | N-CA-C | -6.73 | 92.82 | 111.00 |
| 1 | A | 277 | HIS | N-CA-C | -6.72 | 92.86 | 111.00 |
| 1 | A | 231 | GLU | N-CA-C | 6.72 | 129.13 | 111.00 |
| 2 | F | 318 | ASN | C-N-CA | 6.71 | 138.48 | 121.70 |
| 1 | D | 354 | ASN | N-CA-C | 6.69 | 129.07 | 111.00 |
| 2 | C | 133 | HIS | N-CA-C | 6.68 | 129.05 | 111.00 |
| 1 | D | 1070 | PRO | CA-N-CD | -6.68 | 102.14 | 111.50 |
| 2 | F | 139 | LEU | N-CA-C | 6.68 | 129.03 | 111.00 |
| 1 | A | 92 | GLY | N-CA-C | -6.68 | 96.41 | 113.10 |
| 2 | C | 457 | SER | N-CA-C | 6.66 | 128.99 | 111.00 |
| 1 | D | 516 | GLU | N-CA-C | 6.66 | 128.99 | 111.00 |
| 2 | F | 134 | LYS | N-CA-C | 6.65 | 128.94 | 111.00 |
| 2 | F | 247 | THR | N-CA-C | -6.65 | 93.06 | 111.00 |
| 2 | C | 178 | SER | N-CA-C | 6.63 | 128.89 | 111.00 |
| 1 | D | 248 | GLU | C-N-CA | 6.63 | 138.27 | 121.70 |
| 2 | E | 280 | ASP | N-CA-C | 6.61 | 128.84 | 111.00 |
| 1 | D | 938 | THR | N-CA-C | -6.60 | 93.17 | 111.00 |
| 1 | D | 759 | SER | N-CA-C | 6.56 | 128.70 | 111.00 |
| 1 | A | 1206 | MET | N-CA-C | 6.55 | 128.70 | 111.00 |
| 1 | A | 419 | PRO | N-CA-C | 6.54 | 129.11 | 112.10 |
| 2 | F | 120 | VAL | N-CA-C | 6.54 | 128.65 | 111.00 |
| 1 | D | 272 | SER | N-CA-C | -6.48 | 93.49 | 111.00 |
| 2 | B | 281 | GLU | O-C-N | 6.47 | 133.06 | 122.70 |
| 2 | C | 127 | PRO | N-CA-C | -6.46 | 95.29 | 112.10 |
| 2 | F | 178 | SER | N-CA-C | 6.46 | 128.44 | 111.00 |
| 2 | C | 247 | THR | N-CA-C | -6.46 | 93.57 | 111.00 |
| 2 | C | 459 | ASP | CA-C-N | -6.45 | 103.01 | 117.20 |
| 1 | D | 565 | HIS | N-CA-C | -6.44 | 93.60 | 111.00 |
| 1 | D | 351 | SER | O-C-N | 6.43 | 132.99 | 122.70 |
| 2 | C | 335 | VAL | CB-CA-C | -6.42 | 99.21 | 111.40 |
| 2 | F | 452 | LEU | N-CA-C | -6.41 | 93.69 | 111.00 |
| 1 | D | 193 | ARG | N-CA-C | -6.39 | 93.73 | 111.00 |
| 1 | A | 82 | GLY | N-CA-C | -6.36 | 97.19 | 113.10 |
| 1 | A | 238 | GLN | C-N-CA | 6.34 | 137.55 | 121.70 |
| 1 | A | 346 | ASP | N-CA-C | 6.34 | 128.12 | 111.00 |
| 1 | A | 349 | ASP | N-CA-C | -6.34 | 93.88 | 111.00 |
| 2 | F | 299 | LEU | N-CA-C | 6.33 | 128.10 | 111.00 |
| 1 | A | 1206 | MET | CA-CB-CG | -6.33 | 102.54 | 113.30 |
| 1 | A | 1174 | PRO | N-CA-C | 6.32 | 128.54 | 112.10 |
| 1 | D | 275 | ARG | N-CA-C | -6.32 | 93.92 | 111.00 |
| 2 | C | 428 | LEU | CA-CB-CG | -6.32 | 100.76 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | D | 291 | PHE | N-CA-C | 6.31 | 128.05 | 111.00 |
| 1 | D | 566 | LEU | CA-CB-CG | 6.31 | 129.81 | 115.30 |
| 1 | A | 658 | LYS | N-CA-C | -6.31 | 93.97 | 111.00 |
| 1 | A | 233 | TYR | N-CA-C | 6.30 | 128.02 | 111.00 |
| 2 | B | 309 | HIS | N-CA-C | 6.30 | 128.00 | 111.00 |
| 1 | D | 116 | PRO | N-CA-C | -6.27 | 95.79 | 112.10 |
| 1 | A | 1024 | ASP | N-CA-C | 6.27 | 127.92 | 111.00 |
| 1 | A | 72 | ASN | N-CA-C | -6.26 | 94.11 | 111.00 |
| 1 | A | 956 | GLY | N-CA-C | 6.25 | 128.72 | 113.10 |
| 1 | A | 1198 | LYS | N-CA-C | -6.23 | 94.18 | 111.00 |
| 1 | A | 1209 | ARG | N-CA-C | -6.17 | 94.33 | 111.00 |
| 1 | D | 1008 | LEU | CA-CB-CG | 6.16 | 129.47 | 115.30 |
| 1 | A | 825 | VAL | N-CA-C | -6.16 | 94.37 | 111.00 |
| 1 | D | 579 | ARG | N-CA-C | -6.16 | 94.37 | 111.00 |
| 2 | C | 299 | LEU | N-CA-C | 6.14 | 127.59 | 111.00 |
| 1 | A | 1011 | PRO | N-CA-C | -6.14 | 96.15 | 112.10 |
| 1 | D | 164 | PRO | N-CA-C | -6.13 | 96.15 | 112.10 |
| 2 | C | 134 | LYS | N-CA-C | 6.13 | 127.56 | 111.00 |
| 1 | D | 1179 | PHE | N-CA-C | 6.13 | 127.55 | 111.00 |
| 2 | E | 381 | ILE | CA-C-O | 6.12 | 132.96 | 120.10 |
| 1 | A | 256 | PRO | N-CA-C | -6.11 | 96.22 | 112.10 |
| 1 | A | 466 | LEU | CA-CB-CG | 6.09 | 129.30 | 115.30 |
| 1 | A | 392 | LEU | N-CA-C | 6.08 | 127.42 | 111.00 |
| 1 | A | 951 | TYR | N-CA-C | -6.07 | 94.61 | 111.00 |
| 1 | D | 532 | PRO | N-CA-C | 6.06 | 127.86 | 112.10 |
| 1 | D | 744 | ILE | N-CA-C | 6.05 | 127.33 | 111.00 |
| 1 | D | 364 | VAL | N-CA-C | 6.03 | 127.28 | 111.00 |
| 1 | A | 632 | ALA | N-CA-C | -6.02 | 94.75 | 111.00 |
| 1 | A | 846 | THR | N-CA-C | -6.02 | 94.75 | 111.00 |
| 1 | A | 1026 | ARG | N-CA-CB | -6.02 | 99.76 | 110.60 |
| 1 | D | 192 | GLU | N-CA-C | 6.01 | 127.24 | 111.00 |
| 1 | A | 130 | LEU | N-CA-C | 5.98 | 127.14 | 111.00 |
| 1 | A | 131 | TYR | N-CA-C | 5.97 | 127.13 | 111.00 |
| 2 | E | 281 | GLU | N-CA-C | -5.97 | 94.88 | 111.00 |
| 1 | D | 648 | PRO | N-CA-C | -5.96 | 96.61 | 112.10 |
| 2 | F | 450 | ASN | N-CA-C | -5.93 | 94.98 | 111.00 |
| 1 | D | 348 | LEU | CA-CB-CG | 5.92 | 128.93 | 115.30 |
| 1 | A | 1030 | ARG | N-CA-C | -5.91 | 95.05 | 111.00 |
| 1 | A | 518 | ALA | N-CA-C | 5.90 | 126.94 | 111.00 |
| 1 | A | 226 | GLN | N-CA-C | -5.90 | 95.07 | 111.00 |
| 2 | E | 107 | ARG | NE-CZ-NH1 | 5.89 | 123.25 | 120.30 |
| 1 | D | 346 | ASP | CB-CA-C | 5.89 | 122.17 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 220 | TRP | N-CA-C | 5.88 | 126.89 | 111.00 |
| 1 | A | 383 | LYS | N-CA-C | -5.87 | 95.14 | 111.00 |
| 1 | D | 734 | HIS | N-CA-C | -5.87 | 95.16 | 111.00 |
| 1 | D | 821 | LEU | C-N-CD | -5.87 | 107.70 | 120.60 |
| 1 | A | 121 | PRO | N-CA-C | 5.85 | 127.31 | 112.10 |
| 1 | A | 966 | LEU | CA-CB-CG | 5.85 | 128.75 | 115.30 |
| 2 | C | 236 | GLU | N-CA-C | 5.85 | 126.79 | 111.00 |
| 2 | E | 385 | LEU | C-N-CA | -5.84 | 107.09 | 121.70 |
| 1 | A | 275 | ARG | N-CA-C | -5.84 | 95.24 | 111.00 |
| 1 | D | 537 | GLU | N-CA-C | 5.84 | 126.76 | 111.00 |
| 1 | D | 671 | GLN | C-N-CA | 5.84 | 136.29 | 121.70 |
| 1 | A | 1171 | ASN | N-CA-C | 5.83 | 126.75 | 111.00 |
| 2 | C | 400 | GLN | N-CA-C | -5.82 | 95.29 | 111.00 |
| 1 | A | 1125 | ILE | N-CA-C | 5.82 | 126.70 | 111.00 |
| 1 | D | 418 | CYS | C-N-CD | -5.81 | 107.82 | 120.60 |
| 1 | A | 209 | PRO | N-CA-C | 5.81 | 127.20 | 112.10 |
| 1 | A | 108 | GLN | N-CA-C | -5.80 | 95.33 | 111.00 |
| 2 | B | 260 | LEU | N-CA-C | -5.80 | 95.35 | 111.00 |
| 1 | A | 628 | ARG | N-CA-C | -5.79 | 95.38 | 111.00 |
| 2 | C | 458 | ARG | NE-CZ-NH2 | -5.79 | 117.41 | 120.30 |
| 2 | E | 179 | GLY | N-CA-C | -5.79 | 98.64 | 113.10 |
| 2 | F | 467 | HIS | N-CA-C | -5.79 | 95.38 | 111.00 |
| 1 | A | 418 | CYS | C-N-CD | -5.77 | 107.90 | 120.60 |
| 2 | B | 267 | ALA | N-CA-C | 5.76 | 126.56 | 111.00 |
| 1 | D | 1020 | ILE | N-CA-C | 5.75 | 126.52 | 111.00 |
| 1 | A | 238 | GLN | CB-CA-C | -5.74 | 98.92 | 110.40 |
| 2 | F | 236 | GLU | N-CA-C | 5.72 | 126.45 | 111.00 |
| 2 | C | 139 | LEU | N-CA-C | 5.72 | 126.44 | 111.00 |
| 1 | D | 77 | GLN | N-CA-C | 5.71 | 126.42 | 111.00 |
| 1 | A | 348 | LEU | N-CA-C | -5.70 | 95.61 | 111.00 |
| 1 | A | 1218 | LEU | N-CA-C | 5.70 | 126.39 | 111.00 |
| 1 | A | 498 | LYS | N-CA-C | 5.69 | 126.37 | 111.00 |
| 2 | C | 302 | THR | N-CA-C | 5.68 | 126.34 | 111.00 |
| 1 | A | 784 | GLY | N-CA-C | 5.67 | 127.29 | 113.10 |
| 2 | E | 386 | ASP | N-CA-C | 5.67 | 126.31 | 111.00 |
| 1 | A | 1204 | THR | N-CA-C | 5.67 | 126.31 | 111.00 |
| 1 | D | 874 | LEU | N-CA-C | 5.65 | 126.25 | 111.00 |
| 1 | D | 999 | ASP | N-CA-CB | -5.64 | 100.44 | 110.60 |
| 1 | A | 1213 | PRO | CA-N-CD | -5.63 | 103.61 | 111.50 |
| 1 | D | 1067 | SER | N-CA-C | -5.63 | 95.81 | 111.00 |
| 1 | A | 660 | CYS | N-CA-C | 5.62 | 126.19 | 111.00 |
| 1 | A | 130 | LEU | CA-CB-CG | -5.62 | 102.38 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 872 | SER | C-N-CA | 5.60 | 135.70 | 121.70 |
| 1 | D | 280 | GLU | OE1-CD-OE2 | -5.60 | 116.58 | 123.30 |
| 1 | D | 841 | LEU | CA-CB-CG | 5.60 | 128.17 | 115.30 |
| 1 | D | 735 | GLY | C-N-CA | 5.59 | 135.69 | 121.70 |
| 2 | C | 469 | SER | N-CA-C | 5.59 | 126.09 | 111.00 |
| 1 | D | 651 | ALA | N-CA-C | -5.59 | 95.92 | 111.00 |
| 2 | B | 311 | LEU | N-CA-C | -5.58 | 95.93 | 111.00 |
| 1 | D | 616 | GLU | N-CA-C | 5.58 | 126.07 | 111.00 |
| 1 | A | 1067 | SER | N-CA-C | 5.58 | 126.06 | 111.00 |
| 1 | A | 737 | GLY | N-CA-C | 5.58 | 127.04 | 113.10 |
| 1 | D | 189 | ILE | N-CA-C | -5.57 | 95.96 | 111.00 |
| 1 | A | 560 | PRO | N-CA-C | 5.56 | 126.56 | 112.10 |
| 1 | A | 1158 | LEU | CA-CB-CG | -5.54 | 102.56 | 115.30 |
| 1 | A | 996 | ARG | NE-CZ-NH1 | -5.52 | 117.54 | 120.30 |
| 1 | D | 1179 | PHE | C-N-CA | 5.52 | 135.51 | 121.70 |
| 1 | D | 352 | SER | CA-C-O | 5.52 | 131.70 | 120.10 |
| 1 | D | 510 | ALA | N-CA-C | -5.52 | 96.09 | 111.00 |
| 1 | D | 581 | ASP | N-CA-C | 5.52 | 125.91 | 111.00 |
| 1 | A | 1214 | GLN | N-CA-C | 5.52 | 125.90 | 111.00 |
| 2 | B | 121 | PHE | N-CA-C | 5.51 | 125.89 | 111.00 |
| 1 | A | 180 | PRO | N-CA-C | -5.51 | 97.77 | 112.10 |
| 1 | D | 351 | SER | CA-C-O | -5.50 | 108.54 | 120.10 |
| 1 | A | 610 | PHE | C-N-CA | -5.49 | 98.92 | 122.00 |
| 1 | D | 605 | LEU | C-N-CA | -5.49 | 107.97 | 121.70 |
| 1 | A | 255 | SER | N-CA-C | 5.48 | 125.79 | 111.00 |
| 1 | A | 79 | LEU | CB-CG-CD2 | -5.47 | 101.70 | 111.00 |
| 2 | C | 341 | ASP | N-CA-C | -5.47 | 96.23 | 111.00 |
| 2 | F | 280 | ASP | N-CA-C | 5.47 | 125.77 | 111.00 |
| 2 | F | 445 | GLU | N-CA-C | 5.47 | 125.77 | 111.00 |
| 1 | A | 286 | GLY | N-CA-C | -5.46 | 99.46 | 113.10 |
| 1 | A | 907 | PHE | N-CA-C | -5.45 | 96.28 | 111.00 |
| 1 | A | 218 | SER | N-CA-CB | -5.44 | 102.33 | 110.50 |
| 1 | D | 212 | ALA | N-CA-C | -5.44 | 96.31 | 111.00 |
| 1 | A | 172 | ALA | N-CA-C | 5.43 | 125.66 | 111.00 |
| 1 | A | 581 | ASP | N-CA-C | 5.42 | 125.64 | 111.00 |
| 2 | C | 279 | GLN | CA-C-N | -5.42 | 105.26 | 117.20 |
| 2 | F | 86 | LEU | CB-CG-CD2 | -5.42 | 101.79 | 111.00 |
| 1 | D | 1142 | ARG | N-CA-C | -5.40 | 96.41 | 111.00 |
| 1 | A | 1070 | PRO | CA-N-CD | -5.40 | 103.94 | 111.50 |
| 1 | D | 221 | TYR | N-CA-C | 5.40 | 125.57 | 111.00 |
| 1 | D | 1171 | ASN | N-CA-C | 5.40 | 125.57 | 111.00 |
| 2 | B | 310 | GLU | N-CA-C | -5.39 | 96.44 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | D | 515 | ILE | N-CA-C | 5.38 | 125.53 | 111.00 |
| 2 | C | 129 | ASP | N-CA-C | 5.38 | 125.52 | 111.00 |
| 1 | D | 1177 | VAL | N-CA-C | -5.38 | 96.48 | 111.00 |
| 1 | D | 775 | GLU | N-CA-C | -5.37 | 96.50 | 111.00 |
| 2 | F | 367 | LEU | N-CA-C | -5.37 | 96.51 | 111.00 |
| 1 | A | 238 | GLN | CA-C-N | -5.36 | 105.40 | 117.20 |
| 1 | A | 74 | LEU | C-N-CA | -5.36 | 108.30 | 121.70 |
| 1 | D | 247 | LEU | CB-CG-CD1 | -5.36 | 101.90 | 111.00 |
| 2 | F | 133 | HIS | C-N-CA | 5.34 | 135.05 | 121.70 |
| 2 | F | 355 | GLN | N-CA-C | -5.34 | 96.58 | 111.00 |
| 1 | D | 71 | HIS | N-CA-C | 5.33 | 125.40 | 111.00 |
| 1 | A | 232 | ARG | C-N-CA | 5.33 | 135.03 | 121.70 |
| 1 | D | 1131 | ILE | N-CA-C | 5.33 | 125.38 | 111.00 |
| 1 | A | 919 | MET | N-CA-C | -5.31 | 96.67 | 111.00 |
| 1 | A | 521 | PRO | N-CA-C | 5.30 | 125.88 | 112.10 |
| 1 | D | 1179 | PHE | CA-C-N | -5.29 | 105.55 | 117.20 |
| 1 | D | 919 | MET | N-CA-C | -5.29 | 96.71 | 111.00 |
| 1 | D | 257 | THR | N-CA-C | 5.29 | 125.29 | 111.00 |
| 1 | A | 873 | GLU | N-CA-C | 5.28 | 125.26 | 111.00 |
| 1 | A | 574 | ARG | N-CA-C | 5.28 | 125.25 | 111.00 |
| 1 | D | 528 | GLU | N-CA-C | 5.28 | 125.24 | 111.00 |
| 1 | A | 626 | GLY | N-CA-C | 5.27 | 126.28 | 113.10 |
| 2 | F | 459 | ASP | N-CA-C | 5.27 | 125.22 | 111.00 |
| 1 | D | 74 | LEU | N-CA-C | 5.26 | 125.21 | 111.00 |
| 1 | A | 1193 | VAL | N-CA-C | 5.26 | 125.20 | 111.00 |
| 1 | D | 530 | LEU | CA-CB-CG | 5.26 | 127.39 | 115.30 |
| 1 | D | 1072 | THR | N-CA-C | 5.25 | 125.17 | 111.00 |
| 1 | D | 353 | VAL | N-CA-CB | -5.25 | 99.96 | 111.50 |
| 2 | C | 133 | HIS | CA-C-N | -5.24 | 105.67 | 117.20 |
| 1 | D | 128 | PRO | N-CA-C | 5.23 | 125.71 | 112.10 |
| 1 | D | 239 | LEU | N-CA-C | -5.23 | 96.87 | 111.00 |
| 1 | D | 198 | ASP | N-CA-C | -5.23 | 96.87 | 111.00 |
| 1 | A | 563 | PRO | N-CA-C | 5.23 | 125.69 | 112.10 |
| 1 | A | 522 | GLY | N-CA-C | 5.22 | 126.16 | 113.10 |
| 1 | A | 1001 | GLY | N-CA-C | -5.22 | 100.04 | 113.10 |
| 1 | D | 657 | ARG | N-CA-C | 5.21 | 125.08 | 111.00 |
| 2 | E | 325 | ARG | N-CA-C | 5.21 | 125.08 | 111.00 |
| 1 | A | 183 | GLU | N-CA-C | 5.21 | 125.06 | 111.00 |
| 1 | A | 74 | LEU | CA-CB-CG | 5.21 | 127.28 | 115.30 |
| 1 | A | 1210 | TYR | CA-C-N | -5.20 | 105.80 | 116.20 |
| 1 | D | 881 | PRO | C-N-CD | -5.20 | 109.17 | 120.60 |
| 2 | C | 92 | LEU | CA-CB-CG | -5.20 | 103.35 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | D | 498 | LYS | N-CA-C | 5.20 | 125.03 | 111.00 |
| 2 | E | 432 | TYR | CA-CB-CG | 5.20 | 123.27 | 113.40 |
| 2 | E | 378 | LEU | CB-CG-CD2 | -5.19 | 102.17 | 111.00 |
| 1 | D | 727 | ASP | N-CA-C | -5.19 | 96.98 | 111.00 |
| 1 | A | 757 | GLY | N-CA-C | -5.19 | 100.13 | 113.10 |
| 2 | C | 133 | HIS | C-N-CA | 5.18 | 134.66 | 121.70 |
| 2 | F | 449 | GLU | N-CA-C | 5.18 | 124.99 | 111.00 |
| 1 | A | 606 | THR | CB-CA-C | -5.18 | 97.62 | 111.60 |
| 1 | A | 611 | PRO | N-CA-C | 5.18 | 125.56 | 112.10 |
| 1 | D | 1210 | TYR | N-CA-C | -5.17 | 97.06 | 111.00 |
| 1 | A | 1142 | ARG | N-CA-C | -5.16 | 97.08 | 111.00 |
| 2 | E | 381 | ILE | CB-CA-C | 5.15 | 121.90 | 111.60 |
| 1 | A | 1201 | SER | N-CA-C | -5.15 | 97.09 | 111.00 |
| 1 | D | 130 | LEU | CA-CB-CG | -5.15 | 103.46 | 115.30 |
| 2 | B | 215 | PHE | N-CA-C | 5.15 | 124.89 | 111.00 |
| 1 | D | 1132 | SER | N-CA-C | -5.14 | 97.11 | 111.00 |
| 1 | A | 1231 | LEU | N-CA-C | 5.13 | 124.86 | 111.00 |
| 1 | D | 612 | LEU | CB-CG-CD2 | -5.13 | 102.28 | 111.00 |
| 1 | D | 1021 | SER | N-CA-C | -5.12 | 97.18 | 111.00 |
| 1 | A | 612 | LEU | N-CA-C | -5.12 | 97.18 | 111.00 |
| 1 | D | 292 | LEU | CA-CB-CG | -5.11 | 103.54 | 115.30 |
| 2 | C | 458 | ARG | NE-CZ-NH1 | 5.11 | 122.86 | 120.30 |
| 2 | B | 280 | ASP | N-CA-C | 5.11 | 124.79 | 111.00 |
| 2 | C | 467 | HIS | N-CA-C | -5.09 | 97.26 | 111.00 |
| 1 | D | 1013 | ASP | N-CA-C | 5.08 | 124.73 | 111.00 |
| 1 | D | 411 | LEU | N-CA-C | 5.08 | 124.71 | 111.00 |
| 1 | D | 515 | ILE | CB-CA-C | -5.07 | 101.46 | 111.60 |
| 1 | A | 187 | VAL | N-CA-C | -5.06 | 97.33 | 111.00 |
| 2 | C | 197 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 1 | D | 192 | GLU | CA-C-N | -5.06 | 106.06 | 117.20 |
| 1 | D | 622 | TYR | N-CA-C | 5.06 | 124.67 | 111.00 |
| 1 | D | 992 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 1 | A | 370 | PRO | N-CA-C | -5.06 | 98.95 | 112.10 |
| 1 | D | 609 | GLY | N-CA-C | -5.06 | 100.46 | 113.10 |
| 1 | A | 231 | GLU | CA-C-N | -5.05 | 106.08 | 117.20 |
| 1 | A | 528 | GLU | N-CA-C | 5.03 | 124.58 | 111.00 |
| 1 | A | 189 | ILE | CB-CA-C | -5.03 | 101.55 | 111.60 |
| 2 | B | 281 | GLU | N-CA-C | 5.03 | 124.57 | 111.00 |
| 1 | D | 1031 | GLU | N-CA-C | -5.02 | 97.44 | 111.00 |
| 2 | B | 271 | SER | N-CA-C | -5.02 | 97.44 | 111.00 |
| 1 | A | 224 | CYS | CB-CA-C | -5.02 | 100.36 | 110.40 |
| 1 | A | 229 | VAL | CA-CB-CG2 | -5.01 | 103.38 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|------|------|-----------|------|------------------------|---------------------|
| 1 | D | 1073 | PRO | N-CA-C | 5.01 | 125.13 | 112.10 |
| 2 | C | 138 | LEU | N-CA-C | 5.01 | 124.53 | 111.00 |
| 1 | D | 346 | ASP | CB-CG-OD2 | 5.00 | 122.80 | 118.30 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | D | 249 | VAL | CA |
| 2 | E | 385 | LEU | CA |

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | A | 1179 | PHE | Sidechain |
| 1 | A | 221 | TYR | Sidechain |
| 1 | A | 239 | LEU | Mainchain |
| 1 | A | 395 | TYR | Sidechain |
| 2 | B | 417 | TYR | Sidechain |
| 2 | C | 351 | TYR | Sidechain |
| 1 | D | 368 | PRO | Mainchain |
| 1 | D | 656 | TYR | Sidechain |
| 1 | D | 995 | TYR | Sidechain |
| 2 | E | 432 | TYR | Sidechain |
| 2 | E | 478 | TYR | Sidechain |
| 2 | F | 206 | TYR | Sidechain |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 8681 | 0 | 8521 | 3592 | 8 |
| 1 | D | 8695 | 0 | 8540 | 3900 | 7 |
| 2 | B | 2871 | 0 | 2862 | 809 | 0 |
| 2 | C | 3181 | 0 | 3168 | 1419 | 1 |
| 2 | E | 2871 | 0 | 2862 | 945 | 0 |
| 2 | F | 3181 | 0 | 3168 | 1467 | 4 |
| All | All | 29480 | 0 | 29121 | 11814 | 10 |

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 202.

All (11814) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:352:SER:C | 1:D:352:SER:CA | 1.74 | 1.55 |
| 1:D:460:LYS:N | 1:D:460:LYS:HE2 | 1.20 | 1.48 |
| 2:E:432:TYR:HB2 | 2:E:437:ILE:CD1 | 1.51 | 1.39 |
| 1:D:352:SER:CA | 1:D:358:GLU:OE2 | 1.73 | 1.36 |
| 1:D:914:THR:O | 1:D:918:TRP:HB3 | 1.24 | 1.35 |
| 1:D:352:SER:N | 1:D:358:GLU:OE2 | 1.58 | 1.34 |
| 1:D:995:TYR:CE1 | 1:D:1004:LEU:HB3 | 1.66 | 1.31 |
| 2:C:356:LEU:HB3 | 2:C:359:ASN:ND2 | 1.44 | 1.30 |
| 1:D:460:LYS:H | 1:D:460:LYS:CE | 1.44 | 1.28 |
| 1:A:513:LEU:HB2 | 1:A:568:GLY:CA | 1.64 | 1.28 |
| 1:A:1210:TYR:CE1 | 1:A:1213:PRO:HG2 | 1.68 | 1.28 |
| 2:F:241:TRP:HB2 | 2:F:336:LEU:CD1 | 1.64 | 1.27 |
| 1:A:784:GLY:HA2 | 2:C:362:THR:OG1 | 1.29 | 1.26 |
| 1:D:275:ARG:HB2 | 1:D:843:GLN:CB | 1.64 | 1.25 |
| 1:D:275:ARG:NE | 1:D:843:GLN:H | 1.31 | 1.25 |
| 1:A:669:MET:O | 1:A:673:ALA:HB2 | 1.29 | 1.25 |
| 1:D:1006:ARG:NH1 | 1:D:1006:ARG:HA | 1.49 | 1.25 |
| 1:A:76:ILE:HB | 1:A:911:HIS:NE2 | 1.49 | 1.24 |
| 1:A:210:THR:CB | 1:A:224:CYS:HB2 | 1.66 | 1.24 |
| 1:D:352:SER:C | 1:D:358:GLU:OE2 | 1.75 | 1.23 |
| 1:A:656:TYR:HB3 | 1:A:720:THR:CB | 1.66 | 1.23 |
| 1:D:827:ARG:O | 1:D:829:PRO:HD3 | 1.36 | 1.23 |
| 2:C:241:TRP:HB2 | 2:C:336:LEU:CD1 | 1.69 | 1.23 |
| 2:C:303:LEU:HA | 2:C:337:SER:OG | 1.31 | 1.23 |
| 1:D:891:VAL:HG11 | 1:D:1135:ASP:O | 1.12 | 1.22 |
| 2:E:382:LYS:HE2 | 2:E:412:SER:O | 1.37 | 1.22 |
| 1:D:259:ARG:HA | 1:D:259:ARG:CZ | 1.68 | 1.22 |
| 1:D:1131:ILE:HD11 | 1:D:1138:ARG:N | 1.55 | 1.22 |
| 1:A:389:PHE:HA | 1:A:393:MET:SD | 1.79 | 1.21 |
| 1:D:249:VAL:CG1 | 1:D:252:GLY:H | 1.52 | 1.21 |
| 1:D:367:PRO:CD | 1:D:368:PRO:HD3 | 1.70 | 1.21 |
| 1:D:420:HIS:ND1 | 1:D:421:PRO:HD2 | 1.54 | 1.21 |
| 1:D:801:TRP:CZ3 | 1:D:870:VAL:HG11 | 1.74 | 1.21 |
| 1:D:548:CYS:O | 1:D:552:LEU:HG | 1.35 | 1.21 |
| 2:F:447:THR:O | 2:F:452:LEU:HD12 | 1.40 | 1.21 |
| 2:E:78:PHE:O | 2:E:79:LEU:HG | 1.39 | 1.21 |
| 1:D:1029:GLN:CG | 1:D:1030:ARG:HE | 1.53 | 1.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:477:GLU:CG | 1:A:478:ARG:H | 1.54 | 1.20 |
| 1:D:1020:ILE:HD13 | 1:D:1021:SER:N | 1.54 | 1.20 |
| 1:A:213:VAL:HG12 | 1:A:401:TRP:NE1 | 1.55 | 1.20 |
| 1:D:504:LYS:CB | 1:D:523:ASP:HB2 | 1.71 | 1.20 |
| 1:D:278:ILE:HG22 | 1:D:279:ARG:HD3 | 1.23 | 1.20 |
| 1:D:352:SER:O | 1:D:358:GLU:CD | 1.81 | 1.19 |
| 1:D:604:ALA:HA | 1:D:613:HIS:CE1 | 1.77 | 1.19 |
| 1:A:996:ARG:NH1 | 1:A:1000:GLU:HB3 | 1.58 | 1.19 |
| 1:A:346:ASP:HB3 | 1:A:1040:LYS:HZ3 | 1.03 | 1.19 |
| 1:A:666:GLN:O | 1:A:670:PRO:HD3 | 1.36 | 1.18 |
| 1:A:927:ARG:HG2 | 1:A:928:GLY:H | 1.04 | 1.18 |
| 1:D:275:ARG:CB | 1:D:843:GLN:HB3 | 1.71 | 1.18 |
| 1:D:610:PHE:H | 1:D:611:PRO:HD3 | 1.07 | 1.18 |
| 1:A:1026:ARG:CB | 1:A:1029:GLN:HB2 | 1.74 | 1.18 |
| 1:D:294:THR:HG22 | 1:D:407:PHE:HE2 | 1.06 | 1.18 |
| 1:D:608:ASP:HB3 | 1:D:620:TRP:CD2 | 1.78 | 1.18 |
| 2:E:432:TYR:CB | 2:E:437:ILE:HD11 | 1.73 | 1.18 |
| 2:F:208:LEU:CD1 | 2:F:240:VAL:HB | 1.72 | 1.18 |
| 1:D:992:LEU:HB3 | 1:D:996:ARG:HG2 | 1.18 | 1.18 |
| 1:A:498:LYS:HD2 | 1:A:518:ALA:HB3 | 1.24 | 1.17 |
| 1:D:1027:LYS:NZ | 1:D:1091:GLU:HG2 | 1.60 | 1.17 |
| 2:B:383:VAL:HG13 | 2:B:413:VAL:CG1 | 1.75 | 1.17 |
| 2:C:424:SER:HB3 | 2:C:427:GLN:HE22 | 1.07 | 1.17 |
| 1:D:900:ALA:HB1 | 1:D:915:ALA:HB1 | 1.27 | 1.17 |
| 1:A:1005:VAL:HA | 1:A:1008:LEU:CD1 | 1.73 | 1.17 |
| 1:A:1199:THR:HA | 1:A:1200:PRO:C | 1.64 | 1.17 |
| 2:F:446:THR:HB | 2:F:450:ASN:HB2 | 1.18 | 1.16 |
| 2:B:72:ILE:HA | 2:B:75:ARG:HE | 1.01 | 1.16 |
| 1:D:642:SER:HA | 1:D:645:VAL:HG11 | 1.26 | 1.16 |
| 1:D:891:VAL:CG1 | 1:D:1135:ASP:O | 1.94 | 1.16 |
| 1:D:1165:ALA:HB2 | 1:D:1173:LEU:HD12 | 1.22 | 1.16 |
| 1:A:477:GLU:HG3 | 1:A:478:ARG:N | 1.55 | 1.16 |
| 1:D:420:HIS:CD2 | 1:D:1020:ILE:HD12 | 1.79 | 1.16 |
| 1:A:213:VAL:CG1 | 1:A:401:TRP:HE1 | 1.59 | 1.16 |
| 1:A:612:LEU:HG | 1:A:614:TYR:H | 1.09 | 1.16 |
| 1:A:871:GLY:C | 1:A:873:GLU:H | 1.38 | 1.16 |
| 1:D:1014:ARG:HD2 | 1:D:1014:ARG:O | 1.45 | 1.16 |
| 1:A:593:SER:HA | 1:A:596:MET:HG3 | 1.28 | 1.16 |
| 1:A:823:ARG:HB3 | 1:A:825:VAL:HG23 | 1.20 | 1.15 |
| 1:D:1029:GLN:HG2 | 1:D:1030:ARG:HE | 1.02 | 1.15 |
| 2:F:454:HIS:HB2 | 2:F:466:MET:O | 1.46 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:78:PHE:CE1 | 2:F:103:GLY:HA2 | 1.80 | 1.15 |
| 2:F:454:HIS:HA | 2:F:468:ILE:HD12 | 1.28 | 1.15 |
| 1:D:350:ILE:CG2 | 1:D:352:SER:HB2 | 1.74 | 1.15 |
| 2:E:376:PRO:O | 2:E:380:PRO:HD3 | 1.42 | 1.15 |
| 2:B:383:VAL:CG1 | 2:B:413:VAL:HG13 | 1.76 | 1.15 |
| 2:C:78:PHE:CE1 | 2:C:103:GLY:HA2 | 1.81 | 1.15 |
| 1:D:616:GLU:O | 1:D:725:PRO:HD3 | 1.47 | 1.15 |
| 2:E:372:LEU:HG | 2:E:373:LYS:N | 1.61 | 1.15 |
| 1:A:612:LEU:HD22 | 1:A:621:GLY:N | 1.61 | 1.15 |
| 1:D:891:VAL:HG11 | 1:D:1135:ASP:C | 1.67 | 1.15 |
| 2:C:127:PRO:HD2 | 2:C:210:GLN:HB2 | 1.26 | 1.14 |
| 1:D:548:CYS:C | 1:D:551:LYS:HD3 | 1.67 | 1.14 |
| 1:D:891:VAL:HA | 1:D:894:GLN:CD | 1.66 | 1.14 |
| 1:A:275:ARG:NH2 | 1:A:845:VAL:HA | 1.62 | 1.14 |
| 2:C:386:ASP:HB2 | 2:C:442:LEU:HA | 1.19 | 1.14 |
| 2:C:418:LEU:O | 2:C:421:MET:HG2 | 1.46 | 1.14 |
| 1:A:472:GLN:HG3 | 2:C:460:THR:CA | 1.77 | 1.14 |
| 1:D:509:THR:HB | 1:D:512:LYS:HB3 | 1.27 | 1.14 |
| 1:D:551:LYS:H | 1:D:551:LYS:CD | 1.49 | 1.14 |
| 2:B:309:HIS:HB3 | 2:B:312:LEU:HD22 | 1.29 | 1.14 |
| 1:A:1030:ARG:HG2 | 1:A:1040:LYS:HZ1 | 1.12 | 1.14 |
| 1:D:1131:ILE:CD1 | 1:D:1138:ARG:H | 1.58 | 1.14 |
| 1:D:356:LEU:HD13 | 1:D:369:LEU:CD2 | 1.75 | 1.14 |
| 2:C:443:VAL:HA | 2:C:447:THR:HG21 | 1.28 | 1.14 |
| 1:A:253:ALA:HB2 | 1:A:280:GLU:HB2 | 1.16 | 1.14 |
| 1:A:996:ARG:HH12 | 1:A:1003:TRP:CB | 1.58 | 1.14 |
| 1:D:1204:THR:HA | 1:D:1207:GLU:HB3 | 1.15 | 1.14 |
| 1:D:866:ARG:HG3 | 1:D:1069:ILE:HG21 | 1.15 | 1.14 |
| 1:D:300:ALA:HB2 | 1:D:847:ALA:HB1 | 1.18 | 1.13 |
| 1:D:504:LYS:HD2 | 1:D:523:ASP:HB3 | 1.23 | 1.13 |
| 1:D:81:ARG:NH1 | 1:D:81:ARG:HB2 | 1.63 | 1.13 |
| 1:D:801:TRP:CE3 | 1:D:870:VAL:HG11 | 1.82 | 1.13 |
| 1:A:513:LEU:CB | 1:A:568:GLY:HA2 | 1.78 | 1.13 |
| 2:C:82:SER:HA | 2:C:86:LEU:HD21 | 1.18 | 1.13 |
| 1:D:242:ALA:HB1 | 1:D:245:ILE:HG12 | 1.21 | 1.13 |
| 1:D:267:VAL:HB | 1:D:269:HIS:CD2 | 1.82 | 1.13 |
| 2:F:239:LEU:O | 2:F:338:VAL:HG22 | 1.46 | 1.13 |
| 1:D:1006:ARG:CA | 1:D:1006:ARG:HH11 | 1.61 | 1.13 |
| 2:F:304:TRP:N | 2:F:337:SER:HB2 | 1.60 | 1.13 |
| 2:F:387:VAL:CG2 | 2:F:417:TYR:HA | 1.78 | 1.13 |
| 1:A:618:HIS:N | 1:A:725:PRO:HG2 | 1.64 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:449:GLN:HG2 | 1:D:805:HIS:NE2 | 1.62 | 1.13 |
| 1:D:81:ARG:HH11 | 1:D:81:ARG:HB2 | 1.11 | 1.13 |
| 1:A:253:ALA:HB2 | 1:A:280:GLU:CB | 1.77 | 1.13 |
| 1:A:502:LYS:HG3 | 1:A:503:VAL:H | 1.08 | 1.13 |
| 1:D:275:ARG:HE | 1:D:842:PRO:HA | 1.02 | 1.13 |
| 2:E:213:VAL:HA | 2:E:235:THR:HA | 1.28 | 1.13 |
| 1:D:1006:ARG:NH1 | 1:D:1009:ASN:HB2 | 1.61 | 1.13 |
| 1:D:891:VAL:HG13 | 1:D:1135:ASP:HB3 | 1.28 | 1.13 |
| 1:A:444:TYR:HD2 | 1:A:874:LEU:HD23 | 1.07 | 1.13 |
| 2:C:125:VAL:HG22 | 2:C:208:LEU:HA | 1.16 | 1.13 |
| 1:A:608:ASP:HB3 | 1:A:779:LEU:CD1 | 1.77 | 1.12 |
| 2:B:279:GLN:O | 2:B:280:ASP:HB2 | 1.49 | 1.12 |
| 2:C:351:TYR:C | 2:C:355:GLN:HB2 | 1.68 | 1.12 |
| 1:A:992:LEU:HD23 | 1:A:997:LEU:HD12 | 1.25 | 1.12 |
| 2:E:432:TYR:HA | 2:E:435:MET:HB2 | 1.18 | 1.12 |
| 2:C:236:GLU:HA | 2:C:341:ASP:HB3 | 1.30 | 1.12 |
| 2:C:446:THR:HA | 2:C:450:ASN:CB | 1.78 | 1.12 |
| 1:D:235:TRP:HD1 | 1:D:236:THR:HG22 | 1.06 | 1.12 |
| 1:A:959:GLN:HB2 | 1:A:960:PRO:CD | 1.78 | 1.12 |
| 1:D:797:MET:HB2 | 1:D:869:ARG:HD2 | 1.30 | 1.12 |
| 1:D:1221:TYR:HA | 1:D:1224:ILE:CG2 | 1.80 | 1.12 |
| 1:A:756:ASP:HB3 | 1:A:1057:MET:HG2 | 1.20 | 1.12 |
| 1:A:245:ILE:HG13 | 1:A:246:PRO:HD3 | 1.31 | 1.12 |
| 1:D:652:ILE:HA | 1:D:655:LEU:HG | 1.30 | 1.12 |
| 2:F:203:ARG:CA | 2:F:325:ARG:HD3 | 1.79 | 1.12 |
| 1:A:1043:VAL:HG13 | 1:A:1046:GLU:HB3 | 1.16 | 1.12 |
| 1:A:658:LYS:HG3 | 1:A:713:PRO:HB2 | 1.30 | 1.12 |
| 2:B:285:LYS:HG2 | 2:B:286:GLY:N | 1.56 | 1.12 |
| 2:C:203:ARG:HA | 2:C:325:ARG:HD3 | 1.20 | 1.12 |
| 1:D:668:LEU:O | 1:D:671:GLN:HB2 | 1.46 | 1.12 |
| 1:A:346:ASP:HB3 | 1:A:1040:LYS:NZ | 1.64 | 1.12 |
| 1:D:1133:ILE:HB | 1:D:1136:GLU:HB2 | 1.17 | 1.12 |
| 1:D:235:TRP:CD1 | 1:D:236:THR:HG22 | 1.84 | 1.12 |
| 1:D:203:LEU:H | 1:D:380:GLY:HA2 | 1.02 | 1.12 |
| 1:D:1193:VAL:CG2 | 1:D:1194:THR:H | 1.60 | 1.12 |
| 1:D:591:LEU:HD11 | 1:D:594:LEU:HG | 1.31 | 1.12 |
| 1:D:775:GLU:HG2 | 1:D:780:GLN:HG3 | 1.31 | 1.12 |
| 1:A:503:VAL:HB | 1:A:521:PRO:HA | 1.30 | 1.12 |
| 1:A:79:LEU:HD21 | 1:A:1173:LEU:O | 1.48 | 1.11 |
| 1:A:135:LEU:H | 1:A:135:LEU:HD23 | 1.05 | 1.11 |
| 1:A:210:THR:HB | 1:A:224:CYS:CB | 1.79 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:70:ARG:HB2 | 1:A:81:ARG:HB3 | 1.32 | 1.11 |
| 1:D:649:TYR:HA | 1:D:652:ILE:HB | 1.19 | 1.11 |
| 2:F:387:VAL:HG21 | 2:F:417:TYR:HA | 1.25 | 1.11 |
| 1:D:128:PRO:HA | 1:D:130:LEU:CD2 | 1.80 | 1.11 |
| 1:A:775:GLU:HA | 1:A:780:GLN:HG3 | 1.32 | 1.11 |
| 1:D:367:PRO:HD2 | 1:D:368:PRO:CD | 1.79 | 1.11 |
| 2:F:372:LEU:HD11 | 2:F:436:SER:HB2 | 1.12 | 1.11 |
| 1:A:659:HIS:HB2 | 1:A:719:LEU:HD12 | 1.30 | 1.11 |
| 1:A:854:ALA:HB1 | 1:A:860:LEU:HD13 | 1.30 | 1.11 |
| 1:A:408:GLN:HA | 1:A:411:LEU:HG | 1.26 | 1.11 |
| 1:A:502:LYS:HD2 | 1:A:506:GLU:OE1 | 1.49 | 1.11 |
| 2:C:131:LEU:HG | 2:C:133:HIS:CE1 | 1.85 | 1.11 |
| 1:D:1200:PRO:O | 1:D:1203:PRO:HD2 | 1.47 | 1.11 |
| 1:A:436:PRO:HB3 | 1:A:881:PRO:HD3 | 1.13 | 1.11 |
| 1:D:375:GLU:HG3 | 1:D:379:LYS:HB3 | 1.29 | 1.11 |
| 2:F:247:THR:HB | 2:F:251:TRP:CD1 | 1.85 | 1.11 |
| 1:A:656:TYR:HB3 | 1:A:720:THR:HB | 1.24 | 1.11 |
| 2:F:354:PHE:CE1 | 2:F:370:LYS:HD3 | 1.84 | 1.11 |
| 1:A:758:ASN:HB2 | 1:A:1058:PHE:HZ | 1.09 | 1.11 |
| 1:D:420:HIS:HD2 | 1:D:1020:ILE:HD12 | 0.97 | 1.11 |
| 1:D:1131:ILE:HD11 | 1:D:1138:ARG:H | 1.04 | 1.11 |
| 1:D:781:ALA:HB3 | 1:D:792:LEU:HD21 | 1.31 | 1.11 |
| 1:A:170:ALA:HB1 | 1:A:175:TRP:CZ2 | 1.85 | 1.10 |
| 1:A:612:LEU:HG | 1:A:613:HIS:N | 1.59 | 1.10 |
| 2:C:372:LEU:HD11 | 2:C:436:SER:HB2 | 1.33 | 1.10 |
| 1:D:1204:THR:CA | 1:D:1207:GLU:HB3 | 1.81 | 1.10 |
| 1:D:179:GLY:HA3 | 1:D:182:GLY:HA3 | 1.13 | 1.10 |
| 1:D:592:LEU:HA | 1:D:595:GLN:HG3 | 1.33 | 1.10 |
| 1:A:612:LEU:HG | 1:A:613:HIS:H | 1.06 | 1.10 |
| 1:A:249:VAL:HG11 | 1:A:817:PRO:HG3 | 1.30 | 1.10 |
| 2:B:407:LEU:HD21 | 2:C:120:VAL:HA | 1.23 | 1.10 |
| 1:D:1209:ARG:HH21 | 2:F:253:ASP:HA | 1.01 | 1.10 |
| 1:D:1206:MET:SD | 1:D:1210:TYR:HA | 1.90 | 1.10 |
| 1:A:190:PRO:HB3 | 1:A:192:GLU:HG2 | 1.15 | 1.10 |
| 2:B:117:SER:HB2 | 2:B:262:TRP:NE1 | 1.64 | 1.10 |
| 1:D:242:ALA:HB1 | 1:D:245:ILE:CG1 | 1.80 | 1.10 |
| 1:A:363:ARG:HH22 | 1:A:409:GLN:HB2 | 1.16 | 1.10 |
| 1:D:1231:LEU:HG | 1:D:1232:GLU:H | 0.98 | 1.10 |
| 1:D:212:ALA:O | 1:D:213:VAL:HB | 1.52 | 1.10 |
| 1:D:556:THR:HA | 1:D:559:LEU:HD23 | 1.33 | 1.10 |
| 2:C:203:ARG:CA | 2:C:325:ARG:HD3 | 1.81 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:798:ILE:HG22 | 1:D:869:ARG:HH22 | 1.06 | 1.10 |
| 2:F:241:TRP:CB | 2:F:336:LEU:HD12 | 1.80 | 1.10 |
| 1:A:176:THR:HA | 1:A:218:SER:HB2 | 1.13 | 1.10 |
| 1:A:490:TRP:HA | 1:A:580:LEU:HD22 | 1.29 | 1.10 |
| 1:A:436:PRO:HB2 | 1:A:879:GLN:HA | 1.33 | 1.10 |
| 1:D:1193:VAL:HG22 | 1:D:1194:THR:N | 1.66 | 1.10 |
| 1:D:504:LYS:HB2 | 1:D:523:ASP:HB2 | 1.10 | 1.10 |
| 2:C:382:LYS:HD3 | 2:C:411:ILE:HG13 | 1.34 | 1.10 |
| 1:D:270:ASN:OD1 | 1:D:294:THR:HG21 | 1.51 | 1.10 |
| 2:E:403:PHE:HD1 | 2:E:413:VAL:HB | 1.01 | 1.10 |
| 1:A:1148:ARG:HG2 | 1:A:1148:ARG:HH11 | 1.11 | 1.09 |
| 1:A:575:LYS:HG3 | 1:A:576:LEU:H | 1.11 | 1.09 |
| 1:A:997:LEU:HD22 | 1:A:998:SER:H | 1.00 | 1.09 |
| 2:C:446:THR:O | 2:C:450:ASN:HB3 | 1.49 | 1.09 |
| 1:D:1207:GLU:HA | 1:D:1210:TYR:HB3 | 1.33 | 1.09 |
| 2:E:389:ARG:HE | 2:E:390:GLY:N | 1.48 | 1.09 |
| 1:A:288:ARG:HA | 1:A:288:ARG:HE | 0.96 | 1.09 |
| 2:C:423:SER:OG | 2:C:428:LEU:HD21 | 1.51 | 1.09 |
| 1:D:1210:TYR:OH | 1:D:1212:ILE:HB | 1.52 | 1.09 |
| 2:F:466:MET:HB3 | 2:F:471:LEU:HD22 | 1.12 | 1.09 |
| 2:F:82:SER:HA | 2:F:86:LEU:HD21 | 1.30 | 1.09 |
| 2:C:466:MET:HB3 | 2:C:471:LEU:HD22 | 1.24 | 1.09 |
| 1:D:350:ILE:HG23 | 1:D:352:SER:HB2 | 1.30 | 1.09 |
| 2:F:127:PRO:CD | 2:F:210:GLN:HB2 | 1.82 | 1.09 |
| 1:A:515:ILE:HG21 | 1:A:565:HIS:HA | 1.29 | 1.09 |
| 1:D:551:LYS:H | 1:D:551:LYS:HD2 | 0.95 | 1.09 |
| 1:A:363:ARG:HD2 | 1:A:406:VAL:HB | 1.29 | 1.09 |
| 1:A:606:THR:HG21 | 1:A:612:LEU:HB3 | 1.34 | 1.09 |
| 1:D:607:TRP:HB2 | 1:D:779:LEU:HD23 | 1.33 | 1.09 |
| 1:A:1043:VAL:HA | 1:A:1046:GLU:H | 1.16 | 1.09 |
| 2:F:180:LYS:C | 2:F:180:LYS:HE3 | 1.73 | 1.09 |
| 2:F:276:SER:O | 2:F:287:ASN:HB2 | 1.51 | 1.09 |
| 2:B:204:LEU:HG | 2:B:325:ARG:HH21 | 1.18 | 1.09 |
| 1:D:458:GLU:HA | 1:D:461:LYS:HD3 | 1.30 | 1.09 |
| 1:D:1206:MET:CG | 2:F:257:ARG:HH11 | 1.66 | 1.09 |
| 1:A:190:PRO:HB3 | 1:A:192:GLU:CG | 1.81 | 1.09 |
| 2:F:236:GLU:HA | 2:F:341:ASP:HB3 | 1.33 | 1.09 |
| 2:B:262:TRP:O | 2:B:265:LYS:HB3 | 1.52 | 1.08 |
| 2:B:72:ILE:HA | 2:B:75:ARG:NE | 1.67 | 1.08 |
| 1:D:245:ILE:HG13 | 1:D:246:PRO:N | 1.63 | 1.08 |
| 2:C:456:ARG:HB2 | 2:C:463:LYS:CA | 1.84 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1001:GLY:HA2 | 1:D:1004:LEU:HD22 | 1.09 | 1.08 |
| 2:F:301:GLU:HB3 | 2:F:339:ASN:HB3 | 1.31 | 1.08 |
| 1:A:371:LYS:HD3 | 1:A:396:CYS:HA | 1.30 | 1.08 |
| 2:C:239:LEU:O | 2:C:336:LEU:HD22 | 1.52 | 1.08 |
| 1:D:316:LYS:HG2 | 1:D:348:LEU:HG | 1.36 | 1.08 |
| 1:D:546:ARG:HH21 | 2:F:404:ASN:HB3 | 1.11 | 1.08 |
| 2:E:249:ASN:HD21 | 2:E:285:LYS:HE2 | 1.12 | 1.08 |
| 2:E:322:LEU:O | 2:E:324:GLY:N | 1.86 | 1.08 |
| 2:E:388:GLY:C | 2:E:395:LEU:HD11 | 1.73 | 1.08 |
| 1:D:797:MET:HB2 | 1:D:869:ARG:CD | 1.82 | 1.08 |
| 1:A:228:LEU:HD23 | 1:A:229:VAL:N | 1.68 | 1.08 |
| 1:A:374:ARG:HE | 1:A:392:LEU:HD13 | 1.17 | 1.08 |
| 2:C:421:MET:HG3 | 2:C:422:GLN:H | 1.14 | 1.08 |
| 1:D:888:GLY:HA3 | 1:D:1138:ARG:HD3 | 1.24 | 1.08 |
| 1:A:271:VAL:HG12 | 1:A:272:SER:H | 1.14 | 1.08 |
| 1:A:549:LEU:HD21 | 2:C:398:VAL:HB | 1.12 | 1.08 |
| 2:E:382:LYS:HG2 | 2:E:412:SER:HB2 | 1.31 | 1.08 |
| 1:A:1068:ASP:H | 1:A:1071:ARG:HG2 | 1.16 | 1.08 |
| 2:B:371:VAL:HA | 2:B:433:ASP:HB3 | 1.09 | 1.08 |
| 2:C:435:MET:HE2 | 2:C:435:MET:HA | 1.36 | 1.08 |
| 1:D:612:LEU:HD21 | 1:D:622:TYR:CD1 | 1.89 | 1.08 |
| 1:D:874:LEU:O | 1:D:878:VAL:HG22 | 1.52 | 1.08 |
| 1:A:249:VAL:HG21 | 1:A:817:PRO:HD3 | 1.20 | 1.08 |
| 2:F:127:PRO:HD2 | 2:F:210:GLN:HB2 | 1.30 | 1.08 |
| 2:C:375:HIS:H | 2:C:378:LEU:HD22 | 1.16 | 1.07 |
| 1:D:1141:VAL:HB | 1:D:1146:ARG:NE | 1.68 | 1.07 |
| 1:A:297:MET:SD | 1:A:411:LEU:HD22 | 1.94 | 1.07 |
| 2:C:385:LEU:HD11 | 2:C:402:LEU:HB2 | 1.36 | 1.07 |
| 1:D:1172:ASP:O | 1:D:1173:LEU:HG | 1.54 | 1.07 |
| 1:A:213:VAL:HG13 | 1:A:221:TYR:OH | 1.50 | 1.07 |
| 1:A:606:THR:HG23 | 1:A:613:HIS:C | 1.72 | 1.07 |
| 1:A:439:GLN:HG2 | 1:A:835:GLY:CA | 1.83 | 1.07 |
| 2:E:371:VAL:HA | 2:E:433:ASP:OD2 | 1.53 | 1.07 |
| 2:E:456:ARG:HB2 | 2:E:463:LYS:HG2 | 1.27 | 1.07 |
| 2:F:242:PHE:HB3 | 2:F:333:PRO:HB2 | 1.35 | 1.07 |
| 1:A:802:ARG:O | 1:A:805:HIS:HB3 | 1.53 | 1.07 |
| 1:D:1067:SER:HA | 1:D:1071:ARG:HA | 1.12 | 1.07 |
| 1:D:585:TRP:HB3 | 1:D:587:PRO:HD2 | 1.35 | 1.07 |
| 1:A:170:ALA:HB1 | 1:A:175:TRP:HZ2 | 1.10 | 1.07 |
| 1:A:645:VAL:O | 1:A:646:VAL:HG12 | 1.54 | 1.07 |
| 2:C:208:LEU:CD1 | 2:C:240:VAL:HB | 1.82 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:598:VAL:HA | 1:D:601:LYS:HE2 | 1.36 | 1.07 |
| 1:D:869:ARG:H | 1:D:1200:PRO:CB | 1.66 | 1.07 |
| 1:A:1131:ILE:HG21 | 1:A:1138:ARG:N | 1.70 | 1.07 |
| 1:A:1145:ASP:HB3 | 1:A:1148:ARG:CZ | 1.83 | 1.07 |
| 1:A:603:MET:O | 1:A:605:LEU:HG | 1.53 | 1.07 |
| 2:C:239:LEU:N | 2:C:338:VAL:HG12 | 1.68 | 1.07 |
| 1:D:356:LEU:HD13 | 1:D:369:LEU:HD21 | 1.37 | 1.07 |
| 1:D:389:PHE:HA | 1:D:393:MET:CG | 1.84 | 1.07 |
| 1:D:1069:ILE:HG23 | 1:D:1070:PRO:CD | 1.85 | 1.07 |
| 1:A:249:VAL:HG21 | 1:A:817:PRO:CD | 1.82 | 1.07 |
| 1:D:389:PHE:HA | 1:D:393:MET:HG3 | 1.34 | 1.07 |
| 2:B:323:HIS:HA | 2:B:332:VAL:HA | 1.36 | 1.07 |
| 2:C:301:GLU:HB3 | 2:C:339:ASN:HB3 | 1.36 | 1.07 |
| 1:A:503:VAL:CB | 1:A:521:PRO:HA | 1.85 | 1.07 |
| 1:A:80:SER:N | 1:A:83:LEU:HD11 | 1.69 | 1.07 |
| 2:B:105:GLU:OE1 | 2:B:380:PRO:HA | 1.55 | 1.07 |
| 2:B:309:HIS:HB3 | 2:B:312:LEU:CD2 | 1.83 | 1.07 |
| 1:D:203:LEU:HB3 | 1:D:380:GLY:HA3 | 1.31 | 1.07 |
| 1:D:294:THR:HG22 | 1:D:407:PHE:CE2 | 1.89 | 1.07 |
| 1:D:670:PRO:HG2 | 1:D:673:ALA:HB2 | 1.29 | 1.07 |
| 1:A:996:ARG:HH22 | 1:A:1003:TRP:HB3 | 1.13 | 1.06 |
| 2:B:213:VAL:HA | 2:B:235:THR:O | 1.55 | 1.06 |
| 2:E:418:LEU:HD22 | 2:F:122:ARG:HH21 | 1.14 | 1.06 |
| 2:E:203:ARG:HH12 | 2:F:418:LEU:HD22 | 1.14 | 1.06 |
| 2:F:372:LEU:HD11 | 2:F:436:SER:CB | 1.83 | 1.06 |
| 1:A:232:ARG:HB3 | 1:A:239:LEU:HD22 | 1.13 | 1.06 |
| 1:A:618:HIS:HB2 | 1:A:725:PRO:HB2 | 1.36 | 1.06 |
| 2:C:443:VAL:CA | 2:C:447:THR:HG21 | 1.84 | 1.06 |
| 1:D:181:GLU:HA | 1:D:181:GLU:OE1 | 1.46 | 1.06 |
| 1:A:503:VAL:HG11 | 1:A:520:ALA:C | 1.76 | 1.06 |
| 1:A:893:SER:HB2 | 1:A:896:LEU:HB2 | 1.31 | 1.06 |
| 1:D:107:LEU:HD21 | 1:D:913:CYS:HA | 1.36 | 1.06 |
| 2:E:107:ARG:CG | 2:E:107:ARG:HH11 | 1.67 | 1.06 |
| 1:A:1026:ARG:HB3 | 1:A:1029:GLN:CG | 1.84 | 1.06 |
| 2:B:417:TYR:OH | 2:C:122:ARG:HD3 | 1.52 | 1.06 |
| 1:D:210:THR:HG23 | 1:D:224:CYS:HB3 | 1.36 | 1.06 |
| 1:D:279:ARG:CD | 1:D:841:LEU:HB3 | 1.85 | 1.06 |
| 2:F:234:LYS:HZ3 | 2:F:344:ARG:HD2 | 1.14 | 1.06 |
| 1:A:711:ALA:C | 1:A:713:PRO:HD3 | 1.75 | 1.06 |
| 1:D:856:GLU:OE1 | 1:D:859:TRP:HB2 | 1.54 | 1.06 |
| 1:A:903:GLY:CA | 1:A:1002:GLU:HB3 | 1.85 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:869:ARG:HG2 | 1:A:870:VAL:H | 1.16 | 1.06 |
| 1:A:784:GLY:H | 2:C:363:ARG:CD | 1.69 | 1.06 |
| 1:D:989:THR:HA | 1:D:998:SER:OG | 1.56 | 1.06 |
| 1:A:1014:ARG:HB2 | 1:A:1026:ARG:CZ | 1.85 | 1.06 |
| 1:A:875:LYS:O | 1:A:878:VAL:HG23 | 1.54 | 1.06 |
| 2:B:202:LYS:O | 2:B:325:ARG:HD2 | 1.53 | 1.06 |
| 1:D:1055:SER:HA | 1:D:1058:PHE:HB3 | 1.06 | 1.06 |
| 1:D:177:ARG:HB3 | 1:D:218:SER:HB3 | 1.37 | 1.06 |
| 2:F:247:THR:HB | 2:F:251:TRP:HD1 | 1.15 | 1.06 |
| 2:F:454:HIS:CB | 2:F:466:MET:HB2 | 1.86 | 1.06 |
| 1:A:363:ARG:NH1 | 1:A:406:VAL:HA | 1.70 | 1.06 |
| 1:A:613:HIS:HB3 | 1:A:717:LEU:HG | 1.35 | 1.06 |
| 1:A:845:VAL:HB | 1:A:855:VAL:HB | 1.36 | 1.06 |
| 1:D:1005:VAL:HA | 1:D:1008:LEU:CD1 | 1.85 | 1.06 |
| 1:D:1209:ARG:HH21 | 2:F:253:ASP:CA | 1.67 | 1.06 |
| 1:D:927:ARG:HG2 | 1:D:928:GLY:H | 1.09 | 1.06 |
| 2:E:443:VAL:HG22 | 2:E:453:ILE:HG21 | 1.33 | 1.06 |
| 2:F:406:LEU:HA | 2:F:409:ASN:ND2 | 1.70 | 1.06 |
| 1:D:203:LEU:H | 1:D:380:GLY:CA | 1.69 | 1.06 |
| 2:F:351:TYR:C | 2:F:355:GLN:HB2 | 1.75 | 1.06 |
| 2:C:242:PHE:HB3 | 2:C:333:PRO:HB2 | 1.36 | 1.06 |
| 2:F:125:VAL:HG22 | 2:F:208:LEU:HA | 1.07 | 1.06 |
| 1:A:76:ILE:HG13 | 1:A:77:GLN:HG3 | 1.36 | 1.05 |
| 1:D:504:LYS:HB2 | 1:D:523:ASP:CB | 1.85 | 1.05 |
| 1:D:956:GLY:HA2 | 1:D:1094:THR:HG23 | 1.08 | 1.05 |
| 2:E:390:GLY:N | 2:E:395:LEU:HG | 1.69 | 1.05 |
| 2:F:446:THR:HG21 | 2:F:450:ASN:OD1 | 1.56 | 1.05 |
| 1:D:546:ARG:NH2 | 2:F:404:ASN:HB3 | 1.69 | 1.05 |
| 2:B:285:LYS:CG | 2:B:286:GLY:H | 1.69 | 1.05 |
| 1:D:959:GLN:HB2 | 1:D:960:PRO:HD2 | 1.39 | 1.05 |
| 2:F:239:LEU:O | 2:F:336:LEU:HD22 | 1.56 | 1.05 |
| 1:A:1005:VAL:HA | 1:A:1008:LEU:HD13 | 1.34 | 1.05 |
| 1:A:76:ILE:HG23 | 1:A:77:GLN:H | 0.95 | 1.05 |
| 2:C:180:LYS:HE3 | 2:C:180:LYS:C | 1.77 | 1.05 |
| 2:E:105:GLU:OE2 | 2:E:382:LYS:O | 1.74 | 1.05 |
| 2:E:254:PHE:HA | 2:E:257:ARG:HB3 | 1.37 | 1.05 |
| 2:B:336:LEU:HD21 | 2:B:338:VAL:HG23 | 1.31 | 1.05 |
| 2:C:241:TRP:CB | 2:C:336:LEU:HD12 | 1.85 | 1.05 |
| 1:A:607:TRP:HA | 1:A:610:PHE:O | 1.54 | 1.05 |
| 1:D:885:THR:HB | 1:D:1146:ARG:HD2 | 1.34 | 1.05 |
| 1:D:432:VAL:HG11 | 1:D:1128:ARG:HE | 1.20 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:591:LEU:CD1 | 1:D:594:LEU:HG | 1.86 | 1.05 |
| 1:D:612:LEU:HB2 | 1:D:620:TRP:HB2 | 1.34 | 1.05 |
| 2:F:208:LEU:HD11 | 2:F:240:VAL:HB | 1.38 | 1.05 |
| 1:A:215:ILE:HG23 | 1:A:216:SER:H | 1.20 | 1.05 |
| 1:D:798:ILE:CG2 | 1:D:869:ARG:HH12 | 1.69 | 1.05 |
| 2:B:101:PRO:HA | 2:C:128:VAL:HG21 | 1.34 | 1.05 |
| 1:D:428:LEU:CD1 | 1:D:428:LEU:H | 1.68 | 1.05 |
| 1:D:367:PRO:HD2 | 1:D:368:PRO:HD3 | 1.05 | 1.05 |
| 1:A:1026:ARG:HB3 | 1:A:1029:GLN:CB | 1.86 | 1.04 |
| 1:A:1027:LYS:HB2 | 1:A:1092:PHE:HD2 | 1.22 | 1.04 |
| 2:F:203:ARG:HA | 2:F:325:ARG:HD3 | 1.07 | 1.04 |
| 1:D:620:TRP:O | 1:D:748:TRP:HB2 | 1.56 | 1.04 |
| 2:F:387:VAL:HA | 2:F:443:VAL:HG22 | 1.09 | 1.04 |
| 1:A:167:PRO:HG2 | 1:A:177:ARG:HG3 | 1.38 | 1.04 |
| 2:E:382:LYS:HG3 | 2:E:383:VAL:N | 1.72 | 1.04 |
| 1:A:667:GLN:O | 1:A:670:PRO:HD2 | 1.58 | 1.04 |
| 2:C:431:LYS:HA | 2:C:434:GLU:OE1 | 1.56 | 1.04 |
| 1:D:822:PRO:HD2 | 1:D:825:VAL:CG2 | 1.87 | 1.04 |
| 1:A:728:THR:HG22 | 1:A:729:GLN:H | 1.20 | 1.04 |
| 2:C:85:GLN:HB3 | 2:C:95:CYS:O | 1.56 | 1.04 |
| 1:D:411:LEU:O | 1:D:415:LEU:HB2 | 1.56 | 1.04 |
| 2:C:342:LEU:CD2 | 2:C:345:GLY:H | 1.71 | 1.04 |
| 2:F:203:ARG:HA | 2:F:325:ARG:CD | 1.87 | 1.04 |
| 1:A:239:LEU:O | 1:A:241:PRO:HD2 | 1.58 | 1.04 |
| 1:A:959:GLN:CB | 1:A:960:PRO:HD3 | 1.87 | 1.04 |
| 2:B:74:GLN:HG3 | 2:B:75:ARG:N | 1.66 | 1.04 |
| 1:A:1056:GLU:HA | 1:A:1059:ASN:ND2 | 1.73 | 1.04 |
| 1:A:1208:ARG:NH2 | 2:C:277:ASP:OD2 | 1.91 | 1.04 |
| 1:D:822:PRO:HD2 | 1:D:825:VAL:HG21 | 1.07 | 1.04 |
| 2:E:403:PHE:CD1 | 2:E:413:VAL:HB | 1.92 | 1.04 |
| 1:A:885:THR:CB | 1:A:1146:ARG:HE | 1.70 | 1.04 |
| 2:C:442:LEU:O | 2:C:455:LEU:HD22 | 1.56 | 1.04 |
| 1:D:428:LEU:HD12 | 1:D:428:LEU:H | 0.93 | 1.04 |
| 2:F:342:LEU:CD2 | 2:F:345:GLY:H | 1.71 | 1.04 |
| 1:A:1060:LYS:HE3 | 1:A:1065:ALA:H | 1.18 | 1.03 |
| 2:C:406:LEU:HA | 2:C:409:ASN:ND2 | 1.73 | 1.03 |
| 2:F:239:LEU:H | 2:F:338:VAL:CG1 | 1.70 | 1.03 |
| 1:A:161:GLN:O | 1:A:163:PRO:HD3 | 1.56 | 1.03 |
| 1:D:1029:GLN:NE2 | 1:D:1030:ARG:HH21 | 1.55 | 1.03 |
| 1:D:798:ILE:HG22 | 1:D:869:ARG:NH2 | 1.71 | 1.03 |
| 1:A:608:ASP:CB | 1:A:779:LEU:HD13 | 1.87 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:916:PHE:HA | 1:A:919:MET:HB2 | 1.35 | 1.03 |
| 1:D:157:LEU:HD21 | 1:D:194:ALA:HB3 | 1.37 | 1.03 |
| 1:A:1047:ARG:HA | 1:A:1047:ARG:NH1 | 1.72 | 1.03 |
| 2:B:374:LEU:H | 2:B:458:ARG:NH2 | 1.56 | 1.03 |
| 1:A:1236:GLN:HB3 | 1:A:1237:PRO:HD3 | 1.40 | 1.03 |
| 2:C:244:PRO:HD2 | 2:C:247:THR:HG21 | 1.39 | 1.03 |
| 1:A:1006:ARG:NH2 | 1:A:1010:LEU:HD11 | 1.74 | 1.03 |
| 1:D:348:LEU:HD21 | 1:D:350:ILE:HG13 | 1.35 | 1.03 |
| 1:A:1128:ARG:HG3 | 1:A:1129:PHE:N | 1.69 | 1.03 |
| 1:A:175:TRP:HB3 | 1:A:186:PRO:HD3 | 1.41 | 1.03 |
| 1:A:669:MET:O | 1:A:673:ALA:CB | 2.06 | 1.03 |
| 2:E:107:ARG:HG3 | 2:E:107:ARG:HH11 | 0.89 | 1.03 |
| 2:F:382:LYS:HD3 | 2:F:411:ILE:HG13 | 1.34 | 1.03 |
| 1:A:371:LYS:O | 1:A:373:PRO:HD3 | 1.56 | 1.03 |
| 1:D:371:LYS:HA | 1:D:374:ARG:CD | 1.88 | 1.03 |
| 1:D:798:ILE:HG23 | 1:D:869:ARG:HH12 | 1.17 | 1.03 |
| 1:A:80:SER:H | 1:A:83:LEU:HD11 | 1.19 | 1.03 |
| 2:F:473:ASP:HA | 2:F:476:ILE:CG2 | 1.89 | 1.03 |
| 1:A:249:VAL:CG2 | 1:A:817:PRO:HD3 | 1.89 | 1.02 |
| 1:A:439:GLN:HG2 | 1:A:835:GLY:HA3 | 1.38 | 1.02 |
| 2:C:102:LEU:HD11 | 2:C:435:MET:HE1 | 1.41 | 1.02 |
| 1:D:866:ARG:HB3 | 1:D:867:PRO:HD3 | 1.41 | 1.02 |
| 2:E:262:TRP:HA | 2:E:265:LYS:HE3 | 1.40 | 1.02 |
| 2:F:466:MET:CB | 2:F:471:LEU:HD22 | 1.89 | 1.02 |
| 1:A:997:LEU:CD2 | 1:A:998:SER:H | 1.71 | 1.02 |
| 2:C:236:GLU:HA | 2:C:341:ASP:CB | 1.87 | 1.02 |
| 2:F:386:ASP:O | 2:F:443:VAL:HG13 | 1.59 | 1.02 |
| 1:D:775:GLU:HA | 1:D:780:GLN:HG2 | 1.40 | 1.02 |
| 1:D:815:TRP:HA | 1:D:838:GLY:HA3 | 1.41 | 1.02 |
| 1:A:125:LEU:HD23 | 1:A:125:LEU:H | 1.19 | 1.02 |
| 1:D:1209:ARG:NH1 | 2:F:252:LEU:HD13 | 1.74 | 1.02 |
| 1:D:213:VAL:HG22 | 1:D:401:TRP:CH2 | 1.93 | 1.02 |
| 1:D:854:ALA:HB1 | 1:D:860:LEU:CD1 | 1.88 | 1.02 |
| 1:A:498:LYS:HE3 | 1:A:518:ALA:H | 1.23 | 1.02 |
| 1:A:645:VAL:O | 1:A:650:ARG:HD2 | 1.60 | 1.02 |
| 1:A:76:ILE:HG23 | 1:A:77:GLN:N | 1.73 | 1.02 |
| 1:D:623:LEU:O | 1:D:625:PRO:HD3 | 1.59 | 1.02 |
| 2:E:428:LEU:HD13 | 2:E:428:LEU:H | 1.25 | 1.02 |
| 2:E:447:THR:HG21 | 2:E:453:ILE:HG23 | 1.40 | 1.02 |
| 1:A:288:ARG:HA | 1:A:288:ARG:NE | 1.64 | 1.02 |
| 2:F:200:VAL:HG11 | 2:F:204:LEU:HB2 | 1.38 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:439:PHE:HD1 | 2:F:458:ARG:HB2 | 1.20 | 1.02 |
| 2:C:300:ILE:HG23 | 2:C:342:LEU:HD11 | 1.40 | 1.02 |
| 2:C:430:SER:O | 2:C:434:GLU:HG3 | 1.59 | 1.02 |
| 1:D:420:HIS:HD1 | 1:D:421:PRO:CD | 1.71 | 1.02 |
| 1:D:605:LEU:HD22 | 1:D:781:ALA:CB | 1.88 | 1.02 |
| 2:F:209:ALA:HB1 | 2:F:238:SER:O | 1.60 | 1.02 |
| 1:A:853:ARG:NH1 | 1:A:1105:ALA:HB3 | 1.73 | 1.02 |
| 1:A:479:TYR:O | 1:A:480:LYS:HG2 | 1.57 | 1.02 |
| 1:A:502:LYS:HG3 | 1:A:503:VAL:N | 1.74 | 1.02 |
| 1:A:925:LYS:HG3 | 1:A:926:SER:N | 1.73 | 1.02 |
| 2:E:186:LEU:O | 2:E:190:LEU:HD13 | 1.58 | 1.02 |
| 1:A:1128:ARG:HG3 | 1:A:1129:PHE:H | 0.89 | 1.02 |
| 1:A:192:GLU:HB3 | 1:A:217:PRO:HG2 | 1.39 | 1.02 |
| 1:A:444:TYR:CD2 | 1:A:874:LEU:HD23 | 1.94 | 1.02 |
| 1:D:135:LEU:HD23 | 1:D:135:LEU:H | 1.22 | 1.02 |
| 2:F:386:ASP:HB2 | 2:F:442:LEU:HA | 1.03 | 1.02 |
| 2:F:386:ASP:HB3 | 2:F:442:LEU:HD23 | 1.40 | 1.02 |
| 1:D:1188:CYS:C | 1:D:1189:LEU:HD22 | 1.80 | 1.01 |
| 1:D:351:SER:C | 1:D:358:GLU:OE2 | 1.97 | 1.01 |
| 1:D:297:MET:HG2 | 1:D:411:LEU:HD22 | 1.40 | 1.01 |
| 1:D:717:LEU:O | 1:D:721:ALA:HB2 | 1.59 | 1.01 |
| 1:D:607:TRP:CD1 | 1:D:780:GLN:N | 2.27 | 1.01 |
| 1:D:880:ALA:HB2 | 1:D:1187:ARG:O | 1.58 | 1.01 |
| 1:D:992:LEU:HB3 | 1:D:996:ARG:CG | 1.90 | 1.01 |
| 1:A:612:LEU:HD22 | 1:A:621:GLY:H | 0.85 | 1.01 |
| 1:A:623:LEU:HB3 | 1:A:667:GLN:NE2 | 1.74 | 1.01 |
| 1:D:1014:ARG:CG | 1:D:1026:ARG:HE | 1.72 | 1.01 |
| 1:D:1027:LYS:HZ2 | 1:D:1091:GLU:HG2 | 1.13 | 1.01 |
| 1:D:86:GLN:NE2 | 1:D:132:GLY:H | 1.56 | 1.01 |
| 2:E:266:PHE:HB3 | 2:E:376:PRO:HD3 | 1.39 | 1.01 |
| 1:A:1190:ARG:CZ | 1:A:1197:CYS:HB2 | 1.89 | 1.01 |
| 1:A:408:GLN:HA | 1:A:411:LEU:CG | 1.89 | 1.01 |
| 2:B:419:GLU:HB2 | 2:C:203:ARG:NH2 | 1.75 | 1.01 |
| 1:D:213:VAL:HG21 | 1:D:397:ALA:HB1 | 1.40 | 1.01 |
| 1:D:249:VAL:HG13 | 1:D:252:GLY:H | 0.90 | 1.01 |
| 1:D:577:CYS:O | 1:D:579:ARG:N | 1.93 | 1.01 |
| 1:D:1131:ILE:H | 1:D:1131:ILE:CD1 | 1.73 | 1.01 |
| 1:A:608:ASP:HB3 | 1:A:779:LEU:HD13 | 1.02 | 1.01 |
| 1:D:735:GLY:HA3 | 1:D:749:PHE:HB3 | 1.42 | 1.01 |
| 1:D:275:ARG:NE | 1:D:843:GLN:N | 2.07 | 1.01 |
| 2:F:126:PHE:HA | 2:F:209:ALA:O | 1.58 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1068:ASP:H | 1:A:1071:ARG:CG | 1.73 | 1.01 |
| 2:C:403:PHE:CE1 | 2:C:415:PRO:HG3 | 1.96 | 1.01 |
| 1:A:369:PRO:HB2 | 1:A:372:GLU:HG3 | 1.03 | 1.01 |
| 2:C:200:VAL:HG21 | 2:C:204:LEU:HD22 | 1.42 | 1.01 |
| 2:C:386:ASP:HB3 | 2:C:442:LEU:HD23 | 1.38 | 1.01 |
| 1:D:1141:VAL:HB | 1:D:1146:ARG:HE | 0.87 | 1.01 |
| 1:D:195:LEU:H | 1:D:265:LEU:HD22 | 1.25 | 1.01 |
| 1:D:420:HIS:HD1 | 1:D:421:PRO:HD2 | 0.85 | 1.01 |
| 1:D:503:VAL:O | 1:D:505:LYS:N | 1.92 | 1.01 |
| 1:D:610:PHE:H | 1:D:611:PRO:CD | 1.73 | 1.01 |
| 1:D:249:VAL:HG13 | 1:D:252:GLY:N | 1.75 | 1.01 |
| 1:D:483:PRO:O | 1:D:486:TRP:HB2 | 1.61 | 1.01 |
| 1:A:222:SER:HB2 | 1:A:223:TRP:CD1 | 1.96 | 1.01 |
| 1:A:408:GLN:O | 1:A:412:PRO:HD3 | 1.61 | 1.01 |
| 1:A:615:SER:HB2 | 1:A:725:PRO:HB3 | 1.42 | 1.01 |
| 2:C:341:ASP:O | 2:C:342:LEU:HD13 | 1.60 | 1.01 |
| 1:D:179:GLY:HA3 | 1:D:182:GLY:CA | 1.90 | 1.01 |
| 1:D:870:VAL:O | 1:D:873:GLU:HG2 | 1.60 | 1.01 |
| 2:F:431:LYS:HA | 2:F:434:GLU:OE1 | 1.60 | 1.01 |
| 1:A:1060:LYS:HD3 | 1:A:1073:PRO:CB | 1.90 | 1.01 |
| 2:C:277:ASP:OD2 | 2:C:287:ASN:HB3 | 1.59 | 1.01 |
| 2:C:454:HIS:HB3 | 2:C:466:MET:HB2 | 1.43 | 1.01 |
| 1:D:439:GLN:HE21 | 1:D:835:GLY:HA3 | 1.23 | 1.01 |
| 1:D:612:LEU:HD21 | 1:D:622:TYR:CE1 | 1.95 | 1.01 |
| 1:D:736:ASN:HA | 1:D:750:PHE:CE1 | 1.95 | 1.01 |
| 1:D:904:ASP:HB3 | 1:D:912:GLY:HA3 | 1.38 | 1.01 |
| 1:D:932:HIS:O | 1:D:935:THR:HG22 | 1.59 | 1.01 |
| 2:F:446:THR:HB | 2:F:450:ASN:CB | 1.90 | 1.01 |
| 1:A:1179:PHE:HB3 | 1:A:1220:ILE:HG12 | 1.43 | 1.00 |
| 1:A:118:VAL:N | 1:A:119:PRO:HD3 | 1.73 | 1.00 |
| 1:A:615:SER:CB | 1:A:725:PRO:HB3 | 1.91 | 1.00 |
| 1:D:1019:TRP:CE3 | 1:D:1168:LEU:HG | 1.94 | 1.00 |
| 1:D:1057:MET:HB3 | 1:D:1064:ILE:HD11 | 1.41 | 1.00 |
| 2:F:245:PRO:O | 2:F:248:SER:HB2 | 1.61 | 1.00 |
| 2:F:387:VAL:HG12 | 2:F:443:VAL:HG21 | 1.43 | 1.00 |
| 2:C:393:LEU:HD23 | 2:C:396:ARG:HG2 | 1.42 | 1.00 |
| 2:E:82:SER:H | 2:E:85:GLN:HG3 | 1.26 | 1.00 |
| 1:A:175:TRP:HB2 | 1:A:184:ALA:HA | 1.44 | 1.00 |
| 1:A:420:HIS:CD2 | 1:A:1020:ILE:HG21 | 1.96 | 1.00 |
| 1:A:639:THR:HB | 1:A:640:LEU:HD23 | 1.39 | 1.00 |
| 2:B:268:MET:H | 2:B:270:PRO:HD2 | 1.19 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1131:ILE:HD11 | 1:D:1138:ARG:CA | 1.91 | 1.00 |
| 2:F:190:LEU:O | 2:F:193:TYR:HB3 | 1.62 | 1.00 |
| 2:F:241:TRP:CB | 2:F:336:LEU:HB2 | 1.90 | 1.00 |
| 2:E:78:PHE:HA | 2:E:102:LEU:HB3 | 1.41 | 1.00 |
| 2:F:304:TRP:H | 2:F:337:SER:HB2 | 0.84 | 1.00 |
| 1:A:866:ARG:HG2 | 1:A:1069:ILE:HG21 | 1.42 | 1.00 |
| 1:D:275:ARG:NH1 | 1:D:843:GLN:HG2 | 1.76 | 1.00 |
| 2:E:331:VAL:HG22 | 2:E:333:PRO:HD3 | 1.42 | 1.00 |
| 1:D:1006:ARG:HH12 | 1:D:1009:ASN:HB2 | 0.83 | 1.00 |
| 1:D:269:HIS:O | 1:D:294:THR:HG23 | 1.61 | 1.00 |
| 1:D:441:TRP:CE2 | 1:D:879:GLN:HA | 1.97 | 1.00 |
| 2:E:432:TYR:HA | 2:E:435:MET:CB | 1.91 | 1.00 |
| 2:F:375:HIS:H | 2:F:378:LEU:HD22 | 1.25 | 1.00 |
| 1:A:1047:ARG:HH11 | 1:A:1047:ARG:HA | 1.20 | 1.00 |
| 2:C:234:LYS:HZ3 | 2:C:344:ARG:HD2 | 1.23 | 1.00 |
| 2:C:234:LYS:NZ | 2:C:344:ARG:HD2 | 1.74 | 1.00 |
| 2:E:432:TYR:HB2 | 2:E:437:ILE:HD11 | 1.00 | 1.00 |
| 2:F:125:VAL:HG22 | 2:F:208:LEU:CA | 1.91 | 1.00 |
| 1:A:267:VAL:HG23 | 1:A:291:PHE:CD2 | 1.97 | 1.00 |
| 1:A:213:VAL:HG12 | 1:A:401:TRP:HE1 | 0.83 | 1.00 |
| 1:A:436:PRO:HG2 | 1:A:879:GLN:HB3 | 1.44 | 1.00 |
| 2:C:343:ASP:C | 2:C:347:LEU:HD13 | 1.81 | 1.00 |
| 1:D:1197:CYS:H | 1:D:1204:THR:HG23 | 1.26 | 1.00 |
| 1:D:374:ARG:HD3 | 1:D:392:LEU:HD21 | 1.41 | 1.00 |
| 2:F:301:GLU:CB | 2:F:339:ASN:HB3 | 1.90 | 1.00 |
| 2:C:356:LEU:HB3 | 2:C:359:ASN:HD21 | 1.21 | 1.00 |
| 1:D:1165:ALA:CB | 1:D:1173:LEU:HD12 | 1.90 | 1.00 |
| 1:D:946:ALA:HA | 1:D:949:PHE:CE2 | 1.95 | 1.00 |
| 1:A:175:TRP:HB2 | 1:A:184:ALA:CA | 1.92 | 1.00 |
| 2:C:134:LYS:HB3 | 2:C:180:LYS:HD3 | 1.43 | 1.00 |
| 2:C:301:GLU:CB | 2:C:339:ASN:HB3 | 1.90 | 1.00 |
| 1:D:522:GLY:O | 1:D:524:PRO:HD3 | 1.62 | 1.00 |
| 1:A:1141:VAL:HB | 1:A:1146:ARG:HD2 | 1.44 | 0.99 |
| 1:A:871:GLY:C | 1:A:873:GLU:N | 2.10 | 0.99 |
| 2:B:453:ILE:HD12 | 2:B:468:ILE:HB | 1.43 | 0.99 |
| 1:D:251:THR:OG1 | 1:D:254:SER:HA | 1.62 | 0.99 |
| 1:D:504:LYS:CD | 1:D:523:ASP:HB3 | 1.90 | 0.99 |
| 2:E:128:VAL:HG13 | 2:E:210:GLN:HE21 | 1.24 | 0.99 |
| 2:E:283:GLY:HA3 | 2:E:306:LEU:HA | 1.44 | 0.99 |
| 2:F:386:ASP:HB2 | 2:F:442:LEU:CA | 1.90 | 0.99 |
| 2:F:454:HIS:HB3 | 2:F:466:MET:HB2 | 1.42 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:792:LEU:HD12 | 1:A:793:GLU:H | 1.22 | 0.99 |
| 2:C:325:ARG:HG3 | 2:C:325:ARG:HH11 | 1.23 | 0.99 |
| 1:D:242:ALA:CB | 1:D:245:ILE:HG12 | 1.92 | 0.99 |
| 1:D:775:GLU:HB3 | 1:D:796:LYS:HE2 | 1.44 | 0.99 |
| 2:E:436:SER:C | 2:E:437:ILE:HD12 | 1.82 | 0.99 |
| 2:F:468:ILE:O | 2:F:472:LYS:HG2 | 1.59 | 0.99 |
| 2:B:285:LYS:HG2 | 2:B:286:GLY:H | 0.85 | 0.99 |
| 2:C:387:VAL:HG11 | 2:C:399:CYS:HB3 | 1.44 | 0.99 |
| 1:D:1151:LEU:O | 1:D:1155:ILE:HG12 | 1.63 | 0.99 |
| 1:A:378:VAL:CB | 1:A:381:THR:HG23 | 1.93 | 0.99 |
| 2:B:396:ARG:HD2 | 2:B:417:TYR:HB2 | 1.44 | 0.99 |
| 1:D:1198:LYS:HA | 1:D:1204:THR:OG1 | 1.59 | 0.99 |
| 2:F:473:ASP:HA | 2:F:476:ILE:HG23 | 1.45 | 0.99 |
| 1:A:634:LEU:HB3 | 1:A:635:PRO:HA | 1.45 | 0.99 |
| 2:B:244:PRO:O | 2:B:248:SER:HB2 | 1.61 | 0.99 |
| 2:B:127:PRO:HB2 | 2:C:104:VAL:HG11 | 1.41 | 0.99 |
| 2:F:325:ARG:HG3 | 2:F:325:ARG:HH11 | 1.26 | 0.99 |
| 1:A:152:GLU:HA | 1:A:155:ASN:HD22 | 1.26 | 0.99 |
| 1:A:623:LEU:HB3 | 1:A:667:GLN:HE22 | 1.24 | 0.99 |
| 2:B:374:LEU:HB2 | 2:B:458:ARG:HH12 | 1.26 | 0.99 |
| 1:D:775:GLU:O | 1:D:776:ASP:HB3 | 1.59 | 0.99 |
| 2:F:131:LEU:HG | 2:F:133:HIS:CE1 | 1.97 | 0.99 |
| 1:A:210:THR:O | 1:A:211:LEU:HB2 | 1.62 | 0.99 |
| 1:D:128:PRO:CA | 1:D:130:LEU:HD21 | 1.91 | 0.99 |
| 1:D:641:GLU:C | 1:D:645:VAL:HG21 | 1.81 | 0.99 |
| 2:F:244:PRO:HD2 | 2:F:247:THR:HG21 | 1.42 | 0.99 |
| 1:A:316:LYS:HD2 | 1:A:350:ILE:HG12 | 1.40 | 0.99 |
| 1:A:655:LEU:HB2 | 1:A:719:LEU:HB3 | 1.44 | 0.99 |
| 1:A:962:ALA:HB2 | 1:A:986:TYR:OH | 1.60 | 0.99 |
| 1:D:490:TRP:CZ2 | 1:D:598:VAL:HB | 1.97 | 0.99 |
| 1:D:74:LEU:CD1 | 1:D:77:GLN:HA | 1.93 | 0.99 |
| 1:A:1057:MET:O | 1:A:1064:ILE:HG21 | 1.62 | 0.99 |
| 1:A:624:VAL:O | 1:A:626:GLY:N | 1.95 | 0.99 |
| 1:A:793:GLU:HA | 1:A:796:LYS:HD3 | 1.44 | 0.99 |
| 2:C:466:MET:SD | 2:C:471:LEU:HD23 | 2.03 | 0.99 |
| 1:D:1019:TRP:HE3 | 1:D:1168:LEU:HG | 1.21 | 0.99 |
| 1:D:441:TRP:NE1 | 1:D:879:GLN:HA | 1.74 | 0.99 |
| 2:F:102:LEU:HD11 | 2:F:435:MET:HE1 | 1.41 | 0.99 |
| 1:A:192:GLU:CB | 1:A:217:PRO:HG2 | 1.93 | 0.98 |
| 2:C:396:ARG:HH11 | 2:C:397:GLN:HA | 1.26 | 0.98 |
| 1:D:270:ASN:HA | 1:D:294:THR:CG2 | 1.92 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:375:GLU:O | 1:D:379:LYS:N | 1.96 | 0.98 |
| 1:D:608:ASP:HB3 | 1:D:620:TRP:CE3 | 1.98 | 0.98 |
| 1:D:741:ASP:HB2 | 1:D:748:TRP:HH2 | 1.28 | 0.98 |
| 1:A:879:GLN:HB2 | 1:A:886:LEU:HD11 | 1.45 | 0.98 |
| 1:D:1005:VAL:HA | 1:D:1008:LEU:HD13 | 1.41 | 0.98 |
| 1:D:114:GLY:C | 1:D:116:PRO:HD3 | 1.83 | 0.98 |
| 1:D:994:TRP:O | 1:D:995:TYR:HB3 | 1.62 | 0.98 |
| 2:F:236:GLU:CA | 2:F:341:ASP:HB3 | 1.93 | 0.98 |
| 2:F:454:HIS:HD2 | 2:F:468:ILE:HA | 1.24 | 0.98 |
| 1:A:272:SER:HB3 | 1:A:273:PHE:HD2 | 1.27 | 0.98 |
| 2:C:468:ILE:O | 2:C:472:LYS:HG2 | 1.60 | 0.98 |
| 1:D:1193:VAL:HG22 | 1:D:1194:THR:H | 0.85 | 0.98 |
| 2:F:317:GLY:CA | 2:F:320:SER:HB2 | 1.92 | 0.98 |
| 1:A:192:GLU:OE2 | 1:A:194:ALA:N | 1.97 | 0.98 |
| 1:A:869:ARG:HG2 | 1:A:870:VAL:N | 1.71 | 0.98 |
| 1:D:245:ILE:HG13 | 1:D:246:PRO:CD | 1.92 | 0.98 |
| 1:D:375:GLU:CG | 1:D:379:LYS:HB3 | 1.93 | 0.98 |
| 1:D:551:LYS:N | 1:D:551:LYS:HD2 | 1.63 | 0.98 |
| 1:D:73:PRO:HG3 | 1:D:90:GLN:HG2 | 1.43 | 0.98 |
| 1:A:382:MET:SD | 1:A:383:LYS:N | 2.36 | 0.98 |
| 1:A:621:GLY:HA2 | 1:A:748:TRP:HB3 | 1.42 | 0.98 |
| 2:B:308:ASP:HB3 | 2:B:309:HIS:ND1 | 1.79 | 0.98 |
| 2:C:203:ARG:HA | 2:C:325:ARG:CD | 1.92 | 0.98 |
| 1:A:222:SER:HB2 | 1:A:223:TRP:HD1 | 1.26 | 0.98 |
| 1:A:273:PHE:HA | 1:A:276:ALA:CB | 1.94 | 0.98 |
| 1:A:996:ARG:HB2 | 1:A:1004:LEU:HD22 | 1.44 | 0.98 |
| 2:B:324:GLY:N | 2:B:331:VAL:O | 1.95 | 0.98 |
| 2:B:70:LEU:HD22 | 2:B:88:ARG:HH11 | 1.24 | 0.98 |
| 2:C:247:THR:HB | 2:C:251:TRP:CD1 | 1.99 | 0.98 |
| 2:F:372:LEU:HD21 | 2:F:435:MET:C | 1.84 | 0.98 |
| 2:F:454:HIS:CD2 | 2:F:468:ILE:HA | 1.97 | 0.98 |
| 1:D:886:LEU:C | 1:D:1146:ARG:HH12 | 1.67 | 0.98 |
| 1:A:866:ARG:CG | 1:A:1069:ILE:HG21 | 1.94 | 0.98 |
| 1:A:606:THR:HG23 | 1:A:614:TYR:N | 1.79 | 0.98 |
| 1:A:771:LEU:HD22 | 1:A:771:LEU:H | 1.28 | 0.98 |
| 1:A:815:TRP:HA | 1:A:838:GLY:HA3 | 1.44 | 0.98 |
| 2:B:211:ILE:HA | 2:B:237:ALA:HA | 1.46 | 0.98 |
| 2:F:85:GLN:HB3 | 2:F:95:CYS:O | 1.62 | 0.98 |
| 1:A:1204:THR:O | 1:A:1204:THR:HG22 | 1.61 | 0.98 |
| 1:A:188:ALA:O | 1:A:189:ILE:HG23 | 1.62 | 0.98 |
| 1:A:196:VAL:HG13 | 1:A:269:HIS:CD2 | 1.99 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:372:LEU:HD11 | 2:C:436:SER:CB | 1.94 | 0.98 |
| 2:C:473:ASP:HA | 2:C:476:ILE:CG2 | 1.93 | 0.98 |
| 1:D:1055:SER:CA | 1:D:1058:PHE:HB3 | 1.93 | 0.98 |
| 1:D:1069:ILE:HG23 | 1:D:1070:PRO:HD2 | 1.46 | 0.98 |
| 2:E:262:TRP:O | 2:E:265:LYS:HB3 | 1.64 | 0.98 |
| 2:F:303:LEU:HA | 2:F:337:SER:OG | 1.63 | 0.98 |
| 2:F:236:GLU:HA | 2:F:341:ASP:CB | 1.93 | 0.98 |
| 1:A:297:MET:SD | 1:A:411:LEU:HB2 | 2.04 | 0.98 |
| 1:A:914:THR:HA | 1:A:918:TRP:HB3 | 1.42 | 0.98 |
| 2:C:363:ARG:HH11 | 2:C:363:ARG:HA | 1.28 | 0.98 |
| 2:C:82:SER:CA | 2:C:86:LEU:HD21 | 1.94 | 0.98 |
| 1:D:128:PRO:HA | 1:D:130:LEU:HD21 | 0.99 | 0.98 |
| 1:D:275:ARG:HH11 | 1:D:843:GLN:NE2 | 1.60 | 0.98 |
| 1:D:459:MET:N | 1:D:460:LYS:HZ1 | 1.62 | 0.98 |
| 1:D:926:SER:HB2 | 1:D:930:ASP:HB2 | 1.42 | 0.98 |
| 2:E:107:ARG:NH1 | 2:E:107:ARG:HG3 | 1.64 | 0.98 |
| 2:F:342:LEU:HD23 | 2:F:345:GLY:H | 1.26 | 0.98 |
| 2:F:385:LEU:O | 2:F:416:GLY:HA3 | 1.64 | 0.98 |
| 2:F:372:LEU:CD1 | 2:F:436:SER:HB2 | 1.94 | 0.98 |
| 1:A:498:LYS:HE2 | 1:A:499:LYS:H | 1.29 | 0.97 |
| 2:C:276:SER:O | 2:C:287:ASN:HB2 | 1.62 | 0.97 |
| 2:C:317:GLY:HA3 | 2:C:320:SER:HB2 | 1.46 | 0.97 |
| 1:D:345:TRP:HA | 1:D:1040:LYS:NZ | 1.78 | 0.97 |
| 1:D:428:LEU:HD12 | 1:D:428:LEU:N | 1.78 | 0.97 |
| 1:A:1207:GLU:HB3 | 1:A:1213:PRO:HG3 | 1.42 | 0.97 |
| 1:D:1124:ALA:HB1 | 1:D:1148:ARG:NH1 | 1.79 | 0.97 |
| 2:F:102:LEU:HD11 | 2:F:435:MET:CE | 1.92 | 0.97 |
| 2:F:300:ILE:HG22 | 2:F:301:GLU:HG3 | 1.44 | 0.97 |
| 1:A:959:GLN:HB2 | 1:A:960:PRO:HD3 | 0.99 | 0.97 |
| 1:A:996:ARG:HH12 | 1:A:1003:TRP:HB2 | 1.28 | 0.97 |
| 1:D:1200:PRO:HG2 | 1:D:1203:PRO:HG2 | 1.44 | 0.97 |
| 1:D:959:GLN:HB2 | 1:D:960:PRO:CD | 1.93 | 0.97 |
| 2:E:407:LEU:CD2 | 2:E:412:SER:HA | 1.94 | 0.97 |
| 2:B:106:LEU:HD12 | 2:B:109:ASN:HD22 | 1.27 | 0.97 |
| 2:C:241:TRP:CB | 2:C:336:LEU:HB2 | 1.95 | 0.97 |
| 2:C:439:PHE:CD1 | 2:C:458:ARG:HG3 | 2.00 | 0.97 |
| 1:D:869:ARG:O | 1:D:1200:PRO:HG3 | 1.63 | 0.97 |
| 1:D:1208:ARG:HH12 | 2:F:285:LYS:HD3 | 1.27 | 0.97 |
| 1:D:138:HIS:O | 1:D:142:LEU:HG | 1.64 | 0.97 |
| 2:F:386:ASP:CB | 2:F:442:LEU:HA | 1.93 | 0.97 |
| 1:A:203:LEU:C | 1:A:205:GLU:H | 1.44 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:253:ALA:CB | 1:A:280:GLU:HB2 | 1.94 | 0.97 |
| 2:B:101:PRO:CA | 2:C:128:VAL:HG21 | 1.95 | 0.97 |
| 1:D:219:ALA:O | 1:D:220:TRP:HB2 | 1.61 | 0.97 |
| 1:D:513:LEU:H | 1:D:570:PRO:HG3 | 1.25 | 0.97 |
| 1:A:392:LEU:HG | 1:A:395:TYR:CG | 1.98 | 0.97 |
| 1:A:526:ASP:O | 1:A:527:GLN:HB2 | 1.64 | 0.97 |
| 1:A:76:ILE:CB | 1:A:911:HIS:NE2 | 2.26 | 0.97 |
| 2:E:456:ARG:CZ | 2:E:463:LYS:HE3 | 1.95 | 0.97 |
| 2:F:82:SER:CA | 2:F:86:LEU:HD21 | 1.93 | 0.97 |
| 1:A:308:GLN:NE2 | 1:A:1091:GLU:H | 1.61 | 0.97 |
| 1:A:849:THR:HG22 | 1:A:851:THR:H | 1.29 | 0.97 |
| 2:C:301:GLU:HB3 | 2:C:339:ASN:CB | 1.93 | 0.97 |
| 2:C:419:GLU:OE2 | 2:C:428:LEU:HD13 | 1.64 | 0.97 |
| 1:D:1001:GLY:O | 1:D:1004:LEU:HB2 | 1.64 | 0.97 |
| 1:D:1128:ARG:HG3 | 1:D:1129:PHE:H | 1.28 | 0.97 |
| 1:D:1231:LEU:HD11 | 1:D:1236:GLN:NE2 | 1.80 | 0.97 |
| 1:D:656:TYR:HB3 | 1:D:744:ILE:HG21 | 1.47 | 0.97 |
| 1:D:876:ALA:HA | 1:D:1189:LEU:HB2 | 1.47 | 0.97 |
| 1:A:175:TRP:CB | 1:A:184:ALA:HA | 1.94 | 0.97 |
| 2:C:245:PRO:O | 2:C:248:SER:HB2 | 1.63 | 0.97 |
| 1:D:115:GLN:N | 1:D:116:PRO:HD3 | 1.76 | 0.97 |
| 1:D:1197:CYS:N | 1:D:1204:THR:HG23 | 1.80 | 0.97 |
| 2:E:442:LEU:HD13 | 2:E:443:VAL:N | 1.78 | 0.97 |
| 1:A:927:ARG:O | 1:A:930:ASP:HB3 | 1.65 | 0.97 |
| 1:A:755:LYS:HD3 | 1:A:964:ARG:NH1 | 1.80 | 0.97 |
| 2:C:127:PRO:CD | 2:C:210:GLN:HB2 | 1.94 | 0.97 |
| 1:D:275:ARG:HD2 | 1:D:843:GLN:CD | 1.83 | 0.97 |
| 2:E:377:CYS:C | 2:E:380:PRO:HD2 | 1.83 | 0.97 |
| 1:A:1002:GLU:O | 1:A:1005:VAL:HG22 | 1.63 | 0.97 |
| 1:A:472:GLN:HG3 | 2:C:460:THR:HA | 1.47 | 0.97 |
| 1:A:76:ILE:CG2 | 1:A:77:GLN:H | 1.78 | 0.97 |
| 2:C:236:GLU:CA | 2:C:341:ASP:HB3 | 1.95 | 0.97 |
| 2:C:441:VAL:HG11 | 2:C:454:HIS:CE1 | 1.99 | 0.97 |
| 1:D:350:ILE:H | 1:D:350:ILE:HD12 | 1.30 | 0.97 |
| 1:D:601:LYS:HE3 | 1:D:721:ALA:HB1 | 1.45 | 0.97 |
| 1:D:618:HIS:HB2 | 1:D:725:PRO:HD2 | 1.47 | 0.97 |
| 1:D:996:ARG:NE | 1:D:996:ARG:H | 1.61 | 0.97 |
| 1:D:495:PHE:O | 1:D:496:LYS:HD2 | 1.64 | 0.96 |
| 1:D:801:TRP:CE3 | 1:D:870:VAL:CG1 | 2.46 | 0.96 |
| 2:E:264:ARG:HE | 2:E:273:PHE:HB2 | 1.28 | 0.96 |
| 1:A:1026:ARG:O | 1:A:1030:ARG:N | 1.95 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:225:SER:HA | 1:A:228:LEU:HD13 | 1.46 | 0.96 |
| 1:D:279:ARG:HD2 | 1:D:841:LEU:CB | 1.95 | 0.96 |
| 1:D:302:SER:OG | 1:D:351:SER:HB3 | 1.64 | 0.96 |
| 1:D:900:ALA:CB | 1:D:915:ALA:HB1 | 1.94 | 0.96 |
| 1:A:1198:LYS:HG3 | 1:A:1204:THR:CG2 | 1.94 | 0.96 |
| 1:A:166:PRO:CG | 1:A:398:GLN:HE22 | 1.76 | 0.96 |
| 1:D:1069:ILE:CG2 | 1:D:1070:PRO:HD2 | 1.95 | 0.96 |
| 1:D:375:GLU:HG3 | 1:D:379:LYS:CB | 1.93 | 0.96 |
| 1:D:624:VAL:O | 1:D:626:GLY:N | 1.99 | 0.96 |
| 2:E:254:PHE:HB2 | 2:E:257:ARG:HH11 | 1.26 | 0.96 |
| 1:A:811:GLN:HB2 | 1:A:840:ILE:HG21 | 1.45 | 0.96 |
| 2:C:344:ARG:HA | 2:C:347:LEU:HB2 | 1.45 | 0.96 |
| 2:C:446:THR:HA | 2:C:450:ASN:HB2 | 1.43 | 0.96 |
| 1:D:279:ARG:HD2 | 1:D:841:LEU:HB3 | 0.99 | 0.96 |
| 1:D:887:VAL:HG23 | 1:D:1146:ARG:CZ | 1.95 | 0.96 |
| 2:B:396:ARG:CG | 2:B:417:TYR:HB2 | 1.93 | 0.96 |
| 1:D:101:ARG:HG3 | 1:D:101:ARG:HH11 | 1.30 | 0.96 |
| 1:D:1198:LYS:CA | 1:D:1204:THR:OG1 | 2.14 | 0.96 |
| 1:D:465:ASP:O | 1:D:469:ASP:HB2 | 1.66 | 0.96 |
| 1:D:549:LEU:N | 1:D:551:LYS:NZ | 2.14 | 0.96 |
| 1:D:279:ARG:HB3 | 1:D:841:LEU:HB2 | 1.46 | 0.96 |
| 2:F:127:PRO:HD3 | 2:F:210:GLN:N | 1.80 | 0.96 |
| 1:A:589:PRO:HG3 | 1:A:805:HIS:CD2 | 1.99 | 0.96 |
| 1:A:1038:TRP:O | 1:A:1042:GLU:HG2 | 1.65 | 0.96 |
| 1:A:211:LEU:CD1 | 1:A:221:TYR:HB3 | 1.96 | 0.96 |
| 1:A:605:LEU:HA | 1:A:781:ALA:HB3 | 1.47 | 0.96 |
| 2:C:417:TYR:HD2 | 2:C:417:TYR:N | 1.64 | 0.96 |
| 1:D:1007:GLU:O | 1:D:1011:PRO:HD3 | 1.65 | 0.96 |
| 1:D:798:ILE:HA | 1:D:869:ARG:CZ | 1.95 | 0.96 |
| 1:D:993:ARG:N | 1:D:996:ARG:HD2 | 1.79 | 0.96 |
| 2:F:466:MET:HB3 | 2:F:471:LEU:CD2 | 1.96 | 0.96 |
| 1:A:666:GLN:O | 1:A:670:PRO:CD | 2.14 | 0.96 |
| 2:C:239:LEU:H | 2:C:338:VAL:HG12 | 1.18 | 0.96 |
| 1:D:193:ARG:HA | 1:D:193:ARG:CZ | 1.96 | 0.96 |
| 1:D:866:ARG:HG3 | 1:D:1069:ILE:CG2 | 1.95 | 0.96 |
| 2:E:380:PRO:O | 2:E:382:LYS:HB2 | 1.65 | 0.96 |
| 1:A:493:GLN:O | 1:A:494:GLU:HG2 | 1.65 | 0.96 |
| 2:C:317:GLY:HA3 | 2:C:320:SER:H | 1.29 | 0.96 |
| 1:D:1067:SER:CA | 1:D:1071:ARG:HA | 1.96 | 0.96 |
| 2:E:419:GLU:HA | 2:F:203:ARG:NH2 | 1.81 | 0.96 |
| 1:D:1069:ILE:CB | 1:D:1070:PRO:HD2 | 1.96 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:285:GLN:NE2 | 1:D:1128:ARG:HG2 | 1.80 | 0.96 |
| 1:D:559:LEU:HG | 1:D:560:PRO:HD2 | 1.45 | 0.96 |
| 1:D:604:ALA:HA | 1:D:613:HIS:HE1 | 1.24 | 0.96 |
| 2:F:309:HIS:HA | 2:F:312:LEU:HD12 | 1.43 | 0.96 |
| 2:F:455:LEU:HA | 2:F:456:ARG:HH21 | 1.27 | 0.96 |
| 1:A:660:CYS:SG | 1:A:661:LEU:N | 2.39 | 0.95 |
| 2:C:317:GLY:CA | 2:C:320:SER:HB2 | 1.95 | 0.95 |
| 2:C:454:HIS:HA | 2:C:468:ILE:HD12 | 1.47 | 0.95 |
| 1:D:597:ARG:C | 1:D:616:GLU:OE1 | 2.05 | 0.95 |
| 1:D:605:LEU:O | 1:D:781:ALA:HA | 1.65 | 0.95 |
| 2:B:261:GLN:NE2 | 2:B:264:ARG:HH21 | 1.62 | 0.95 |
| 2:B:311:LEU:CG | 2:B:312:LEU:H | 1.78 | 0.95 |
| 2:B:86:LEU:HD23 | 2:B:96:HIS:HB2 | 1.48 | 0.95 |
| 2:F:114:TRP:HE1 | 2:F:259:ARG:CZ | 1.78 | 0.95 |
| 2:F:241:TRP:N | 2:F:336:LEU:CB | 2.29 | 0.95 |
| 2:F:241:TRP:CD1 | 2:F:243:THR:HG23 | 2.01 | 0.95 |
| 1:D:1208:ARG:HH22 | 2:F:285:LYS:CD | 1.78 | 0.95 |
| 2:F:423:SER:OG | 2:F:428:LEU:HD21 | 1.66 | 0.95 |
| 2:F:453:ILE:HG22 | 2:F:455:LEU:H | 1.30 | 0.95 |
| 2:B:301:GLU:HA | 2:B:340:GLY:HA3 | 1.47 | 0.95 |
| 2:C:431:LYS:NZ | 2:C:435:MET:HG2 | 1.80 | 0.95 |
| 1:D:1138:ARG:HH11 | 1:D:1138:ARG:HG2 | 1.29 | 0.95 |
| 1:D:849:THR:HB | 1:D:852:ARG:H | 1.31 | 0.95 |
| 1:A:176:THR:CA | 1:A:218:SER:HB2 | 1.96 | 0.95 |
| 1:A:758:ASN:HB2 | 1:A:1058:PHE:CZ | 2.00 | 0.95 |
| 1:A:927:ARG:HG2 | 1:A:928:GLY:N | 1.81 | 0.95 |
| 2:B:260:LEU:C | 2:B:264:ARG:HD3 | 1.86 | 0.95 |
| 1:D:1023:GLN:OE1 | 1:D:1100:VAL:HA | 1.64 | 0.95 |
| 1:D:241:PRO:O | 1:D:244:LEU:HG | 1.65 | 0.95 |
| 1:D:203:LEU:N | 1:D:380:GLY:HA2 | 1.79 | 0.95 |
| 2:E:187:HIS:HA | 2:E:190:LEU:HD22 | 1.47 | 0.95 |
| 2:F:134:LYS:HB3 | 2:F:180:LYS:HD3 | 1.49 | 0.95 |
| 2:E:181:LEU:HB3 | 2:E:215:PHE:HE1 | 1.28 | 0.95 |
| 2:F:127:PRO:HD3 | 2:F:209:ALA:C | 1.87 | 0.95 |
| 2:F:350:LEU:HD12 | 2:F:350:LEU:N | 1.80 | 0.95 |
| 2:F:435:MET:HE2 | 2:F:435:MET:HA | 1.46 | 0.95 |
| 1:A:1218:LEU:O | 1:A:1219:ASP:HB2 | 1.64 | 0.95 |
| 1:A:169:TRP:CZ3 | 1:A:391:ASP:HA | 2.01 | 0.95 |
| 2:B:372:LEU:HD13 | 2:B:434:GLU:HA | 1.45 | 0.95 |
| 2:C:206:TYR:HD2 | 2:C:206:TYR:H | 0.96 | 0.95 |
| 2:C:466:MET:CB | 2:C:471:LEU:HD22 | 1.97 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1006:ARG:HH12 | 1:D:1009:ASN:CB | 1.79 | 0.95 |
| 1:D:576:LEU:CG | 1:D:577:CYS:H | 1.80 | 0.95 |
| 1:A:1131:ILE:HD13 | 1:A:1138:ARG:N | 1.82 | 0.95 |
| 1:A:490:TRP:HH2 | 1:A:598:VAL:HB | 1.28 | 0.95 |
| 1:A:549:LEU:HD21 | 2:C:398:VAL:CB | 1.97 | 0.95 |
| 1:D:486:TRP:HZ2 | 1:D:722:ARG:HA | 1.31 | 0.95 |
| 1:A:1131:ILE:HD11 | 1:A:1133:ILE:HG22 | 1.49 | 0.95 |
| 1:A:996:ARG:NH2 | 1:A:1003:TRP:HB3 | 1.81 | 0.95 |
| 2:E:255:TRP:O | 2:E:259:ARG:HB2 | 1.66 | 0.95 |
| 2:E:382:LYS:HG2 | 2:E:412:SER:CB | 1.96 | 0.95 |
| 2:E:449:GLU:HA | 2:E:449:GLU:OE1 | 1.61 | 0.95 |
| 1:A:203:LEU:C | 1:A:205:GLU:N | 2.19 | 0.95 |
| 1:A:194:ALA:HA | 1:A:265:LEU:HB2 | 1.45 | 0.95 |
| 1:A:580:LEU:HD12 | 1:A:581:ASP:H | 1.32 | 0.95 |
| 1:A:853:ARG:HH12 | 1:A:1105:ALA:HB3 | 1.29 | 0.95 |
| 1:A:176:THR:HG23 | 1:A:177:ARG:H | 1.31 | 0.95 |
| 1:A:210:THR:HB | 1:A:224:CYS:HB2 | 0.95 | 0.95 |
| 1:D:513:LEU:HB2 | 1:D:568:GLY:HA2 | 1.45 | 0.95 |
| 2:E:431:LYS:HA | 2:E:434:GLU:CG | 1.95 | 0.95 |
| 1:A:1069:ILE:HG22 | 1:A:1070:PRO:HD3 | 1.47 | 0.94 |
| 1:A:348:LEU:HA | 1:A:350:ILE:HD13 | 1.46 | 0.94 |
| 1:A:454:GLU:O | 1:A:458:GLU:HG3 | 1.67 | 0.94 |
| 2:B:323:HIS:CA | 2:B:332:VAL:HA | 1.97 | 0.94 |
| 1:D:145:LYS:O | 1:D:149:PRO:HD2 | 1.67 | 0.94 |
| 1:D:621:GLY:HA2 | 1:D:748:TRP:CB | 1.96 | 0.94 |
| 1:D:441:TRP:HE1 | 1:D:880:ALA:H | 1.14 | 0.94 |
| 2:E:117:SER:HA | 2:E:121:PHE:CE1 | 2.01 | 0.94 |
| 1:A:756:ASP:CB | 1:A:1057:MET:HG2 | 1.97 | 0.94 |
| 1:A:170:ALA:CB | 1:A:175:TRP:HZ2 | 1.79 | 0.94 |
| 1:A:272:SER:HA | 1:A:275:ARG:HB2 | 1.49 | 0.94 |
| 1:D:429:GLU:HG3 | 1:D:1128:ARG:NH2 | 1.82 | 0.94 |
| 1:D:607:TRP:HD1 | 1:D:780:GLN:H | 1.00 | 0.94 |
| 1:D:914:THR:O | 1:D:918:TRP:CB | 2.15 | 0.94 |
| 1:A:645:VAL:HG13 | 1:A:650:ARG:HB2 | 1.48 | 0.94 |
| 2:C:467:HIS:O | 2:C:471:LEU:CD1 | 2.15 | 0.94 |
| 1:D:452:TYR:CB | 1:D:801:TRP:HE1 | 1.79 | 0.94 |
| 1:D:490:TRP:HE3 | 1:D:580:LEU:HD22 | 1.29 | 0.94 |
| 1:D:813:VAL:HB | 1:D:840:ILE:HG13 | 1.49 | 0.94 |
| 1:D:824:ALA:HA | 1:D:827:ARG:CG | 1.96 | 0.94 |
| 1:A:1236:GLN:HB3 | 1:A:1237:PRO:CD | 1.97 | 0.94 |
| 1:A:225:SER:OG | 1:A:386:ARG:HB2 | 1.67 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:378:VAL:C | 1:A:380:GLY:N | 2.19 | 0.94 |
| 1:D:1118:TRP:O | 1:D:1121:GLU:HG3 | 1.68 | 0.94 |
| 1:D:259:ARG:HA | 1:D:259:ARG:NH1 | 1.80 | 0.94 |
| 2:E:447:THR:CG2 | 2:E:453:ILE:HG23 | 1.97 | 0.94 |
| 2:F:214:CYS:SG | 2:F:236:GLU:HG3 | 2.07 | 0.94 |
| 2:C:471:LEU:HD12 | 2:C:471:LEU:N | 1.82 | 0.94 |
| 1:D:1069:ILE:O | 1:D:1071:ARG:HG3 | 1.66 | 0.94 |
| 1:D:79:LEU:HD23 | 1:D:83:LEU:HD12 | 1.49 | 0.94 |
| 2:E:456:ARG:HD3 | 2:E:463:LYS:HG3 | 1.48 | 0.94 |
| 1:D:1029:GLN:HG2 | 1:D:1030:ARG:NE | 1.82 | 0.94 |
| 1:D:933:SER:HB2 | 1:D:943:ARG:HD3 | 1.45 | 0.94 |
| 1:A:515:ILE:HG22 | 1:A:516:GLU:H | 1.26 | 0.94 |
| 2:C:190:LEU:O | 2:C:193:TYR:HB3 | 1.67 | 0.94 |
| 2:C:303:LEU:CA | 2:C:337:SER:OG | 2.14 | 0.94 |
| 1:A:784:GLY:HA2 | 2:C:362:THR:HG1 | 1.20 | 0.94 |
| 2:C:439:PHE:HB3 | 2:C:457:SER:O | 1.67 | 0.94 |
| 1:D:922:GLN:HG2 | 1:D:931:LEU:HD13 | 1.48 | 0.94 |
| 2:E:264:ARG:NE | 2:E:273:PHE:HB2 | 1.82 | 0.94 |
| 2:E:266:PHE:HB3 | 2:E:376:PRO:CD | 1.96 | 0.94 |
| 2:E:425:LEU:HB3 | 2:E:426:GLU:OE2 | 1.68 | 0.94 |
| 2:F:466:MET:SD | 2:F:471:LEU:HD23 | 2.08 | 0.94 |
| 2:B:343:ASP:HB3 | 2:B:344:ARG:HE | 1.33 | 0.94 |
| 2:B:105:GLU:HB3 | 2:B:380:PRO:HB3 | 1.50 | 0.94 |
| 1:D:1155:ILE:HA | 1:D:1158:LEU:HD21 | 1.49 | 0.94 |
| 1:D:274:ASP:OD2 | 1:D:293:ASP:HA | 1.66 | 0.94 |
| 1:A:1001:GLY:O | 1:A:1005:VAL:HG13 | 1.67 | 0.94 |
| 2:C:200:VAL:CG2 | 2:C:204:LEU:HD22 | 1.98 | 0.94 |
| 2:C:127:PRO:HD3 | 2:C:210:GLN:N | 1.81 | 0.94 |
| 2:C:69:LEU:HD23 | 2:C:351:TYR:CE1 | 2.02 | 0.94 |
| 2:C:443:VAL:HA | 2:C:447:THR:CG2 | 1.98 | 0.94 |
| 1:D:577:CYS:C | 1:D:579:ARG:H | 1.70 | 0.94 |
| 2:F:125:VAL:HG23 | 2:F:126:PHE:N | 1.81 | 0.94 |
| 1:A:490:TRP:CH2 | 1:A:598:VAL:HB | 2.02 | 0.94 |
| 2:C:357:THR:O | 2:C:358:GLU:HG2 | 1.68 | 0.94 |
| 1:D:735:GLY:HA3 | 1:D:749:PHE:CB | 1.97 | 0.94 |
| 2:E:430:SER:O | 2:E:433:ASP:HB3 | 1.65 | 0.94 |
| 1:A:1023:GLN:NE2 | 1:A:1103:SER:OG | 2.01 | 0.94 |
| 1:A:288:ARG:HE | 1:A:288:ARG:CA | 1.81 | 0.94 |
| 1:A:640:LEU:H | 1:A:640:LEU:HD23 | 1.33 | 0.94 |
| 1:A:893:SER:HB2 | 1:A:896:LEU:CB | 1.97 | 0.94 |
| 2:C:125:VAL:HG22 | 2:C:208:LEU:CA | 1.97 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:455:LEU:HD12 | 1:D:869:ARG:NH1 | 1.83 | 0.94 |
| 1:D:623:LEU:HB3 | 1:D:667:GLN:NE2 | 1.83 | 0.94 |
| 1:A:1128:ARG:CG | 1:A:1129:PHE:H | 1.77 | 0.93 |
| 1:A:201:VAL:HG22 | 1:A:208:CYS:O | 1.69 | 0.93 |
| 1:A:166:PRO:HG3 | 1:A:398:GLN:NE2 | 1.83 | 0.93 |
| 1:A:897:TRP:O | 1:A:900:ALA:HB3 | 1.68 | 0.93 |
| 2:B:72:ILE:O | 2:B:75:ARG:HG3 | 1.67 | 0.93 |
| 1:D:887:VAL:N | 1:D:1146:ARG:HH12 | 1.66 | 0.93 |
| 1:D:309:ARG:O | 1:D:313:ILE:HG23 | 1.68 | 0.93 |
| 1:D:392:LEU:O | 1:D:395:TYR:HB2 | 1.65 | 0.93 |
| 1:D:780:GLN:OE1 | 1:D:780:GLN:HA | 1.67 | 0.93 |
| 2:F:353:SER:HB2 | 2:F:373:LYS:H | 1.31 | 0.93 |
| 1:A:1006:ARG:HA | 1:A:1006:ARG:NH1 | 1.83 | 0.93 |
| 1:A:298:HIS:CD2 | 1:A:358:LEU:HD22 | 2.02 | 0.93 |
| 2:B:114:TRP:HA | 2:B:262:TRP:CZ2 | 2.03 | 0.93 |
| 1:D:1200:PRO:CG | 1:D:1203:PRO:HG2 | 1.97 | 0.93 |
| 1:D:275:ARG:HH21 | 1:D:842:PRO:CB | 1.81 | 0.93 |
| 1:D:356:LEU:HD13 | 1:D:369:LEU:HD22 | 1.50 | 0.93 |
| 1:D:407:PHE:O | 1:D:411:LEU:HG | 1.68 | 0.93 |
| 1:D:275:ARG:HH21 | 1:D:842:PRO:HB3 | 1.32 | 0.93 |
| 1:A:1043:VAL:CG1 | 1:A:1046:GLU:HB3 | 1.97 | 0.93 |
| 1:A:1124:ALA:HB1 | 1:A:1148:ARG:NH1 | 1.82 | 0.93 |
| 1:A:196:VAL:HB | 1:A:401:TRP:HZ3 | 1.29 | 0.93 |
| 1:A:485:LEU:HD12 | 1:A:489:GLU:OE2 | 1.69 | 0.93 |
| 1:A:566:LEU:HB3 | 1:A:567:PRO:HD3 | 1.51 | 0.93 |
| 1:A:893:SER:CB | 1:A:896:LEU:HB2 | 1.98 | 0.93 |
| 2:C:322:LEU:HD13 | 2:C:322:LEU:O | 1.68 | 0.93 |
| 2:E:277:ASP:HA | 2:E:287:ASN:OD1 | 1.68 | 0.93 |
| 2:F:238:SER:HA | 2:F:338:VAL:HG11 | 1.48 | 0.93 |
| 2:F:289:LEU:HD12 | 2:F:301:GLU:HB2 | 1.48 | 0.93 |
| 2:F:391:PRO:HB2 | 2:F:394:GLU:OE2 | 1.68 | 0.93 |
| 1:A:582:ASP:N | 1:A:583:PRO:HD2 | 1.83 | 0.93 |
| 2:C:376:PRO:HG3 | 2:C:482:ALA:HB1 | 1.49 | 0.93 |
| 1:D:1204:THR:HA | 1:D:1207:GLU:CB | 1.99 | 0.93 |
| 1:D:606:THR:HG21 | 1:D:612:LEU:O | 1.66 | 0.93 |
| 2:F:234:LYS:NZ | 2:F:344:ARG:HD2 | 1.82 | 0.93 |
| 2:F:387:VAL:CA | 2:F:443:VAL:HG22 | 1.97 | 0.93 |
| 1:A:1026:ARG:HB2 | 1:A:1029:GLN:HB2 | 1.49 | 0.93 |
| 1:A:1131:ILE:HG23 | 1:A:1132:SER:H | 1.31 | 0.93 |
| 1:A:925:LYS:HG3 | 1:A:926:SER:H | 1.32 | 0.93 |
| 1:D:1025:LEU:HD13 | 1:D:1027:LYS:HE2 | 1.47 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1051:GLY:HA2 | 1:D:1054:GLU:HG3 | 1.49 | 0.93 |
| 1:D:1231:LEU:HG | 1:D:1232:GLU:N | 1.81 | 0.93 |
| 2:F:456:ARG:HG2 | 2:F:457:SER:H | 1.33 | 0.93 |
| 1:A:309:ARG:O | 1:A:313:ILE:HG23 | 1.68 | 0.93 |
| 2:B:396:ARG:CD | 2:B:417:TYR:HB2 | 1.97 | 0.93 |
| 1:A:556:THR:HG23 | 2:C:452:LEU:HB3 | 1.50 | 0.93 |
| 1:D:768:LYS:HA | 1:D:772:PRO:HG3 | 1.51 | 0.93 |
| 1:A:744:ILE:HB | 1:A:745:PRO:HD3 | 1.50 | 0.93 |
| 1:D:1116:MET:HE3 | 1:D:1153:LEU:HA | 1.46 | 0.93 |
| 2:F:203:ARG:HB3 | 2:F:204:LEU:CD1 | 1.97 | 0.93 |
| 1:A:1057:MET:C | 1:A:1064:ILE:HG21 | 1.89 | 0.93 |
| 1:A:606:THR:HG22 | 1:A:620:TRP:HE3 | 1.29 | 0.93 |
| 2:B:323:HIS:HB2 | 2:B:331:VAL:C | 1.88 | 0.93 |
| 1:D:436:PRO:O | 1:D:879:GLN:HB2 | 1.67 | 0.93 |
| 2:E:407:LEU:HD23 | 2:E:411:ILE:O | 1.67 | 0.93 |
| 1:D:1206:MET:HG2 | 2:F:257:ARG:NH1 | 1.83 | 0.93 |
| 1:A:1188:CYS:C | 1:A:1189:LEU:HD22 | 1.90 | 0.93 |
| 1:D:1231:LEU:HD11 | 1:D:1236:GLN:HE21 | 1.33 | 0.93 |
| 1:D:666:GLN:C | 1:D:669:MET:O | 2.07 | 0.93 |
| 2:F:299:LEU:N | 2:F:299:LEU:HD23 | 1.81 | 0.93 |
| 2:F:447:THR:O | 2:F:452:LEU:HA | 1.68 | 0.93 |
| 1:A:273:PHE:HA | 1:A:276:ALA:HB2 | 1.46 | 0.93 |
| 1:D:1223:ILE:HG13 | 1:D:1224:ILE:N | 1.83 | 0.93 |
| 1:D:509:THR:CB | 1:D:512:LYS:HB3 | 1.97 | 0.93 |
| 1:D:580:LEU:HD11 | 1:D:593:SER:OG | 1.67 | 0.93 |
| 1:D:608:ASP:OD1 | 1:D:611:PRO:HD2 | 1.69 | 0.93 |
| 1:D:549:LEU:HD21 | 2:F:398:VAL:HA | 1.49 | 0.93 |
| 1:A:411:LEU:HD12 | 1:A:412:PRO:N | 1.84 | 0.92 |
| 1:A:886:LEU:N | 1:A:1146:ARG:NH2 | 2.17 | 0.92 |
| 2:C:454:HIS:HB2 | 2:C:468:ILE:HA | 1.47 | 0.92 |
| 2:C:467:HIS:HB3 | 2:C:470:LYS:HE2 | 1.50 | 0.92 |
| 1:D:897:TRP:CH2 | 1:D:1173:LEU:HD13 | 2.04 | 0.92 |
| 1:D:217:PRO:O | 1:D:218:SER:OG | 1.87 | 0.92 |
| 1:D:269:HIS:CD2 | 1:D:291:PHE:HD2 | 1.85 | 0.92 |
| 1:D:808:ILE:O | 1:D:811:GLN:HB2 | 1.69 | 0.92 |
| 2:F:127:PRO:CD | 2:F:128:VAL:H | 1.78 | 0.92 |
| 2:F:301:GLU:CG | 2:F:339:ASN:HB3 | 1.99 | 0.92 |
| 1:A:1131:ILE:HD13 | 1:A:1138:ARG:H | 1.32 | 0.92 |
| 1:A:223:TRP:CD1 | 1:A:223:TRP:N | 2.36 | 0.92 |
| 1:A:451:THR:OG1 | 1:A:1202:ASN:CG | 2.07 | 0.92 |
| 2:C:350:LEU:N | 2:C:350:LEU:HD12 | 1.82 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:592:LEU:HA | 1:D:595:GLN:CG | 1.98 | 0.92 |
| 1:A:657:ARG:O | 1:A:660:CYS:HB3 | 1.68 | 0.92 |
| 1:D:270:ASN:HA | 1:D:294:THR:HG23 | 1.49 | 0.92 |
| 1:D:371:LYS:HA | 1:D:374:ARG:HD2 | 1.51 | 0.92 |
| 1:D:795:ASN:N | 1:D:795:ASN:HD22 | 1.59 | 0.92 |
| 1:A:1030:ARG:CG | 1:A:1040:LYS:HZ1 | 1.83 | 0.92 |
| 1:A:434:TYR:O | 1:A:435:LEU:HG | 1.68 | 0.92 |
| 1:D:633:LYS:CB | 1:D:638:THR:HG21 | 1.99 | 0.92 |
| 2:E:247:THR:HG22 | 2:E:250:GLN:HE21 | 1.32 | 0.92 |
| 1:A:245:ILE:CG1 | 1:A:246:PRO:HD3 | 2.00 | 0.92 |
| 1:A:468:ASN:ND2 | 2:C:460:THR:HG21 | 1.84 | 0.92 |
| 2:C:303:LEU:C | 2:C:337:SER:HB2 | 1.90 | 0.92 |
| 1:D:412:PRO:HG2 | 1:D:413:LEU:HG | 1.51 | 0.92 |
| 2:E:431:LYS:C | 2:E:433:ASP:H | 1.67 | 0.92 |
| 2:F:453:ILE:HD13 | 2:F:465:MET:HB3 | 1.51 | 0.92 |
| 1:A:112:LEU:HD23 | 1:A:920:THR:HB | 1.50 | 0.92 |
| 1:A:125:LEU:H | 1:A:125:LEU:CD2 | 1.82 | 0.92 |
| 1:A:169:TRP:HZ3 | 1:A:391:ASP:HA | 1.32 | 0.92 |
| 2:C:341:ASP:CG | 2:C:342:LEU:N | 2.20 | 0.92 |
| 1:D:1131:ILE:H | 1:D:1131:ILE:HD12 | 1.35 | 0.92 |
| 1:D:1208:ARG:NH1 | 2:F:285:LYS:HD3 | 1.83 | 0.92 |
| 1:D:127:LEU:HD22 | 1:D:129:PRO:HD3 | 1.51 | 0.92 |
| 1:D:438:ASN:O | 1:D:441:TRP:HB2 | 1.69 | 0.92 |
| 1:D:275:ARG:NE | 1:D:842:PRO:HA | 1.84 | 0.92 |
| 1:A:107:LEU:HB2 | 1:A:113:TRP:CD1 | 2.03 | 0.92 |
| 1:A:213:VAL:HA | 1:A:221:TYR:HE2 | 1.35 | 0.92 |
| 2:C:209:ALA:HB1 | 2:C:238:SER:O | 1.69 | 0.92 |
| 2:C:126:PHE:HA | 2:C:209:ALA:O | 1.70 | 0.92 |
| 2:F:317:GLY:HA2 | 2:F:320:SER:HB2 | 1.52 | 0.92 |
| 2:F:368:HIS:NE2 | 2:F:370:LYS:HD2 | 1.84 | 0.92 |
| 1:A:891:VAL:HA | 1:A:1180:PHE:HE1 | 1.35 | 0.92 |
| 1:A:412:PRO:HG2 | 1:A:413:LEU:H | 1.31 | 0.92 |
| 1:A:887:VAL:CG2 | 1:A:1146:ARG:HH11 | 1.83 | 0.92 |
| 1:D:1027:LYS:HB3 | 1:D:1091:GLU:HB3 | 1.52 | 0.92 |
| 1:D:849:THR:HB | 1:D:852:ARG:N | 1.85 | 0.92 |
| 2:F:222:LYS:O | 2:F:223:GLN:HB2 | 1.70 | 0.92 |
| 1:D:1116:MET:CE | 1:D:1153:LEU:HA | 2.00 | 0.92 |
| 1:D:113:TRP:HE3 | 1:D:114:GLY:H | 1.09 | 0.92 |
| 1:D:85:GLU:CD | 1:D:130:LEU:HD22 | 1.90 | 0.92 |
| 1:D:283:LEU:HD23 | 1:D:839:ALA:HB3 | 1.52 | 0.92 |
| 2:C:421:MET:HG3 | 2:C:422:GLN:N | 1.85 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1190:ARG:HD3 | 1:D:1195:MET:HE3 | 1.52 | 0.91 |
| 1:D:743:ASP:C | 1:D:744:ILE:HD13 | 1.91 | 0.91 |
| 2:F:256:LEU:HD11 | 2:F:287:ASN:OD1 | 1.71 | 0.91 |
| 1:A:195:LEU:CD2 | 1:A:217:PRO:HD2 | 2.01 | 0.91 |
| 1:D:873:GLU:HB3 | 1:D:1200:PRO:CD | 2.00 | 0.91 |
| 1:D:470:ALA:O | 1:D:474:LEU:HD13 | 1.71 | 0.91 |
| 1:D:513:LEU:H | 1:D:570:PRO:CG | 1.83 | 0.91 |
| 1:A:1010:LEU:O | 1:A:1096:ARG:NH2 | 2.02 | 0.91 |
| 2:C:342:LEU:HD23 | 2:C:345:GLY:H | 1.33 | 0.91 |
| 1:D:374:ARG:HB3 | 1:D:392:LEU:HD11 | 1.52 | 0.91 |
| 1:D:457:ARG:HA | 1:D:460:LYS:HD2 | 1.52 | 0.91 |
| 1:D:272:SER:HB3 | 1:D:843:GLN:CD | 1.91 | 0.91 |
| 1:A:634:LEU:CB | 1:A:635:PRO:HA | 1.99 | 0.91 |
| 1:A:885:THR:C | 1:A:886:LEU:HD23 | 1.91 | 0.91 |
| 2:C:303:LEU:HA | 2:C:337:SER:HG | 1.10 | 0.91 |
| 1:A:784:GLY:H | 2:C:363:ARG:HD3 | 1.32 | 0.91 |
| 1:D:350:ILE:O | 1:D:361:ARG:HB2 | 1.70 | 0.91 |
| 1:D:424:LEU:O | 1:D:428:LEU:HD11 | 1.69 | 0.91 |
| 2:E:383:VAL:O | 2:E:384:ALA:CB | 2.17 | 0.91 |
| 2:F:439:PHE:CD1 | 2:F:458:ARG:HB2 | 2.03 | 0.91 |
| 1:A:228:LEU:CD1 | 1:A:386:ARG:HB3 | 2.01 | 0.91 |
| 1:A:618:HIS:HB2 | 1:A:725:PRO:CB | 2.00 | 0.91 |
| 2:B:202:LYS:O | 2:B:325:ARG:NH1 | 2.04 | 0.91 |
| 1:D:1218:LEU:HB3 | 1:D:1223:ILE:HG22 | 1.52 | 0.91 |
| 1:D:278:ILE:CG2 | 1:D:279:ARG:HD3 | 2.00 | 0.91 |
| 1:D:618:HIS:HB2 | 1:D:725:PRO:CD | 2.00 | 0.91 |
| 1:D:73:PRO:CG | 1:D:90:GLN:HG2 | 2.00 | 0.91 |
| 2:F:303:LEU:HA | 2:F:337:SER:HG | 1.32 | 0.91 |
| 1:A:1060:LYS:CE | 1:A:1065:ALA:H | 1.82 | 0.91 |
| 1:A:240:SER:HA | 1:A:243:ASP:OD2 | 1.70 | 0.91 |
| 1:A:316:LYS:CD | 1:A:350:ILE:HG12 | 1.99 | 0.91 |
| 2:B:204:LEU:HD12 | 2:B:325:ARG:H | 1.35 | 0.91 |
| 1:D:190:PRO:C | 1:D:192:GLU:H | 1.72 | 0.91 |
| 1:D:891:VAL:CG1 | 1:D:1135:ASP:HB3 | 2.00 | 0.91 |
| 2:E:128:VAL:HG13 | 2:E:210:GLN:NE2 | 1.84 | 0.91 |
| 2:F:125:VAL:CG2 | 2:F:208:LEU:HA | 1.97 | 0.91 |
| 1:A:1046:GLU:O | 1:A:1049:TRP:HD1 | 1.52 | 0.91 |
| 1:A:203:LEU:CD1 | 1:A:379:LYS:C | 2.38 | 0.91 |
| 1:A:997:LEU:HD22 | 1:A:998:SER:N | 1.85 | 0.91 |
| 2:C:454:HIS:N | 2:C:466:MET:O | 2.02 | 0.91 |
| 1:D:1002:GLU:O | 1:D:1005:VAL:HG22 | 1.69 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:634:LEU:HD13 | 1:D:635:PRO:O | 1.69 | 0.91 |
| 1:D:649:TYR:CA | 1:D:652:ILE:HB | 2.01 | 0.91 |
| 1:A:996:ARG:NH1 | 1:A:1003:TRP:CB | 2.33 | 0.91 |
| 1:A:163:PRO:HB3 | 1:A:164:PRO:HD3 | 1.52 | 0.91 |
| 1:A:374:ARG:HH11 | 1:A:374:ARG:HG2 | 1.35 | 0.91 |
| 1:A:498:LYS:CD | 1:A:518:ALA:HB3 | 2.00 | 0.91 |
| 1:A:618:HIS:CB | 1:A:725:PRO:HB2 | 2.00 | 0.91 |
| 2:C:241:TRP:HB2 | 2:C:336:LEU:HD12 | 0.94 | 0.91 |
| 2:C:306:LEU:N | 2:C:335:VAL:HG11 | 1.85 | 0.91 |
| 2:C:302:THR:H | 2:C:339:ASN:HA | 1.36 | 0.91 |
| 1:A:784:GLY:CA | 2:C:362:THR:OG1 | 2.18 | 0.91 |
| 2:C:471:LEU:HA | 2:C:474:PHE:HB3 | 1.52 | 0.91 |
| 1:D:605:LEU:HD22 | 1:D:781:ALA:HB1 | 1.52 | 0.91 |
| 1:D:1209:ARG:HH22 | 2:F:252:LEU:HD22 | 1.33 | 0.91 |
| 1:A:1200:PRO:HB2 | 1:A:1202:ASN:C | 1.90 | 0.91 |
| 1:A:1236:GLN:H | 1:A:1236:GLN:NE2 | 1.68 | 0.91 |
| 1:A:851:THR:HG22 | 1:A:853:ARG:H | 1.36 | 0.91 |
| 2:B:211:ILE:HG12 | 2:B:237:ALA:HB1 | 1.51 | 0.91 |
| 2:C:435:MET:CE | 2:C:435:MET:HA | 2.01 | 0.91 |
| 2:C:81:GLY:HA3 | 2:C:97:PRO:HB2 | 1.53 | 0.91 |
| 1:D:449:GLN:HA | 1:D:452:TYR:HE2 | 1.32 | 0.91 |
| 2:E:428:LEU:CD1 | 2:E:428:LEU:H | 1.83 | 0.91 |
| 2:F:342:LEU:HB2 | 2:F:344:ARG:CG | 2.00 | 0.91 |
| 1:A:436:PRO:HD2 | 1:A:879:GLN:NE2 | 1.86 | 0.91 |
| 1:A:503:VAL:CG2 | 1:A:521:PRO:HA | 2.01 | 0.91 |
| 1:A:774:MET:HA | 1:A:777:GLY:HA3 | 1.52 | 0.91 |
| 2:C:374:LEU:HB3 | 2:C:378:LEU:HB3 | 1.51 | 0.91 |
| 1:D:630:ASN:HB2 | 1:D:744:ILE:C | 1.91 | 0.91 |
| 1:D:436:PRO:O | 1:D:879:GLN:CB | 2.19 | 0.91 |
| 1:A:1191:LYS:O | 1:A:1192:GLU:HB3 | 1.71 | 0.90 |
| 1:A:961:PHE:H | 1:A:961:PHE:HD1 | 1.16 | 0.90 |
| 1:D:105:GLU:O | 1:D:109:LYS:HG2 | 1.70 | 0.90 |
| 1:D:1157:ASN:HB3 | 1:D:1161:ARG:NH1 | 1.85 | 0.90 |
| 1:D:297:MET:HG2 | 1:D:411:LEU:CD2 | 2.00 | 0.90 |
| 1:D:556:THR:O | 1:D:559:LEU:HB3 | 1.71 | 0.90 |
| 2:E:422:GLN:HG2 | 2:E:424:SER:H | 1.32 | 0.90 |
| 2:E:374:LEU:H | 2:E:458:ARG:NH2 | 1.67 | 0.90 |
| 2:F:241:TRP:N | 2:F:336:LEU:HB3 | 1.86 | 0.90 |
| 1:A:1212:ILE:HG22 | 1:A:1213:PRO:N | 1.81 | 0.90 |
| 1:D:279:ARG:O | 1:D:841:LEU:HG | 1.69 | 0.90 |
| 2:F:241:TRP:HB2 | 2:F:336:LEU:HD12 | 0.91 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1027:LYS:HB2 | 1:A:1092:PHE:CD2 | 2.05 | 0.90 |
| 1:A:477:GLU:HG2 | 1:A:482:ASP:CG | 1.92 | 0.90 |
| 2:C:354:PHE:CE1 | 2:C:370:LYS:HD3 | 2.06 | 0.90 |
| 2:C:61:GLY:O | 2:C:64:GLU:HG2 | 1.70 | 0.90 |
| 1:D:1131:ILE:N | 1:D:1131:ILE:CD1 | 2.28 | 0.90 |
| 2:F:291:TYR:OH | 2:F:355:GLN:HG3 | 1.71 | 0.90 |
| 1:A:107:LEU:HB2 | 1:A:113:TRP:NE1 | 1.85 | 0.90 |
| 1:A:79:LEU:HB3 | 1:A:89:GLY:HA2 | 1.52 | 0.90 |
| 1:A:275:ARG:HH21 | 1:A:845:VAL:HA | 1.23 | 0.90 |
| 2:C:454:HIS:HB3 | 2:C:466:MET:CB | 2.01 | 0.90 |
| 1:D:503:VAL:C | 1:D:505:LYS:H | 1.74 | 0.90 |
| 2:E:181:LEU:HB3 | 2:E:215:PHE:CE1 | 2.05 | 0.90 |
| 2:F:351:TYR:O | 2:F:355:GLN:N | 2.05 | 0.90 |
| 1:A:612:LEU:HB3 | 1:A:620:TRP:HB2 | 1.51 | 0.90 |
| 1:A:612:LEU:CD2 | 1:A:621:GLY:H | 1.81 | 0.90 |
| 2:B:202:LYS:O | 2:B:325:ARG:CD | 2.18 | 0.90 |
| 1:D:74:LEU:HD12 | 1:D:77:GLN:HA | 1.51 | 0.90 |
| 2:F:203:ARG:HB3 | 2:F:204:LEU:HD13 | 1.54 | 0.90 |
| 1:A:87:ILE:HG22 | 1:A:88:PHE:N | 1.86 | 0.90 |
| 2:B:347:LEU:O | 2:B:350:LEU:HB3 | 1.71 | 0.90 |
| 1:D:371:LYS:HA | 1:D:374:ARG:HD3 | 1.53 | 0.90 |
| 1:D:407:PHE:CD1 | 1:D:411:LEU:HD21 | 2.07 | 0.90 |
| 1:D:413:LEU:HA | 1:D:416:GLU:OE1 | 1.70 | 0.90 |
| 1:A:1231:LEU:HD11 | 1:A:1236:GLN:HE22 | 1.36 | 0.90 |
| 1:A:370:PRO:HB2 | 1:A:399:ASP:HB2 | 1.54 | 0.90 |
| 1:A:468:ASN:ND2 | 1:A:578:PRO:HG2 | 1.86 | 0.90 |
| 2:C:341:ASP:CG | 2:C:342:LEU:H | 1.72 | 0.90 |
| 2:C:388:GLY:O | 2:C:444:THR:HA | 1.70 | 0.90 |
| 2:C:446:THR:C | 2:C:450:ASN:HB3 | 1.92 | 0.90 |
| 2:E:325:ARG:HG2 | 2:E:330:ASN:HA | 1.54 | 0.90 |
| 1:A:177:ARG:HA | 1:A:182:GLY:O | 1.69 | 0.90 |
| 2:B:374:LEU:H | 2:B:458:ARG:HH22 | 1.12 | 0.90 |
| 1:D:175:TRP:CE3 | 1:D:184:ALA:HA | 2.06 | 0.90 |
| 1:D:214:ALA:N | 1:D:401:TRP:CZ2 | 2.40 | 0.90 |
| 1:A:241:PRO:HA | 1:A:244:LEU:HB2 | 1.53 | 0.90 |
| 1:A:197:PHE:N | 1:A:269:HIS:NE2 | 2.19 | 0.90 |
| 2:C:336:LEU:HD23 | 2:C:337:SER:N | 1.87 | 0.90 |
| 1:D:1020:ILE:HD13 | 1:D:1021:SER:CA | 2.02 | 0.90 |
| 1:D:1014:ARG:HD3 | 1:D:1026:ARG:HG3 | 1.54 | 0.90 |
| 1:D:823:ARG:HA | 1:D:826:ILE:HD11 | 1.51 | 0.90 |
| 2:E:270:PRO:HA | 2:E:273:PHE:CE2 | 2.05 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1224:ILE:O | 1:A:1224:ILE:HD12 | 1.71 | 0.90 |
| 1:A:276:ALA:HA | 1:A:279:ARG:HD3 | 1.53 | 0.90 |
| 2:C:395:LEU:HD21 | 2:C:443:VAL:HG12 | 1.52 | 0.90 |
| 1:D:1208:ARG:HH22 | 2:F:285:LYS:HD3 | 1.36 | 0.90 |
| 1:D:265:LEU:HG | 1:D:266:VAL:N | 1.86 | 0.90 |
| 1:D:966:LEU:HD23 | 1:D:970:ASN:HD21 | 1.34 | 0.90 |
| 2:E:456:ARG:HB2 | 2:E:463:LYS:CG | 2.02 | 0.90 |
| 2:F:208:LEU:HD12 | 2:F:208:LEU:O | 1.72 | 0.90 |
| 2:F:447:THR:CA | 2:F:452:LEU:HA | 2.02 | 0.90 |
| 1:A:653:GLU:HA | 1:A:656:TYR:CZ | 2.06 | 0.89 |
| 1:D:515:ILE:HD11 | 1:D:568:GLY:O | 1.72 | 0.89 |
| 1:D:486:TRP:CZ2 | 1:D:722:ARG:HA | 2.07 | 0.89 |
| 1:D:795:ASN:H | 1:D:795:ASN:ND2 | 1.68 | 0.89 |
| 2:F:61:GLY:O | 2:F:64:GLU:HG2 | 1.72 | 0.89 |
| 2:C:208:LEU:HD13 | 2:C:240:VAL:HB | 1.53 | 0.89 |
| 2:C:350:LEU:HD12 | 2:C:350:LEU:H | 1.37 | 0.89 |
| 1:D:956:GLY:CA | 1:D:1094:THR:HG23 | 2.00 | 0.89 |
| 1:D:460:LYS:N | 1:D:460:LYS:CE | 2.16 | 0.89 |
| 1:D:548:CYS:CA | 1:D:551:LYS:HD3 | 2.01 | 0.89 |
| 2:F:305:ASN:C | 2:F:335:VAL:HG11 | 1.92 | 0.89 |
| 2:F:341:ASP:CG | 2:F:342:LEU:N | 2.22 | 0.89 |
| 1:A:564:GLN:HA | 1:A:567:PRO:HD2 | 1.53 | 0.89 |
| 2:C:256:LEU:HD11 | 2:C:287:ASN:OD1 | 1.73 | 0.89 |
| 2:C:241:TRP:N | 2:C:336:LEU:CB | 2.36 | 0.89 |
| 1:D:548:CYS:N | 1:D:551:LYS:HZ3 | 1.70 | 0.89 |
| 1:D:614:TYR:CE2 | 1:D:620:TRP:CE3 | 2.60 | 0.89 |
| 2:E:128:VAL:HB | 2:E:208:LEU:HB3 | 1.53 | 0.89 |
| 1:A:1146:ARG:NH1 | 1:A:1185:ILE:HG23 | 1.86 | 0.89 |
| 1:A:214:ALA:HA | 1:A:401:TRP:CZ2 | 2.07 | 0.89 |
| 2:B:324:GLY:HA2 | 2:B:325:ARG:CZ | 2.01 | 0.89 |
| 2:C:102:LEU:HD11 | 2:C:435:MET:CE | 2.01 | 0.89 |
| 2:C:396:ARG:NH1 | 2:C:397:GLN:HA | 1.86 | 0.89 |
| 1:D:1206:MET:O | 1:D:1210:TYR:N | 2.06 | 0.89 |
| 2:E:431:LYS:HA | 2:E:434:GLU:HG2 | 1.52 | 0.89 |
| 2:F:403:PHE:CE1 | 2:F:415:PRO:HG3 | 2.06 | 0.89 |
| 1:A:1043:VAL:CA | 1:A:1046:GLU:H | 1.85 | 0.89 |
| 1:A:127:LEU:HD22 | 1:A:129:PRO:HD3 | 1.54 | 0.89 |
| 1:D:1066:THR:HG23 | 1:D:1068:ASP:OD1 | 1.71 | 0.89 |
| 1:D:179:GLY:CA | 1:D:182:GLY:HA3 | 2.02 | 0.89 |
| 1:D:504:LYS:HD2 | 1:D:523:ASP:CB | 2.01 | 0.89 |
| 1:D:767:ALA:CB | 1:D:771:LEU:HD22 | 2.03 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:804:ALA:O | 1:D:808:ILE:HG13 | 1.72 | 0.89 |
| 2:B:396:ARG:NH1 | 2:B:417:TYR:CD2 | 2.40 | 0.89 |
| 1:D:457:ARG:N | 1:D:460:LYS:HZ2 | 1.71 | 0.89 |
| 1:D:795:ASN:O | 1:D:798:ILE:HG12 | 1.73 | 0.89 |
| 2:F:322:LEU:O | 2:F:322:LEU:HD13 | 1.72 | 0.89 |
| 2:F:336:LEU:HD23 | 2:F:337:SER:N | 1.87 | 0.89 |
| 1:A:1066:THR:HG1 | 1:A:1071:ARG:HB3 | 1.37 | 0.89 |
| 1:A:256:PRO:HD2 | 1:A:257:THR:H | 1.38 | 0.89 |
| 1:A:608:ASP:CA | 1:A:779:LEU:HB2 | 2.03 | 0.89 |
| 1:A:621:GLY:CA | 1:A:748:TRP:HB3 | 2.02 | 0.89 |
| 2:C:82:SER:HA | 2:C:86:LEU:CD2 | 2.01 | 0.89 |
| 1:D:366:GLY:N | 1:D:367:PRO:HD3 | 1.88 | 0.89 |
| 1:D:371:LYS:O | 1:D:373:PRO:HD3 | 1.72 | 0.89 |
| 1:D:213:VAL:HG22 | 1:D:401:TRP:CZ2 | 2.08 | 0.89 |
| 1:D:634:LEU:HD22 | 1:D:635:PRO:HD2 | 1.53 | 0.89 |
| 1:A:1011:PRO:O | 1:A:1028:VAL:HG21 | 1.71 | 0.89 |
| 1:A:604:ALA:HA | 1:A:717:LEU:HD22 | 1.54 | 0.89 |
| 1:A:623:LEU:O | 1:A:623:LEU:HG | 1.73 | 0.89 |
| 1:A:912:GLY:C | 1:A:917:GLY:HA3 | 1.92 | 0.89 |
| 1:D:1166:TYR:HD1 | 1:D:1166:TYR:N | 1.69 | 0.89 |
| 1:D:869:ARG:H | 1:D:1200:PRO:HB3 | 1.37 | 0.89 |
| 1:D:95:PRO:HG2 | 1:D:99:ALA:HB3 | 1.54 | 0.89 |
| 1:A:297:MET:CE | 1:A:411:LEU:HD13 | 2.03 | 0.89 |
| 1:A:425:ALA:HA | 1:A:428:LEU:HD12 | 1.54 | 0.89 |
| 1:A:613:HIS:CB | 1:A:717:LEU:HG | 2.01 | 0.89 |
| 2:C:458:ARG:HH11 | 2:C:458:ARG:HG2 | 1.38 | 0.89 |
| 1:D:213:VAL:HG13 | 1:D:401:TRP:CZ2 | 2.07 | 0.89 |
| 1:D:267:VAL:HB | 1:D:269:HIS:HD2 | 1.28 | 0.89 |
| 1:D:374:ARG:CD | 1:D:392:LEU:HD21 | 2.02 | 0.89 |
| 1:D:472:GLN:HB3 | 2:F:460:THR:O | 1.72 | 0.89 |
| 1:D:772:PRO:HA | 1:D:775:GLU:HB2 | 1.54 | 0.89 |
| 1:D:1209:ARG:NH2 | 2:F:253:ASP:HA | 1.86 | 0.89 |
| 2:F:395:LEU:O | 2:F:398:VAL:HB | 1.73 | 0.89 |
| 1:A:253:ALA:HB3 | 1:A:256:PRO:HB3 | 1.55 | 0.89 |
| 1:A:612:LEU:CG | 1:A:613:HIS:N | 2.33 | 0.89 |
| 1:A:656:TYR:HB3 | 1:A:720:THR:OG1 | 1.72 | 0.89 |
| 2:B:117:SER:HB2 | 2:B:262:TRP:CE2 | 2.07 | 0.89 |
| 2:C:254:PHE:HA | 2:C:257:ARG:HH21 | 1.36 | 0.89 |
| 1:D:486:TRP:HA | 1:D:489:GLU:OE2 | 1.73 | 0.89 |
| 1:D:608:ASP:O | 1:D:609:GLY:C | 2.12 | 0.89 |
| 1:D:879:GLN:OE1 | 1:D:1189:LEU:HD21 | 1.71 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:201:ASN:OD1 | 2:F:422:GLN:HB2 | 1.72 | 0.89 |
| 1:A:1005:VAL:HA | 1:A:1008:LEU:HD12 | 1.55 | 0.88 |
| 1:A:173:GLU:OE2 | 1:A:223:TRP:HZ2 | 1.55 | 0.88 |
| 1:A:352:SER:O | 1:A:358:LEU:HD21 | 1.73 | 0.88 |
| 1:A:815:TRP:HA | 1:A:838:GLY:CA | 2.03 | 0.88 |
| 2:B:106:LEU:HD12 | 2:B:109:ASN:ND2 | 1.88 | 0.88 |
| 2:B:311:LEU:HG | 2:B:312:LEU:H | 1.35 | 0.88 |
| 1:D:348:LEU:CD2 | 1:D:350:ILE:HG13 | 2.02 | 0.88 |
| 1:D:448:ALA:HB1 | 1:D:870:VAL:HB | 1.51 | 0.88 |
| 1:D:914:THR:CB | 1:D:999:ASP:HB3 | 2.03 | 0.88 |
| 2:E:185:LEU:HD11 | 2:E:236:GLU:O | 1.73 | 0.88 |
| 2:F:474:PHE:HA | 2:F:477:LYS:CD | 2.01 | 0.88 |
| 1:A:638:THR:HG23 | 1:A:642:SER:OG | 1.73 | 0.88 |
| 1:A:996:ARG:NH1 | 1:A:1003:TRP:HB2 | 1.89 | 0.88 |
| 2:B:115:TRP:O | 2:B:119:VAL:HB | 1.71 | 0.88 |
| 2:C:125:VAL:HG23 | 2:C:126:PHE:N | 1.88 | 0.88 |
| 2:C:386:ASP:HB2 | 2:C:442:LEU:CA | 2.02 | 0.88 |
| 1:D:1069:ILE:CG1 | 1:D:1070:PRO:HD2 | 2.02 | 0.88 |
| 1:D:349:ASP:O | 1:D:361:ARG:HD3 | 1.73 | 0.88 |
| 2:F:454:HIS:N | 2:F:466:MET:O | 2.06 | 0.88 |
| 1:A:202:CYS:SG | 1:A:210:THR:HG21 | 2.14 | 0.88 |
| 1:D:895:GLU:OE1 | 1:D:896:LEU:HD22 | 1.71 | 0.88 |
| 1:A:360:GLU:O | 1:A:364:LEU:HD23 | 1.73 | 0.88 |
| 1:A:477:GLU:HG3 | 1:A:478:ARG:H | 0.72 | 0.88 |
| 1:D:1131:ILE:HD12 | 1:D:1131:ILE:N | 1.87 | 0.88 |
| 1:D:179:GLY:C | 1:D:181:GLU:N | 2.17 | 0.88 |
| 1:D:569:HIS:N | 1:D:570:PRO:HD2 | 1.88 | 0.88 |
| 2:F:467:HIS:O | 2:F:471:LEU:CD1 | 2.21 | 0.88 |
| 1:A:215:ILE:CG2 | 1:A:216:SER:H | 1.86 | 0.88 |
| 1:A:871:GLY:O | 1:A:873:GLU:N | 2.07 | 0.88 |
| 1:D:1208:ARG:NH2 | 2:F:285:LYS:HD3 | 1.89 | 0.88 |
| 1:D:352:SER:O | 1:D:358:GLU:OE2 | 1.82 | 0.88 |
| 1:D:601:LYS:HD2 | 1:D:616:GLU:HG2 | 1.56 | 0.88 |
| 2:F:390:GLY:HA2 | 2:F:391:PRO:C | 1.94 | 0.88 |
| 2:F:424:SER:HB3 | 2:F:427:GLN:HE22 | 1.39 | 0.88 |
| 2:F:471:LEU:HD12 | 2:F:471:LEU:N | 1.88 | 0.88 |
| 2:B:186:LEU:HD11 | 2:B:337:SER:HB2 | 1.55 | 0.88 |
| 1:D:1010:LEU:CD2 | 1:D:1015:THR:HA | 2.03 | 0.88 |
| 1:D:359:VAL:O | 1:D:359:VAL:HG12 | 1.71 | 0.88 |
| 1:D:463:LEU:HA | 1:D:466:LEU:CD2 | 2.04 | 0.88 |
| 1:D:656:TYR:HB3 | 1:D:744:ILE:CG2 | 2.04 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:83:LEU:HG | 1:D:89:GLY:HA2 | 1.53 | 0.88 |
| 2:E:432:TYR:HB2 | 2:E:437:ILE:HD13 | 1.54 | 0.88 |
| 1:A:1026:ARG:HB3 | 1:A:1029:GLN:CD | 1.93 | 0.88 |
| 1:A:1124:ALA:HB1 | 1:A:1148:ARG:HH11 | 1.38 | 0.88 |
| 1:A:606:THR:CG2 | 1:A:620:TRP:HE3 | 1.86 | 0.88 |
| 1:A:925:LYS:CG | 1:A:926:SER:H | 1.85 | 0.88 |
| 2:B:67:GLU:HB3 | 2:B:70:LEU:HB2 | 1.53 | 0.88 |
| 1:D:1028:VAL:HG22 | 1:D:1096:ARG:NH1 | 1.87 | 0.88 |
| 1:D:1198:LYS:HA | 1:D:1204:THR:CB | 2.03 | 0.88 |
| 1:D:1206:MET:CG | 2:F:257:ARG:NH1 | 2.36 | 0.88 |
| 1:D:214:ALA:HB3 | 1:D:218:SER:C | 1.94 | 0.88 |
| 1:D:458:GLU:O | 1:D:461:LYS:HG2 | 1.72 | 0.88 |
| 1:D:73:PRO:C | 1:D:74:LEU:HD22 | 1.93 | 0.88 |
| 2:F:406:LEU:HA | 2:F:409:ASN:HD21 | 1.39 | 0.88 |
| 1:A:515:ILE:HD11 | 1:A:568:GLY:O | 1.72 | 0.88 |
| 1:A:792:LEU:HD12 | 1:A:793:GLU:N | 1.88 | 0.88 |
| 2:B:400:GLN:N | 2:B:400:GLN:OE1 | 2.07 | 0.88 |
| 2:C:342:LEU:HB2 | 2:C:344:ARG:CG | 2.01 | 0.88 |
| 1:D:278:ILE:O | 1:D:282:TYR:CD1 | 2.27 | 0.88 |
| 1:D:504:LYS:CB | 1:D:523:ASP:CB | 2.49 | 0.88 |
| 1:D:645:VAL:O | 1:D:645:VAL:HG13 | 1.74 | 0.88 |
| 1:D:737:GLY:H | 1:D:750:PHE:HZ | 1.16 | 0.88 |
| 1:A:243:ASP:O | 1:A:246:PRO:HD2 | 1.73 | 0.88 |
| 1:A:297:MET:HE1 | 1:A:411:LEU:HD13 | 1.55 | 0.88 |
| 1:A:575:LYS:CG | 1:A:576:LEU:H | 1.86 | 0.88 |
| 2:B:447:THR:HG23 | 2:B:452:LEU:N | 1.88 | 0.88 |
| 1:D:163:PRO:HB2 | 1:D:165:LYS:HG3 | 1.56 | 0.88 |
| 1:D:352:SER:O | 1:D:358:GLU:CG | 2.20 | 0.88 |
| 1:D:368:PRO:HA | 1:D:369:LEU:HD23 | 1.56 | 0.88 |
| 1:D:611:PRO:HB2 | 1:D:612:LEU:HD13 | 1.56 | 0.88 |
| 1:D:854:ALA:HB1 | 1:D:860:LEU:HD12 | 1.55 | 0.88 |
| 1:A:1007:GLU:O | 1:A:1011:PRO:HD3 | 1.73 | 0.88 |
| 1:A:436:PRO:HB3 | 1:A:881:PRO:CD | 2.03 | 0.88 |
| 1:A:744:ILE:CB | 1:A:745:PRO:HD3 | 2.04 | 0.88 |
| 2:B:277:ASP:OD1 | 2:B:287:ASN:ND2 | 2.06 | 0.88 |
| 2:C:320:SER:HB3 | 2:C:321:LYS:HG3 | 1.54 | 0.88 |
| 1:D:1220:ILE:O | 1:D:1223:ILE:HG23 | 1.75 | 0.88 |
| 2:E:302:THR:C | 2:E:303:LEU:HD12 | 1.94 | 0.88 |
| 1:A:276:ALA:O | 1:A:279:ARG:HB2 | 1.73 | 0.87 |
| 1:A:656:TYR:CB | 1:A:720:THR:HB | 2.05 | 0.87 |
| 1:A:845:VAL:HB | 1:A:855:VAL:CB | 2.04 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:849:THR:HG22 | 1:D:851:THR:H | 1.38 | 0.87 |
| 1:D:441:TRP:HE1 | 1:D:880:ALA:N | 1.71 | 0.87 |
| 2:F:217:PRO:HB2 | 2:F:219:PHE:CE1 | 2.10 | 0.87 |
| 1:A:1041:TRP:NE1 | 1:A:1043:VAL:HB | 1.90 | 0.87 |
| 1:A:296:SER:HB2 | 1:A:847:ALA:HB3 | 1.53 | 0.87 |
| 1:A:440:ASN:HB2 | 1:A:877:MET:SD | 2.14 | 0.87 |
| 1:A:869:ARG:HA | 1:A:1201:SER:H | 1.36 | 0.87 |
| 2:C:241:TRP:N | 2:C:336:LEU:HB2 | 1.89 | 0.87 |
| 1:D:1014:ARG:HG2 | 1:D:1026:ARG:HE | 1.38 | 0.87 |
| 1:D:79:LEU:HD11 | 1:D:1173:LEU:O | 1.74 | 0.87 |
| 1:D:897:TRP:CH2 | 1:D:1177:VAL:HG11 | 2.10 | 0.87 |
| 2:C:301:GLU:CG | 2:C:339:ASN:HB3 | 2.04 | 0.87 |
| 1:D:1141:VAL:CB | 1:D:1146:ARG:HE | 1.82 | 0.87 |
| 1:D:599:THR:O | 1:D:603:MET:HG3 | 1.74 | 0.87 |
| 1:D:989:THR:HG22 | 1:D:999:ASP:OD2 | 1.74 | 0.87 |
| 1:D:997:LEU:HD22 | 1:D:998:SER:H | 1.38 | 0.87 |
| 2:F:341:ASP:O | 2:F:342:LEU:HD13 | 1.74 | 0.87 |
| 1:A:444:TYR:HE1 | 1:A:1206:MET:SD | 1.98 | 0.87 |
| 2:B:453:ILE:HG21 | 2:B:468:ILE:HD12 | 1.57 | 0.87 |
| 2:C:243:THR:OG1 | 2:C:334:CYS:HB2 | 1.73 | 0.87 |
| 2:C:304:TRP:N | 2:C:337:SER:HB2 | 1.90 | 0.87 |
| 2:C:455:LEU:C | 2:C:456:ARG:HE | 1.78 | 0.87 |
| 1:D:358:GLU:O | 1:D:361:ARG:HB3 | 1.72 | 0.87 |
| 1:D:420:HIS:NE2 | 1:D:1020:ILE:HG21 | 1.88 | 0.87 |
| 1:D:610:PHE:N | 1:D:611:PRO:HD3 | 1.85 | 0.87 |
| 2:F:417:TYR:HD2 | 2:F:417:TYR:N | 1.71 | 0.87 |
| 2:F:424:SER:CB | 2:F:427:GLN:HE22 | 1.87 | 0.87 |
| 1:A:869:ARG:C | 1:A:1200:PRO:HA | 1.94 | 0.87 |
| 1:A:215:ILE:HG23 | 1:A:216:SER:N | 1.85 | 0.87 |
| 2:B:261:GLN:HE21 | 2:B:264:ARG:NH2 | 1.71 | 0.87 |
| 2:B:83:LYS:HD2 | 2:B:83:LYS:H | 1.36 | 0.87 |
| 2:C:113:GLU:O | 2:C:116:THR:HG23 | 1.75 | 0.87 |
| 2:C:244:PRO:HD2 | 2:C:247:THR:CG2 | 2.05 | 0.87 |
| 2:C:471:LEU:HD12 | 2:C:471:LEU:H | 1.33 | 0.87 |
| 1:D:196:VAL:HG21 | 1:D:215:ILE:HD12 | 1.53 | 0.87 |
| 1:D:198:ASP:CB | 1:D:400:VAL:HG11 | 2.04 | 0.87 |
| 2:E:114:TRP:HE1 | 2:E:259:ARG:NH2 | 1.71 | 0.87 |
| 2:F:419:GLU:OE2 | 2:F:428:LEU:HD13 | 1.73 | 0.87 |
| 1:A:1046:GLU:O | 1:A:1049:TRP:CD1 | 2.28 | 0.87 |
| 1:A:612:LEU:CG | 1:A:614:TYR:H | 1.87 | 0.87 |
| 1:A:741:ASP:OD1 | 1:A:742:VAL:HG23 | 1.75 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:989:THR:HA | 1:A:998:SER:OG | 1.74 | 0.87 |
| 2:B:261:GLN:HE21 | 2:B:264:ARG:HH21 | 0.88 | 0.87 |
| 2:B:261:GLN:HA | 2:B:264:ARG:HE | 1.38 | 0.87 |
| 1:D:1029:GLN:CG | 1:D:1030:ARG:NE | 2.38 | 0.87 |
| 1:D:449:GLN:HA | 1:D:452:TYR:CE2 | 2.09 | 0.87 |
| 1:D:621:GLY:HA2 | 1:D:748:TRP:HB3 | 1.57 | 0.87 |
| 1:D:992:LEU:CB | 1:D:996:ARG:HG2 | 2.04 | 0.87 |
| 1:A:1011:PRO:HD2 | 1:A:1012:VAL:HG22 | 1.54 | 0.87 |
| 1:A:249:VAL:HG23 | 1:A:815:TRP:O | 1.75 | 0.87 |
| 1:A:502:LYS:CG | 1:A:503:VAL:H | 1.87 | 0.87 |
| 1:A:618:HIS:H | 1:A:725:PRO:HG2 | 1.30 | 0.87 |
| 2:C:317:GLY:C | 2:C:319:VAL:H | 1.76 | 0.87 |
| 1:D:1067:SER:HA | 1:D:1071:ARG:CA | 2.03 | 0.87 |
| 1:D:612:LEU:CB | 1:D:620:TRP:HB2 | 2.05 | 0.87 |
| 1:D:845:VAL:HB | 1:D:855:VAL:HG21 | 1.57 | 0.87 |
| 1:D:798:ILE:CG2 | 1:D:869:ARG:NH1 | 2.36 | 0.87 |
| 2:E:418:LEU:HD22 | 2:F:122:ARG:NH2 | 1.87 | 0.87 |
| 1:A:653:GLU:O | 1:A:657:ARG:HG3 | 1.75 | 0.87 |
| 2:B:254:PHE:O | 2:B:257:ARG:HB3 | 1.73 | 0.87 |
| 2:C:456:ARG:HB2 | 2:C:463:LYS:HA | 1.55 | 0.87 |
| 1:D:1019:TRP:HE3 | 1:D:1168:LEU:CG | 1.88 | 0.87 |
| 1:D:193:ARG:HA | 1:D:193:ARG:NH1 | 1.90 | 0.87 |
| 1:D:249:VAL:CG2 | 1:D:250:PRO:HD2 | 2.04 | 0.87 |
| 1:D:95:PRO:HG2 | 1:D:99:ALA:CB | 2.05 | 0.87 |
| 1:A:515:ILE:HG12 | 1:A:565:HIS:O | 1.75 | 0.87 |
| 2:B:261:GLN:HA | 2:B:264:ARG:NE | 1.89 | 0.87 |
| 2:C:77:HIS:O | 2:C:100:GLY:HA3 | 1.75 | 0.87 |
| 1:D:576:LEU:HG | 1:D:577:CYS:H | 1.37 | 0.87 |
| 1:D:660:CYS:CB | 1:D:745:PRO:HG3 | 2.04 | 0.87 |
| 1:D:812:MET:O | 1:D:840:ILE:HG23 | 1.73 | 0.87 |
| 1:D:815:TRP:HE3 | 1:D:838:GLY:H | 1.19 | 0.87 |
| 1:D:927:ARG:HG2 | 1:D:928:GLY:N | 1.88 | 0.87 |
| 2:E:205:PRO:HB3 | 2:E:243:THR:HA | 1.57 | 0.87 |
| 1:A:230:GLU:CD | 1:A:231:GLU:N | 2.28 | 0.86 |
| 1:A:869:ARG:HG2 | 1:A:870:VAL:HG23 | 1.55 | 0.86 |
| 2:C:208:LEU:HD22 | 2:C:242:PHE:CE2 | 2.10 | 0.86 |
| 1:D:456:GLN:C | 1:D:460:LYS:NZ | 2.29 | 0.86 |
| 1:D:768:LYS:HD3 | 1:D:769:ASP:N | 1.87 | 0.86 |
| 1:D:795:ASN:H | 1:D:795:ASN:HD22 | 0.88 | 0.86 |
| 1:D:996:ARG:CD | 1:D:996:ARG:H | 1.87 | 0.86 |
| 1:D:1209:ARG:HG3 | 2:F:249:ASN:HB3 | 1.55 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:348:LEU:C | 1:A:350:ILE:N | 2.18 | 0.86 |
| 1:A:576:LEU:HD23 | 2:C:481:SER:OG | 1.73 | 0.86 |
| 2:B:72:ILE:CA | 2:B:75:ARG:HE | 1.85 | 0.86 |
| 1:A:613:HIS:HB3 | 1:A:717:LEU:CG | 2.04 | 0.86 |
| 2:B:396:ARG:HG3 | 2:B:417:TYR:HB2 | 1.56 | 0.86 |
| 1:D:452:TYR:HB3 | 1:D:801:TRP:HE1 | 1.38 | 0.86 |
| 1:D:452:TYR:HB3 | 1:D:801:TRP:NE1 | 1.89 | 0.86 |
| 1:D:772:PRO:O | 1:D:775:GLU:O | 1.93 | 0.86 |
| 2:E:78:PHE:CD2 | 2:E:102:LEU:HD12 | 2.10 | 0.86 |
| 1:A:903:GLY:HA2 | 1:A:1002:GLU:HB3 | 1.54 | 0.86 |
| 1:A:310:SER:O | 1:A:313:ILE:HG13 | 1.75 | 0.86 |
| 2:C:252:LEU:HD12 | 2:C:305:ASN:HB2 | 1.56 | 0.86 |
| 1:D:1006:ARG:HA | 1:D:1006:ARG:HH11 | 0.73 | 0.86 |
| 1:D:163:PRO:HG2 | 1:D:165:LYS:HE3 | 1.57 | 0.86 |
| 2:F:439:PHE:HD1 | 2:F:458:ARG:CB | 1.88 | 0.86 |
| 1:A:1146:ARG:CZ | 1:A:1185:ILE:HG23 | 2.06 | 0.86 |
| 1:A:135:LEU:H | 1:A:135:LEU:CD2 | 1.83 | 0.86 |
| 1:A:184:ALA:O | 1:A:185:VAL:HG12 | 1.75 | 0.86 |
| 1:D:995:TYR:O | 1:D:1004:LEU:HD23 | 1.75 | 0.86 |
| 1:D:1066:THR:O | 1:D:1073:PRO:HD3 | 1.76 | 0.86 |
| 1:D:1208:ARG:HH12 | 2:F:285:LYS:CD | 1.88 | 0.86 |
| 2:E:455:LEU:O | 2:E:463:LYS:HA | 1.75 | 0.86 |
| 1:A:190:PRO:CB | 1:A:192:GLU:HG2 | 2.03 | 0.86 |
| 1:A:412:PRO:HG2 | 1:A:413:LEU:HG | 1.54 | 0.86 |
| 1:D:1019:TRP:CD1 | 1:D:1020:ILE:HG22 | 2.10 | 0.86 |
| 1:D:300:ALA:HB2 | 1:D:847:ALA:CB | 2.03 | 0.86 |
| 1:D:439:GLN:NE2 | 1:D:835:GLY:HA3 | 1.90 | 0.86 |
| 1:D:891:VAL:HA | 1:D:894:GLN:NE2 | 1.91 | 0.86 |
| 2:F:114:TRP:HB2 | 2:F:262:TRP:CZ2 | 2.10 | 0.86 |
| 2:F:238:SER:CA | 2:F:338:VAL:HG11 | 2.06 | 0.86 |
| 1:D:549:LEU:HD11 | 2:F:401:GLY:HA3 | 1.57 | 0.86 |
| 1:A:1158:LEU:O | 1:A:1162:CYS:SG | 2.33 | 0.86 |
| 1:A:293:ASP:HB3 | 1:A:296:SER:H | 1.40 | 0.86 |
| 1:A:472:GLN:NE2 | 2:C:460:THR:O | 2.07 | 0.86 |
| 2:C:326:ASP:OD2 | 2:C:329:LYS:N | 2.08 | 0.86 |
| 2:C:390:GLY:HA2 | 2:C:391:PRO:C | 1.95 | 0.86 |
| 2:C:391:PRO:HB2 | 2:C:394:GLU:OE2 | 1.76 | 0.86 |
| 1:D:485:LEU:HD12 | 1:D:489:GLU:OE2 | 1.76 | 0.86 |
| 1:D:490:TRP:CE3 | 1:D:580:LEU:HD22 | 2.10 | 0.86 |
| 2:F:203:ARG:HE | 2:F:204:LEU:CD1 | 1.87 | 0.86 |
| 2:F:241:TRP:CZ3 | 2:F:255:TRP:NE1 | 2.43 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:F:418:LEU:O | 2:F:421:MET:HG2 | 1.74 | 0.86 |
| 2:C:289:LEU:HD12 | 2:C:301:GLU:HB2 | 1.56 | 0.86 |
| 2:C:387:VAL:HG12 | 2:C:395:LEU:CD2 | 2.06 | 0.86 |
| 1:D:1055:SER:HA | 1:D:1058:PHE:CB | 2.01 | 0.86 |
| 1:D:284:ILE:HD12 | 1:D:284:ILE:H | 1.38 | 0.86 |
| 1:D:824:ALA:HA | 1:D:827:ARG:HG3 | 1.55 | 0.86 |
| 2:E:270:PRO:HA | 2:E:273:PHE:CD2 | 2.09 | 0.86 |
| 2:E:374:LEU:O | 2:E:375:HIS:HB2 | 1.74 | 0.86 |
| 2:E:387:VAL:HG12 | 2:E:416:GLY:HA3 | 1.57 | 0.86 |
| 2:C:385:LEU:O | 2:C:416:GLY:HA3 | 1.76 | 0.86 |
| 1:D:995:TYR:HE1 | 1:D:1004:LEU:HB3 | 1.41 | 0.86 |
| 1:D:242:ALA:HB1 | 1:D:245:ILE:CD1 | 2.05 | 0.86 |
| 1:D:383:LYS:O | 1:D:386:ARG:HG3 | 1.76 | 0.86 |
| 1:D:457:ARG:HH22 | 2:F:485:VAL:HG23 | 1.40 | 0.86 |
| 1:D:869:ARG:N | 1:D:1200:PRO:CB | 2.38 | 0.86 |
| 2:E:387:VAL:HG12 | 2:E:416:GLY:CA | 2.04 | 0.86 |
| 2:E:420:THR:HG23 | 2:E:421:MET:H | 1.40 | 0.86 |
| 1:A:1020:ILE:HD12 | 1:A:1021:SER:H | 1.40 | 0.86 |
| 1:A:378:VAL:O | 1:A:380:GLY:N | 2.09 | 0.86 |
| 1:A:556:THR:HG23 | 2:C:452:LEU:CB | 2.05 | 0.86 |
| 1:A:617:ARG:O | 1:A:762:VAL:HG23 | 1.76 | 0.86 |
| 2:B:267:ALA:HB2 | 2:B:270:PRO:HB2 | 1.56 | 0.86 |
| 1:D:459:MET:H | 1:D:460:LYS:HZ1 | 1.20 | 0.86 |
| 1:D:869:ARG:N | 1:D:1200:PRO:HB3 | 1.89 | 0.86 |
| 2:F:343:ASP:C | 2:F:347:LEU:HD13 | 1.94 | 0.86 |
| 1:A:145:LYS:HG3 | 1:A:1118:TRP:CH2 | 2.11 | 0.85 |
| 1:A:272:SER:HB3 | 1:A:273:PHE:CD2 | 2.11 | 0.85 |
| 2:C:446:THR:OG1 | 2:C:455:LEU:HD21 | 1.76 | 0.85 |
| 1:A:472:GLN:HG3 | 2:C:460:THR:CB | 2.05 | 0.85 |
| 1:D:189:ILE:CG2 | 1:D:258:GLN:HB3 | 2.05 | 0.85 |
| 1:D:293:ASP:O | 1:D:296:SER:HB3 | 1.76 | 0.85 |
| 1:D:564:GLN:HA | 1:D:566:LEU:O | 1.75 | 0.85 |
| 1:D:598:VAL:HA | 1:D:601:LYS:CE | 2.06 | 0.85 |
| 2:F:190:LEU:HB2 | 2:F:314:MET:HE1 | 1.56 | 0.85 |
| 1:A:576:LEU:HD12 | 1:A:577:CYS:N | 1.91 | 0.85 |
| 2:C:375:HIS:HB3 | 2:C:378:LEU:HD13 | 1.55 | 0.85 |
| 2:C:385:LEU:HD21 | 2:C:402:LEU:HD23 | 1.57 | 0.85 |
| 1:D:876:ALA:HB1 | 1:D:1188:CYS:SG | 2.16 | 0.85 |
| 1:D:635:PRO:HA | 1:D:639:THR:OG1 | 1.77 | 0.85 |
| 1:D:801:TRP:CH2 | 1:D:805:HIS:CG | 2.65 | 0.85 |
| 2:F:306:LEU:O | 2:F:306:LEU:HG | 1.76 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:369:PRO:CB | 1:A:372:GLU:HG3 | 1.98 | 0.85 |
| 2:B:102:LEU:H | 2:B:102:LEU:HD12 | 1.41 | 0.85 |
| 2:C:127:PRO:HD3 | 2:C:209:ALA:C | 1.97 | 0.85 |
| 1:D:249:VAL:CG1 | 1:D:252:GLY:N | 2.34 | 0.85 |
| 1:D:302:SER:HB2 | 1:D:351:SER:OG | 1.76 | 0.85 |
| 1:D:612:LEU:HG | 1:D:621:GLY:C | 1.97 | 0.85 |
| 1:D:652:ILE:HA | 1:D:655:LEU:CG | 2.06 | 0.85 |
| 2:E:101:PRO:CD | 2:F:128:VAL:HG21 | 2.06 | 0.85 |
| 2:F:215:PHE:CD2 | 2:F:233:GLU:HG2 | 2.11 | 0.85 |
| 1:D:1209:ARG:NH2 | 2:F:252:LEU:HD22 | 1.90 | 0.85 |
| 2:F:387:VAL:O | 2:F:420:THR:OG1 | 1.94 | 0.85 |
| 1:A:369:PRO:HB2 | 1:A:372:GLU:CG | 1.98 | 0.85 |
| 1:A:359:ALA:HB2 | 1:A:407:PHE:HE2 | 1.39 | 0.85 |
| 1:A:604:ALA:HA | 1:A:717:LEU:CD2 | 2.07 | 0.85 |
| 1:A:629:ASP:HB3 | 1:A:744:ILE:O | 1.76 | 0.85 |
| 2:B:472:LYS:HG3 | 2:B:473:ASP:N | 1.90 | 0.85 |
| 2:C:129:ASP:OD1 | 2:C:131:LEU:HD22 | 1.76 | 0.85 |
| 2:C:446:THR:HB | 2:C:450:ASN:OD1 | 1.76 | 0.85 |
| 1:D:78:MET:SD | 1:D:1175:GLN:NE2 | 2.49 | 0.85 |
| 1:D:1138:ARG:HH22 | 1:D:1191:LYS:CE | 1.88 | 0.85 |
| 1:D:242:ALA:O | 1:D:246:PRO:HD3 | 1.76 | 0.85 |
| 2:F:471:LEU:N | 2:F:471:LEU:CD1 | 2.36 | 0.85 |
| 1:A:1141:VAL:HB | 1:A:1146:ARG:CD | 2.07 | 0.85 |
| 1:A:445:LEU:O | 1:A:448:ALA:HB3 | 1.77 | 0.85 |
| 1:A:921:LEU:HD12 | 1:A:921:LEU:H | 1.39 | 0.85 |
| 2:C:473:ASP:HA | 2:C:476:ILE:HG23 | 1.56 | 0.85 |
| 1:D:1191:LYS:O | 1:D:1192:GLU:HB3 | 1.74 | 0.85 |
| 1:D:1212:ILE:HG23 | 1:D:1214:GLN:H | 1.41 | 0.85 |
| 1:D:741:ASP:HB2 | 1:D:748:TRP:CH2 | 2.11 | 0.85 |
| 1:A:670:PRO:HG2 | 1:A:671:GLN:HE21 | 1.38 | 0.85 |
| 1:A:741:ASP:O | 1:A:742:VAL:HB | 1.77 | 0.85 |
| 1:D:175:TRP:CZ3 | 1:D:184:ALA:HA | 2.10 | 0.85 |
| 1:D:309:ARG:HA | 1:D:312:TRP:HB2 | 1.58 | 0.85 |
| 2:F:326:ASP:OD1 | 2:F:329:LYS:HG2 | 1.76 | 0.85 |
| 2:F:387:VAL:HG21 | 2:F:417:TYR:CA | 2.07 | 0.85 |
| 2:F:394:GLU:HA | 2:F:397:GLN:OE1 | 1.75 | 0.85 |
| 1:A:1158:LEU:HD21 | 1:A:1178:ALA:O | 1.77 | 0.85 |
| 1:A:784:GLY:N | 2:C:363:ARG:CD | 2.39 | 0.85 |
| 1:A:832:ASP:O | 1:A:833:GLU:HB2 | 1.77 | 0.85 |
| 2:B:311:LEU:HG | 2:B:312:LEU:N | 1.89 | 0.85 |
| 2:C:244:PRO:CD | 2:C:247:THR:HG21 | 2.05 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:444:TYR:OH | 1:D:1206:MET:HB3 | 1.75 | 0.85 |
| 1:D:1221:TYR:HA | 1:D:1224:ILE:HG23 | 1.59 | 0.85 |
| 1:D:524:PRO:O | 1:D:525:MET:HB3 | 1.74 | 0.85 |
| 1:D:564:GLN:CA | 1:D:566:LEU:O | 2.25 | 0.85 |
| 1:D:569:HIS:H | 1:D:570:PRO:HD2 | 1.40 | 0.85 |
| 1:D:995:TYR:H | 1:D:996:ARG:NH1 | 1.74 | 0.85 |
| 1:A:127:LEU:HD23 | 1:A:128:PRO:HD2 | 1.57 | 0.85 |
| 1:A:606:THR:CG2 | 1:A:613:HIS:N | 2.40 | 0.85 |
| 1:A:744:ILE:CG1 | 1:A:745:PRO:HD3 | 2.05 | 0.85 |
| 1:A:98:ALA:O | 1:A:102:ARG:HG2 | 1.77 | 0.85 |
| 2:C:180:LYS:HE3 | 2:C:181:LEU:N | 1.91 | 0.85 |
| 2:C:342:LEU:HG | 2:C:344:ARG:HB2 | 1.57 | 0.85 |
| 1:D:1025:LEU:O | 1:D:1027:LYS:HD3 | 1.75 | 0.85 |
| 2:F:317:GLY:HA3 | 2:F:320:SER:H | 1.40 | 0.85 |
| 2:F:342:LEU:HB2 | 2:F:344:ARG:HB2 | 1.59 | 0.85 |
| 1:A:1145:ASP:HA | 1:A:1148:ARG:HB2 | 1.59 | 0.85 |
| 1:A:1210:TYR:HE1 | 1:A:1213:PRO:HG2 | 1.35 | 0.85 |
| 1:A:612:LEU:HG | 1:A:614:TYR:N | 1.89 | 0.85 |
| 1:A:85:GLU:OE1 | 1:A:128:PRO:HA | 1.76 | 0.85 |
| 2:F:326:ASP:OD2 | 2:F:329:LYS:N | 2.08 | 0.85 |
| 1:A:503:VAL:HG21 | 1:A:520:ALA:O | 1.77 | 0.85 |
| 1:A:767:ALA:HB3 | 1:A:771:LEU:HD23 | 1.59 | 0.85 |
| 1:D:1222:GLN:O | 1:D:1226:LEU:HD22 | 1.74 | 0.85 |
| 1:D:504:LYS:HB2 | 1:D:523:ASP:O | 1.76 | 0.85 |
| 1:D:549:LEU:H | 1:D:551:LYS:NZ | 1.71 | 0.85 |
| 1:D:559:LEU:HD12 | 1:D:560:PRO:HD3 | 1.57 | 0.85 |
| 2:E:109:ASN:HB2 | 2:E:378:LEU:CA | 2.07 | 0.85 |
| 1:A:223:TRP:N | 1:A:223:TRP:HD1 | 1.74 | 0.84 |
| 1:A:232:ARG:CB | 1:A:239:LEU:HD22 | 2.04 | 0.84 |
| 1:A:452:TYR:HA | 1:A:869:ARG:HH21 | 1.40 | 0.84 |
| 1:A:659:HIS:O | 1:A:663:GLN:HG3 | 1.76 | 0.84 |
| 2:C:471:LEU:CD1 | 2:C:471:LEU:H | 1.66 | 0.84 |
| 1:D:171:TRP:O | 1:D:172:ALA:HB2 | 1.77 | 0.84 |
| 1:D:513:LEU:N | 1:D:570:PRO:HG3 | 1.90 | 0.84 |
| 1:D:529:ASP:O | 1:D:530:LEU:HB3 | 1.75 | 0.84 |
| 1:D:612:LEU:CD1 | 1:D:612:LEU:H | 1.89 | 0.84 |
| 1:D:775:GLU:HA | 1:D:780:GLN:CG | 2.06 | 0.84 |
| 2:F:454:HIS:O | 2:F:455:LEU:HB2 | 1.73 | 0.84 |
| 1:A:97:GLU:O | 1:A:101:ARG:HB2 | 1.77 | 0.84 |
| 1:A:1131:ILE:HG21 | 1:A:1137:VAL:C | 1.96 | 0.84 |
| 1:A:213:VAL:HA | 1:A:221:TYR:CE2 | 2.12 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:203:LEU:HD12 | 1:A:380:GLY:N | 1.92 | 0.84 |
| 1:A:869:ARG:CG | 1:A:870:VAL:H | 1.89 | 0.84 |
| 1:A:992:LEU:CD1 | 1:A:993:ARG:H | 1.90 | 0.84 |
| 2:C:354:PHE:HB2 | 2:C:372:LEU:HA | 1.59 | 0.84 |
| 1:D:442:GLU:OE2 | 1:D:442:GLU:HA | 1.77 | 0.84 |
| 2:E:328:ARG:N | 2:E:328:ARG:HD2 | 1.90 | 0.84 |
| 2:F:342:LEU:HB2 | 2:F:344:ARG:CB | 2.06 | 0.84 |
| 1:A:569:HIS:CD2 | 1:A:570:PRO:HD2 | 2.13 | 0.84 |
| 1:A:612:LEU:CG | 1:A:613:HIS:H | 1.83 | 0.84 |
| 1:A:854:ALA:CB | 1:A:860:LEU:HD13 | 2.07 | 0.84 |
| 1:D:797:MET:C | 1:D:869:ARG:HD3 | 1.97 | 0.84 |
| 1:D:887:VAL:HG22 | 1:D:1185:ILE:HG22 | 1.57 | 0.84 |
| 2:E:432:TYR:CA | 2:E:435:MET:HB2 | 2.05 | 0.84 |
| 2:F:130:ALA:HB1 | 2:F:182:ARG:HH12 | 1.42 | 0.84 |
| 2:F:214:CYS:SG | 2:F:236:GLU:CG | 2.65 | 0.84 |
| 1:A:1200:PRO:HB2 | 1:A:1203:PRO:N | 1.90 | 0.84 |
| 1:A:308:GLN:HA | 1:A:311:LEU:HD12 | 1.60 | 0.84 |
| 1:A:400:VAL:O | 1:A:403:THR:HG23 | 1.77 | 0.84 |
| 2:C:291:TYR:OH | 2:C:355:GLN:HG3 | 1.77 | 0.84 |
| 2:C:397:GLN:O | 2:C:398:VAL:HG22 | 1.78 | 0.84 |
| 2:C:73:CYS:HB3 | 2:C:79:LEU:HD23 | 1.57 | 0.84 |
| 1:D:269:HIS:C | 1:D:294:THR:HG23 | 1.97 | 0.84 |
| 1:D:576:LEU:O | 1:D:577:CYS:O | 1.95 | 0.84 |
| 2:F:268:MET:HB2 | 2:F:352:ASP:OD1 | 1.76 | 0.84 |
| 1:A:879:GLN:HG2 | 1:A:1189:LEU:CD2 | 2.06 | 0.84 |
| 1:A:448:ALA:HB1 | 1:A:870:VAL:CG1 | 2.07 | 0.84 |
| 1:D:1197:CYS:O | 1:D:1204:THR:OG1 | 1.95 | 0.84 |
| 1:D:1221:TYR:HA | 1:D:1224:ILE:HG22 | 1.58 | 0.84 |
| 1:D:223:TRP:O | 1:D:227:ARG:HD2 | 1.78 | 0.84 |
| 2:F:374:LEU:HB3 | 2:F:378:LEU:HB3 | 1.57 | 0.84 |
| 2:F:440:THR:O | 2:F:457:SER:HB2 | 1.77 | 0.84 |
| 2:F:471:LEU:HA | 2:F:474:PHE:HD2 | 1.41 | 0.84 |
| 1:A:286:GLY:N | 1:A:1128:ARG:HH22 | 1.76 | 0.84 |
| 1:A:1145:ASP:HB3 | 1:A:1148:ARG:NH1 | 1.93 | 0.84 |
| 1:A:606:THR:HG22 | 1:A:620:TRP:CE3 | 2.12 | 0.84 |
| 1:A:655:LEU:O | 1:A:659:HIS:HB2 | 1.77 | 0.84 |
| 1:A:842:PRO:HB2 | 1:A:856:GLU:OE1 | 1.77 | 0.84 |
| 1:D:74:LEU:HA | 1:D:76:ILE:O | 1.77 | 0.84 |
| 1:D:779:LEU:HD22 | 1:D:780:GLN:N | 1.92 | 0.84 |
| 1:D:987:ALA:O | 1:D:991:GLY:N | 2.10 | 0.84 |
| 1:A:118:VAL:H | 1:A:119:PRO:HD3 | 1.42 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:854:ALA:HB1 | 1:A:860:LEU:CD1 | 2.07 | 0.84 |
| 1:A:904:ASP:HB2 | 1:A:910:MET:O | 1.77 | 0.84 |
| 1:D:210:THR:O | 1:D:211:LEU:HB2 | 1.78 | 0.84 |
| 1:D:617:ARG:O | 1:D:762:VAL:HG23 | 1.77 | 0.84 |
| 1:D:770:PHE:O | 1:D:774:MET:HG2 | 1.77 | 0.84 |
| 2:F:180:LYS:HE3 | 2:F:181:LEU:N | 1.91 | 0.84 |
| 2:F:347:LEU:C | 2:F:350:LEU:HD11 | 1.98 | 0.84 |
| 2:F:346:MET:CE | 2:F:347:LEU:HD12 | 2.08 | 0.84 |
| 1:A:175:TRP:H | 1:A:186:PRO:HB3 | 1.41 | 0.84 |
| 1:A:618:HIS:HA | 1:A:762:VAL:CG2 | 2.08 | 0.84 |
| 1:A:825:VAL:O | 1:A:829:PRO:CD | 2.26 | 0.84 |
| 1:A:850:ILE:HD11 | 1:A:1099:TRP:CZ2 | 2.13 | 0.84 |
| 2:B:204:LEU:HG | 2:B:325:ARG:NH2 | 1.91 | 0.84 |
| 2:C:129:ASP:OD1 | 2:C:131:LEU:HD13 | 1.77 | 0.84 |
| 1:D:1027:LYS:HB3 | 1:D:1091:GLU:CB | 2.08 | 0.84 |
| 1:D:80:SER:HB2 | 1:D:125:LEU:HB2 | 1.60 | 0.84 |
| 2:E:377:CYS:O | 2:E:380:PRO:HD2 | 1.76 | 0.84 |
| 2:E:200:VAL:HG12 | 2:F:418:LEU:CD2 | 2.08 | 0.84 |
| 1:A:256:PRO:CD | 1:A:257:THR:H | 1.87 | 0.84 |
| 1:A:397:ALA:O | 1:A:400:VAL:HB | 1.77 | 0.84 |
| 2:B:257:ARG:O | 2:B:260:LEU:HB3 | 1.76 | 0.84 |
| 1:D:157:LEU:CD2 | 1:D:194:ALA:HB3 | 2.08 | 0.84 |
| 1:D:257:THR:HG22 | 1:D:257:THR:O | 1.77 | 0.84 |
| 1:D:282:TYR:HE2 | 1:D:432:VAL:HG22 | 1.41 | 0.84 |
| 1:D:302:SER:O | 1:D:1024:ASP:OD2 | 1.95 | 0.84 |
| 1:D:854:ALA:HB1 | 1:D:860:LEU:HD13 | 1.58 | 0.84 |
| 2:F:336:LEU:HD23 | 2:F:336:LEU:C | 1.98 | 0.84 |
| 1:A:308:GLN:HE21 | 1:A:1091:GLU:H | 1.26 | 0.84 |
| 1:A:166:PRO:HG3 | 1:A:398:GLN:HE22 | 1.39 | 0.84 |
| 1:A:652:ILE:HA | 1:A:655:LEU:HD21 | 1.60 | 0.84 |
| 1:A:801:TRP:CZ3 | 1:A:808:ILE:HD12 | 2.13 | 0.84 |
| 1:D:1236:GLN:HB2 | 1:D:1237:PRO:CD | 2.07 | 0.84 |
| 1:D:513:LEU:CB | 1:D:568:GLY:HA2 | 2.07 | 0.84 |
| 2:F:197:LEU:HD11 | 2:F:322:LEU:HG | 1.60 | 0.84 |
| 2:F:317:GLY:HA3 | 2:F:320:SER:HB2 | 1.60 | 0.84 |
| 2:F:357:THR:HA | 2:F:370:LYS:HZ1 | 1.43 | 0.84 |
| 1:A:135:LEU:N | 1:A:135:LEU:HD23 | 1.91 | 0.83 |
| 1:A:176:THR:HA | 1:A:218:SER:CB | 2.04 | 0.83 |
| 1:A:213:VAL:CG1 | 1:A:401:TRP:NE1 | 2.27 | 0.83 |
| 1:A:210:THR:CA | 1:A:224:CYS:HB2 | 2.08 | 0.83 |
| 2:C:131:LEU:C | 2:C:182:ARG:HD3 | 1.98 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:194:ALA:HB1 | 1:D:265:LEU:CD1 | 2.08 | 0.83 |
| 2:F:306:LEU:N | 2:F:335:VAL:HG11 | 1.92 | 0.83 |
| 1:A:195:LEU:HG | 1:A:265:LEU:HD22 | 1.60 | 0.83 |
| 1:A:192:GLU:CD | 1:A:265:LEU:HD23 | 1.99 | 0.83 |
| 2:C:197:LEU:HD11 | 2:C:322:LEU:CG | 2.08 | 0.83 |
| 1:A:784:GLY:N | 2:C:363:ARG:HD2 | 1.94 | 0.83 |
| 1:D:607:TRP:HD1 | 1:D:780:GLN:N | 1.65 | 0.83 |
| 1:D:455:LEU:CD1 | 1:D:869:ARG:NH1 | 2.40 | 0.83 |
| 2:E:86:LEU:HA | 2:E:90:SER:HB3 | 1.60 | 0.83 |
| 1:A:346:ASP:CB | 1:A:1040:LYS:HZ3 | 1.88 | 0.83 |
| 1:A:1140:LEU:HD23 | 1:A:1141:VAL:H | 1.43 | 0.83 |
| 1:A:192:GLU:CB | 1:A:195:LEU:HD21 | 2.08 | 0.83 |
| 1:A:660:CYS:SG | 1:A:745:PRO:HG3 | 2.18 | 0.83 |
| 1:A:608:ASP:HA | 1:A:779:LEU:HB2 | 1.58 | 0.83 |
| 2:B:323:HIS:CB | 2:B:332:VAL:HA | 2.08 | 0.83 |
| 2:B:440:THR:HG22 | 2:B:441:VAL:H | 1.42 | 0.83 |
| 1:D:195:LEU:H | 1:D:265:LEU:CD2 | 1.90 | 0.83 |
| 1:D:547:ALA:HA | 1:D:551:LYS:HE2 | 1.60 | 0.83 |
| 2:E:259:ARG:CZ | 2:E:263:TRP:HE1 | 1.91 | 0.83 |
| 2:E:402:LEU:HD22 | 2:E:468:ILE:HD11 | 1.59 | 0.83 |
| 2:F:444:THR:O | 2:F:447:THR:CG2 | 2.26 | 0.83 |
| 2:F:460:THR:HG23 | 2:F:462:MET:HB2 | 1.60 | 0.83 |
| 2:F:483:LYS:O | 2:F:483:LYS:HE2 | 1.77 | 0.83 |
| 2:B:383:VAL:HG13 | 2:B:413:VAL:HG13 | 0.87 | 0.83 |
| 2:C:217:PRO:HB2 | 2:C:219:PHE:CE1 | 2.13 | 0.83 |
| 1:D:1206:MET:SD | 1:D:1210:TYR:CA | 2.66 | 0.83 |
| 1:D:1208:ARG:HG3 | 1:D:1209:ARG:H | 1.43 | 0.83 |
| 1:D:185:VAL:HG23 | 1:D:186:PRO:O | 1.79 | 0.83 |
| 1:D:285:GLN:HE22 | 1:D:1128:ARG:HG2 | 1.38 | 0.83 |
| 1:D:436:PRO:HG3 | 1:D:881:PRO:HD3 | 1.60 | 0.83 |
| 1:D:959:GLN:O | 1:D:963:GLU:HG2 | 1.78 | 0.83 |
| 2:F:417:TYR:HD2 | 2:F:417:TYR:H | 0.89 | 0.83 |
| 2:F:451:GLY:O | 2:F:452:LEU:HB2 | 1.77 | 0.83 |
| 1:A:1026:ARG:HB3 | 1:A:1029:GLN:HB2 | 1.44 | 0.83 |
| 1:A:823:ARG:CB | 1:A:825:VAL:HG23 | 2.06 | 0.83 |
| 1:A:83:LEU:HD22 | 1:A:89:GLY:HA2 | 1.60 | 0.83 |
| 2:B:323:HIS:HA | 2:B:333:PRO:HD2 | 1.60 | 0.83 |
| 2:C:208:LEU:HD11 | 2:C:240:VAL:HB | 1.59 | 0.83 |
| 1:D:1020:ILE:CD1 | 1:D:1021:SER:N | 2.41 | 0.83 |
| 2:F:200:VAL:O | 2:F:203:ARG:HB2 | 1.78 | 0.83 |
| 2:F:276:SER:O | 2:F:287:ASN:CB | 2.26 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1041:TRP:C | 1:A:1041:TRP:CD1 | 2.50 | 0.83 |
| 1:A:271:VAL:HG22 | 1:A:295:MET:SD | 2.19 | 0.83 |
| 1:A:305:SER:HB2 | 1:A:308:GLN:CG | 2.09 | 0.83 |
| 1:A:382:MET:SD | 1:A:385:ILE:HG22 | 2.18 | 0.83 |
| 1:A:789:PRO:HA | 1:A:792:LEU:HD11 | 1.60 | 0.83 |
| 2:B:269:SER:H | 2:B:270:PRO:HD3 | 1.43 | 0.83 |
| 2:B:373:LYS:HE2 | 2:B:459:ASP:HA | 1.61 | 0.83 |
| 2:C:364:LYS:HD3 | 2:C:364:LYS:H | 1.42 | 0.83 |
| 2:C:395:LEU:HD21 | 2:C:443:VAL:CG1 | 2.08 | 0.83 |
| 2:C:424:SER:HB3 | 2:C:427:GLN:NE2 | 1.91 | 0.83 |
| 1:D:1027:LYS:HD2 | 1:D:1091:GLU:OE2 | 1.79 | 0.83 |
| 1:D:208:CYS:SG | 1:D:244:LEU:HD12 | 2.19 | 0.83 |
| 1:D:887:VAL:HG23 | 1:D:1146:ARG:NH2 | 1.93 | 0.83 |
| 1:A:1043:VAL:HA | 1:A:1046:GLU:N | 1.92 | 0.83 |
| 1:A:393:MET:N | 1:A:393:MET:SD | 2.52 | 0.83 |
| 1:A:468:ASN:O | 1:A:472:GLN:HG2 | 1.79 | 0.83 |
| 1:A:916:PHE:HA | 1:A:919:MET:CB | 2.09 | 0.83 |
| 2:C:308:ASP:OD1 | 2:C:332:VAL:O | 1.95 | 0.83 |
| 2:C:483:LYS:HE2 | 2:C:483:LYS:O | 1.78 | 0.83 |
| 1:D:1206:MET:O | 1:D:1206:MET:SD | 2.37 | 0.83 |
| 1:D:436:PRO:CG | 1:D:881:PRO:HD3 | 2.08 | 0.83 |
| 1:D:83:LEU:HD13 | 1:D:83:LEU:H | 1.42 | 0.83 |
| 2:E:378:LEU:O | 2:E:381:ILE:O | 1.97 | 0.83 |
| 2:F:241:TRP:N | 2:F:336:LEU:HB2 | 1.93 | 0.83 |
| 1:A:1046:GLU:OE1 | 1:A:1049:TRP:HB3 | 1.79 | 0.83 |
| 1:A:1133:ILE:HG23 | 1:A:1136:GLU:HB2 | 1.61 | 0.83 |
| 1:D:990:LYS:HE2 | 1:D:1000:GLU:CD | 1.99 | 0.83 |
| 1:D:670:PRO:HG2 | 1:D:673:ALA:CB | 2.09 | 0.83 |
| 2:E:106:LEU:HA | 2:E:109:ASN:OD1 | 1.79 | 0.83 |
| 2:E:249:ASN:ND2 | 2:E:285:LYS:HE2 | 1.93 | 0.83 |
| 2:F:197:LEU:HD11 | 2:F:322:LEU:CG | 2.07 | 0.83 |
| 1:A:1148:ARG:CG | 1:A:1148:ARG:HH11 | 1.91 | 0.83 |
| 1:A:138:HIS:O | 1:A:142:LEU:HG | 1.77 | 0.83 |
| 1:A:573:TYR:O | 1:A:574:ARG:HG3 | 1.78 | 0.83 |
| 1:A:664:GLY:O | 1:A:667:GLN:HG2 | 1.79 | 0.83 |
| 1:A:853:ARG:CZ | 1:A:1105:ALA:HB3 | 2.08 | 0.83 |
| 2:C:126:PHE:C | 2:C:128:VAL:N | 2.31 | 0.83 |
| 2:C:264:ARG:HA | 2:C:270:PRO:HB3 | 1.60 | 0.83 |
| 1:D:408:GLN:O | 1:D:412:PRO:HD3 | 1.79 | 0.83 |
| 1:D:434:TYR:O | 1:D:1130:CYS:HB3 | 1.79 | 0.83 |
| 2:E:347:LEU:O | 2:E:350:LEU:HB3 | 1.79 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:197:LEU:HD23 | 2:F:198:ASP:N | 1.93 | 0.83 |
| 1:A:408:GLN:HA | 1:A:411:LEU:CD2 | 2.09 | 0.83 |
| 1:A:786:ALA:HB1 | 1:A:790:ARG:NH1 | 1.94 | 0.83 |
| 1:D:380:GLY:O | 1:D:381:THR:HG22 | 1.77 | 0.83 |
| 1:A:462:SER:O | 1:A:466:LEU:HD23 | 1.78 | 0.82 |
| 1:A:484:TRP:O | 1:A:488:LEU:HG | 1.78 | 0.82 |
| 1:A:452:TYR:CA | 1:A:869:ARG:HH21 | 1.91 | 0.82 |
| 1:A:927:ARG:CG | 1:A:928:GLY:H | 1.91 | 0.82 |
| 2:C:197:LEU:HD11 | 2:C:322:LEU:HG | 1.58 | 0.82 |
| 2:C:431:LYS:HZ1 | 2:C:435:MET:HG2 | 1.40 | 0.82 |
| 1:D:270:ASN:O | 1:D:272:SER:O | 1.97 | 0.82 |
| 1:D:316:LYS:NZ | 1:D:348:LEU:HD23 | 1.94 | 0.82 |
| 1:D:345:TRP:HA | 1:D:1040:LYS:HZ3 | 1.40 | 0.82 |
| 1:D:475:SER:O | 1:D:711:ALA:HB1 | 1.77 | 0.82 |
| 1:D:486:TRP:HZ2 | 1:D:722:ARG:CA | 1.92 | 0.82 |
| 1:D:995:TYR:CD1 | 1:D:1004:LEU:HB3 | 2.14 | 0.82 |
| 1:D:914:THR:OG1 | 1:D:999:ASP:OD1 | 1.97 | 0.82 |
| 2:F:239:LEU:N | 2:F:338:VAL:CG1 | 2.42 | 0.82 |
| 2:F:387:VAL:HG12 | 2:F:443:VAL:CG2 | 2.09 | 0.82 |
| 2:F:445:GLU:O | 2:F:448:LEU:N | 2.12 | 0.82 |
| 1:A:1113:LEU:HB3 | 1:A:1117:LYS:HE3 | 1.61 | 0.82 |
| 1:A:1166:TYR:CD1 | 1:A:1166:TYR:N | 2.46 | 0.82 |
| 1:A:379:LYS:HG2 | 1:A:379:LYS:O | 1.79 | 0.82 |
| 1:A:490:TRP:O | 1:A:580:LEU:HD13 | 1.78 | 0.82 |
| 1:A:743:ASP:C | 1:A:744:ILE:HD13 | 1.99 | 0.82 |
| 2:B:261:GLN:HA | 2:B:264:ARG:CD | 2.09 | 0.82 |
| 2:B:313:HIS:O | 2:B:316:PRO:HD3 | 1.79 | 0.82 |
| 2:C:247:THR:HB | 2:C:251:TRP:HD1 | 1.40 | 0.82 |
| 2:C:356:LEU:HB3 | 2:C:359:ASN:CG | 1.99 | 0.82 |
| 1:A:783:PRO:HG2 | 2:C:363:ARG:CZ | 2.09 | 0.82 |
| 1:D:167:PRO:C | 1:D:169:TRP:H | 1.79 | 0.82 |
| 1:D:271:VAL:HG12 | 1:D:272:SER:N | 1.92 | 0.82 |
| 1:D:304:LEU:H | 1:D:309:ARG:NH2 | 1.77 | 0.82 |
| 1:D:414:PHE:HA | 1:D:417:ARG:HH11 | 1.42 | 0.82 |
| 1:A:1047:ARG:NH2 | 1:A:1050:LYS:HD2 | 1.94 | 0.82 |
| 1:A:1060:LYS:HD3 | 1:A:1073:PRO:HB2 | 1.60 | 0.82 |
| 1:A:1109:LEU:HD12 | 1:A:1113:LEU:HD21 | 1.60 | 0.82 |
| 2:B:269:SER:N | 2:B:270:PRO:CD | 2.42 | 0.82 |
| 2:C:455:LEU:HB3 | 2:C:456:ARG:NE | 1.94 | 0.82 |
| 1:D:1065:ALA:C | 1:D:1073:PRO:HG3 | 1.99 | 0.82 |
| 1:D:256:PRO:HG2 | 1:D:284:ILE:CD1 | 2.09 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:350:ILE:HG22 | 1:D:352:SER:HB2 | 1.57 | 0.82 |
| 1:D:496:LYS:HE3 | 1:D:571:GLY:CA | 2.09 | 0.82 |
| 2:E:428:LEU:O | 2:E:431:LYS:HB3 | 1.78 | 0.82 |
| 2:F:453:ILE:CG2 | 2:F:455:LEU:H | 1.92 | 0.82 |
| 2:F:454:HIS:HA | 2:F:468:ILE:CD1 | 2.08 | 0.82 |
| 1:A:996:ARG:CZ | 1:A:1000:GLU:HB3 | 2.09 | 0.82 |
| 1:A:213:VAL:C | 1:A:401:TRP:HZ2 | 1.83 | 0.82 |
| 1:A:490:TRP:HA | 1:A:580:LEU:CD2 | 2.07 | 0.82 |
| 1:A:649:TYR:O | 1:A:653:GLU:N | 2.11 | 0.82 |
| 1:A:827:ARG:HA | 1:A:831:TYR:CZ | 2.15 | 0.82 |
| 1:A:897:TRP:HE1 | 1:A:901:VAL:CG1 | 1.93 | 0.82 |
| 1:D:213:VAL:C | 1:D:401:TRP:HZ2 | 1.82 | 0.82 |
| 2:E:377:CYS:SG | 2:E:378:LEU:HD12 | 2.18 | 0.82 |
| 2:E:389:ARG:C | 2:E:395:LEU:HG | 1.98 | 0.82 |
| 2:E:451:GLY:O | 2:E:452:LEU:HD13 | 1.79 | 0.82 |
| 2:F:320:SER:HB3 | 2:F:321:LYS:HG3 | 1.60 | 0.82 |
| 2:F:447:THR:HA | 2:F:452:LEU:HA | 1.61 | 0.82 |
| 1:A:223:TRP:O | 1:A:227:ARG:HB2 | 1.79 | 0.82 |
| 1:A:601:LYS:NZ | 1:A:721:ALA:HB1 | 1.95 | 0.82 |
| 2:C:208:LEU:HD11 | 2:C:240:VAL:C | 1.99 | 0.82 |
| 2:C:398:VAL:O | 2:C:402:LEU:HD13 | 1.79 | 0.82 |
| 2:C:446:THR:CA | 2:C:450:ASN:HB3 | 2.09 | 0.82 |
| 1:D:367:PRO:CG | 1:D:368:PRO:HD3 | 2.09 | 0.82 |
| 1:A:1047:ARG:HD3 | 1:A:1047:ARG:O | 1.78 | 0.82 |
| 1:A:260:ASP:H | 1:A:264:GLN:NE2 | 1.77 | 0.82 |
| 1:A:275:ARG:NH2 | 1:A:845:VAL:CA | 2.43 | 0.82 |
| 1:A:471:CYS:HB3 | 1:A:472:GLN:OE1 | 1.78 | 0.82 |
| 1:D:312:TRP:C | 1:D:316:LYS:HD3 | 2.00 | 0.82 |
| 1:D:960:PRO:HA | 1:D:963:GLU:HG3 | 1.60 | 0.82 |
| 2:F:341:ASP:C | 2:F:342:LEU:HD13 | 1.99 | 0.82 |
| 1:A:1025:LEU:C | 1:A:1026:ARG:HG3 | 2.00 | 0.82 |
| 1:A:1198:LYS:HG3 | 1:A:1204:THR:HG21 | 1.60 | 0.82 |
| 1:D:1203:PRO:O | 1:D:1207:GLU:N | 2.12 | 0.82 |
| 1:D:1207:GLU:CA | 1:D:1210:TYR:HD2 | 1.93 | 0.82 |
| 1:A:1114:VAL:HA | 1:A:1117:LYS:HD2 | 1.61 | 0.82 |
| 1:A:1131:ILE:CD1 | 1:A:1133:ILE:HG22 | 2.09 | 0.82 |
| 1:A:1220:ILE:N | 1:A:1220:ILE:HD12 | 1.95 | 0.82 |
| 1:A:658:LYS:HG3 | 1:A:713:PRO:CB | 2.06 | 0.82 |
| 2:C:372:LEU:CD1 | 2:C:436:SER:HB2 | 2.09 | 0.82 |
| 2:C:471:LEU:O | 2:C:475:LEU:HG | 1.80 | 0.82 |
| 1:D:1052:GLY:HA2 | 1:D:1055:SER:HB3 | 1.61 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:869:ARG:O | 1:D:1200:PRO:CG | 2.26 | 0.82 |
| 1:D:1207:GLU:O | 1:D:1210:TYR:CD2 | 2.33 | 0.82 |
| 1:D:438:ASN:N | 1:D:441:TRP:CD1 | 2.48 | 0.82 |
| 2:E:407:LEU:HD23 | 2:E:412:SER:HA | 1.61 | 0.82 |
| 2:F:253:ASP:O | 2:F:257:ARG:HD2 | 1.79 | 0.82 |
| 1:D:1206:MET:HG2 | 2:F:257:ARG:HH11 | 1.40 | 0.82 |
| 2:F:455:LEU:C | 2:F:456:ARG:HE | 1.83 | 0.82 |
| 1:A:885:THR:HB | 1:A:1146:ARG:HE | 1.44 | 0.82 |
| 1:A:165:LYS:HB2 | 1:A:178:TYR:HA | 1.62 | 0.82 |
| 1:A:175:TRP:CD1 | 1:A:183:GLU:HB2 | 2.14 | 0.82 |
| 1:A:190:PRO:CB | 1:A:192:GLU:CG | 2.56 | 0.82 |
| 2:C:115:TRP:HH2 | 2:C:210:GLN:HG2 | 1.44 | 0.82 |
| 2:C:326:ASP:OD1 | 2:C:329:LYS:HG2 | 1.80 | 0.82 |
| 2:C:344:ARG:HA | 2:C:347:LEU:HD22 | 1.62 | 0.82 |
| 1:D:890:ASP:OD1 | 1:D:1191:LYS:HD3 | 1.79 | 0.82 |
| 1:D:175:TRP:HB2 | 1:D:185:VAL:HG13 | 1.60 | 0.82 |
| 1:D:193:ARG:HA | 1:D:193:ARG:NE | 1.88 | 0.82 |
| 1:D:275:ARG:CD | 1:D:843:GLN:H | 1.92 | 0.82 |
| 1:D:375:GLU:O | 1:D:379:LYS:HG3 | 1.79 | 0.82 |
| 1:D:498:LYS:HG2 | 1:D:499:LYS:H | 1.45 | 0.82 |
| 1:D:549:LEU:H | 1:D:551:LYS:HZ3 | 1.26 | 0.82 |
| 1:D:768:LYS:CE | 1:D:769:ASP:H | 1.93 | 0.82 |
| 1:D:808:ILE:O | 1:D:811:GLN:CB | 2.27 | 0.82 |
| 2:F:415:PRO:HB3 | 2:F:417:TYR:CE2 | 2.15 | 0.82 |
| 2:F:471:LEU:O | 2:F:475:LEU:HG | 1.80 | 0.82 |
| 1:A:228:LEU:HD12 | 1:A:386:ARG:HB3 | 1.62 | 0.82 |
| 1:A:626:GLY:HA3 | 1:A:628:ARG:O | 1.80 | 0.82 |
| 1:A:784:GLY:H | 2:C:363:ARG:HD2 | 1.41 | 0.82 |
| 1:D:1069:ILE:O | 1:D:1071:ARG:CG | 2.26 | 0.82 |
| 1:D:112:LEU:CD2 | 1:D:917:GLY:O | 2.28 | 0.82 |
| 1:D:364:VAL:HG12 | 1:D:364:VAL:O | 1.80 | 0.82 |
| 1:D:869:ARG:H | 1:D:1200:PRO:HB2 | 1.45 | 0.82 |
| 1:A:1208:ARG:N | 1:A:1210:TYR:CD1 | 2.48 | 0.81 |
| 1:D:422:VAL:HG11 | 1:D:1111:LEU:HD12 | 1.60 | 0.81 |
| 2:F:375:HIS:H | 2:F:378:LEU:CD2 | 1.93 | 0.81 |
| 2:F:447:THR:O | 2:F:452:LEU:CD1 | 2.26 | 0.81 |
| 1:A:1040:LYS:HB3 | 1:A:1044:VAL:CG1 | 2.09 | 0.81 |
| 1:A:1160:THR:O | 1:A:1164:PHE:HD1 | 1.63 | 0.81 |
| 1:A:115:GLN:N | 1:A:116:PRO:HD2 | 1.93 | 0.81 |
| 1:A:490:TRP:CA | 1:A:580:LEU:HD22 | 2.08 | 0.81 |
| 2:C:421:MET:HE2 | 2:C:422:GLN:HB2 | 1.62 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:851:THR:HG23 | 1:D:1102:GLN:HB3 | 1.63 | 0.81 |
| 1:D:931:LEU:HB3 | 1:D:934:LYS:HZ2 | 1.45 | 0.81 |
| 1:A:213:VAL:CG1 | 1:A:397:ALA:HB1 | 2.10 | 0.81 |
| 1:A:512:LYS:O | 1:A:513:LEU:HD23 | 1.80 | 0.81 |
| 2:C:402:LEU:HG | 2:C:472:LYS:NZ | 1.95 | 0.81 |
| 2:C:446:THR:CA | 2:C:450:ASN:CB | 2.58 | 0.81 |
| 2:C:467:HIS:O | 2:C:471:LEU:HD11 | 1.80 | 0.81 |
| 1:D:1137:VAL:HG12 | 1:D:1139:TYR:CE1 | 2.15 | 0.81 |
| 1:D:196:VAL:CG2 | 1:D:215:ILE:HD12 | 2.11 | 0.81 |
| 1:D:233:TYR:O | 1:D:234:SER:HB2 | 1.79 | 0.81 |
| 1:D:847:ALA:HA | 1:D:852:ARG:HA | 1.62 | 0.81 |
| 2:F:125:VAL:HG23 | 2:F:126:PHE:H | 1.42 | 0.81 |
| 2:F:455:LEU:CA | 2:F:456:ARG:HE | 1.92 | 0.81 |
| 1:A:608:ASP:O | 1:A:620:TRP:CH2 | 2.33 | 0.81 |
| 1:A:794:ILE:HA | 1:A:797:MET:SD | 2.20 | 0.81 |
| 2:B:101:PRO:HA | 2:C:128:VAL:CG2 | 2.09 | 0.81 |
| 2:B:192:HIS:CE1 | 2:C:80:SER:HB3 | 2.16 | 0.81 |
| 2:C:299:LEU:HD23 | 2:C:299:LEU:N | 1.95 | 0.81 |
| 2:C:344:ARG:HA | 2:C:347:LEU:CB | 2.11 | 0.81 |
| 1:D:1157:ASN:O | 1:D:1161:ARG:HD2 | 1.80 | 0.81 |
| 1:D:1206:MET:HG3 | 2:F:257:ARG:HH11 | 1.46 | 0.81 |
| 1:D:347:TRP:CD1 | 1:D:349:ASP:OD2 | 2.32 | 0.81 |
| 1:D:457:ARG:HH11 | 1:D:457:ARG:HB3 | 1.44 | 0.81 |
| 1:D:618:HIS:HB2 | 1:D:725:PRO:CG | 2.08 | 0.81 |
| 2:E:432:TYR:CB | 2:E:437:ILE:CD1 | 2.44 | 0.81 |
| 1:A:282:TYR:O | 1:A:283:LEU:HB2 | 1.79 | 0.81 |
| 1:A:575:LYS:HG3 | 1:A:576:LEU:N | 1.94 | 0.81 |
| 1:A:628:ARG:O | 1:A:629:ASP:HB2 | 1.79 | 0.81 |
| 1:A:653:GLU:HG3 | 1:A:656:TYR:CE1 | 2.15 | 0.81 |
| 1:A:866:ARG:HB3 | 1:A:867:PRO:HD3 | 1.59 | 0.81 |
| 1:A:900:ALA:HA | 1:A:915:ALA:CB | 2.11 | 0.81 |
| 2:B:133:HIS:CD2 | 2:C:231:ILE:HG21 | 2.14 | 0.81 |
| 2:B:344:ARG:H | 2:B:344:ARG:HD2 | 1.43 | 0.81 |
| 2:C:384:ALA:HB2 | 2:C:437:ILE:HD12 | 1.60 | 0.81 |
| 1:D:718:ALA:O | 1:D:722:ARG:HD2 | 1.80 | 0.81 |
| 1:D:798:ILE:HG23 | 1:D:869:ARG:NH1 | 1.95 | 0.81 |
| 2:F:208:LEU:HD22 | 2:F:242:PHE:CE2 | 2.15 | 0.81 |
| 2:F:341:ASP:CG | 2:F:342:LEU:H | 1.83 | 0.81 |
| 1:D:572:TRP:HZ2 | 2:F:470:LYS:HB3 | 1.45 | 0.81 |
| 1:A:1066:THR:OG1 | 1:A:1073:PRO:HD2 | 1.81 | 0.81 |
| 1:A:655:LEU:HD13 | 1:A:719:LEU:C | 2.00 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:74:GLN:O | 2:B:77:HIS:HA | 1.80 | 0.81 |
| 1:D:265:LEU:HD21 | 1:D:267:VAL:HG13 | 1.61 | 0.81 |
| 1:D:375:GLU:C | 1:D:379:LYS:HG3 | 2.01 | 0.81 |
| 1:D:493:GLN:O | 1:D:494:GLU:HG2 | 1.81 | 0.81 |
| 1:A:1060:LYS:HD3 | 1:A:1073:PRO:HB3 | 1.62 | 0.81 |
| 1:A:249:VAL:CG1 | 1:A:817:PRO:HG3 | 2.11 | 0.81 |
| 1:A:869:ARG:HH11 | 1:A:869:ARG:HG3 | 1.46 | 0.81 |
| 1:A:883:GLY:C | 1:A:884:TYR:HD1 | 1.83 | 0.81 |
| 1:D:1218:LEU:CB | 1:D:1223:ILE:HG22 | 2.09 | 0.81 |
| 1:D:275:ARG:HE | 1:D:842:PRO:CA | 1.91 | 0.81 |
| 1:D:439:GLN:HG2 | 1:D:835:GLY:CA | 2.11 | 0.81 |
| 1:D:903:GLY:HA3 | 1:D:1002:GLU:HB2 | 1.63 | 0.81 |
| 2:F:78:PHE:CD1 | 2:F:103:GLY:HA2 | 2.15 | 0.81 |
| 1:A:81:ARG:CZ | 1:A:126:ARG:HA | 2.09 | 0.81 |
| 2:B:323:HIS:HB2 | 2:B:331:VAL:O | 1.80 | 0.81 |
| 2:C:374:LEU:HD12 | 2:C:379:ALA:HA | 1.61 | 0.81 |
| 1:D:120:LEU:H | 1:D:120:LEU:HD22 | 1.45 | 0.81 |
| 1:D:962:ALA:HB3 | 1:D:982:ALA:HB1 | 1.63 | 0.81 |
| 2:F:300:ILE:HG22 | 2:F:301:GLU:N | 1.96 | 0.81 |
| 2:F:447:THR:HG23 | 2:F:448:LEU:HG | 1.63 | 0.81 |
| 1:A:1158:LEU:CD2 | 1:A:1178:ALA:O | 2.29 | 0.81 |
| 1:A:424:LEU:N | 1:A:424:LEU:HD23 | 1.96 | 0.81 |
| 1:A:604:ALA:HB1 | 1:A:717:LEU:HD11 | 1.63 | 0.81 |
| 2:C:134:LYS:HB3 | 2:C:180:LYS:CD | 2.09 | 0.81 |
| 2:C:467:HIS:O | 2:C:471:LEU:HD13 | 1.78 | 0.81 |
| 1:D:1128:ARG:HG3 | 1:D:1129:PHE:N | 1.95 | 0.81 |
| 1:D:1208:ARG:CZ | 2:F:285:LYS:HD3 | 2.11 | 0.81 |
| 1:D:135:LEU:CD2 | 1:D:135:LEU:H | 1.94 | 0.81 |
| 2:E:79:LEU:HA | 2:E:100:GLY:N | 1.95 | 0.81 |
| 2:F:363:ARG:NH1 | 2:F:363:ARG:HB3 | 1.96 | 0.81 |
| 2:F:447:THR:C | 2:F:452:LEU:HA | 2.00 | 0.81 |
| 2:F:467:HIS:O | 2:F:471:LEU:HD13 | 1.80 | 0.81 |
| 1:A:370:PRO:O | 1:A:371:LYS:HG2 | 1.79 | 0.81 |
| 1:A:665:LYS:HG2 | 1:A:666:GLN:N | 1.96 | 0.81 |
| 2:B:267:ALA:CB | 2:B:270:PRO:HB2 | 2.10 | 0.81 |
| 2:C:78:PHE:HE1 | 2:C:103:GLY:HA2 | 1.46 | 0.81 |
| 2:C:130:ALA:HB1 | 2:C:182:ARG:HH12 | 1.46 | 0.81 |
| 1:D:170:ALA:HB1 | 1:D:171:TRP:O | 1.81 | 0.81 |
| 1:D:177:ARG:HG3 | 1:D:178:TYR:N | 1.96 | 0.81 |
| 1:D:549:LEU:N | 1:D:551:LYS:HZ2 | 1.77 | 0.81 |
| 1:D:556:THR:HA | 1:D:559:LEU:CD2 | 2.10 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:575:LYS:HE3 | 1:D:581:ASP:O | 1.81 | 0.81 |
| 1:D:667:GLN:O | 1:D:671:GLN:HG2 | 1.80 | 0.81 |
| 1:D:78:MET:O | 1:D:79:LEU:HD12 | 1.79 | 0.81 |
| 1:A:163:PRO:CB | 1:A:164:PRO:HD3 | 2.11 | 0.81 |
| 1:A:363:ARG:NH2 | 1:A:409:GLN:HB2 | 1.93 | 0.81 |
| 1:A:925:LYS:CG | 1:A:926:SER:N | 2.41 | 0.81 |
| 2:C:275:SER:HB2 | 2:C:287:ASN:ND2 | 1.95 | 0.81 |
| 1:D:1029:GLN:HG3 | 1:D:1030:ARG:HE | 1.46 | 0.81 |
| 1:D:194:ALA:HA | 1:D:265:LEU:CB | 2.10 | 0.81 |
| 1:D:350:ILE:C | 1:D:352:SER:H | 1.83 | 0.81 |
| 1:D:715:GLN:HG2 | 1:D:717:LEU:HG | 1.62 | 0.81 |
| 1:D:116:PRO:HA | 1:D:921:LEU:HD13 | 1.62 | 0.81 |
| 2:E:77:HIS:HB3 | 2:E:101:PRO:HD2 | 1.61 | 0.81 |
| 2:F:247:THR:CB | 2:F:251:TRP:HD1 | 1.93 | 0.81 |
| 1:A:606:THR:OG1 | 1:A:612:LEU:C | 2.20 | 0.80 |
| 1:A:955:TYR:HB3 | 1:A:1098:ASN:CG | 2.01 | 0.80 |
| 1:A:988:ALA:O | 1:A:998:SER:OG | 1.97 | 0.80 |
| 1:D:190:PRO:HB3 | 1:D:217:PRO:HB2 | 1.63 | 0.80 |
| 1:D:246:PRO:C | 1:D:247:LEU:HD12 | 2.00 | 0.80 |
| 1:D:269:HIS:CE1 | 1:D:291:PHE:HA | 2.16 | 0.80 |
| 1:D:435:LEU:O | 1:D:839:ALA:HB1 | 1.81 | 0.80 |
| 1:D:719:LEU:HD12 | 1:D:720:THR:N | 1.95 | 0.80 |
| 1:D:797:MET:CB | 1:D:869:ARG:CD | 2.59 | 0.80 |
| 2:F:299:LEU:HD23 | 2:F:299:LEU:H | 1.45 | 0.80 |
| 1:A:312:TRP:HZ2 | 1:A:346:ASP:O | 1.63 | 0.80 |
| 1:A:633:LYS:HD2 | 1:A:633:LYS:C | 2.00 | 0.80 |
| 1:A:711:ALA:O | 1:A:713:PRO:HD3 | 1.79 | 0.80 |
| 1:A:931:LEU:HD23 | 1:A:932:HIS:N | 1.96 | 0.80 |
| 2:B:448:LEU:O | 2:B:448:LEU:HD23 | 1.81 | 0.80 |
| 1:D:737:GLY:N | 1:D:750:PHE:CZ | 2.48 | 0.80 |
| 1:D:916:PHE:O | 1:D:920:THR:N | 2.14 | 0.80 |
| 1:A:147:SER:O | 1:A:151:LEU:HG | 1.80 | 0.80 |
| 1:A:228:LEU:C | 1:A:228:LEU:HD23 | 2.00 | 0.80 |
| 1:A:848:GLY:O | 1:A:852:ARG:HA | 1.81 | 0.80 |
| 1:D:107:LEU:CD2 | 1:D:913:CYS:HA | 2.12 | 0.80 |
| 1:D:134:ASN:HB3 | 1:D:137:GLN:HB2 | 1.62 | 0.80 |
| 1:D:256:PRO:HG2 | 1:D:284:ILE:HD11 | 1.62 | 0.80 |
| 1:D:288:ARG:HH11 | 1:D:288:ARG:HG3 | 1.46 | 0.80 |
| 1:D:389:PHE:HD1 | 1:D:390:GLN:N | 1.77 | 0.80 |
| 1:D:717:LEU:HD23 | 1:D:717:LEU:N | 1.95 | 0.80 |
| 1:D:767:ALA:HB2 | 1:D:771:LEU:HD22 | 1.60 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:430:SER:O | 2:F:434:GLU:HG3 | 1.81 | 0.80 |
| 1:A:552:LEU:HD22 | 2:C:448:LEU:HD23 | 1.62 | 0.80 |
| 2:C:310:GLU:O | 2:C:313:HIS:HB3 | 1.81 | 0.80 |
| 1:D:1065:ALA:O | 1:D:1073:PRO:HG3 | 1.81 | 0.80 |
| 1:D:173:GLU:O | 1:D:220:TRP:HB3 | 1.81 | 0.80 |
| 1:D:597:ARG:NH1 | 1:D:724:GLY:O | 2.14 | 0.80 |
| 1:D:612:LEU:CD1 | 1:D:612:LEU:N | 2.44 | 0.80 |
| 2:E:382:LYS:CE | 2:E:412:SER:O | 2.25 | 0.80 |
| 1:A:166:PRO:HG2 | 1:A:398:GLN:HE22 | 1.46 | 0.80 |
| 1:A:606:THR:CG2 | 1:A:613:HIS:H | 1.95 | 0.80 |
| 1:A:607:TRP:CZ2 | 1:A:671:GLN:HA | 2.16 | 0.80 |
| 1:A:793:GLU:CA | 1:A:796:LYS:HD3 | 2.11 | 0.80 |
| 2:B:262:TRP:O | 2:B:265:LYS:CB | 2.29 | 0.80 |
| 2:B:385:LEU:HB3 | 2:B:441:VAL:HG23 | 1.63 | 0.80 |
| 1:D:1138:ARG:CG | 1:D:1138:ARG:HH11 | 1.94 | 0.80 |
| 1:D:298:HIS:CD2 | 1:D:407:PHE:HB2 | 2.17 | 0.80 |
| 1:D:608:ASP:OD1 | 1:D:611:PRO:CD | 2.30 | 0.80 |
| 1:D:608:ASP:HA | 1:D:620:TRP:CH2 | 2.16 | 0.80 |
| 1:D:917:GLY:O | 1:D:920:THR:HB | 1.81 | 0.80 |
| 1:D:992:LEU:CD1 | 1:D:993:ARG:H | 1.93 | 0.80 |
| 1:A:1030:ARG:HG2 | 1:A:1040:LYS:NZ | 1.97 | 0.80 |
| 1:A:577:CYS:HB3 | 1:A:578:PRO:CD | 2.10 | 0.80 |
| 2:B:117:SER:CB | 2:B:262:TRP:NE1 | 2.44 | 0.80 |
| 2:C:203:ARG:O | 2:C:204:LEU:CB | 2.29 | 0.80 |
| 2:C:397:GLN:HG2 | 2:C:398:VAL:HG13 | 1.62 | 0.80 |
| 2:C:454:HIS:CB | 2:C:466:MET:O | 2.30 | 0.80 |
| 1:D:1025:LEU:O | 1:D:1026:ARG:C | 2.17 | 0.80 |
| 1:D:1202:ASN:O | 1:D:1206:MET:N | 2.15 | 0.80 |
| 1:D:194:ALA:HB1 | 1:D:265:LEU:HD13 | 1.63 | 0.80 |
| 1:D:255:SER:HB3 | 1:D:256:PRO:C | 2.02 | 0.80 |
| 1:D:252:GLY:O | 1:D:256:PRO:HG3 | 1.82 | 0.80 |
| 1:D:282:TYR:CE2 | 1:D:432:VAL:HA | 2.16 | 0.80 |
| 1:D:81:ARG:HG3 | 1:D:82:GLY:N | 1.97 | 0.80 |
| 1:D:887:VAL:O | 1:D:1139:TYR:N | 2.15 | 0.80 |
| 2:E:247:THR:CG2 | 2:E:250:GLN:HE21 | 1.95 | 0.80 |
| 2:E:283:GLY:CA | 2:E:306:LEU:HA | 2.11 | 0.80 |
| 2:E:320:SER:O | 2:E:323:HIS:CD2 | 2.35 | 0.80 |
| 2:E:388:GLY:C | 2:E:395:LEU:CD1 | 2.49 | 0.80 |
| 1:A:114:GLY:N | 1:A:116:PRO:HD2 | 1.97 | 0.80 |
| 1:A:1196:ASP:HA | 1:A:1207:GLU:OE1 | 1.81 | 0.80 |
| 1:A:176:THR:HG23 | 1:A:177:ARG:N | 1.97 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:76:ILE:HB | 1:A:911:HIS:CE1 | 2.16 | 0.80 |
| 2:B:402:LEU:O | 2:B:406:LEU:HD23 | 1.80 | 0.80 |
| 1:D:424:LEU:O | 1:D:428:LEU:CD1 | 2.29 | 0.80 |
| 1:D:621:GLY:HA2 | 1:D:748:TRP:HB2 | 1.62 | 0.80 |
| 2:E:384:ALA:O | 2:E:414:TRP:CB | 2.30 | 0.80 |
| 2:F:244:PRO:CD | 2:F:247:THR:HG21 | 2.10 | 0.80 |
| 2:F:317:GLY:HA3 | 2:F:320:SER:N | 1.96 | 0.80 |
| 1:A:897:TRP:HZ3 | 1:A:1108:TYR:HE1 | 1.29 | 0.80 |
| 2:C:357:THR:HA | 2:C:370:LYS:NZ | 1.96 | 0.80 |
| 1:D:1010:LEU:HD13 | 1:D:1100:VAL:HG21 | 1.62 | 0.80 |
| 1:D:1124:ALA:HB1 | 1:D:1148:ARG:HH11 | 1.46 | 0.80 |
| 1:D:302:SER:CB | 1:D:351:SER:HB3 | 2.11 | 0.80 |
| 1:D:823:ARG:HA | 1:D:826:ILE:CD1 | 2.11 | 0.80 |
| 1:D:926:SER:CB | 1:D:930:ASP:HB2 | 2.12 | 0.80 |
| 2:E:199:LEU:HG | 2:E:200:VAL:HG23 | 1.64 | 0.80 |
| 1:A:1006:ARG:HA | 1:A:1006:ARG:CZ | 2.12 | 0.80 |
| 1:A:211:LEU:HG | 1:A:221:TYR:CG | 2.16 | 0.80 |
| 1:A:213:VAL:CA | 1:A:221:TYR:HE2 | 1.93 | 0.80 |
| 1:A:606:THR:HG21 | 1:A:612:LEU:CB | 2.10 | 0.80 |
| 1:A:863:SER:O | 1:A:873:GLU:HG3 | 1.81 | 0.80 |
| 2:B:72:ILE:HG13 | 2:B:73:CYS:N | 1.97 | 0.80 |
| 2:C:432:TYR:CG | 2:C:437:ILE:HD11 | 2.17 | 0.80 |
| 1:D:1010:LEU:HD23 | 1:D:1015:THR:HA | 1.64 | 0.80 |
| 1:D:267:VAL:CB | 1:D:269:HIS:CD2 | 2.64 | 0.80 |
| 1:D:271:VAL:HG12 | 1:D:272:SER:H | 1.46 | 0.80 |
| 2:E:380:PRO:N | 2:E:438:LEU:HD11 | 1.97 | 0.80 |
| 2:F:357:THR:HA | 2:F:370:LYS:NZ | 1.96 | 0.80 |
| 1:A:365:TYR:O | 1:A:366:VAL:HG22 | 1.82 | 0.80 |
| 1:A:725:PRO:O | 1:A:726:LYS:HB2 | 1.81 | 0.80 |
| 2:C:474:PHE:HA | 2:C:477:LYS:CD | 2.12 | 0.80 |
| 1:D:1026:ARG:N | 1:D:1026:ARG:HD3 | 1.97 | 0.80 |
| 1:D:1165:ALA:HB3 | 1:D:1166:TYR:CE1 | 2.16 | 0.80 |
| 1:D:259:ARG:HG3 | 1:D:261:TRP:HD1 | 1.46 | 0.80 |
| 1:D:256:PRO:HB3 | 1:D:281:GLN:HG3 | 1.64 | 0.80 |
| 1:D:636:THR:O | 1:D:640:LEU:HG | 1.82 | 0.80 |
| 2:F:241:TRP:HZ3 | 2:F:255:TRP:NE1 | 1.79 | 0.80 |
| 2:F:244:PRO:HD2 | 2:F:247:THR:CG2 | 2.12 | 0.80 |
| 1:A:821:LEU:O | 1:A:826:ILE:HG23 | 1.80 | 0.79 |
| 1:A:893:SER:HA | 1:A:896:LEU:HD23 | 1.64 | 0.79 |
| 1:A:898:ILE:HD11 | 1:A:1101:VAL:HG13 | 1.64 | 0.79 |
| 2:C:336:LEU:HD23 | 2:C:336:LEU:C | 2.03 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:446:THR:HA | 2:C:450:ASN:HB3 | 1.62 | 0.79 |
| 1:D:201:VAL:HG22 | 1:D:208:CYS:O | 1.81 | 0.79 |
| 1:D:606:THR:HG23 | 1:D:607:TRP:N | 1.96 | 0.79 |
| 2:E:293:PHE:O | 2:E:296:GLY:N | 2.14 | 0.79 |
| 2:F:346:MET:HE3 | 2:F:347:LEU:HD12 | 1.63 | 0.79 |
| 1:A:1041:TRP:O | 1:A:1042:GLU:HB2 | 1.81 | 0.79 |
| 1:A:486:TRP:CZ3 | 1:A:598:VAL:HG21 | 2.16 | 0.79 |
| 1:A:656:TYR:CD1 | 1:A:744:ILE:HD12 | 2.17 | 0.79 |
| 2:C:78:PHE:CD1 | 2:C:103:GLY:HA2 | 2.17 | 0.79 |
| 2:C:300:ILE:HG22 | 2:C:301:GLU:HG3 | 1.61 | 0.79 |
| 2:C:300:ILE:HG23 | 2:C:342:LEU:CD1 | 2.10 | 0.79 |
| 2:C:403:PHE:HE1 | 2:C:415:PRO:HG3 | 1.47 | 0.79 |
| 1:D:78:MET:HB3 | 1:D:1175:GLN:HB3 | 1.64 | 0.79 |
| 1:D:914:THR:HG21 | 1:D:999:ASP:HB3 | 1.63 | 0.79 |
| 1:A:670:PRO:HG2 | 1:A:671:GLN:NE2 | 1.96 | 0.79 |
| 1:A:81:ARG:HD3 | 1:A:125:LEU:O | 1.82 | 0.79 |
| 2:B:385:LEU:HD23 | 2:B:414:TRP:O | 1.82 | 0.79 |
| 2:B:450:ASN:HD22 | 2:B:452:LEU:HD23 | 1.47 | 0.79 |
| 2:C:300:ILE:CG2 | 2:C:342:LEU:HD11 | 2.11 | 0.79 |
| 2:C:344:ARG:CA | 2:C:347:LEU:HD22 | 2.11 | 0.79 |
| 1:D:1027:LYS:HB3 | 1:D:1091:GLU:CA | 2.11 | 0.79 |
| 1:D:1180:PHE:O | 1:D:1182:ALA:N | 2.15 | 0.79 |
| 1:D:1213:PRO:O | 1:D:1214:GLN:HB2 | 1.82 | 0.79 |
| 1:D:271:VAL:CG1 | 1:D:272:SER:H | 1.87 | 0.79 |
| 1:D:459:MET:HE2 | 1:D:594:LEU:HD11 | 1.64 | 0.79 |
| 1:D:649:TYR:CD2 | 1:D:652:ILE:HG21 | 2.16 | 0.79 |
| 1:D:741:ASP:CB | 1:D:748:TRP:HH2 | 1.94 | 0.79 |
| 1:A:196:VAL:CB | 1:A:401:TRP:HZ3 | 1.95 | 0.79 |
| 1:A:513:LEU:HB2 | 1:A:568:GLY:HA2 | 0.85 | 0.79 |
| 1:A:78:MET:HG2 | 1:A:79:LEU:N | 1.97 | 0.79 |
| 1:A:843:GLN:O | 1:A:843:GLN:HG2 | 1.80 | 0.79 |
| 2:B:259:ARG:O | 2:B:260:LEU:C | 2.17 | 0.79 |
| 2:B:268:MET:N | 2:B:270:PRO:HD2 | 1.97 | 0.79 |
| 2:C:303:LEU:HA | 2:C:337:SER:CB | 2.11 | 0.79 |
| 2:C:456:ARG:HB2 | 2:C:463:LYS:C | 2.02 | 0.79 |
| 1:D:206:GLY:HA2 | 1:D:245:ILE:CG2 | 2.12 | 0.79 |
| 1:D:797:MET:HB2 | 1:D:869:ARG:HD3 | 1.64 | 0.79 |
| 2:E:376:PRO:O | 2:E:380:PRO:CD | 2.26 | 0.79 |
| 2:F:417:TYR:CD2 | 2:F:417:TYR:N | 2.43 | 0.79 |
| 1:A:1126:ASP:HB3 | 1:A:1141:VAL:HG13 | 1.64 | 0.79 |
| 1:A:1166:TYR:N | 1:A:1166:TYR:HD1 | 1.79 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:374:ARG:HE | 1:A:392:LEU:CD1 | 1.94 | 0.79 |
| 1:D:1133:ILE:O | 1:D:1135:ASP:N | 2.16 | 0.79 |
| 1:D:913:CYS:SG | 1:D:914:THR:N | 2.56 | 0.79 |
| 1:A:1047:ARG:CA | 1:A:1047:ARG:HH11 | 1.96 | 0.79 |
| 1:A:176:THR:CG2 | 1:A:177:ARG:H | 1.87 | 0.79 |
| 1:A:273:PHE:O | 1:A:276:ALA:HB3 | 1.83 | 0.79 |
| 1:A:150:TYR:OH | 1:A:288:ARG:O | 2.01 | 0.79 |
| 1:A:605:LEU:CA | 1:A:781:ALA:HB3 | 2.13 | 0.79 |
| 1:A:944:GLU:HA | 1:A:947:LYS:HE3 | 1.64 | 0.79 |
| 1:A:95:PRO:O | 1:A:100:VAL:HG23 | 1.82 | 0.79 |
| 1:D:1141:VAL:N | 1:D:1146:ARG:HH21 | 1.80 | 0.79 |
| 2:E:372:LEU:HG | 2:E:373:LYS:H | 1.46 | 0.79 |
| 2:F:328:ARG:O | 2:F:329:LYS:HD2 | 1.82 | 0.79 |
| 2:F:442:LEU:N | 2:F:455:LEU:HD22 | 1.97 | 0.79 |
| 2:F:454:HIS:CB | 2:F:466:MET:O | 2.29 | 0.79 |
| 1:A:468:ASN:ND2 | 1:A:578:PRO:CG | 2.45 | 0.79 |
| 1:A:448:ALA:HB1 | 1:A:870:VAL:HG12 | 1.61 | 0.79 |
| 1:A:999:ASP:O | 1:A:1000:GLU:HG3 | 1.83 | 0.79 |
| 2:B:412:SER:O | 2:B:413:VAL:HG22 | 1.82 | 0.79 |
| 2:C:114:TRP:HE1 | 2:C:259:ARG:CZ | 1.95 | 0.79 |
| 1:D:167:PRO:C | 1:D:169:TRP:N | 2.34 | 0.79 |
| 1:D:87:ILE:HG21 | 1:D:1166:TYR:OH | 1.82 | 0.79 |
| 1:D:1209:ARG:HH22 | 2:F:256:LEU:HD22 | 1.48 | 0.79 |
| 1:A:1041:TRP:CD1 | 1:A:1043:VAL:HB | 2.18 | 0.79 |
| 1:A:1131:ILE:CG1 | 1:A:1133:ILE:HG22 | 2.13 | 0.79 |
| 1:A:118:VAL:N | 1:A:119:PRO:CD | 2.46 | 0.79 |
| 2:C:241:TRP:CZ3 | 2:C:255:TRP:NE1 | 2.51 | 0.79 |
| 2:C:251:TRP:HA | 2:C:251:TRP:CE3 | 2.17 | 0.79 |
| 1:D:1207:GLU:HA | 1:D:1210:TYR:CB | 2.12 | 0.79 |
| 1:D:177:ARG:CG | 1:D:178:TYR:N | 2.45 | 0.79 |
| 1:D:284:ILE:HD12 | 1:D:284:ILE:N | 1.98 | 0.79 |
| 1:D:645:VAL:HG13 | 1:D:650:ARG:HG2 | 1.64 | 0.79 |
| 1:D:649:TYR:HA | 1:D:652:ILE:CB | 2.09 | 0.79 |
| 1:D:768:LYS:CD | 1:D:769:ASP:H | 1.94 | 0.79 |
| 2:E:284:ARG:O | 2:E:285:LYS:HB3 | 1.83 | 0.79 |
| 2:F:453:ILE:HG22 | 2:F:455:LEU:N | 1.98 | 0.79 |
| 1:A:1060:LYS:HE3 | 1:A:1065:ALA:N | 1.96 | 0.79 |
| 1:A:1155:ILE:HA | 1:A:1158:LEU:HD12 | 1.64 | 0.79 |
| 1:A:371:LYS:C | 1:A:372:GLU:HG2 | 2.02 | 0.79 |
| 1:A:608:ASP:HA | 1:A:779:LEU:CB | 2.12 | 0.79 |
| 2:B:437:ILE:HG22 | 2:B:438:LEU:H | 1.46 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:115:TRP:CH2 | 2:C:210:GLN:HG2 | 2.18 | 0.79 |
| 1:D:1027:LYS:HB2 | 1:D:1096:ARG:HE | 1.48 | 0.79 |
| 1:D:135:LEU:HD23 | 1:D:135:LEU:N | 1.98 | 0.79 |
| 1:D:845:VAL:HG12 | 1:D:846:THR:O | 1.83 | 0.79 |
| 2:E:384:ALA:O | 2:E:414:TRP:HB3 | 1.82 | 0.79 |
| 2:E:448:LEU:HD23 | 2:E:449:GLU:N | 1.97 | 0.79 |
| 1:A:1110:HIS:O | 1:A:1114:VAL:HG23 | 1.82 | 0.79 |
| 1:A:253:ALA:HB3 | 1:A:256:PRO:CB | 2.13 | 0.79 |
| 1:A:455:LEU:HD12 | 1:A:798:ILE:HG22 | 1.65 | 0.79 |
| 2:C:203:ARG:O | 2:C:204:LEU:HB2 | 1.83 | 0.79 |
| 2:C:387:VAL:HG11 | 2:C:399:CYS:CB | 2.11 | 0.79 |
| 1:D:1026:ARG:NE | 1:D:1029:GLN:OE1 | 2.16 | 0.79 |
| 1:D:195:LEU:N | 1:D:265:LEU:HD22 | 1.98 | 0.79 |
| 1:D:546:ARG:C | 1:D:551:LYS:HZ1 | 1.86 | 0.79 |
| 1:D:656:TYR:CD1 | 1:D:744:ILE:HD12 | 2.18 | 0.79 |
| 1:D:618:HIS:HA | 1:D:762:VAL:CG2 | 2.13 | 0.79 |
| 2:E:123:GLU:HG2 | 2:F:415:PRO:HG2 | 1.64 | 0.79 |
| 2:F:241:TRP:HB3 | 2:F:336:LEU:HB2 | 1.65 | 0.79 |
| 2:F:303:LEU:CA | 2:F:337:SER:OG | 2.31 | 0.79 |
| 2:F:454:HIS:HB2 | 2:F:466:MET:C | 2.02 | 0.79 |
| 1:A:1016:GLU:HA | 1:A:1021:SER:O | 1.83 | 0.78 |
| 1:D:1189:LEU:N | 1:D:1189:LEU:HD22 | 1.97 | 0.78 |
| 1:D:612:LEU:N | 1:D:612:LEU:HD13 | 1.98 | 0.78 |
| 1:D:605:LEU:HD22 | 1:D:781:ALA:HB2 | 1.63 | 0.78 |
| 1:D:996:ARG:N | 1:D:996:ARG:CD | 2.46 | 0.78 |
| 2:E:369:ARG:HA | 2:E:430:SER:HB3 | 1.63 | 0.78 |
| 2:F:389:ARG:HG3 | 2:F:445:GLU:OE2 | 1.83 | 0.78 |
| 1:A:411:LEU:O | 1:A:415:LEU:HD22 | 1.83 | 0.78 |
| 1:A:477:GLU:HG2 | 1:A:482:ASP:OD2 | 1.83 | 0.78 |
| 1:A:653:GLU:HA | 1:A:656:TYR:CE1 | 2.18 | 0.78 |
| 1:D:212:ALA:O | 1:D:213:VAL:CB | 2.31 | 0.78 |
| 1:D:412:PRO:O | 1:D:416:GLU:HG3 | 1.84 | 0.78 |
| 1:D:586:THR:N | 1:D:587:PRO:CD | 2.45 | 0.78 |
| 1:D:995:TYR:CD2 | 1:D:995:TYR:O | 2.35 | 0.78 |
| 2:F:245:PRO:HG2 | 2:F:246:ARG:HD3 | 1.64 | 0.78 |
| 1:A:1206:MET:N | 1:A:1209:ARG:HB2 | 1.98 | 0.78 |
| 1:A:276:ALA:HA | 1:A:279:ARG:CD | 2.14 | 0.78 |
| 2:C:354:PHE:HE1 | 2:C:370:LYS:HB3 | 1.48 | 0.78 |
| 1:D:851:THR:CG2 | 1:D:1102:GLN:HB3 | 2.13 | 0.78 |
| 1:D:352:SER:CB | 1:D:352:SER:C | 2.51 | 0.78 |
| 1:D:559:LEU:CG | 1:D:560:PRO:HD2 | 2.13 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:775:GLU:CA | 1:D:780:GLN:HG2 | 2.13 | 0.78 |
| 2:E:109:ASN:HB2 | 2:E:378:LEU:HA | 1.65 | 0.78 |
| 2:E:188:GLY:O | 2:E:191:GLU:HG2 | 1.82 | 0.78 |
| 1:A:996:ARG:NH1 | 1:A:1004:LEU:N | 2.31 | 0.78 |
| 1:A:1006:ARG:HH12 | 1:A:1009:ASN:HB2 | 1.48 | 0.78 |
| 1:A:1157:ASN:HB3 | 1:A:1161:ARG:CZ | 2.12 | 0.78 |
| 1:A:316:LYS:HZ3 | 1:A:350:ILE:HG13 | 1.48 | 0.78 |
| 1:A:497:GLN:HA | 1:A:516:GLU:HB3 | 1.63 | 0.78 |
| 1:A:563:PRO:C | 1:A:564:GLN:HE21 | 1.86 | 0.78 |
| 2:B:110:LEU:CD2 | 2:B:342:LEU:HD21 | 2.14 | 0.78 |
| 2:C:317:GLY:HA3 | 2:C:320:SER:N | 1.98 | 0.78 |
| 2:C:439:PHE:HD1 | 2:C:458:ARG:HB2 | 1.47 | 0.78 |
| 1:D:101:ARG:CG | 1:D:101:ARG:HH11 | 1.97 | 0.78 |
| 1:D:273:PHE:H | 1:D:275:ARG:HB3 | 1.48 | 0.78 |
| 1:D:269:HIS:CD2 | 1:D:291:PHE:CD2 | 2.71 | 0.78 |
| 1:D:613:HIS:CE1 | 1:D:717:LEU:HD13 | 2.18 | 0.78 |
| 2:E:389:ARG:NH2 | 2:E:391:PRO:O | 2.16 | 0.78 |
| 2:E:456:ARG:HA | 2:E:462:MET:O | 1.82 | 0.78 |
| 2:E:67:GLU:HG2 | 2:E:70:LEU:HD11 | 1.64 | 0.78 |
| 2:E:68:ALA:O | 2:E:72:ILE:HD13 | 1.82 | 0.78 |
| 1:A:1026:ARG:O | 1:A:1030:ARG:HB2 | 1.83 | 0.78 |
| 1:A:879:GLN:HG2 | 1:A:1189:LEU:HG | 1.63 | 0.78 |
| 2:B:99:PHE:HD2 | 2:C:129:ASP:CG | 1.86 | 0.78 |
| 1:D:1056:GLU:HA | 1:D:1059:ASN:HD21 | 1.47 | 0.78 |
| 1:D:282:TYR:CD2 | 1:D:432:VAL:HG13 | 2.18 | 0.78 |
| 1:D:549:LEU:HA | 1:D:552:LEU:HD12 | 1.66 | 0.78 |
| 1:D:616:GLU:HG3 | 1:D:724:GLY:O | 1.82 | 0.78 |
| 2:E:193:TYR:CE2 | 2:E:322:LEU:HD22 | 2.19 | 0.78 |
| 2:E:199:LEU:HB2 | 2:F:77:HIS:NE2 | 1.98 | 0.78 |
| 1:A:1226:LEU:HD22 | 1:A:1226:LEU:H | 1.47 | 0.78 |
| 1:A:472:GLN:HG3 | 2:C:460:THR:HB | 1.65 | 0.78 |
| 1:A:249:VAL:HG21 | 1:A:817:PRO:CG | 2.13 | 0.78 |
| 2:C:375:HIS:O | 2:C:378:LEU:HB2 | 1.84 | 0.78 |
| 1:D:289:MET:C | 1:D:289:MET:SD | 2.62 | 0.78 |
| 1:D:879:GLN:OE1 | 1:D:1189:LEU:CD2 | 2.30 | 0.78 |
| 1:D:927:ARG:CG | 1:D:928:GLY:H | 1.92 | 0.78 |
| 2:F:78:PHE:HE1 | 2:F:103:GLY:HA2 | 1.49 | 0.78 |
| 2:F:354:PHE:HB2 | 2:F:372:LEU:HA | 1.65 | 0.78 |
| 1:A:1231:LEU:HD11 | 1:A:1236:GLN:NE2 | 1.98 | 0.78 |
| 1:A:392:LEU:HG | 1:A:395:TYR:CD1 | 2.18 | 0.78 |
| 1:A:601:LYS:HG2 | 1:A:721:ALA:CB | 2.13 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:622:TYR:O | 1:A:746:GLY:HA3 | 1.83 | 0.78 |
| 2:C:376:PRO:CG | 2:C:482:ALA:HB1 | 2.13 | 0.78 |
| 2:C:424:SER:CB | 2:C:427:GLN:HE22 | 1.93 | 0.78 |
| 2:C:472:LYS:HA | 2:C:475:LEU:HD11 | 1.66 | 0.78 |
| 1:D:659:HIS:ND1 | 1:D:719:LEU:HD22 | 1.99 | 0.78 |
| 2:E:115:TRP:O | 2:E:116:THR:HG23 | 1.83 | 0.78 |
| 1:A:996:ARG:HH12 | 1:A:1003:TRP:CA | 1.97 | 0.78 |
| 1:A:1041:TRP:C | 1:A:1041:TRP:HD1 | 1.88 | 0.78 |
| 1:A:1131:ILE:CD1 | 1:A:1138:ARG:H | 1.95 | 0.78 |
| 1:A:795:ASN:ND2 | 1:A:796:LYS:N | 2.30 | 0.78 |
| 1:A:439:GLN:CG | 1:A:836:LEU:H | 1.96 | 0.78 |
| 1:A:933:SER:HB2 | 1:A:943:ARG:HD3 | 1.66 | 0.78 |
| 2:C:206:TYR:HD2 | 2:C:206:TYR:N | 1.79 | 0.78 |
| 2:C:303:LEU:CD1 | 2:C:339:ASN:OD1 | 2.31 | 0.78 |
| 2:C:375:HIS:H | 2:C:378:LEU:CD2 | 1.94 | 0.78 |
| 1:A:468:ASN:CG | 2:C:460:THR:HG21 | 2.03 | 0.78 |
| 1:D:580:LEU:C | 1:D:580:LEU:HD12 | 2.04 | 0.78 |
| 1:D:645:VAL:O | 1:D:645:VAL:CG1 | 2.31 | 0.78 |
| 1:D:717:LEU:HD23 | 1:D:717:LEU:H | 1.46 | 0.78 |
| 2:E:389:ARG:NE | 2:E:390:GLY:N | 2.29 | 0.78 |
| 2:E:432:TYR:O | 2:E:437:ILE:HD13 | 1.84 | 0.78 |
| 2:F:310:GLU:O | 2:F:313:HIS:HB3 | 1.83 | 0.78 |
| 1:A:1131:ILE:CG2 | 1:A:1137:VAL:HA | 2.14 | 0.78 |
| 1:A:271:VAL:HG12 | 1:A:272:SER:N | 1.96 | 0.78 |
| 1:A:371:LYS:C | 1:A:373:PRO:HD3 | 2.04 | 0.78 |
| 1:A:371:LYS:NZ | 1:A:400:VAL:HG23 | 1.99 | 0.78 |
| 1:A:408:GLN:CA | 1:A:411:LEU:HG | 2.12 | 0.78 |
| 1:A:559:LEU:HB3 | 1:A:560:PRO:HD2 | 1.65 | 0.78 |
| 1:A:779:LEU:O | 1:A:780:GLN:HG2 | 1.84 | 0.78 |
| 2:C:395:LEU:HD21 | 2:C:443:VAL:CB | 2.12 | 0.78 |
| 1:D:194:ALA:HA | 1:D:265:LEU:HB2 | 1.64 | 0.78 |
| 1:D:369:LEU:HB3 | 1:D:372:GLU:CG | 2.14 | 0.78 |
| 1:D:613:HIS:CG | 1:D:717:LEU:HD22 | 2.18 | 0.78 |
| 2:F:304:TRP:H | 2:F:337:SER:CB | 1.81 | 0.78 |
| 2:F:305:ASN:CA | 2:F:335:VAL:HG11 | 2.14 | 0.78 |
| 2:F:375:HIS:O | 2:F:378:LEU:HB2 | 1.84 | 0.78 |
| 2:F:385:LEU:HD11 | 2:F:402:LEU:HB2 | 1.66 | 0.78 |
| 2:F:435:MET:O | 2:F:436:SER:CB | 2.31 | 0.78 |
| 1:A:482:ASP:HB2 | 1:A:483:PRO:CD | 2.13 | 0.78 |
| 1:A:804:ALA:O | 1:A:808:ILE:HG13 | 1.84 | 0.78 |
| 1:A:845:VAL:CB | 1:A:855:VAL:HB | 2.12 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:893:SER:HB2 | 1:A:896:LEU:CG | 2.13 | 0.78 |
| 1:A:924:ARG:O | 1:A:925:LYS:HG2 | 1.83 | 0.78 |
| 1:D:1132:SER:HA | 1:D:1136:GLU:O | 1.83 | 0.78 |
| 1:D:1141:VAL:HG12 | 1:D:1142:ARG:O | 1.84 | 0.78 |
| 1:D:660:CYS:HB2 | 1:D:745:PRO:HG3 | 1.65 | 0.78 |
| 1:D:275:ARG:HH11 | 1:D:843:GLN:CD | 1.87 | 0.78 |
| 1:D:887:VAL:H | 1:D:1146:ARG:HH22 | 1.31 | 0.78 |
| 1:D:76:ILE:HA | 1:D:911:HIS:NE2 | 1.97 | 0.78 |
| 2:F:239:LEU:N | 2:F:338:VAL:HG11 | 1.98 | 0.78 |
| 2:F:431:LYS:NZ | 2:F:435:MET:HG2 | 1.98 | 0.78 |
| 2:F:82:SER:HA | 2:F:86:LEU:CD2 | 2.10 | 0.78 |
| 1:A:1041:TRP:O | 1:A:1041:TRP:CD1 | 2.37 | 0.77 |
| 1:A:241:PRO:HA | 1:A:244:LEU:CB | 2.14 | 0.77 |
| 1:D:900:ALA:CA | 1:D:915:ALA:HB1 | 2.13 | 0.77 |
| 1:D:922:GLN:HG2 | 1:D:931:LEU:CD1 | 2.13 | 0.77 |
| 2:F:182:ARG:NH2 | 2:F:213:VAL:O | 2.15 | 0.77 |
| 1:A:758:ASN:CB | 1:A:1058:PHE:HZ | 1.95 | 0.77 |
| 1:A:1166:TYR:H | 1:A:1166:TYR:HD1 | 1.31 | 0.77 |
| 1:A:238:GLN:HB2 | 1:A:239:LEU:HG | 1.65 | 0.77 |
| 1:A:83:LEU:HD13 | 1:A:89:GLY:CA | 2.15 | 0.77 |
| 1:D:206:GLY:HA2 | 1:D:245:ILE:HG22 | 1.65 | 0.77 |
| 1:D:371:LYS:NZ | 1:D:396:CYS:HB2 | 1.99 | 0.77 |
| 1:D:414:PHE:HA | 1:D:417:ARG:NH1 | 1.98 | 0.77 |
| 1:D:824:ALA:HA | 1:D:827:ARG:CB | 2.13 | 0.77 |
| 1:D:883:GLY:O | 1:D:1143:GLU:HB2 | 1.84 | 0.77 |
| 2:E:94:GLY:HA2 | 2:E:96:HIS:CE1 | 2.20 | 0.77 |
| 2:E:418:LEU:CD1 | 2:F:122:ARG:HE | 1.97 | 0.77 |
| 1:A:196:VAL:HB | 1:A:401:TRP:CZ3 | 2.18 | 0.77 |
| 1:A:213:VAL:HG13 | 1:A:397:ALA:HB1 | 1.67 | 0.77 |
| 1:A:813:VAL:CG2 | 1:A:814:VAL:N | 2.47 | 0.77 |
| 2:B:231:ILE:CG1 | 2:C:135:PRO:HG3 | 2.14 | 0.77 |
| 1:D:1001:GLY:HA2 | 1:D:1004:LEU:CD2 | 2.04 | 0.77 |
| 1:D:1134:HIS:O | 1:D:1135:ASP:HB2 | 1.83 | 0.77 |
| 1:D:578:PRO:O | 1:D:580:LEU:N | 2.18 | 0.77 |
| 1:D:624:VAL:C | 1:D:626:GLY:H | 1.86 | 0.77 |
| 1:D:903:GLY:CA | 1:D:1002:GLU:HB2 | 2.13 | 0.77 |
| 2:F:134:LYS:HB3 | 2:F:180:LYS:CD | 2.13 | 0.77 |
| 2:B:323:HIS:HB2 | 2:B:332:VAL:CA | 2.14 | 0.77 |
| 2:C:126:PHE:C | 2:C:128:VAL:H | 1.80 | 0.77 |
| 2:C:367:LEU:O | 2:C:369:ARG:HD2 | 1.83 | 0.77 |
| 2:C:439:PHE:HD1 | 2:C:458:ARG:CB | 1.98 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1072:THR:N | 1:D:1073:PRO:HD2 | 2.00 | 0.77 |
| 1:D:177:ARG:CG | 1:D:178:TYR:H | 1.97 | 0.77 |
| 1:D:247:LEU:O | 1:D:248:GLU:HB2 | 1.85 | 0.77 |
| 1:D:348:LEU:O | 1:D:348:LEU:HD13 | 1.84 | 0.77 |
| 1:D:775:GLU:HG2 | 1:D:780:GLN:CG | 2.12 | 0.77 |
| 1:D:80:SER:O | 1:D:82:GLY:N | 2.17 | 0.77 |
| 2:E:254:PHE:O | 2:E:258:HIS:N | 2.17 | 0.77 |
| 2:F:114:TRP:HE1 | 2:F:259:ARG:NH1 | 1.82 | 0.77 |
| 2:F:233:GLU:O | 2:F:234:LYS:HG2 | 1.85 | 0.77 |
| 2:F:243:THR:O | 2:F:334:CYS:N | 2.16 | 0.77 |
| 2:F:471:LEU:HA | 2:F:474:PHE:CD2 | 2.19 | 0.77 |
| 1:A:869:ARG:HA | 1:A:1201:SER:N | 1.98 | 0.77 |
| 1:A:175:TRP:CB | 1:A:186:PRO:HD3 | 2.15 | 0.77 |
| 2:C:200:VAL:HG21 | 2:C:204:LEU:CD2 | 2.14 | 0.77 |
| 1:D:866:ARG:CG | 1:D:1069:ILE:HG21 | 2.08 | 0.77 |
| 1:D:214:ALA:N | 1:D:401:TRP:HZ2 | 1.82 | 0.77 |
| 1:D:916:PHE:O | 1:D:920:THR:CA | 2.32 | 0.77 |
| 2:F:356:LEU:O | 2:F:370:LYS:HE2 | 1.84 | 0.77 |
| 2:F:81:GLY:HA3 | 2:F:97:PRO:HD2 | 1.65 | 0.77 |
| 1:A:308:GLN:NE2 | 1:A:1091:GLU:N | 2.33 | 0.77 |
| 1:A:460:LYS:N | 1:A:460:LYS:HD2 | 1.98 | 0.77 |
| 1:A:550:GLN:O | 1:A:554:GLY:N | 2.17 | 0.77 |
| 1:A:608:ASP:O | 1:A:620:TRP:HH2 | 1.67 | 0.77 |
| 1:A:728:THR:HG22 | 1:A:729:GLN:N | 1.99 | 0.77 |
| 1:A:805:HIS:ND1 | 1:A:806:LYS:N | 2.32 | 0.77 |
| 2:C:81:GLY:CA | 2:C:97:PRO:HB2 | 2.13 | 0.77 |
| 1:D:1166:TYR:CD1 | 1:D:1166:TYR:N | 2.43 | 0.77 |
| 1:D:504:LYS:HB3 | 1:D:523:ASP:HB2 | 1.66 | 0.77 |
| 2:E:309:HIS:ND1 | 2:E:310:GLU:HG2 | 2.00 | 0.77 |
| 2:E:431:LYS:HA | 2:E:434:GLU:HG3 | 1.64 | 0.77 |
| 1:A:79:LEU:CD2 | 1:A:1173:LEU:O | 2.29 | 0.77 |
| 1:A:1221:TYR:O | 1:A:1224:ILE:HG22 | 1.83 | 0.77 |
| 1:A:498:LYS:NZ | 1:A:519:GLY:H | 1.83 | 0.77 |
| 1:A:640:LEU:N | 1:A:640:LEU:HD23 | 1.98 | 0.77 |
| 1:A:448:ALA:HA | 1:A:870:VAL:HG13 | 1.65 | 0.77 |
| 1:A:962:ALA:HB2 | 1:A:986:TYR:CZ | 2.19 | 0.77 |
| 2:B:324:GLY:CA | 2:B:325:ARG:CZ | 2.62 | 0.77 |
| 2:C:382:LYS:HD3 | 2:C:411:ILE:CG1 | 2.13 | 0.77 |
| 1:D:1221:TYR:HD1 | 1:D:1222:GLN:H | 1.33 | 0.77 |
| 1:D:195:LEU:N | 1:D:265:LEU:HD13 | 1.99 | 0.77 |
| 2:E:67:GLU:HG2 | 2:E:70:LEU:CD1 | 2.14 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:305:ASN:HA | 2:F:335:VAL:HG11 | 1.65 | 0.77 |
| 1:A:77:GLN:CB | 1:A:1174:PRO:HB3 | 2.14 | 0.77 |
| 1:A:1175:GLN:HG3 | 1:A:1176:SER:N | 2.00 | 0.77 |
| 1:A:358:LEU:O | 1:A:361:VAL:HG13 | 1.85 | 0.77 |
| 1:A:460:LYS:O | 1:A:464:MET:HG3 | 1.84 | 0.77 |
| 1:A:711:ALA:O | 1:A:712:VAL:HG23 | 1.83 | 0.77 |
| 2:B:233:GLU:C | 2:B:234:LYS:HE2 | 2.03 | 0.77 |
| 2:B:478:TYR:O | 2:B:482:ALA:HB2 | 1.84 | 0.77 |
| 2:B:233:GLU:OE2 | 2:C:133:HIS:N | 2.15 | 0.77 |
| 1:D:869:ARG:O | 1:D:1200:PRO:CB | 2.32 | 0.77 |
| 1:D:302:SER:HB2 | 1:D:351:SER:CB | 2.15 | 0.77 |
| 2:E:78:PHE:O | 2:E:79:LEU:CG | 2.27 | 0.77 |
| 2:F:435:MET:CE | 2:F:435:MET:HA | 2.14 | 0.77 |
| 2:F:435:MET:O | 2:F:436:SER:HB3 | 1.84 | 0.77 |
| 1:A:1040:LYS:CG | 1:A:1044:VAL:HG11 | 2.15 | 0.77 |
| 1:A:1210:TYR:CE1 | 1:A:1213:PRO:CG | 2.61 | 0.77 |
| 2:B:311:LEU:CG | 2:B:312:LEU:N | 2.47 | 0.77 |
| 1:D:346:ASP:H | 1:D:1040:LYS:HD3 | 1.48 | 0.77 |
| 1:D:294:THR:CG2 | 1:D:407:PHE:HE2 | 1.93 | 0.77 |
| 1:D:512:LYS:O | 1:D:513:LEU:HD23 | 1.84 | 0.77 |
| 1:D:885:THR:C | 1:D:886:LEU:HD23 | 2.05 | 0.77 |
| 2:E:69:LEU:H | 2:E:69:LEU:HD12 | 1.48 | 0.77 |
| 1:A:885:THR:HB | 1:A:1146:ARG:NE | 1.99 | 0.77 |
| 1:A:608:ASP:CB | 1:A:779:LEU:HB2 | 2.14 | 0.77 |
| 1:A:827:ARG:HH11 | 1:A:827:ARG:HG2 | 1.50 | 0.77 |
| 2:C:79:LEU:HA | 2:C:99:PHE:HA | 1.67 | 0.77 |
| 1:D:1008:LEU:C | 1:D:1011:PRO:HD2 | 2.05 | 0.77 |
| 1:D:1143:GLU:O | 1:D:1146:ARG:HG3 | 1.85 | 0.77 |
| 1:D:797:MET:CB | 1:D:869:ARG:HD3 | 2.14 | 0.77 |
| 1:D:610:PHE:CE1 | 1:D:972:ARG:NH2 | 2.52 | 0.77 |
| 2:E:375:HIS:CD2 | 2:E:376:PRO:HB3 | 2.20 | 0.77 |
| 2:E:373:LYS:HB2 | 2:E:459:ASP:OD1 | 1.84 | 0.77 |
| 2:F:342:LEU:HG | 2:F:344:ARG:HB2 | 1.67 | 0.77 |
| 1:A:1037:GLN:C | 1:A:1039:LYS:H | 1.84 | 0.76 |
| 1:A:562:ARG:HB3 | 1:A:565:HIS:CE1 | 2.21 | 0.76 |
| 1:A:584:ALA:C | 1:A:585:TRP:HE3 | 1.87 | 0.76 |
| 1:A:593:SER:CA | 1:A:596:MET:HG3 | 2.12 | 0.76 |
| 1:A:624:VAL:C | 1:A:626:GLY:H | 1.88 | 0.76 |
| 2:B:112:ALA:O | 2:B:115:TRP:HB3 | 1.85 | 0.76 |
| 2:C:208:LEU:HD12 | 2:C:208:LEU:O | 1.85 | 0.76 |
| 2:C:215:PHE:CD2 | 2:C:233:GLU:HG2 | 2.21 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:824:ALA:HA | 1:D:827:ARG:HB3 | 1.67 | 0.76 |
| 2:F:383:VAL:HG23 | 2:F:439:PHE:O | 1.83 | 0.76 |
| 1:A:192:GLU:O | 1:A:193:ARG:HG3 | 1.84 | 0.76 |
| 1:A:213:VAL:O | 1:A:401:TRP:HZ2 | 1.68 | 0.76 |
| 1:A:462:SER:C | 1:A:466:LEU:HD23 | 2.06 | 0.76 |
| 1:A:617:ARG:HG2 | 1:A:765:PRO:HD3 | 1.66 | 0.76 |
| 1:A:601:LYS:HA | 1:A:717:LEU:HB3 | 1.65 | 0.76 |
| 1:A:732:TYR:HE1 | 1:A:755:LYS:CB | 1.98 | 0.76 |
| 2:C:300:ILE:HG22 | 2:C:301:GLU:H | 1.49 | 0.76 |
| 2:C:393:LEU:O | 2:C:396:ARG:HG3 | 1.86 | 0.76 |
| 1:D:167:PRO:HD2 | 1:D:168:ALA:N | 1.99 | 0.76 |
| 1:D:441:TRP:NE1 | 1:D:879:GLN:CA | 2.48 | 0.76 |
| 2:E:389:ARG:N | 2:E:395:LEU:HD11 | 2.00 | 0.76 |
| 2:F:302:THR:C | 2:F:303:LEU:HD12 | 2.06 | 0.76 |
| 1:A:1119:LEU:HA | 1:A:1122:GLU:CG | 2.15 | 0.76 |
| 1:A:441:TRP:NE1 | 1:A:877:MET:HB3 | 2.00 | 0.76 |
| 1:A:643:ALA:O | 1:A:645:VAL:HG23 | 1.85 | 0.76 |
| 1:A:989:THR:HG22 | 1:A:999:ASP:HB2 | 1.65 | 0.76 |
| 2:B:69:LEU:O | 2:B:72:ILE:HG12 | 1.83 | 0.76 |
| 2:C:201:ASN:C | 2:C:203:ARG:H | 1.88 | 0.76 |
| 2:C:301:GLU:HB3 | 2:C:339:ASN:CG | 2.06 | 0.76 |
| 2:C:328:ARG:O | 2:C:329:LYS:HD2 | 1.86 | 0.76 |
| 2:C:81:GLY:HA3 | 2:C:97:PRO:CB | 2.15 | 0.76 |
| 1:D:289:MET:SD | 1:D:290:ARG:N | 2.58 | 0.76 |
| 1:D:605:LEU:CD2 | 1:D:781:ALA:HB1 | 2.14 | 0.76 |
| 1:D:611:PRO:HB2 | 1:D:612:LEU:CD1 | 2.15 | 0.76 |
| 1:D:928:GLY:HA2 | 1:D:931:LEU:HD12 | 1.65 | 0.76 |
| 2:F:301:GLU:HB3 | 2:F:339:ASN:CB | 2.12 | 0.76 |
| 1:A:1041:TRP:O | 1:A:1041:TRP:HD1 | 1.68 | 0.76 |
| 1:A:152:GLU:HA | 1:A:155:ASN:ND2 | 2.00 | 0.76 |
| 2:B:323:HIS:HB2 | 2:B:332:VAL:N | 2.00 | 0.76 |
| 2:C:258:HIS:HA | 2:C:261:GLN:OE1 | 1.85 | 0.76 |
| 2:C:241:TRP:N | 2:C:336:LEU:HB3 | 2.00 | 0.76 |
| 2:C:389:ARG:CG | 2:C:390:GLY:H | 1.98 | 0.76 |
| 1:D:1158:LEU:H | 1:D:1158:LEU:HD23 | 1.50 | 0.76 |
| 1:D:842:PRO:HB2 | 1:D:856:GLU:CD | 2.05 | 0.76 |
| 2:E:194:VAL:HG13 | 2:E:195:ASN:N | 2.01 | 0.76 |
| 2:F:394:GLU:N | 2:F:394:GLU:CD | 2.39 | 0.76 |
| 1:A:887:VAL:HG23 | 1:A:1146:ARG:HH11 | 1.50 | 0.76 |
| 1:A:885:THR:CB | 1:A:1146:ARG:NE | 2.48 | 0.76 |
| 1:A:1179:PHE:CD1 | 1:A:1220:ILE:HG21 | 2.20 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:244:LEU:O | 1:A:247:LEU:HB3 | 1.86 | 0.76 |
| 1:A:591:LEU:HD12 | 1:A:594:LEU:HG | 1.67 | 0.76 |
| 1:A:868:ASP:HB3 | 1:A:1199:THR:HB | 1.68 | 0.76 |
| 2:B:74:GLN:O | 2:B:77:HIS:CA | 2.33 | 0.76 |
| 2:C:182:ARG:NH2 | 2:C:213:VAL:O | 2.18 | 0.76 |
| 2:C:416:GLY:O | 2:C:419:GLU:HB3 | 1.85 | 0.76 |
| 1:D:137:GLN:O | 1:D:141:LEU:HD12 | 1.86 | 0.76 |
| 1:D:513:LEU:O | 1:D:570:PRO:HD2 | 1.86 | 0.76 |
| 1:D:522:GLY:O | 1:D:524:PRO:CD | 2.33 | 0.76 |
| 1:D:649:TYR:HD2 | 1:D:652:ILE:HG21 | 1.50 | 0.76 |
| 1:D:823:ARG:O | 1:D:826:ILE:HG12 | 1.85 | 0.76 |
| 1:D:556:THR:HB | 2:F:467:HIS:NE2 | 1.99 | 0.76 |
| 1:A:582:ASP:HB3 | 1:A:592:LEU:HD22 | 1.68 | 0.76 |
| 1:A:600:PRO:O | 1:A:602:LEU:O | 2.04 | 0.76 |
| 1:A:79:LEU:HD12 | 1:A:89:GLY:O | 1.85 | 0.76 |
| 2:C:241:TRP:HB3 | 2:C:336:LEU:HB2 | 1.67 | 0.76 |
| 1:D:437:VAL:HA | 1:D:441:TRP:HD1 | 1.50 | 0.76 |
| 1:D:659:HIS:CD2 | 1:D:719:LEU:HB2 | 2.21 | 0.76 |
| 2:F:208:LEU:HD13 | 2:F:240:VAL:HB | 1.64 | 0.76 |
| 1:A:610:PHE:N | 1:A:610:PHE:HD2 | 1.83 | 0.76 |
| 2:C:239:LEU:N | 2:C:338:VAL:CG1 | 2.46 | 0.76 |
| 2:C:352:ASP:N | 2:C:355:GLN:HB2 | 2.00 | 0.76 |
| 2:C:466:MET:HB3 | 2:C:471:LEU:CD2 | 2.10 | 0.76 |
| 1:D:1207:GLU:HA | 1:D:1210:TYR:CD2 | 2.21 | 0.76 |
| 1:D:130:LEU:O | 1:D:131:TYR:CD2 | 2.39 | 0.76 |
| 1:D:140:ARG:O | 1:D:144:GLN:HB2 | 1.85 | 0.76 |
| 1:D:375:GLU:HG3 | 1:D:379:LYS:CG | 2.16 | 0.76 |
| 1:D:456:GLN:C | 1:D:460:LYS:HZ3 | 1.88 | 0.76 |
| 1:D:547:ALA:CA | 1:D:551:LYS:HE2 | 2.16 | 0.76 |
| 1:D:606:THR:CG2 | 1:D:612:LEU:O | 2.34 | 0.76 |
| 1:D:83:LEU:HG | 1:D:89:GLY:CA | 2.16 | 0.76 |
| 2:F:201:ASN:C | 2:F:203:ARG:H | 1.89 | 0.76 |
| 2:F:347:LEU:CA | 2:F:350:LEU:HD11 | 2.15 | 0.76 |
| 2:F:350:LEU:H | 2:F:350:LEU:HD12 | 1.51 | 0.76 |
| 2:F:449:GLU:O | 2:F:450:ASN:C | 2.24 | 0.76 |
| 1:A:498:LYS:HE3 | 1:A:518:ALA:N | 2.01 | 0.76 |
| 2:C:444:THR:O | 2:C:447:THR:N | 2.18 | 0.76 |
| 2:C:452:LEU:HD12 | 2:C:453:ILE:N | 2.01 | 0.76 |
| 1:D:1102:GLN:O | 1:D:1106:VAL:HG23 | 1.85 | 0.76 |
| 1:D:1165:ALA:C | 1:D:1166:TYR:HD1 | 1.89 | 0.76 |
| 1:D:275:ARG:HD2 | 1:D:843:GLN:OE1 | 1.85 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:604:ALA:CA | 1:D:613:HIS:CE1 | 2.67 | 0.76 |
| 1:D:630:ASN:HB2 | 1:D:744:ILE:O | 1.86 | 0.76 |
| 1:D:645:VAL:CG1 | 1:D:650:ARG:HG2 | 2.15 | 0.76 |
| 1:D:717:LEU:CD2 | 1:D:717:LEU:H | 1.92 | 0.76 |
| 1:D:748:TRP:CH2 | 1:D:750:PHE:HE2 | 2.02 | 0.76 |
| 1:D:914:THR:CG2 | 1:D:999:ASP:HB3 | 2.15 | 0.76 |
| 2:E:213:VAL:HG13 | 2:E:235:THR:HG22 | 1.67 | 0.76 |
| 2:F:197:LEU:O | 2:F:202:LYS:HA | 1.85 | 0.76 |
| 2:F:444:THR:O | 2:F:447:THR:HG22 | 1.86 | 0.76 |
| 1:A:1112:MET:HA | 1:A:1156:THR:CG2 | 2.16 | 0.76 |
| 1:A:175:TRP:HB3 | 1:A:186:PRO:CD | 2.15 | 0.76 |
| 1:A:274:ASP:N | 1:A:276:ALA:H | 1.83 | 0.76 |
| 1:A:618:HIS:HB2 | 1:A:725:PRO:CG | 2.16 | 0.76 |
| 1:A:77:GLN:OE1 | 1:A:1174:PRO:CB | 2.34 | 0.76 |
| 2:B:260:LEU:O | 2:B:264:ARG:HD3 | 1.86 | 0.76 |
| 2:B:440:THR:HG22 | 2:B:441:VAL:N | 2.01 | 0.76 |
| 2:C:244:PRO:CD | 2:C:247:THR:CG2 | 2.64 | 0.76 |
| 2:C:300:ILE:HG22 | 2:C:301:GLU:N | 2.00 | 0.76 |
| 2:C:303:LEU:HD11 | 2:C:339:ASN:OD1 | 1.86 | 0.76 |
| 2:C:385:LEU:HD11 | 2:C:402:LEU:CB | 2.14 | 0.76 |
| 2:C:474:PHE:HE1 | 2:C:478:TYR:CD2 | 2.04 | 0.76 |
| 2:C:484:ASN:O | 2:C:485:VAL:HG13 | 1.86 | 0.76 |
| 1:D:192:GLU:O | 1:D:217:PRO:HD3 | 1.86 | 0.76 |
| 1:D:549:LEU:CA | 1:D:551:LYS:HZ2 | 1.99 | 0.76 |
| 1:D:656:TYR:O | 1:D:659:HIS:CE1 | 2.38 | 0.76 |
| 1:D:966:LEU:HD23 | 1:D:970:ASN:ND2 | 2.00 | 0.76 |
| 2:F:208:LEU:HD11 | 2:F:240:VAL:CB | 2.16 | 0.76 |
| 2:F:241:TRP:HB2 | 2:F:336:LEU:CG | 2.14 | 0.76 |
| 2:F:374:LEU:HD12 | 2:F:379:ALA:HA | 1.65 | 0.76 |
| 1:A:120:LEU:H | 1:A:120:LEU:HD22 | 1.50 | 0.76 |
| 1:A:354:ASN:OD1 | 1:A:355:SER:N | 2.18 | 0.76 |
| 1:A:471:CYS:CB | 1:A:472:GLN:OE1 | 2.34 | 0.76 |
| 1:A:667:GLN:O | 1:A:671:GLN:HG2 | 1.86 | 0.76 |
| 2:B:417:TYR:HH | 2:C:122:ARG:HD3 | 1.48 | 0.76 |
| 1:D:903:GLY:HA3 | 1:D:1002:GLU:CB | 2.16 | 0.76 |
| 2:E:336:LEU:HD22 | 2:E:338:VAL:HG23 | 1.67 | 0.76 |
| 2:F:393:LEU:O | 2:F:396:ARG:HG3 | 1.85 | 0.76 |
| 1:A:1069:ILE:CG2 | 1:A:1070:PRO:HD3 | 2.15 | 0.75 |
| 1:A:1169:GLY:O | 1:A:1170:LEU:HB3 | 1.86 | 0.75 |
| 1:A:913:CYS:C | 1:A:918:TRP:H | 1.89 | 0.75 |
| 2:C:254:PHE:CA | 2:C:257:ARG:HH21 | 1.98 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:907:PHE:CZ | 1:D:1002:GLU:HB3 | 2.20 | 0.75 |
| 1:D:1027:LYS:HZ3 | 1:D:1091:GLU:HG2 | 1.48 | 0.75 |
| 1:D:1165:ALA:O | 1:D:1169:GLY:HA3 | 1.87 | 0.75 |
| 1:D:203:LEU:C | 1:D:203:LEU:HD23 | 2.07 | 0.75 |
| 1:D:463:LEU:HA | 1:D:466:LEU:HD22 | 1.68 | 0.75 |
| 1:D:671:GLN:NE2 | 1:D:671:GLN:HA | 2.00 | 0.75 |
| 1:D:865:ALA:HA | 1:D:872:SER:HA | 1.68 | 0.75 |
| 1:D:993:ARG:C | 1:D:996:ARG:HD2 | 2.05 | 0.75 |
| 2:E:102:LEU:HD13 | 2:E:102:LEU:O | 1.87 | 0.75 |
| 2:E:383:VAL:O | 2:E:384:ALA:HB2 | 1.85 | 0.75 |
| 2:F:200:VAL:CG1 | 2:F:204:LEU:HB2 | 2.15 | 0.75 |
| 1:A:112:LEU:HD21 | 1:A:918:TRP:HA | 1.69 | 0.75 |
| 2:C:415:PRO:HB3 | 2:C:417:TYR:CE2 | 2.21 | 0.75 |
| 2:C:382:LYS:O | 2:C:438:LEU:HB2 | 1.86 | 0.75 |
| 1:A:560:PRO:HD2 | 2:C:452:LEU:HD23 | 1.66 | 0.75 |
| 1:D:948:ILE:HG23 | 1:D:1071:ARG:HB2 | 1.69 | 0.75 |
| 1:D:1145:ASP:HA | 1:D:1148:ARG:CD | 2.16 | 0.75 |
| 1:D:352:SER:O | 1:D:358:GLU:HG2 | 1.85 | 0.75 |
| 1:D:389:PHE:CA | 1:D:393:MET:HG3 | 2.16 | 0.75 |
| 2:E:336:LEU:HD23 | 2:E:337:SER:N | 2.00 | 0.75 |
| 2:E:371:VAL:HA | 2:E:433:ASP:CG | 2.05 | 0.75 |
| 1:A:142:LEU:HD22 | 1:A:1118:TRP:CD1 | 2.21 | 0.75 |
| 1:A:374:ARG:NE | 1:A:392:LEU:HD13 | 1.98 | 0.75 |
| 1:A:601:LYS:HG2 | 1:A:721:ALA:HB1 | 1.68 | 0.75 |
| 1:A:914:THR:O | 1:A:915:ALA:CB | 2.34 | 0.75 |
| 2:B:201:ASN:HB2 | 2:C:421:MET:HE1 | 1.68 | 0.75 |
| 2:B:269:SER:H | 2:B:270:PRO:CD | 1.98 | 0.75 |
| 1:D:432:VAL:HB | 1:D:1128:ARG:HH21 | 1.51 | 0.75 |
| 1:D:744:ILE:HG12 | 1:D:745:PRO:HD2 | 1.68 | 0.75 |
| 1:D:823:ARG:NE | 1:D:824:ALA:H | 1.85 | 0.75 |
| 1:D:83:LEU:N | 1:D:83:LEU:HD13 | 2.01 | 0.75 |
| 2:F:484:ASN:O | 2:F:485:VAL:HG13 | 1.87 | 0.75 |
| 1:A:1026:ARG:CB | 1:A:1029:GLN:CB | 2.49 | 0.75 |
| 1:A:1151:LEU:HG | 1:A:1223:ILE:HD11 | 1.68 | 0.75 |
| 1:A:879:GLN:CG | 1:A:1189:LEU:HD21 | 2.15 | 0.75 |
| 1:A:1207:GLU:HA | 1:A:1210:TYR:HD1 | 1.51 | 0.75 |
| 1:A:1231:LEU:HG | 1:A:1232:GLU:H | 1.51 | 0.75 |
| 2:B:90:SER:HA | 2:B:93:SER:OG | 1.85 | 0.75 |
| 2:B:99:PHE:CD2 | 2:C:129:ASP:CG | 2.60 | 0.75 |
| 2:C:425:LEU:HD21 | 2:C:429:TYR:OH | 1.86 | 0.75 |
| 2:C:372:LEU:HD21 | 2:C:435:MET:C | 2.07 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1006:ARG:CZ | 1:D:1010:LEU:HD11 | 2.15 | 0.75 |
| 1:D:1028:VAL:HG22 | 1:D:1096:ARG:CZ | 2.16 | 0.75 |
| 1:D:113:TRP:HE3 | 1:D:114:GLY:N | 1.81 | 0.75 |
| 1:D:239:LEU:CB | 1:D:242:ALA:HB3 | 2.15 | 0.75 |
| 1:D:459:MET:N | 1:D:460:LYS:NZ | 2.34 | 0.75 |
| 1:D:956:GLY:HA2 | 1:D:1094:THR:CG2 | 2.04 | 0.75 |
| 2:E:351:TYR:C | 2:E:353:SER:H | 1.89 | 0.75 |
| 2:F:251:TRP:CE3 | 2:F:251:TRP:HA | 2.20 | 0.75 |
| 1:A:1041:TRP:CE2 | 1:A:1043:VAL:HB | 2.21 | 0.75 |
| 1:A:594:LEU:HD23 | 1:A:594:LEU:N | 2.01 | 0.75 |
| 1:A:940:GLY:O | 1:A:941:ILE:HD12 | 1.86 | 0.75 |
| 1:A:961:PHE:N | 1:A:961:PHE:CD1 | 2.51 | 0.75 |
| 2:C:128:VAL:HG12 | 2:C:192:HIS:CD2 | 2.21 | 0.75 |
| 2:C:239:LEU:O | 2:C:338:VAL:CG1 | 2.34 | 0.75 |
| 2:F:243:THR:O | 2:F:334:CYS:HB2 | 1.87 | 0.75 |
| 2:F:454:HIS:HD2 | 2:F:468:ILE:CA | 1.99 | 0.75 |
| 2:F:73:CYS:HB3 | 2:F:79:LEU:HD23 | 1.69 | 0.75 |
| 2:B:306:LEU:HD22 | 2:B:310:GLU:HG2 | 1.67 | 0.75 |
| 1:D:1236:GLN:HB2 | 1:D:1237:PRO:HD3 | 1.68 | 0.75 |
| 1:D:134:ASN:HB3 | 1:D:137:GLN:H | 1.51 | 0.75 |
| 1:D:259:ARG:HG3 | 1:D:261:TRP:CD1 | 2.22 | 0.75 |
| 1:D:434:TYR:O | 1:D:435:LEU:HG | 1.86 | 0.75 |
| 1:D:608:ASP:HB3 | 1:D:620:TRP:CE2 | 2.22 | 0.75 |
| 1:D:865:ALA:HB3 | 1:D:1197:CYS:SG | 2.26 | 0.75 |
| 2:E:253:ASP:O | 2:E:257:ARG:N | 2.20 | 0.75 |
| 2:F:385:LEU:HD11 | 2:F:402:LEU:CB | 2.17 | 0.75 |
| 1:A:1175:GLN:HG3 | 1:A:1176:SER:H | 1.49 | 0.75 |
| 1:A:412:PRO:O | 1:A:415:LEU:HB2 | 1.86 | 0.75 |
| 1:A:652:ILE:HA | 1:A:655:LEU:CD2 | 2.16 | 0.75 |
| 1:A:823:ARG:HG3 | 1:A:823:ARG:O | 1.87 | 0.75 |
| 1:D:1029:GLN:NE2 | 1:D:1030:ARG:NH2 | 2.32 | 0.75 |
| 1:D:1131:ILE:H | 1:D:1131:ILE:HD13 | 1.51 | 0.75 |
| 1:D:1154:GLN:OE1 | 1:D:1220:ILE:HA | 1.85 | 0.75 |
| 1:D:249:VAL:HG23 | 1:D:250:PRO:HD2 | 1.66 | 0.75 |
| 1:D:279:ARG:HG3 | 1:D:841:LEU:O | 1.87 | 0.75 |
| 1:D:213:VAL:HG13 | 1:D:401:TRP:CE2 | 2.21 | 0.75 |
| 1:D:881:PRO:O | 1:D:884:TYR:HB2 | 1.86 | 0.75 |
| 2:F:114:TRP:HE1 | 2:F:259:ARG:NH2 | 1.85 | 0.75 |
| 2:F:131:LEU:HB3 | 2:F:133:HIS:CG | 2.21 | 0.75 |
| 2:F:239:LEU:H | 2:F:338:VAL:CG2 | 1.99 | 0.75 |
| 1:A:879:GLN:HG2 | 1:A:1189:LEU:CG | 2.17 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:172:ALA:HA | 1:A:221:TYR:O | 1.85 | 0.75 |
| 1:A:256:PRO:HB2 | 1:A:281:GLN:HA | 1.67 | 0.75 |
| 1:A:473:LEU:HD23 | 1:A:473:LEU:H | 1.50 | 0.75 |
| 1:A:539:PHE:O | 1:A:540:GLN:CG | 2.35 | 0.75 |
| 1:A:922:GLN:HG3 | 1:A:923:GLY:N | 2.01 | 0.75 |
| 1:A:926:SER:O | 1:A:927:ARG:HB2 | 1.86 | 0.75 |
| 2:B:104:VAL:HG21 | 2:C:128:VAL:O | 1.87 | 0.75 |
| 1:D:356:LEU:CD1 | 1:D:369:LEU:HD22 | 2.16 | 0.75 |
| 1:D:417:ARG:O | 1:D:418:CYS:SG | 2.45 | 0.75 |
| 1:D:584:ALA:C | 1:D:585:TRP:HE3 | 1.90 | 0.75 |
| 1:D:247:LEU:HA | 1:D:815:TRP:CD1 | 2.22 | 0.75 |
| 2:F:277:ASP:OD2 | 2:F:287:ASN:HB3 | 1.87 | 0.75 |
| 2:F:446:THR:CA | 2:F:450:ASN:H | 1.99 | 0.75 |
| 1:A:1011:PRO:HG2 | 1:A:1012:VAL:HG13 | 1.68 | 0.75 |
| 1:A:1119:LEU:HA | 1:A:1122:GLU:HG2 | 1.69 | 0.75 |
| 1:A:870:VAL:HG22 | 1:A:1202:ASN:HD22 | 1.52 | 0.75 |
| 1:A:266:VAL:HG23 | 1:A:290:ARG:O | 1.86 | 0.75 |
| 1:A:610:PHE:N | 1:A:610:PHE:CD2 | 2.52 | 0.75 |
| 1:A:825:VAL:O | 1:A:829:PRO:HD3 | 1.85 | 0.75 |
| 2:C:344:ARG:N | 2:C:347:LEU:HD13 | 2.01 | 0.75 |
| 1:A:576:LEU:HD21 | 2:C:482:ALA:HB2 | 1.67 | 0.75 |
| 1:D:249:VAL:HG22 | 1:D:250:PRO:CD | 2.16 | 0.75 |
| 1:D:623:LEU:O | 1:D:625:PRO:CD | 2.34 | 0.75 |
| 1:D:642:SER:CA | 1:D:645:VAL:HG11 | 2.13 | 0.75 |
| 1:D:665:LYS:O | 1:D:669:MET:HG2 | 1.87 | 0.75 |
| 2:E:78:PHE:CA | 2:E:102:LEU:HB3 | 2.17 | 0.75 |
| 2:E:353:SER:OG | 2:E:372:LEU:HD11 | 1.86 | 0.75 |
| 2:E:422:GLN:C | 2:E:424:SER:H | 1.89 | 0.75 |
| 2:F:203:ARG:HE | 2:F:204:LEU:HD13 | 1.48 | 0.75 |
| 2:F:254:PHE:CA | 2:F:257:ARG:HH21 | 2.00 | 0.75 |
| 1:A:481:GLU:HB3 | 1:A:482:ASP:OD1 | 1.86 | 0.74 |
| 1:A:608:ASP:C | 1:A:620:TRP:HH2 | 1.90 | 0.74 |
| 1:A:821:LEU:HG | 1:A:826:ILE:HG23 | 1.69 | 0.74 |
| 1:A:897:TRP:NE1 | 1:A:901:VAL:HG13 | 2.02 | 0.74 |
| 1:A:933:SER:HB2 | 1:A:943:ARG:CZ | 2.17 | 0.74 |
| 1:A:933:SER:HB2 | 1:A:943:ARG:CD | 2.15 | 0.74 |
| 1:A:958:GLY:O | 1:A:961:PHE:CD1 | 2.39 | 0.74 |
| 1:A:958:GLY:O | 1:A:961:PHE:HD1 | 1.69 | 0.74 |
| 2:C:386:ASP:CB | 2:C:442:LEU:HA | 2.10 | 0.74 |
| 1:D:242:ALA:HA | 1:D:245:ILE:HG23 | 1.68 | 0.74 |
| 1:D:352:SER:C | 1:D:358:GLU:CD | 2.37 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:542:ASP:O | 1:D:546:ARG:N | 2.18 | 0.74 |
| 1:D:275:ARG:NH1 | 1:D:843:GLN:CG | 2.50 | 0.74 |
| 1:D:798:ILE:HG22 | 1:D:869:ARG:CZ | 2.17 | 0.74 |
| 2:E:185:LEU:HD13 | 2:E:238:SER:OG | 1.87 | 0.74 |
| 2:F:395:LEU:HB3 | 2:F:443:VAL:CG2 | 2.15 | 0.74 |
| 2:F:471:LEU:HA | 2:F:474:PHE:HB3 | 1.69 | 0.74 |
| 2:F:402:LEU:HG | 2:F:472:LYS:HZ3 | 1.52 | 0.74 |
| 1:A:1015:THR:HA | 1:A:1016:GLU:OE2 | 1.86 | 0.74 |
| 1:A:1148:ARG:HG2 | 1:A:1148:ARG:NH1 | 1.90 | 0.74 |
| 1:A:76:ILE:HG13 | 1:A:77:GLN:CG | 2.15 | 0.74 |
| 1:A:879:GLN:CB | 1:A:886:LEU:HD11 | 2.16 | 0.74 |
| 2:B:306:LEU:C | 2:B:308:ASP:N | 2.37 | 0.74 |
| 2:B:344:ARG:CD | 2:B:344:ARG:H | 1.99 | 0.74 |
| 2:C:342:LEU:HB2 | 2:C:344:ARG:CB | 2.17 | 0.74 |
| 1:D:1025:LEU:HD22 | 1:D:1025:LEU:O | 1.87 | 0.74 |
| 1:D:1045:ALA:HB1 | 1:D:1090:GLU:HG2 | 1.69 | 0.74 |
| 1:D:131:TYR:CB | 1:D:138:HIS:CE1 | 2.70 | 0.74 |
| 1:D:176:THR:N | 1:D:185:VAL:HG11 | 2.01 | 0.74 |
| 1:D:865:ALA:HB1 | 1:D:872:SER:OG | 1.86 | 0.74 |
| 1:D:904:ASP:OD2 | 1:D:915:ALA:HB3 | 1.86 | 0.74 |
| 2:E:215:PHE:HB3 | 2:E:233:GLU:HA | 1.70 | 0.74 |
| 2:F:447:THR:HA | 2:F:452:LEU:CA | 2.17 | 0.74 |
| 2:F:445:GLU:HA | 2:F:448:LEU:HD12 | 1.69 | 0.74 |
| 2:F:446:THR:HG22 | 2:F:449:GLU:OE1 | 1.87 | 0.74 |
| 1:A:261:TRP:HA | 1:A:261:TRP:CE3 | 2.21 | 0.74 |
| 1:A:665:LYS:CG | 1:A:666:GLN:N | 2.50 | 0.74 |
| 1:A:717:LEU:O | 1:A:721:ALA:HB3 | 1.88 | 0.74 |
| 1:A:813:VAL:HB | 1:A:840:ILE:HG12 | 1.70 | 0.74 |
| 1:A:897:TRP:CZ3 | 1:A:1108:TYR:HE1 | 2.05 | 0.74 |
| 2:B:74:GLN:CG | 2:B:75:ARG:N | 2.50 | 0.74 |
| 2:C:273:PHE:CE1 | 2:C:291:TYR:HD1 | 2.04 | 0.74 |
| 1:D:885:THR:CB | 1:D:1146:ARG:HD2 | 2.15 | 0.74 |
| 1:D:660:CYS:HB2 | 1:D:745:PRO:HD3 | 1.68 | 0.74 |
| 1:D:622:TYR:O | 1:D:746:GLY:CA | 2.36 | 0.74 |
| 2:E:380:PRO:O | 2:E:382:LYS:CB | 2.34 | 0.74 |
| 2:F:241:TRP:CA | 2:F:336:LEU:HB2 | 2.18 | 0.74 |
| 2:F:351:TYR:O | 2:F:352:ASP:C | 2.24 | 0.74 |
| 1:A:622:TYR:HB2 | 1:A:747:CYS:O | 1.87 | 0.74 |
| 2:C:276:SER:O | 2:C:287:ASN:CB | 2.36 | 0.74 |
| 2:C:343:ASP:O | 2:C:347:LEU:HD13 | 1.87 | 0.74 |
| 1:D:872:SER:OG | 1:D:1200:PRO:HD3 | 1.86 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:348:LEU:CD1 | 1:D:350:ILE:HD11 | 2.17 | 0.74 |
| 1:D:900:ALA:HB1 | 1:D:915:ALA:CB | 2.13 | 0.74 |
| 2:F:389:ARG:HG3 | 2:F:390:GLY:H | 1.52 | 0.74 |
| 1:A:282:TYR:CZ | 1:A:432:VAL:HG22 | 2.21 | 0.74 |
| 1:A:451:THR:C | 1:A:869:ARG:NH2 | 2.40 | 0.74 |
| 1:A:468:ASN:HD21 | 1:A:578:PRO:CG | 2.00 | 0.74 |
| 1:A:490:TRP:CZ2 | 1:A:596:MET:HB3 | 2.22 | 0.74 |
| 1:A:601:LYS:HZ3 | 1:A:616:GLU:HG2 | 1.52 | 0.74 |
| 1:A:720:THR:CG2 | 1:A:721:ALA:N | 2.51 | 0.74 |
| 1:A:932:HIS:HB3 | 1:A:947:LYS:HG2 | 1.68 | 0.74 |
| 1:A:958:GLY:HA2 | 1:A:986:TYR:CE2 | 2.22 | 0.74 |
| 2:B:284:ARG:O | 2:B:285:LYS:HB3 | 1.87 | 0.74 |
| 2:C:194:VAL:O | 2:C:197:LEU:HD22 | 1.86 | 0.74 |
| 2:C:207:GLY:HA3 | 2:C:239:LEU:HD11 | 1.69 | 0.74 |
| 1:D:1031:GLU:HG3 | 1:D:1031:GLU:O | 1.87 | 0.74 |
| 1:D:1202:ASN:O | 1:D:1203:PRO:C | 2.25 | 0.74 |
| 1:D:220:TRP:CD1 | 1:D:221:TYR:HD2 | 2.05 | 0.74 |
| 1:D:269:HIS:HB3 | 1:D:277:HIS:CD2 | 2.22 | 0.74 |
| 1:D:513:LEU:H | 1:D:570:PRO:CD | 1.99 | 0.74 |
| 1:D:622:TYR:O | 1:D:746:GLY:HA3 | 1.87 | 0.74 |
| 2:F:245:PRO:O | 2:F:248:SER:CB | 2.35 | 0.74 |
| 1:A:247:LEU:HD12 | 1:A:251:THR:CG2 | 2.17 | 0.74 |
| 1:A:448:ALA:O | 1:A:870:VAL:HG11 | 1.87 | 0.74 |
| 2:B:350:LEU:O | 2:B:350:LEU:HD13 | 1.88 | 0.74 |
| 2:C:387:VAL:O | 2:C:420:THR:OG1 | 2.06 | 0.74 |
| 1:D:1014:ARG:CD | 1:D:1026:ARG:NE | 2.50 | 0.74 |
| 1:D:308:GLN:CD | 1:D:1027:LYS:HZ1 | 1.91 | 0.74 |
| 1:D:569:HIS:H | 1:D:570:PRO:CD | 2.01 | 0.74 |
| 1:D:610:PHE:HE1 | 1:D:972:ARG:NH2 | 1.86 | 0.74 |
| 1:D:744:ILE:HB | 1:D:745:PRO:HD3 | 1.70 | 0.74 |
| 2:F:299:LEU:N | 2:F:299:LEU:CD2 | 2.50 | 0.74 |
| 1:A:1026:ARG:N | 1:A:1091:GLU:OE2 | 2.21 | 0.74 |
| 1:A:435:LEU:HD23 | 1:A:879:GLN:OE1 | 1.86 | 0.74 |
| 2:B:236:GLU:HG2 | 2:B:341:ASP:HB2 | 1.69 | 0.74 |
| 2:C:403:PHE:CD1 | 2:C:417:TYR:OH | 2.41 | 0.74 |
| 1:D:1069:ILE:HG12 | 1:D:1070:PRO:HD2 | 1.68 | 0.74 |
| 1:D:80:SER:HB2 | 1:D:125:LEU:HG | 1.69 | 0.74 |
| 1:D:220:TRP:CD1 | 1:D:221:TYR:CD2 | 2.76 | 0.74 |
| 1:D:312:TRP:CZ2 | 1:D:347:TRP:HA | 2.21 | 0.74 |
| 1:D:551:LYS:N | 1:D:551:LYS:CD | 2.30 | 0.74 |
| 1:D:807:ARG:HB2 | 1:D:858:THR:HG23 | 1.69 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:931:LEU:O | 1:D:934:LYS:HD2 | 1.88 | 0.74 |
| 1:D:972:ARG:O | 1:D:974:THR:HG23 | 1.88 | 0.74 |
| 2:E:128:VAL:CG1 | 2:E:210:GLN:HE21 | 1.98 | 0.74 |
| 2:E:432:TYR:HD2 | 2:E:437:ILE:HG12 | 1.53 | 0.74 |
| 2:E:442:LEU:HD12 | 2:E:454:HIS:CE1 | 2.23 | 0.74 |
| 2:F:455:LEU:CB | 2:F:456:ARG:HE | 2.00 | 0.74 |
| 2:F:476:ILE:HD13 | 2:F:477:LYS:N | 2.02 | 0.74 |
| 1:A:297:MET:HG3 | 1:A:298:HIS:N | 2.03 | 0.74 |
| 1:A:452:TYR:N | 1:A:869:ARG:HH21 | 1.86 | 0.74 |
| 1:A:497:GLN:HA | 1:A:516:GLU:CB | 2.18 | 0.74 |
| 1:A:606:THR:OG1 | 1:A:613:HIS:N | 2.21 | 0.74 |
| 1:A:624:VAL:HG11 | 1:A:747:CYS:SG | 2.26 | 0.74 |
| 2:B:311:LEU:CD1 | 2:B:312:LEU:H | 2.00 | 0.74 |
| 1:D:879:GLN:O | 1:D:1189:LEU:HD21 | 1.87 | 0.74 |
| 1:D:209:PRO:O | 1:D:224:CYS:SG | 2.45 | 0.74 |
| 1:D:189:ILE:HG23 | 1:D:258:GLN:HB3 | 1.67 | 0.74 |
| 2:E:373:LYS:HA | 2:E:458:ARG:CZ | 2.17 | 0.74 |
| 2:F:243:THR:OG1 | 2:F:334:CYS:HB2 | 1.87 | 0.74 |
| 2:F:344:ARG:HA | 2:F:347:LEU:HD22 | 1.68 | 0.74 |
| 1:A:903:GLY:HA3 | 1:A:1002:GLU:HB3 | 1.70 | 0.74 |
| 1:A:1014:ARG:HB2 | 1:A:1026:ARG:NH1 | 2.03 | 0.74 |
| 1:A:145:LYS:HG3 | 1:A:1118:TRP:HH2 | 1.51 | 0.74 |
| 1:A:252:GLY:O | 1:A:280:GLU:HB3 | 1.88 | 0.74 |
| 1:A:261:TRP:HE3 | 1:A:261:TRP:HA | 1.52 | 0.74 |
| 1:A:196:VAL:O | 1:A:401:TRP:HH2 | 1.70 | 0.74 |
| 1:A:612:LEU:CB | 1:A:620:TRP:HB2 | 2.17 | 0.74 |
| 1:A:765:PRO:HG2 | 1:A:766:PHE:CD1 | 2.23 | 0.74 |
| 1:A:873:GLU:OE1 | 1:A:875:LYS:CG | 2.36 | 0.74 |
| 2:C:356:LEU:CB | 2:C:359:ASN:HD21 | 2.00 | 0.74 |
| 1:D:1005:VAL:O | 1:D:1009:ASN:N | 2.21 | 0.74 |
| 1:D:101:ARG:HG3 | 1:D:101:ARG:NH1 | 1.91 | 0.74 |
| 1:D:897:TRP:CZ3 | 1:D:1177:VAL:HG11 | 2.22 | 0.74 |
| 1:D:1185:ILE:HD12 | 1:D:1185:ILE:O | 1.87 | 0.74 |
| 1:D:1236:GLN:CB | 1:D:1237:PRO:CD | 2.66 | 0.74 |
| 1:D:189:ILE:HG21 | 1:D:258:GLN:HB3 | 1.70 | 0.74 |
| 1:D:270:ASN:CG | 1:D:294:THR:HG21 | 2.08 | 0.74 |
| 1:D:614:TYR:HE2 | 1:D:620:TRP:CE3 | 2.05 | 0.74 |
| 1:D:842:PRO:HB2 | 1:D:856:GLU:OE2 | 1.88 | 0.74 |
| 2:F:193:TYR:HB2 | 2:F:242:PHE:CE2 | 2.22 | 0.74 |
| 2:F:389:ARG:CG | 2:F:390:GLY:H | 2.00 | 0.74 |
| 2:F:464:GLU:OE2 | 2:F:466:MET:HG2 | 1.87 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:348:LEU:O | 1:A:349:ASP:C | 2.26 | 0.74 |
| 1:A:392:LEU:CD2 | 1:A:395:TYR:HB2 | 2.18 | 0.74 |
| 1:A:85:GLU:OE2 | 1:A:127:LEU:O | 2.05 | 0.74 |
| 2:B:279:GLN:O | 2:B:280:ASP:CB | 2.30 | 0.74 |
| 2:B:110:LEU:HD21 | 2:B:342:LEU:HD21 | 1.70 | 0.74 |
| 2:B:342:LEU:O | 2:B:345:GLY:N | 2.21 | 0.74 |
| 1:A:1209:ARG:NH2 | 2:C:256:LEU:HD23 | 2.03 | 0.74 |
| 1:D:195:LEU:O | 1:D:267:VAL:HA | 1.88 | 0.74 |
| 1:D:452:TYR:CG | 1:D:801:TRP:NE1 | 2.55 | 0.74 |
| 1:D:478:ARG:NE | 1:D:481:GLU:OE1 | 2.21 | 0.74 |
| 1:D:572:TRP:CZ2 | 2:F:470:LYS:HB3 | 2.23 | 0.74 |
| 1:D:913:CYS:O | 1:D:917:GLY:HA3 | 1.88 | 0.74 |
| 2:F:387:VAL:HG23 | 2:F:417:TYR:HA | 1.68 | 0.74 |
| 1:A:1236:GLN:CB | 1:A:1237:PRO:CD | 2.64 | 0.73 |
| 1:A:257:THR:HG23 | 1:A:258:GLN:O | 1.87 | 0.73 |
| 1:A:581:ASP:C | 1:A:583:PRO:HD2 | 2.08 | 0.73 |
| 2:C:197:LEU:HD23 | 2:C:198:ASP:N | 2.03 | 0.73 |
| 2:C:394:GLU:CD | 2:C:394:GLU:H | 1.91 | 0.73 |
| 1:D:360:HIS:O | 1:D:364:VAL:HG22 | 1.88 | 0.73 |
| 1:D:554:GLY:HA2 | 1:D:557:GLU:HG3 | 1.68 | 0.73 |
| 1:D:577:CYS:HB3 | 1:D:578:PRO:HD2 | 1.70 | 0.73 |
| 2:F:344:ARG:N | 2:F:347:LEU:HD13 | 2.03 | 0.73 |
| 1:A:1205:GLY:O | 1:A:1208:ARG:HB3 | 1.88 | 0.73 |
| 1:A:593:SER:HA | 1:A:596:MET:CG | 2.15 | 0.73 |
| 1:A:669:MET:C | 1:A:673:ALA:HB2 | 2.09 | 0.73 |
| 1:A:815:TRP:CA | 1:A:838:GLY:HA3 | 2.17 | 0.73 |
| 1:A:87:ILE:HG22 | 1:A:88:PHE:H | 1.48 | 0.73 |
| 2:C:290:TYR:HA | 2:C:298:GLU:O | 1.88 | 0.73 |
| 2:C:323:HIS:O | 2:C:333:PRO:HD3 | 1.88 | 0.73 |
| 1:D:1072:THR:HG21 | 1:D:1134:HIS:CE1 | 2.23 | 0.73 |
| 1:D:1142:ARG:O | 1:D:1144:GLU:O | 2.06 | 0.73 |
| 1:D:556:THR:OG1 | 2:F:452:LEU:HD22 | 1.88 | 0.73 |
| 1:D:926:SER:HB2 | 1:D:930:ASP:CB | 2.17 | 0.73 |
| 2:E:428:LEU:HD13 | 2:E:428:LEU:N | 2.02 | 0.73 |
| 2:F:432:TYR:HB3 | 2:F:437:ILE:HD11 | 1.70 | 0.73 |
| 1:A:1024:ASP:HA | 1:A:1026:ARG:NH1 | 2.03 | 0.73 |
| 1:A:887:VAL:HG22 | 1:A:1146:ARG:HH11 | 1.51 | 0.73 |
| 1:A:503:VAL:HB | 1:A:521:PRO:CA | 2.16 | 0.73 |
| 1:A:845:VAL:HB | 1:A:855:VAL:CG2 | 2.19 | 0.73 |
| 2:B:306:LEU:C | 2:B:308:ASP:H | 1.91 | 0.73 |
| 2:C:192:HIS:O | 2:C:196:CYS:SG | 2.46 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:200:VAL:HG11 | 2:C:204:LEU:HD13 | 1.70 | 0.73 |
| 2:C:301:GLU:HG2 | 2:C:339:ASN:HB3 | 1.70 | 0.73 |
| 1:D:1005:VAL:HA | 1:D:1008:LEU:HD12 | 1.68 | 0.73 |
| 2:E:93:SER:C | 2:E:95:CYS:H | 1.90 | 0.73 |
| 2:F:115:TRP:CH2 | 2:F:210:GLN:HG2 | 2.22 | 0.73 |
| 2:F:431:LYS:HE2 | 2:F:435:MET:HB2 | 1.70 | 0.73 |
| 1:A:1200:PRO:O | 1:A:1204:THR:OG1 | 2.06 | 0.73 |
| 1:A:205:GLU:HA | 1:A:205:GLU:OE1 | 1.87 | 0.73 |
| 1:A:739:TYR:HA | 1:A:742:VAL:HB | 1.71 | 0.73 |
| 1:A:904:ASP:C | 1:A:910:MET:HA | 2.08 | 0.73 |
| 1:A:933:SER:HB2 | 1:A:943:ARG:NE | 2.03 | 0.73 |
| 2:B:123:GLU:HB2 | 2:C:403:PHE:HZ | 1.53 | 0.73 |
| 2:B:396:ARG:HD2 | 2:B:418:LEU:H | 1.52 | 0.73 |
| 2:C:300:ILE:HA | 2:C:342:LEU:HD12 | 1.69 | 0.73 |
| 1:D:888:GLY:HA3 | 1:D:1138:ARG:HA | 1.70 | 0.73 |
| 1:D:271:VAL:O | 1:D:274:ASP:HB2 | 1.88 | 0.73 |
| 1:D:293:ASP:CG | 1:D:296:SER:HB2 | 2.08 | 0.73 |
| 1:D:805:HIS:O | 1:D:809:SER:N | 2.20 | 0.73 |
| 1:D:992:LEU:HD12 | 1:D:993:ARG:H | 1.52 | 0.73 |
| 2:F:247:THR:CB | 2:F:251:TRP:CD1 | 2.67 | 0.73 |
| 2:F:353:SER:HB3 | 2:F:373:LYS:O | 1.88 | 0.73 |
| 1:A:897:TRP:HZ3 | 1:A:1108:TYR:CE1 | 2.07 | 0.73 |
| 1:A:1160:THR:HG22 | 1:A:1164:PHE:HE1 | 1.51 | 0.73 |
| 1:A:297:MET:HG3 | 1:A:298:HIS:H | 1.52 | 0.73 |
| 1:A:498:LYS:HZ2 | 1:A:519:GLY:H | 1.35 | 0.73 |
| 1:A:500:ALA:HB1 | 1:A:520:ALA:HB3 | 1.70 | 0.73 |
| 1:D:1069:ILE:HG23 | 1:D:1070:PRO:N | 2.02 | 0.73 |
| 1:D:86:GLN:NE2 | 1:D:132:GLY:N | 2.34 | 0.73 |
| 1:D:179:GLY:CA | 1:D:182:GLY:CA | 2.65 | 0.73 |
| 1:D:369:LEU:O | 1:D:371:LYS:O | 2.05 | 0.73 |
| 1:D:598:VAL:CA | 1:D:601:LYS:HE2 | 2.16 | 0.73 |
| 1:D:658:LYS:CE | 1:D:713:PRO:HB2 | 2.19 | 0.73 |
| 1:D:891:VAL:O | 1:D:894:GLN:HG2 | 1.88 | 0.73 |
| 1:D:996:ARG:N | 1:D:996:ARG:NE | 2.36 | 0.73 |
| 2:E:117:SER:HA | 2:E:121:PHE:CD1 | 2.24 | 0.73 |
| 2:E:383:VAL:O | 2:E:384:ALA:HB3 | 1.87 | 0.73 |
| 1:A:145:LYS:O | 1:A:149:PRO:HD2 | 1.88 | 0.73 |
| 1:A:166:PRO:HG3 | 1:A:398:GLN:CD | 2.08 | 0.73 |
| 1:A:278:ILE:HG12 | 1:A:291:PHE:CE1 | 2.22 | 0.73 |
| 1:A:386:ARG:HD3 | 1:A:387:GLU:H | 1.53 | 0.73 |
| 1:A:712:VAL:O | 1:A:719:LEU:HD22 | 1.88 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:868:ASP:O | 1:A:869:ARG:HB2 | 1.88 | 0.73 |
| 1:A:875:LYS:C | 1:A:878:VAL:HG23 | 2.09 | 0.73 |
| 1:A:87:ILE:CG2 | 1:A:88:PHE:H | 2.01 | 0.73 |
| 2:B:128:VAL:HB | 2:B:208:LEU:HB2 | 1.70 | 0.73 |
| 2:C:267:ALA:HB3 | 2:C:270:PRO:HB3 | 1.70 | 0.73 |
| 2:C:363:ARG:HH11 | 2:C:363:ARG:CA | 1.99 | 0.73 |
| 1:D:429:GLU:HG3 | 1:D:1128:ARG:CZ | 2.18 | 0.73 |
| 1:D:474:LEU:N | 1:D:474:LEU:HD12 | 2.02 | 0.73 |
| 1:D:546:ARG:HH21 | 2:F:404:ASN:CB | 1.95 | 0.73 |
| 1:D:546:ARG:O | 1:D:551:LYS:NZ | 2.19 | 0.73 |
| 1:D:618:HIS:NE2 | 1:D:761:ASN:HB3 | 2.02 | 0.73 |
| 1:D:761:ASN:O | 1:D:763:GLY:N | 2.21 | 0.73 |
| 1:D:989:THR:CA | 1:D:998:SER:OG | 2.34 | 0.73 |
| 1:D:993:ARG:CA | 1:D:996:ARG:HD2 | 2.19 | 0.73 |
| 2:E:102:LEU:HD13 | 2:E:102:LEU:C | 2.09 | 0.73 |
| 2:F:202:LYS:O | 2:F:325:ARG:HG2 | 1.88 | 0.73 |
| 1:A:1109:LEU:O | 1:A:1112:MET:HG3 | 1.89 | 0.73 |
| 1:A:273:PHE:C | 1:A:276:ALA:H | 1.92 | 0.73 |
| 1:A:600:PRO:C | 1:A:602:LEU:O | 2.27 | 0.73 |
| 1:A:634:LEU:HD12 | 1:A:638:THR:CB | 2.19 | 0.73 |
| 2:B:75:ARG:HD2 | 2:B:434:GLU:OE2 | 1.87 | 0.73 |
| 2:C:347:LEU:CA | 2:C:350:LEU:HD11 | 2.18 | 0.73 |
| 1:D:410:GLN:O | 1:D:412:PRO:HD2 | 1.88 | 0.73 |
| 1:A:1029:GLN:C | 1:A:1031:GLU:O | 2.26 | 0.73 |
| 1:A:1131:ILE:HG21 | 1:A:1137:VAL:CA | 2.19 | 0.73 |
| 1:A:259:ARG:HA | 1:A:259:ARG:NE | 2.04 | 0.73 |
| 1:A:439:GLN:CG | 1:A:835:GLY:HA3 | 2.17 | 0.73 |
| 2:C:347:LEU:HA | 2:C:350:LEU:HD11 | 1.69 | 0.73 |
| 2:C:356:LEU:O | 2:C:370:LYS:HE2 | 1.88 | 0.73 |
| 1:D:495:PHE:HB2 | 1:D:573:TYR:CE1 | 2.23 | 0.73 |
| 1:D:515:ILE:CD1 | 1:D:568:GLY:O | 2.37 | 0.73 |
| 1:D:645:VAL:O | 1:D:650:ARG:HB3 | 1.88 | 0.73 |
| 2:E:218:VAL:H | 2:E:231:ILE:HA | 1.53 | 0.73 |
| 2:E:272:ASN:HA | 2:E:292:ASN:ND2 | 2.04 | 0.73 |
| 2:F:452:LEU:O | 2:F:453:ILE:HG13 | 1.88 | 0.73 |
| 1:A:1118:TRP:O | 1:A:1122:GLU:HG2 | 1.89 | 0.73 |
| 1:A:219:ALA:O | 1:A:220:TRP:CE3 | 2.41 | 0.73 |
| 1:A:79:LEU:CD1 | 1:A:89:GLY:O | 2.37 | 0.73 |
| 2:B:99:PHE:CD2 | 2:C:129:ASP:OD2 | 2.42 | 0.73 |
| 1:A:1208:ARG:NH2 | 2:C:277:ASP:CG | 2.42 | 0.73 |
| 2:C:398:VAL:HA | 2:C:401:GLY:HA3 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:463:LYS:O | 2:C:465:MET:HE2 | 1.88 | 0.73 |
| 1:D:308:GLN:OE1 | 1:D:1027:LYS:NZ | 2.21 | 0.73 |
| 1:D:1138:ARG:NH2 | 1:D:1191:LYS:CE | 2.51 | 0.73 |
| 1:D:779:LEU:C | 1:D:779:LEU:HD22 | 2.09 | 0.73 |
| 1:D:948:ILE:CG2 | 1:D:1071:ARG:HB2 | 2.19 | 0.73 |
| 1:A:241:PRO:HA | 1:A:244:LEU:CG | 2.18 | 0.73 |
| 1:A:436:PRO:CB | 1:A:881:PRO:HD3 | 2.08 | 0.73 |
| 1:A:930:ASP:HA | 1:A:933:SER:HB3 | 1.70 | 0.73 |
| 2:B:304:TRP:CE3 | 2:B:304:TRP:HA | 2.24 | 0.73 |
| 2:B:400:GLN:NE2 | 2:B:417:TYR:CG | 2.55 | 0.73 |
| 2:C:342:LEU:HB2 | 2:C:344:ARG:HD3 | 1.70 | 0.73 |
| 1:D:1195:MET:HB3 | 1:D:1196:ASP:O | 1.89 | 0.73 |
| 1:D:257:THR:OG1 | 1:D:281:GLN:NE2 | 2.21 | 0.73 |
| 1:D:278:ILE:O | 1:D:282:TYR:HD1 | 1.72 | 0.73 |
| 1:D:432:VAL:CG1 | 1:D:1128:ARG:HE | 1.99 | 0.73 |
| 1:D:81:ARG:HG2 | 1:D:125:LEU:O | 1.88 | 0.73 |
| 2:E:377:CYS:SG | 2:E:378:LEU:CD1 | 2.77 | 0.73 |
| 2:F:473:ASP:CA | 2:F:476:ILE:HG23 | 2.17 | 0.73 |
| 1:A:1165:ALA:O | 1:A:1170:LEU:N | 2.22 | 0.72 |
| 1:A:223:TRP:H | 1:A:223:TRP:HD1 | 1.32 | 0.72 |
| 1:A:821:LEU:HD12 | 1:A:825:VAL:HB | 1.69 | 0.72 |
| 1:D:1151:LEU:HD23 | 1:D:1223:ILE:HD11 | 1.71 | 0.72 |
| 1:D:547:ALA:O | 1:D:551:LYS:HG2 | 1.89 | 0.72 |
| 1:D:918:TRP:C | 1:D:920:THR:N | 2.41 | 0.72 |
| 2:E:431:LYS:C | 2:E:433:ASP:N | 2.38 | 0.72 |
| 2:E:76:ARG:HG3 | 2:E:435:MET:SD | 2.29 | 0.72 |
| 2:F:342:LEU:O | 2:F:342:LEU:HD22 | 1.88 | 0.72 |
| 1:A:449:GLN:HA | 1:A:452:TYR:CE1 | 2.24 | 0.72 |
| 1:A:580:LEU:HD12 | 1:A:581:ASP:N | 2.04 | 0.72 |
| 1:A:616:GLU:HG2 | 1:A:724:GLY:HA3 | 1.71 | 0.72 |
| 1:A:615:SER:HB3 | 1:A:725:PRO:HB3 | 1.69 | 0.72 |
| 2:B:324:GLY:N | 2:B:333:PRO:HD3 | 2.03 | 0.72 |
| 2:B:99:PHE:HE2 | 2:C:131:LEU:HD11 | 1.54 | 0.72 |
| 1:A:1209:ARG:HH22 | 2:C:256:LEU:HD23 | 1.54 | 0.72 |
| 1:A:784:GLY:N | 2:C:363:ARG:HD3 | 2.02 | 0.72 |
| 1:D:1113:LEU:N | 1:D:1113:LEU:HD23 | 2.04 | 0.72 |
| 1:D:897:TRP:HH2 | 1:D:1173:LEU:HD13 | 1.50 | 0.72 |
| 2:F:403:PHE:HD1 | 2:F:417:TYR:HH | 1.32 | 0.72 |
| 2:F:416:GLY:O | 2:F:419:GLU:HB3 | 1.88 | 0.72 |
| 2:F:424:SER:HB3 | 2:F:427:GLN:NE2 | 2.03 | 0.72 |
| 1:A:1026:ARG:O | 1:A:1030:ARG:CB | 2.37 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1193:VAL:HG23 | 1:A:1194:THR:N | 2.03 | 0.72 |
| 1:A:247:LEU:HD12 | 1:A:251:THR:HG21 | 1.71 | 0.72 |
| 1:A:913:CYS:N | 1:A:917:GLY:HA3 | 2.03 | 0.72 |
| 2:B:114:TRP:CA | 2:B:262:TRP:CZ2 | 2.71 | 0.72 |
| 1:D:239:LEU:HB3 | 1:D:242:ALA:HB3 | 1.72 | 0.72 |
| 1:D:242:ALA:CA | 1:D:245:ILE:HG12 | 2.17 | 0.72 |
| 1:D:453:GLU:O | 1:D:457:ARG:HG2 | 1.90 | 0.72 |
| 1:D:670:PRO:HB2 | 1:D:672:GLU:O | 1.89 | 0.72 |
| 1:D:735:GLY:CA | 1:D:749:PHE:HB3 | 2.18 | 0.72 |
| 2:E:115:TRP:HZ3 | 2:E:210:GLN:HA | 1.54 | 0.72 |
| 2:E:122:ARG:HD2 | 2:E:122:ARG:H | 1.54 | 0.72 |
| 2:E:213:VAL:HG13 | 2:E:235:THR:CG2 | 2.18 | 0.72 |
| 2:F:120:VAL:HG23 | 2:F:121:PHE:N | 2.03 | 0.72 |
| 1:D:553:LYS:HD3 | 2:F:468:ILE:HG22 | 1.70 | 0.72 |
| 1:A:1131:ILE:HD11 | 1:A:1133:ILE:CG2 | 2.18 | 0.72 |
| 1:A:652:ILE:C | 1:A:655:LEU:HG | 2.09 | 0.72 |
| 1:A:73:PRO:O | 1:A:74:LEU:HD13 | 1.90 | 0.72 |
| 1:A:87:ILE:CG2 | 1:A:88:PHE:N | 2.51 | 0.72 |
| 2:B:304:TRP:HE3 | 2:B:304:TRP:HA | 1.54 | 0.72 |
| 2:C:325:ARG:HG3 | 2:C:325:ARG:NH1 | 1.99 | 0.72 |
| 1:D:115:GLN:HE22 | 1:D:924:ARG:NH1 | 1.86 | 0.72 |
| 1:D:633:LYS:HB2 | 1:D:638:THR:HG21 | 1.70 | 0.72 |
| 2:F:77:HIS:O | 2:F:100:GLY:HA3 | 1.89 | 0.72 |
| 2:F:186:LEU:HD23 | 2:F:187:HIS:N | 2.03 | 0.72 |
| 2:F:342:LEU:O | 2:F:342:LEU:CD2 | 2.37 | 0.72 |
| 2:F:402:LEU:HG | 2:F:472:LYS:NZ | 2.03 | 0.72 |
| 1:A:1002:GLU:HG3 | 1:A:1003:TRP:CE3 | 2.24 | 0.72 |
| 1:A:1068:ASP:C | 1:A:1070:PRO:HD3 | 2.10 | 0.72 |
| 1:A:87:ILE:HG21 | 1:A:1166:TYR:OH | 1.89 | 0.72 |
| 1:A:1179:PHE:CB | 1:A:1220:ILE:HG12 | 2.19 | 0.72 |
| 1:A:451:THR:HG21 | 1:A:1202:ASN:HB3 | 1.72 | 0.72 |
| 1:A:80:SER:OG | 1:A:125:LEU:HD11 | 1.89 | 0.72 |
| 1:A:175:TRP:HB2 | 1:A:184:ALA:C | 2.10 | 0.72 |
| 1:A:175:TRP:N | 1:A:186:PRO:HB3 | 2.03 | 0.72 |
| 1:A:566:LEU:HB3 | 1:A:567:PRO:CD | 2.19 | 0.72 |
| 1:A:615:SER:HB2 | 1:A:725:PRO:CB | 2.19 | 0.72 |
| 1:A:753:PRO:HD2 | 1:A:770:PHE:CG | 2.23 | 0.72 |
| 1:A:873:GLU:HB3 | 1:A:875:LYS:HG3 | 1.70 | 0.72 |
| 1:D:1000:GLU:O | 1:D:1004:LEU:HD13 | 1.88 | 0.72 |
| 1:D:1005:VAL:CA | 1:D:1008:LEU:HD13 | 2.15 | 0.72 |
| 1:D:429:GLU:HG2 | 1:D:1117:LYS:HE2 | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1126:ASP:OD2 | 1:D:1145:ASP:HB3 | 1.89 | 0.72 |
| 1:D:283:LEU:CD2 | 1:D:839:ALA:HB3 | 2.18 | 0.72 |
| 1:D:269:HIS:NE2 | 1:D:291:PHE:HD2 | 1.88 | 0.72 |
| 1:D:443:ARG:HG2 | 1:D:443:ARG:HH11 | 1.55 | 0.72 |
| 1:D:597:ARG:O | 1:D:599:THR:N | 2.22 | 0.72 |
| 1:D:600:PRO:HG2 | 1:D:616:GLU:HB3 | 1.72 | 0.72 |
| 1:D:657:ARG:O | 1:D:660:CYS:HB3 | 1.89 | 0.72 |
| 1:D:997:LEU:CD2 | 1:D:998:SER:H | 2.02 | 0.72 |
| 2:E:307:GLY:HA2 | 2:E:334:CYS:HB3 | 1.71 | 0.72 |
| 2:F:403:PHE:CD1 | 2:F:417:TYR:OH | 2.43 | 0.72 |
| 2:F:485:VAL:OXT | 2:F:485:VAL:CG2 | 2.38 | 0.72 |
| 1:A:1020:ILE:CD1 | 1:A:1021:SER:H | 2.02 | 0.72 |
| 2:B:78:PHE:HE1 | 2:B:103:GLY:HA2 | 1.52 | 0.72 |
| 2:C:247:THR:CB | 2:C:251:TRP:CD1 | 2.71 | 0.72 |
| 2:C:356:LEU:CB | 2:C:359:ASN:ND2 | 2.39 | 0.72 |
| 2:B:199:LEU:HD23 | 2:C:77:HIS:HD2 | 1.53 | 0.72 |
| 1:D:907:PHE:HZ | 1:D:1002:GLU:HB3 | 1.53 | 0.72 |
| 1:D:513:LEU:O | 1:D:568:GLY:CA | 2.38 | 0.72 |
| 1:D:943:ARG:O | 1:D:946:ALA:HB3 | 1.90 | 0.72 |
| 1:D:1209:ARG:NH2 | 2:F:256:LEU:HD22 | 2.05 | 0.72 |
| 1:A:439:GLN:HG3 | 1:A:836:LEU:N | 2.04 | 0.72 |
| 1:A:618:HIS:HA | 1:A:762:VAL:HG21 | 1.72 | 0.72 |
| 1:A:621:GLY:N | 1:A:748:TRP:HB3 | 2.03 | 0.72 |
| 1:A:786:ALA:O | 1:A:789:PRO:HD2 | 1.90 | 0.72 |
| 2:B:469:SER:C | 2:B:471:LEU:H | 1.91 | 0.72 |
| 2:C:303:LEU:N | 2:C:303:LEU:HD12 | 2.05 | 0.72 |
| 2:C:355:GLN:O | 2:C:357:THR:N | 2.22 | 0.72 |
| 2:C:375:HIS:N | 2:C:378:LEU:HD22 | 2.00 | 0.72 |
| 2:C:394:GLU:CD | 2:C:394:GLU:N | 2.43 | 0.72 |
| 2:C:485:VAL:CG2 | 2:C:485:VAL:OXT | 2.38 | 0.72 |
| 1:D:1113:LEU:HD23 | 1:D:1113:LEU:H | 1.54 | 0.72 |
| 1:D:389:PHE:CD1 | 1:D:390:GLN:N | 2.57 | 0.72 |
| 1:D:452:TYR:CB | 1:D:801:TRP:NE1 | 2.48 | 0.72 |
| 1:D:599:THR:HB | 1:D:600:PRO:HD3 | 1.72 | 0.72 |
| 1:D:656:TYR:HB3 | 1:D:744:ILE:HD12 | 1.70 | 0.72 |
| 2:E:114:TRP:CH2 | 2:E:238:SER:O | 2.42 | 0.72 |
| 2:E:448:LEU:C | 2:E:448:LEU:HD23 | 2.09 | 0.72 |
| 1:A:879:GLN:HG2 | 1:A:1189:LEU:HD21 | 1.72 | 0.72 |
| 1:A:228:LEU:HD11 | 1:A:386:ARG:HB3 | 1.70 | 0.72 |
| 1:A:286:GLY:N | 1:A:1128:ARG:NH2 | 2.37 | 0.72 |
| 1:A:436:PRO:CG | 1:A:879:GLN:HB3 | 2.19 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:503:VAL:HG11 | 1:A:521:PRO:N | 2.04 | 0.72 |
| 1:A:539:PHE:O | 1:A:540:GLN:HG2 | 1.88 | 0.72 |
| 1:A:634:LEU:HB3 | 1:A:635:PRO:CA | 2.19 | 0.72 |
| 1:A:658:LYS:CG | 1:A:713:PRO:HB2 | 2.17 | 0.72 |
| 1:A:613:HIS:HB3 | 1:A:717:LEU:CD2 | 2.19 | 0.72 |
| 1:A:739:TYR:C | 1:A:741:ASP:H | 1.92 | 0.72 |
| 1:A:913:CYS:O | 1:A:918:TRP:N | 2.20 | 0.72 |
| 2:B:299:LEU:HD21 | 2:B:302:THR:HG23 | 1.72 | 0.72 |
| 2:B:67:GLU:HB2 | 2:B:88:ARG:NH1 | 2.03 | 0.72 |
| 2:C:272:ASN:HB3 | 2:C:292:ASN:HB2 | 1.72 | 0.72 |
| 2:C:243:THR:O | 2:C:334:CYS:N | 2.22 | 0.72 |
| 1:D:1116:MET:SD | 1:D:1153:LEU:HD22 | 2.30 | 0.72 |
| 1:D:177:ARG:NE | 1:D:216:SER:H | 1.87 | 0.72 |
| 1:D:265:LEU:HD21 | 1:D:267:VAL:HA | 1.72 | 0.72 |
| 1:D:421:PRO:O | 1:D:425:ALA:HB3 | 1.90 | 0.72 |
| 1:D:620:TRP:NE1 | 1:D:751:LYS:HB2 | 2.04 | 0.72 |
| 1:D:795:ASN:HA | 1:D:798:ILE:CD1 | 2.20 | 0.72 |
| 1:D:967:MET:HA | 1:D:967:MET:HE3 | 1.72 | 0.72 |
| 2:F:114:TRP:NE1 | 2:F:259:ARG:NH1 | 2.36 | 0.72 |
| 2:F:209:ALA:CB | 2:F:238:SER:O | 2.38 | 0.72 |
| 2:F:305:ASN:HA | 2:F:335:VAL:CG1 | 2.19 | 0.72 |
| 2:F:357:THR:O | 2:F:358:GLU:HG2 | 1.90 | 0.72 |
| 2:F:423:SER:HB2 | 2:F:427:GLN:OE1 | 1.90 | 0.72 |
| 1:A:1113:LEU:HD23 | 1:A:1113:LEU:N | 2.05 | 0.72 |
| 1:A:410:GLN:O | 1:A:414:PHE:CD2 | 2.43 | 0.72 |
| 1:A:618:HIS:CE1 | 1:A:761:ASN:HD22 | 2.08 | 0.72 |
| 1:A:918:TRP:O | 1:A:920:THR:HG22 | 1.90 | 0.72 |
| 2:B:468:ILE:O | 2:B:468:ILE:HG23 | 1.89 | 0.72 |
| 2:C:454:HIS:HB3 | 2:C:466:MET:O | 1.89 | 0.72 |
| 1:D:1014:ARG:CD | 1:D:1026:ARG:HE | 2.02 | 0.72 |
| 1:D:368:PRO:CA | 1:D:369:LEU:HD23 | 2.19 | 0.72 |
| 1:D:550:GLN:CB | 1:D:551:LYS:HE3 | 2.19 | 0.72 |
| 1:D:623:LEU:HB3 | 1:D:667:GLN:CD | 2.10 | 0.72 |
| 1:D:726:LYS:O | 1:D:727:ASP:CG | 2.28 | 0.72 |
| 1:D:959:GLN:CB | 1:D:960:PRO:CD | 2.67 | 0.72 |
| 2:E:382:LYS:CG | 2:E:383:VAL:N | 2.47 | 0.72 |
| 2:F:360:SER:HB3 | 2:F:364:LYS:HD2 | 1.72 | 0.72 |
| 2:E:203:ARG:NH1 | 2:F:418:LEU:HD22 | 1.99 | 0.72 |
| 1:A:1056:GLU:HA | 1:A:1059:ASN:HD21 | 1.52 | 0.72 |
| 1:A:955:TYR:CD2 | 1:A:1098:ASN:OD1 | 2.42 | 0.72 |
| 1:A:887:VAL:CG2 | 1:A:1146:ARG:NH1 | 2.51 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1170:LEU:O | 1:A:1170:LEU:HD13 | 1.87 | 0.72 |
| 1:A:402:ALA:C | 1:A:406:VAL:HG13 | 2.10 | 0.72 |
| 1:A:866:ARG:HD3 | 1:A:866:ARG:O | 1.89 | 0.72 |
| 1:A:893:SER:HB2 | 1:A:896:LEU:HD23 | 1.71 | 0.72 |
| 2:B:131:LEU:C | 2:B:182:ARG:HH21 | 1.94 | 0.72 |
| 2:B:403:PHE:CE1 | 2:B:415:PRO:HD3 | 2.24 | 0.72 |
| 2:B:371:VAL:CA | 2:B:433:ASP:HB3 | 2.04 | 0.72 |
| 2:C:180:LYS:O | 2:C:181:LEU:HD23 | 1.88 | 0.72 |
| 2:C:186:LEU:HD23 | 2:C:187:HIS:N | 2.05 | 0.72 |
| 2:C:374:LEU:CD1 | 2:C:379:ALA:HA | 2.19 | 0.72 |
| 1:D:1006:ARG:NH2 | 1:D:1010:LEU:HD11 | 2.05 | 0.72 |
| 1:D:371:LYS:HG3 | 1:D:396:CYS:CA | 2.19 | 0.72 |
| 1:D:719:LEU:HG | 1:D:720:THR:H | 1.55 | 0.72 |
| 2:E:79:LEU:HA | 2:E:100:GLY:H | 1.55 | 0.72 |
| 2:E:255:TRP:CE3 | 2:E:255:TRP:HA | 2.23 | 0.72 |
| 2:E:391:PRO:HG2 | 2:E:395:LEU:H | 1.54 | 0.72 |
| 2:E:423:SER:O | 2:E:424:SER:HB3 | 1.89 | 0.72 |
| 2:F:342:LEU:HB2 | 2:F:344:ARG:CD | 2.20 | 0.72 |
| 1:A:1187:ARG:NH2 | 1:A:1212:ILE:O | 2.23 | 0.71 |
| 1:A:452:TYR:N | 1:A:869:ARG:NH2 | 2.37 | 0.71 |
| 1:A:955:TYR:CE2 | 1:A:1102:GLN:NE2 | 2.58 | 0.71 |
| 1:A:955:TYR:HD2 | 1:A:1098:ASN:OD1 | 1.72 | 0.71 |
| 2:B:234:LYS:O | 2:B:236:GLU:HG3 | 1.89 | 0.71 |
| 2:C:344:ARG:HA | 2:C:347:LEU:CG | 2.20 | 0.71 |
| 2:C:372:LEU:HD21 | 2:C:436:SER:HB2 | 1.72 | 0.71 |
| 2:C:383:VAL:HG23 | 2:C:439:PHE:O | 1.89 | 0.71 |
| 2:C:430:SER:O | 2:C:434:GLU:CG | 2.37 | 0.71 |
| 2:C:92:LEU:HD21 | 2:C:344:ARG:HE | 1.55 | 0.71 |
| 1:D:1015:THR:HG23 | 1:D:1026:ARG:HB2 | 1.70 | 0.71 |
| 1:D:884:TYR:OH | 1:D:1142:ARG:NH1 | 2.23 | 0.71 |
| 1:D:865:ALA:CB | 1:D:1197:CYS:SG | 2.78 | 0.71 |
| 1:D:744:ILE:HG12 | 1:D:745:PRO:CD | 2.20 | 0.71 |
| 1:D:275:ARG:CZ | 1:D:843:GLN:H | 2.01 | 0.71 |
| 1:D:960:PRO:HA | 1:D:963:GLU:CG | 2.19 | 0.71 |
| 1:D:976:GLN:O | 1:D:980:GLU:HG3 | 1.89 | 0.71 |
| 2:F:127:PRO:CD | 2:F:128:VAL:N | 2.48 | 0.71 |
| 2:F:185:LEU:HD12 | 2:F:236:GLU:HB2 | 1.72 | 0.71 |
| 2:F:402:LEU:O | 2:F:406:LEU:HD13 | 1.89 | 0.71 |
| 1:A:515:ILE:HG22 | 1:A:516:GLU:N | 2.04 | 0.71 |
| 1:A:564:GLN:N | 1:A:564:GLN:HE21 | 1.87 | 0.71 |
| 1:A:73:PRO:C | 1:A:74:LEU:HD22 | 2.09 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:277:ASP:CG | 2:B:287:ASN:HD21 | 1.93 | 0.71 |
| 2:B:475:LEU:O | 2:B:479:ILE:N | 2.19 | 0.71 |
| 2:C:78:PHE:C | 2:C:100:GLY:H | 1.93 | 0.71 |
| 2:C:476:ILE:HD13 | 2:C:477:LYS:N | 2.03 | 0.71 |
| 1:D:145:LYS:O | 1:D:149:PRO:CD | 2.37 | 0.71 |
| 1:D:281:GLN:HE21 | 1:D:287:SER:CB | 2.03 | 0.71 |
| 1:D:845:VAL:HB | 1:D:855:VAL:CG2 | 2.20 | 0.71 |
| 1:D:865:ALA:HA | 1:D:872:SER:CA | 2.20 | 0.71 |
| 2:E:336:LEU:HD23 | 2:E:337:SER:H | 1.54 | 0.71 |
| 2:E:350:LEU:HD23 | 2:E:350:LEU:O | 1.90 | 0.71 |
| 2:E:431:LYS:O | 2:E:433:ASP:N | 2.23 | 0.71 |
| 2:F:458:ARG:NE | 2:F:459:ASP:O | 2.20 | 0.71 |
| 1:A:1025:LEU:O | 1:A:1026:ARG:HG3 | 1.89 | 0.71 |
| 1:A:129:PRO:O | 1:A:131:TYR:CZ | 2.44 | 0.71 |
| 1:A:157:LEU:HD11 | 1:A:195:LEU:HA | 1.70 | 0.71 |
| 1:A:389:PHE:CD1 | 1:A:390:GLN:N | 2.58 | 0.71 |
| 2:B:122:ARG:HB2 | 2:B:124:GLN:HE21 | 1.55 | 0.71 |
| 2:B:199:LEU:HD13 | 2:B:200:VAL:HG13 | 1.70 | 0.71 |
| 2:B:417:TYR:O | 2:B:419:GLU:N | 2.22 | 0.71 |
| 2:B:213:VAL:HG11 | 2:C:132:HIS:CE1 | 2.25 | 0.71 |
| 1:D:1027:LYS:HB2 | 1:D:1096:ARG:HG3 | 1.70 | 0.71 |
| 1:D:626:GLY:O | 1:D:627:ARG:HB3 | 1.89 | 0.71 |
| 1:D:279:ARG:HH21 | 1:D:844:VAL:CG2 | 2.02 | 0.71 |
| 2:F:354:PHE:CZ | 2:F:370:LYS:HD3 | 2.25 | 0.71 |
| 1:A:1040:LYS:HB3 | 1:A:1044:VAL:HG11 | 1.72 | 0.71 |
| 1:A:444:TYR:CE1 | 1:A:1206:MET:SD | 2.83 | 0.71 |
| 1:A:612:LEU:CD2 | 1:A:620:TRP:HA | 2.20 | 0.71 |
| 1:A:753:PRO:HB2 | 1:A:770:PHE:CZ | 2.24 | 0.71 |
| 1:A:897:TRP:HE1 | 1:A:901:VAL:HG13 | 1.54 | 0.71 |
| 2:B:78:PHE:O | 2:B:79:LEU:HB2 | 1.89 | 0.71 |
| 1:D:1108:TYR:HA | 1:D:1164:PHE:CE1 | 2.25 | 0.71 |
| 1:D:260:ASP:OD2 | 1:D:261:TRP:CE2 | 2.44 | 0.71 |
| 1:D:367:PRO:CD | 1:D:368:PRO:CD | 2.54 | 0.71 |
| 1:D:457:ARG:CB | 1:D:457:ARG:HH11 | 2.04 | 0.71 |
| 1:D:714:GLY:O | 1:D:716:PRO:HD3 | 1.89 | 0.71 |
| 2:F:115:TRP:HH2 | 2:F:210:GLN:HG2 | 1.53 | 0.71 |
| 1:A:1141:VAL:HG12 | 1:A:1142:ARG:O | 1.91 | 0.71 |
| 1:A:348:LEU:HD13 | 1:A:350:ILE:HD13 | 1.72 | 0.71 |
| 1:A:476:GLY:CA | 1:A:711:ALA:HB1 | 2.19 | 0.71 |
| 2:B:308:ASP:HB3 | 2:B:309:HIS:CE1 | 2.25 | 0.71 |
| 2:C:317:GLY:HA3 | 2:C:320:SER:CB | 2.19 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:396:ARG:HH11 | 2:C:397:GLN:CA | 2.02 | 0.71 |
| 1:D:1008:LEU:O | 1:D:1012:VAL:HG22 | 1.89 | 0.71 |
| 1:D:415:LEU:C | 1:D:417:ARG:H | 1.93 | 0.71 |
| 1:D:474:LEU:H | 1:D:474:LEU:HD12 | 1.55 | 0.71 |
| 2:F:254:PHE:HE2 | 2:F:255:TRP:CE2 | 2.09 | 0.71 |
| 2:F:354:PHE:HE1 | 2:F:370:LYS:HB3 | 1.55 | 0.71 |
| 1:A:1019:TRP:HD1 | 1:A:1020:ILE:HG22 | 1.55 | 0.71 |
| 1:A:605:LEU:HA | 1:A:781:ALA:CB | 2.20 | 0.71 |
| 1:A:623:LEU:HD22 | 1:A:667:GLN:OE1 | 1.90 | 0.71 |
| 1:A:80:SER:OG | 1:A:125:LEU:HD21 | 1.90 | 0.71 |
| 2:C:242:PHE:HA | 2:C:334:CYS:O | 1.91 | 0.71 |
| 2:C:317:GLY:HA2 | 2:C:320:SER:HB2 | 1.73 | 0.71 |
| 2:C:468:ILE:HG13 | 2:C:472:LYS:HE3 | 1.72 | 0.71 |
| 1:D:1186:ASP:OD1 | 1:D:1187:ARG:N | 2.23 | 0.71 |
| 1:D:739:TYR:CG | 1:D:740:ASN:N | 2.59 | 0.71 |
| 2:E:441:VAL:HG12 | 2:E:442:LEU:N | 2.06 | 0.71 |
| 2:F:131:LEU:C | 2:F:182:ARG:HD3 | 2.10 | 0.71 |
| 2:F:267:ALA:HB3 | 2:F:270:PRO:HB3 | 1.72 | 0.71 |
| 2:F:67:GLU:O | 2:F:71:GLU:HB3 | 1.90 | 0.71 |
| 1:A:297:MET:SD | 1:A:411:LEU:CD2 | 2.77 | 0.71 |
| 1:A:496:LYS:O | 1:A:516:GLU:HB2 | 1.90 | 0.71 |
| 1:A:576:LEU:HD12 | 1:A:577:CYS:HB2 | 1.71 | 0.71 |
| 1:A:606:THR:HG23 | 1:A:613:HIS:N | 2.05 | 0.71 |
| 2:B:231:ILE:HD11 | 2:C:135:PRO:HG3 | 1.72 | 0.71 |
| 2:C:388:GLY:CA | 2:C:444:THR:HG22 | 2.20 | 0.71 |
| 2:C:396:ARG:HD2 | 2:C:396:ARG:C | 2.10 | 0.71 |
| 1:D:1206:MET:CE | 1:D:1210:TYR:HA | 2.20 | 0.71 |
| 1:D:275:ARG:CZ | 1:D:843:GLN:N | 2.53 | 0.71 |
| 1:D:553:LYS:HD3 | 2:F:468:ILE:CG2 | 2.20 | 0.71 |
| 1:D:827:ARG:HD3 | 1:D:828:HIS:N | 2.06 | 0.71 |
| 1:D:885:THR:HG22 | 1:D:1186:ASP:O | 1.91 | 0.71 |
| 2:F:190:LEU:CB | 2:F:314:MET:HE1 | 2.20 | 0.71 |
| 1:A:1068:ASP:N | 1:A:1071:ARG:CG | 2.50 | 0.71 |
| 1:A:1153:LEU:HD13 | 1:A:1157:ASN:HD21 | 1.55 | 0.71 |
| 1:A:348:LEU:O | 1:A:350:ILE:N | 2.23 | 0.71 |
| 1:A:458:GLU:O | 1:A:461:LYS:HG2 | 1.90 | 0.71 |
| 1:A:482:ASP:OD2 | 1:A:483:PRO:HD2 | 1.89 | 0.71 |
| 2:B:114:TRP:HE1 | 2:B:259:ARG:NE | 1.88 | 0.71 |
| 2:B:211:ILE:HG12 | 2:B:237:ALA:CB | 2.18 | 0.71 |
| 2:C:342:LEU:HB2 | 2:C:344:ARG:CD | 2.19 | 0.71 |
| 1:D:1197:CYS:C | 1:D:1204:THR:OG1 | 2.29 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:305:SER:HB2 | 1:D:308:GLN:OE1 | 1.89 | 0.71 |
| 1:D:858:THR:HB | 1:D:859:TRP:CD1 | 2.25 | 0.71 |
| 2:E:254:PHE:CE1 | 2:E:258:HIS:HB2 | 2.26 | 0.71 |
| 2:E:422:GLN:HG2 | 2:E:424:SER:N | 2.03 | 0.71 |
| 2:E:86:LEU:HA | 2:E:90:SER:CB | 2.20 | 0.71 |
| 2:F:209:ALA:CB | 2:F:239:LEU:HA | 2.21 | 0.71 |
| 2:F:456:ARG:CG | 2:F:457:SER:H | 1.94 | 0.71 |
| 2:F:485:VAL:HG22 | 2:F:485:VAL:OXT | 1.90 | 0.71 |
| 1:A:853:ARG:HH22 | 1:A:1105:ALA:CB | 2.04 | 0.71 |
| 1:A:1200:PRO:HB2 | 1:A:1202:ASN:O | 1.89 | 0.71 |
| 1:A:174:GLY:HA2 | 1:A:220:TRP:N | 2.04 | 0.71 |
| 1:A:577:CYS:CB | 1:A:578:PRO:HD3 | 2.21 | 0.71 |
| 1:A:468:ASN:HD21 | 1:A:578:PRO:HG3 | 1.56 | 0.71 |
| 1:A:719:LEU:HD23 | 1:A:719:LEU:N | 2.04 | 0.71 |
| 2:B:248:SER:O | 2:B:252:LEU:HB2 | 1.91 | 0.71 |
| 2:C:125:VAL:CG2 | 2:C:208:LEU:HA | 2.09 | 0.71 |
| 2:C:354:PHE:CZ | 2:C:370:LYS:HD3 | 2.26 | 0.71 |
| 1:D:1023:GLN:HE22 | 1:D:1099:TRP:C | 1.93 | 0.71 |
| 1:D:1131:ILE:HD11 | 1:D:1138:ARG:CB | 2.19 | 0.71 |
| 1:D:255:SER:OG | 1:D:258:GLN:N | 2.21 | 0.71 |
| 1:D:277:HIS:HB3 | 1:D:291:PHE:CE2 | 2.26 | 0.71 |
| 1:D:345:TRP:HA | 1:D:1040:LYS:HZ2 | 1.53 | 0.71 |
| 1:D:633:LYS:HB3 | 1:D:638:THR:HG21 | 1.72 | 0.71 |
| 1:D:798:ILE:CG2 | 1:D:869:ARG:HH22 | 1.97 | 0.71 |
| 2:E:199:LEU:HG | 2:E:200:VAL:N | 2.04 | 0.71 |
| 2:E:387:VAL:O | 2:E:442:LEU:HD22 | 1.91 | 0.71 |
| 2:E:456:ARG:HG3 | 2:E:462:MET:C | 2.10 | 0.71 |
| 2:F:306:LEU:HD21 | 2:F:310:GLU:CD | 2.10 | 0.71 |
| 1:A:1066:THR:OG1 | 1:A:1073:PRO:CD | 2.39 | 0.71 |
| 1:A:1141:VAL:HG11 | 1:A:1146:ARG:HA | 1.73 | 0.71 |
| 1:A:1124:ALA:HB1 | 1:A:1148:ARG:HG2 | 1.71 | 0.71 |
| 1:A:188:ALA:O | 1:A:189:ILE:CG2 | 2.37 | 0.71 |
| 1:A:298:HIS:ND1 | 1:A:299:MET:N | 2.38 | 0.71 |
| 1:A:436:PRO:HB2 | 1:A:879:GLN:CA | 2.15 | 0.71 |
| 1:A:444:TYR:OH | 1:A:1200:PRO:HG3 | 1.90 | 0.71 |
| 2:C:120:VAL:HG23 | 2:C:121:PHE:N | 2.06 | 0.71 |
| 2:C:240:VAL:HA | 2:C:336:LEU:HB3 | 1.73 | 0.71 |
| 2:C:247:THR:CB | 2:C:251:TRP:HD1 | 2.03 | 0.71 |
| 2:C:241:TRP:CA | 2:C:336:LEU:HB2 | 2.21 | 0.71 |
| 1:D:1165:ALA:HB3 | 1:D:1166:TYR:HE1 | 1.56 | 0.71 |
| 1:D:193:ARG:CA | 1:D:193:ARG:NH1 | 2.54 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:420:HIS:NE2 | 1:D:1020:ILE:CG2 | 2.53 | 0.71 |
| 1:D:479:TYR:CD1 | 1:D:480:LYS:HG3 | 2.26 | 0.71 |
| 1:D:510:ALA:O | 1:D:512:LYS:N | 2.24 | 0.71 |
| 1:D:547:ALA:C | 1:D:551:LYS:HE2 | 2.11 | 0.71 |
| 1:D:656:TYR:HD1 | 1:D:744:ILE:HD12 | 1.53 | 0.71 |
| 1:D:765:PRO:HG2 | 1:D:766:PHE:CD1 | 2.26 | 0.71 |
| 1:D:78:MET:CB | 1:D:1175:GLN:HB3 | 2.19 | 0.71 |
| 1:D:815:TRP:HA | 1:D:838:GLY:CA | 2.20 | 0.71 |
| 2:E:353:SER:OG | 2:E:374:LEU:HG | 1.88 | 0.71 |
| 2:E:382:LYS:CG | 2:E:412:SER:HB2 | 2.16 | 0.71 |
| 2:E:377:CYS:HB3 | 2:E:483:LYS:HE3 | 1.72 | 0.71 |
| 2:F:421:MET:HG3 | 2:F:422:GLN:H | 1.56 | 0.71 |
| 1:A:1008:LEU:C | 1:A:1008:LEU:HD22 | 2.11 | 0.70 |
| 1:A:1029:GLN:NE2 | 1:A:1096:ARG:CZ | 2.54 | 0.70 |
| 1:A:1043:VAL:HG22 | 1:A:1046:GLU:HB2 | 1.72 | 0.70 |
| 1:A:214:ALA:CB | 1:A:219:ALA:HB3 | 2.20 | 0.70 |
| 1:A:247:LEU:HD23 | 1:A:248:GLU:OE1 | 1.91 | 0.70 |
| 1:A:767:ALA:O | 1:A:771:LEU:HB2 | 1.91 | 0.70 |
| 1:A:950:ASN:HA | 1:A:953:ARG:HG3 | 1.73 | 0.70 |
| 2:B:259:ARG:HH11 | 2:B:259:ARG:HB3 | 1.56 | 0.70 |
| 2:C:200:VAL:O | 2:C:203:ARG:HB2 | 1.90 | 0.70 |
| 2:C:241:TRP:HB2 | 2:C:336:LEU:CG | 2.21 | 0.70 |
| 1:D:550:GLN:N | 1:D:551:LYS:CE | 2.54 | 0.70 |
| 1:D:754:HIS:O | 1:D:758:ASN:N | 2.21 | 0.70 |
| 1:D:79:LEU:HB3 | 1:D:83:LEU:HD11 | 1.73 | 0.70 |
| 1:D:922:GLN:CG | 1:D:931:LEU:HD13 | 2.18 | 0.70 |
| 2:E:79:LEU:O | 2:E:100:GLY:HA3 | 1.91 | 0.70 |
| 2:E:239:LEU:HD23 | 2:E:338:VAL:HG21 | 1.72 | 0.70 |
| 2:E:294:PRO:HD2 | 2:E:351:TYR:CE2 | 2.25 | 0.70 |
| 2:E:307:GLY:HA2 | 2:E:334:CYS:CB | 2.21 | 0.70 |
| 1:D:458:GLU:OE2 | 2:F:264:ARG:HB3 | 1.90 | 0.70 |
| 1:A:630:ASN:HD22 | 1:A:631:LEU:N | 1.90 | 0.70 |
| 2:B:202:LYS:O | 2:B:325:ARG:CZ | 2.39 | 0.70 |
| 2:B:383:VAL:HG22 | 2:B:384:ALA:H | 1.56 | 0.70 |
| 2:B:387:VAL:HG11 | 2:B:396:ARG:HB2 | 1.73 | 0.70 |
| 1:D:1014:ARG:HD3 | 1:D:1026:ARG:NE | 2.06 | 0.70 |
| 1:D:1232:GLU:HG3 | 1:D:1234:ARG:NE | 2.06 | 0.70 |
| 1:D:265:LEU:HD21 | 1:D:267:VAL:CA | 2.21 | 0.70 |
| 1:D:297:MET:SD | 1:D:415:LEU:HD22 | 2.31 | 0.70 |
| 2:E:320:SER:O | 2:E:323:HIS:HD2 | 1.73 | 0.70 |
| 1:A:439:GLN:CG | 1:A:836:LEU:N | 2.54 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:549:LEU:HD23 | 1:A:552:LEU:HD12 | 1.73 | 0.70 |
| 1:A:634:LEU:HD12 | 1:A:638:THR:HB | 1.72 | 0.70 |
| 1:A:601:LYS:HZ1 | 1:A:721:ALA:HB1 | 1.55 | 0.70 |
| 1:A:608:ASP:HB3 | 1:A:779:LEU:CG | 2.21 | 0.70 |
| 1:A:813:VAL:HG22 | 1:A:814:VAL:N | 2.06 | 0.70 |
| 1:A:933:SER:HA | 1:A:943:ARG:HG2 | 1.71 | 0.70 |
| 2:B:373:LYS:HA | 2:B:458:ARG:CZ | 2.22 | 0.70 |
| 2:C:239:LEU:O | 2:C:338:VAL:HG12 | 1.92 | 0.70 |
| 1:A:472:GLN:CG | 2:C:460:THR:HA | 2.20 | 0.70 |
| 1:D:576:LEU:HD12 | 1:D:577:CYS:N | 2.06 | 0.70 |
| 1:D:732:TYR:CD2 | 1:D:732:TYR:N | 2.59 | 0.70 |
| 1:D:801:TRP:HH2 | 1:D:805:HIS:CG | 2.08 | 0.70 |
| 2:E:203:ARG:HH12 | 2:F:418:LEU:CD2 | 1.99 | 0.70 |
| 2:F:254:PHE:N | 2:F:257:ARG:HH21 | 1.89 | 0.70 |
| 2:F:243:THR:OG1 | 2:F:334:CYS:CB | 2.39 | 0.70 |
| 1:A:247:LEU:CD1 | 1:A:251:THR:HG21 | 2.21 | 0.70 |
| 1:A:355:SER:HA | 1:A:407:PHE:CE1 | 2.26 | 0.70 |
| 1:A:515:ILE:CD1 | 1:A:568:GLY:O | 2.40 | 0.70 |
| 1:A:627:ARG:O | 1:A:628:ARG:HB3 | 1.90 | 0.70 |
| 1:A:655:LEU:O | 1:A:719:LEU:HD12 | 1.91 | 0.70 |
| 1:A:771:LEU:H | 1:A:771:LEU:CD2 | 2.02 | 0.70 |
| 2:C:299:LEU:H | 2:C:299:LEU:HD23 | 1.54 | 0.70 |
| 2:C:439:PHE:CD1 | 2:C:458:ARG:HB2 | 2.25 | 0.70 |
| 2:C:470:LYS:HE3 | 2:C:471:LEU:HD21 | 1.74 | 0.70 |
| 1:D:1192:GLU:O | 1:D:1192:GLU:HG2 | 1.89 | 0.70 |
| 1:D:225:SER:HA | 1:D:228:LEU:HD21 | 1.72 | 0.70 |
| 1:D:203:LEU:CB | 1:D:380:GLY:HA3 | 2.17 | 0.70 |
| 1:D:374:ARG:CB | 1:D:392:LEU:HD11 | 2.21 | 0.70 |
| 1:D:598:VAL:HG12 | 1:D:602:LEU:HD11 | 1.73 | 0.70 |
| 1:D:885:THR:HB | 1:D:1146:ARG:CD | 2.17 | 0.70 |
| 2:E:109:ASN:ND2 | 2:E:378:LEU:HB3 | 2.06 | 0.70 |
| 2:E:249:ASN:HD21 | 2:E:285:LYS:CE | 1.97 | 0.70 |
| 2:F:239:LEU:H | 2:F:338:VAL:HG13 | 1.55 | 0.70 |
| 2:F:454:HIS:CB | 2:F:466:MET:CB | 2.66 | 0.70 |
| 1:A:1212:ILE:CG2 | 1:A:1213:PRO:N | 2.55 | 0.70 |
| 2:C:214:CYS:SG | 2:C:236:GLU:HG3 | 2.32 | 0.70 |
| 2:C:471:LEU:HA | 2:C:474:PHE:HD2 | 1.54 | 0.70 |
| 1:D:1158:LEU:HG | 1:D:1159:LEU:H | 1.56 | 0.70 |
| 1:D:190:PRO:C | 1:D:192:GLU:N | 2.44 | 0.70 |
| 1:D:266:VAL:O | 1:D:266:VAL:HG13 | 1.91 | 0.70 |
| 1:D:278:ILE:HD13 | 1:D:291:PHE:HD1 | 1.55 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:401:TRP:HA | 1:D:404:HIS:CD2 | 2.26 | 0.70 |
| 1:D:576:LEU:CG | 1:D:579:ARG:HE | 2.05 | 0.70 |
| 1:D:623:LEU:HG | 1:D:623:LEU:O | 1.89 | 0.70 |
| 2:E:441:VAL:HG12 | 2:E:442:LEU:H | 1.57 | 0.70 |
| 2:F:394:GLU:CD | 2:F:394:GLU:H | 1.92 | 0.70 |
| 1:A:1066:THR:OG1 | 1:A:1071:ARG:HB3 | 1.91 | 0.70 |
| 1:A:1019:TRP:HZ3 | 1:A:1164:PHE:HA | 1.56 | 0.70 |
| 1:A:125:LEU:N | 1:A:125:LEU:CD2 | 2.50 | 0.70 |
| 1:A:239:LEU:O | 1:A:241:PRO:CD | 2.38 | 0.70 |
| 2:C:125:VAL:HG23 | 2:C:126:PHE:H | 1.57 | 0.70 |
| 1:D:127:LEU:CD2 | 1:D:129:PRO:HD3 | 2.20 | 0.70 |
| 1:D:474:LEU:CD1 | 1:D:474:LEU:H | 2.04 | 0.70 |
| 1:D:603:MET:HB3 | 1:D:605:LEU:CD2 | 2.22 | 0.70 |
| 1:D:601:LYS:HG2 | 1:D:721:ALA:CB | 2.21 | 0.70 |
| 1:D:810:SER:OG | 1:D:811:GLN:N | 2.24 | 0.70 |
| 2:E:118:VAL:HG13 | 2:E:119:VAL:H | 1.57 | 0.70 |
| 2:F:326:ASP:CG | 2:F:327:GLY:N | 2.42 | 0.70 |
| 1:A:169:TRP:CE3 | 1:A:390:GLN:O | 2.45 | 0.70 |
| 1:A:606:THR:HG22 | 1:A:614:TYR:CD2 | 2.27 | 0.70 |
| 1:A:869:ARG:HG3 | 1:A:869:ARG:NH1 | 2.06 | 0.70 |
| 1:A:883:GLY:C | 1:A:884:TYR:CD1 | 2.64 | 0.70 |
| 2:B:199:LEU:CD1 | 2:B:200:VAL:HG13 | 2.22 | 0.70 |
| 2:C:207:GLY:HA2 | 2:C:240:VAL:O | 1.91 | 0.70 |
| 2:C:342:LEU:HB2 | 2:C:344:ARG:HB2 | 1.74 | 0.70 |
| 2:C:351:TYR:O | 2:C:352:ASP:C | 2.27 | 0.70 |
| 2:C:393:LEU:O | 2:C:397:GLN:N | 2.23 | 0.70 |
| 2:C:455:LEU:CA | 2:C:456:ARG:HE | 2.04 | 0.70 |
| 1:D:597:ARG:HH11 | 1:D:724:GLY:C | 1.94 | 0.70 |
| 1:D:612:LEU:HD13 | 1:D:612:LEU:H | 1.53 | 0.70 |
| 2:E:114:TRP:HH2 | 2:E:238:SER:O | 1.75 | 0.70 |
| 2:E:326:ASP:H | 2:E:331:VAL:HG12 | 1.55 | 0.70 |
| 2:E:430:SER:O | 2:E:434:GLU:HG2 | 1.91 | 0.70 |
| 1:A:273:PHE:C | 1:A:276:ALA:HB3 | 2.12 | 0.70 |
| 1:A:282:TYR:O | 1:A:283:LEU:CB | 2.39 | 0.70 |
| 1:A:412:PRO:CG | 1:A:413:LEU:H | 2.05 | 0.70 |
| 1:A:448:ALA:CA | 1:A:870:VAL:HG13 | 2.21 | 0.70 |
| 1:A:783:PRO:HG2 | 2:C:363:ARG:NH1 | 2.07 | 0.70 |
| 2:B:204:LEU:HD12 | 2:B:325:ARG:N | 2.05 | 0.70 |
| 1:D:371:LYS:CA | 1:D:374:ARG:HD2 | 2.22 | 0.70 |
| 1:D:420:HIS:CD2 | 1:D:1020:ILE:CD1 | 2.69 | 0.70 |
| 1:D:607:TRP:HD1 | 1:D:779:LEU:HA | 1.56 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:892:ASP:OD2 | 1:D:892:ASP:C | 2.30 | 0.70 |
| 2:F:446:THR:CG2 | 2:F:450:ASN:OD1 | 2.35 | 0.70 |
| 2:F:452:LEU:O | 2:F:453:ILE:CG1 | 2.39 | 0.70 |
| 1:A:192:GLU:HB3 | 1:A:217:PRO:CG | 2.18 | 0.70 |
| 1:A:211:LEU:HD12 | 1:A:221:TYR:HB3 | 1.73 | 0.70 |
| 1:A:402:ALA:O | 1:A:406:VAL:HG13 | 1.92 | 0.70 |
| 1:A:417:ARG:HH11 | 1:A:417:ARG:HG2 | 1.57 | 0.70 |
| 1:A:451:THR:HG21 | 1:A:1202:ASN:CB | 2.22 | 0.70 |
| 1:A:831:TYR:CD1 | 1:A:831:TYR:N | 2.59 | 0.70 |
| 1:A:900:ALA:CA | 1:A:915:ALA:HB1 | 2.22 | 0.70 |
| 2:B:215:PHE:O | 2:B:216:HIS:HB2 | 1.91 | 0.70 |
| 2:B:117:SER:HB2 | 2:B:262:TRP:HE1 | 1.54 | 0.70 |
| 2:C:200:VAL:HG11 | 2:C:204:LEU:HB2 | 1.74 | 0.70 |
| 2:C:263:TRP:CZ2 | 2:C:301:GLU:OE2 | 2.45 | 0.70 |
| 2:C:344:ARG:HA | 2:C:347:LEU:CD2 | 2.22 | 0.70 |
| 2:C:375:HIS:ND1 | 2:C:376:PRO:HD2 | 2.06 | 0.70 |
| 2:C:389:ARG:CZ | 2:C:390:GLY:HA3 | 2.20 | 0.70 |
| 1:D:107:LEU:HD23 | 1:D:107:LEU:N | 2.06 | 0.70 |
| 1:D:1118:TRP:O | 1:D:1122:GLU:HG2 | 1.92 | 0.70 |
| 1:D:889:ALA:HB3 | 1:D:1180:PHE:CE1 | 2.27 | 0.70 |
| 1:D:121:PRO:CB | 1:D:1175:GLN:HE22 | 2.04 | 0.70 |
| 1:D:633:LYS:CD | 1:D:638:THR:HG21 | 2.22 | 0.70 |
| 1:D:737:GLY:O | 1:D:741:ASP:OD1 | 2.10 | 0.70 |
| 1:D:774:MET:O | 1:D:779:LEU:O | 2.10 | 0.70 |
| 1:D:832:ASP:O | 1:D:833:GLU:HB2 | 1.92 | 0.70 |
| 1:D:993:ARG:HD3 | 1:D:993:ARG:O | 1.92 | 0.70 |
| 2:F:241:TRP:HZ3 | 2:F:255:TRP:CE2 | 2.08 | 0.70 |
| 1:A:1031:GLU:O | 1:A:1032:THR:HB | 1.91 | 0.70 |
| 1:A:174:GLY:O | 1:A:175:TRP:CG | 2.44 | 0.70 |
| 1:A:603:MET:HE3 | 1:A:791:ALA:HB1 | 1.74 | 0.70 |
| 1:A:821:LEU:CD1 | 1:A:825:VAL:HB | 2.22 | 0.70 |
| 1:A:827:ARG:HA | 1:A:831:TYR:OH | 1.91 | 0.70 |
| 2:C:127:PRO:CD | 2:C:128:VAL:H | 1.98 | 0.70 |
| 1:D:1014:ARG:HD3 | 1:D:1026:ARG:CG | 2.21 | 0.70 |
| 1:D:1175:GLN:C | 1:D:1177:VAL:H | 1.94 | 0.70 |
| 1:D:1198:LYS:HD2 | 1:D:1204:THR:HB | 1.73 | 0.70 |
| 1:D:267:VAL:HG21 | 1:D:291:PHE:HE2 | 1.56 | 0.70 |
| 1:D:374:ARG:HG2 | 1:D:374:ARG:HH11 | 1.57 | 0.70 |
| 1:D:294:THR:CG2 | 1:D:407:PHE:CE2 | 2.70 | 0.70 |
| 1:D:500:ALA:HB2 | 1:D:521:PRO:HG3 | 1.72 | 0.70 |
| 1:D:527:GLN:HE21 | 1:D:528:GLU:HB3 | 1.56 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:569:HIS:N | 1:D:570:PRO:CD | 2.55 | 0.70 |
| 1:D:933:SER:HB2 | 1:D:943:ARG:CD | 2.20 | 0.70 |
| 1:D:944:GLU:HB3 | 1:D:1071:ARG:HD3 | 1.74 | 0.70 |
| 2:E:437:ILE:HD12 | 2:E:437:ILE:N | 2.04 | 0.70 |
| 2:F:213:VAL:HA | 2:F:235:THR:HA | 1.72 | 0.70 |
| 2:F:342:LEU:HB2 | 2:F:344:ARG:HD3 | 1.72 | 0.70 |
| 2:F:382:LYS:HD3 | 2:F:411:ILE:CG1 | 2.18 | 0.70 |
| 2:F:467:HIS:HB3 | 2:F:470:LYS:HE2 | 1.74 | 0.70 |
| 2:F:471:LEU:H | 2:F:471:LEU:CD1 | 1.67 | 0.70 |
| 1:A:107:LEU:HB2 | 1:A:113:TRP:HE1 | 1.54 | 0.69 |
| 1:A:77:GLN:HB2 | 1:A:1174:PRO:HB3 | 1.72 | 0.69 |
| 1:A:211:LEU:HG | 1:A:221:TYR:HB3 | 1.74 | 0.69 |
| 1:A:886:LEU:HD23 | 1:A:886:LEU:N | 2.07 | 0.69 |
| 1:A:927:ARG:CG | 1:A:928:GLY:N | 2.53 | 0.69 |
| 1:D:370:GLU:O | 1:D:371:LYS:HB2 | 1.92 | 0.69 |
| 1:D:600:PRO:CG | 1:D:616:GLU:HB3 | 2.21 | 0.69 |
| 2:E:88:ARG:HD3 | 2:E:88:ARG:N | 2.07 | 0.69 |
| 2:F:342:LEU:CB | 2:F:344:ARG:HD3 | 2.22 | 0.69 |
| 1:A:891:VAL:CA | 1:A:1180:PHE:HE1 | 2.03 | 0.69 |
| 1:A:1209:ARG:HH12 | 2:C:256:LEU:HB3 | 1.57 | 0.69 |
| 1:A:869:ARG:CA | 1:A:1200:PRO:HA | 2.22 | 0.69 |
| 2:B:394:GLU:O | 2:B:398:VAL:HG23 | 1.92 | 0.69 |
| 2:C:241:TRP:HZ3 | 2:C:255:TRP:NE1 | 1.89 | 0.69 |
| 1:D:1008:LEU:HA | 1:D:1011:PRO:HG3 | 1.73 | 0.69 |
| 1:D:205:GLU:HA | 1:D:205:GLU:OE1 | 1.91 | 0.69 |
| 1:D:256:PRO:HB3 | 1:D:281:GLN:CG | 2.22 | 0.69 |
| 1:D:381:THR:CG2 | 1:D:385:ILE:HB | 2.21 | 0.69 |
| 1:D:547:ALA:C | 1:D:551:LYS:CE | 2.61 | 0.69 |
| 1:D:660:CYS:HB2 | 1:D:745:PRO:CD | 2.21 | 0.69 |
| 1:D:658:LYS:HE3 | 1:D:713:PRO:CB | 2.21 | 0.69 |
| 1:D:845:VAL:HG23 | 1:D:855:VAL:HB | 1.74 | 0.69 |
| 1:D:436:PRO:O | 1:D:879:GLN:HB3 | 1.92 | 0.69 |
| 2:F:94:GLY:HA2 | 2:F:96:HIS:CE1 | 2.27 | 0.69 |
| 2:F:81:GLY:HA3 | 2:F:97:PRO:HB2 | 1.75 | 0.69 |
| 1:A:483:PRO:HB3 | 1:A:712:VAL:HG11 | 1.73 | 0.69 |
| 1:A:540:GLN:O | 1:A:543:VAL:HG12 | 1.93 | 0.69 |
| 1:A:869:ARG:O | 1:A:1200:PRO:HA | 1.91 | 0.69 |
| 1:A:886:LEU:N | 1:A:1146:ARG:HH21 | 1.88 | 0.69 |
| 1:A:992:LEU:HD12 | 1:A:993:ARG:H | 1.56 | 0.69 |
| 2:C:251:TRP:HA | 2:C:251:TRP:HE3 | 1.57 | 0.69 |
| 2:C:363:ARG:NH1 | 2:C:363:ARG:HA | 2.05 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:435:MET:O | 2:C:436:SER:HB3 | 1.90 | 0.69 |
| 1:D:1111:LEU:HD22 | 1:D:1164:PHE:CE1 | 2.28 | 0.69 |
| 1:D:177:ARG:O | 1:D:179:GLY:N | 2.25 | 0.69 |
| 1:D:656:TYR:HE1 | 1:D:743:ASP:CG | 1.96 | 0.69 |
| 1:D:798:ILE:CA | 1:D:869:ARG:CZ | 2.69 | 0.69 |
| 1:D:891:VAL:HG11 | 1:D:1135:ASP:CA | 2.22 | 0.69 |
| 2:E:214:CYS:HB2 | 2:E:236:GLU:HB2 | 1.73 | 0.69 |
| 2:E:387:VAL:CG1 | 2:E:416:GLY:HA3 | 2.23 | 0.69 |
| 2:F:113:GLU:O | 2:F:116:THR:HG23 | 1.93 | 0.69 |
| 2:F:389:ARG:O | 2:F:392:THR:HA | 1.92 | 0.69 |
| 2:F:371:VAL:HG23 | 2:F:433:ASP:C | 2.12 | 0.69 |
| 1:A:211:LEU:CG | 1:A:221:TYR:HB3 | 2.22 | 0.69 |
| 1:A:195:LEU:HD23 | 1:A:217:PRO:HD2 | 1.73 | 0.69 |
| 1:A:634:LEU:CG | 1:A:635:PRO:HA | 2.22 | 0.69 |
| 1:A:658:LYS:O | 1:A:662:GLU:HG2 | 1.93 | 0.69 |
| 1:A:737:GLY:O | 1:A:741:ASP:OD2 | 2.10 | 0.69 |
| 1:A:827:ARG:HG3 | 1:A:828:HIS:N | 2.08 | 0.69 |
| 2:B:269:SER:HB2 | 2:B:352:ASP:OD1 | 1.92 | 0.69 |
| 2:C:134:LYS:HB3 | 2:C:180:LYS:CE | 2.23 | 0.69 |
| 2:C:403:PHE:O | 2:C:407:LEU:N | 2.23 | 0.69 |
| 1:D:457:ARG:C | 1:D:460:LYS:CE | 2.60 | 0.69 |
| 1:D:556:THR:OG1 | 2:F:452:LEU:CD2 | 2.41 | 0.69 |
| 1:D:516:GLU:HA | 1:D:565:HIS:CE1 | 2.26 | 0.69 |
| 2:E:455:LEU:HD23 | 2:E:464:GLU:O | 1.91 | 0.69 |
| 1:A:1199:THR:CA | 1:A:1200:PRO:C | 2.52 | 0.69 |
| 1:A:192:GLU:CA | 1:A:217:PRO:HG2 | 2.22 | 0.69 |
| 1:A:667:GLN:C | 1:A:670:PRO:HD2 | 2.12 | 0.69 |
| 1:A:732:TYR:HE1 | 1:A:755:LYS:CA | 2.03 | 0.69 |
| 2:B:261:GLN:CA | 2:B:264:ARG:HE | 2.05 | 0.69 |
| 2:B:72:ILE:HD12 | 2:B:372:LEU:HD11 | 1.74 | 0.69 |
| 2:C:341:ASP:C | 2:C:342:LEU:HD13 | 2.13 | 0.69 |
| 1:D:887:VAL:CG2 | 1:D:1146:ARG:CZ | 2.69 | 0.69 |
| 1:D:348:LEU:HD11 | 1:D:350:ILE:HD11 | 1.75 | 0.69 |
| 1:D:788:GLY:O | 1:D:791:ALA:N | 2.24 | 0.69 |
| 2:E:116:THR:O | 2:E:120:VAL:HG12 | 1.92 | 0.69 |
| 2:E:85:GLN:HB3 | 2:E:97:PRO:HG3 | 1.75 | 0.69 |
| 1:D:1209:ARG:NH2 | 2:F:253:ASP:N | 2.40 | 0.69 |
| 2:F:254:PHE:HE2 | 2:F:255:TRP:CZ2 | 2.11 | 0.69 |
| 1:A:115:GLN:N | 1:A:116:PRO:CD | 2.56 | 0.69 |
| 1:A:1199:THR:HA | 1:A:1201:SER:N | 2.07 | 0.69 |
| 1:A:624:VAL:C | 1:A:626:GLY:N | 2.43 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:653:GLU:HG3 | 1:A:656:TYR:HE1 | 1.58 | 0.69 |
| 1:A:769:ASP:O | 1:A:773:LYS:HG3 | 1.91 | 0.69 |
| 1:A:792:LEU:HA | 1:A:795:ASN:OD1 | 1.91 | 0.69 |
| 2:B:78:PHE:CG | 2:B:102:LEU:HB2 | 2.27 | 0.69 |
| 2:B:324:GLY:CA | 2:B:325:ARG:NH2 | 2.55 | 0.69 |
| 2:C:455:LEU:HD12 | 2:C:455:LEU:N | 2.08 | 0.69 |
| 2:C:439:PHE:HD1 | 2:C:458:ARG:HG3 | 1.54 | 0.69 |
| 1:D:1192:GLU:OE2 | 1:D:1195:MET:SD | 2.51 | 0.69 |
| 1:D:1197:CYS:N | 1:D:1204:THR:CG2 | 2.54 | 0.69 |
| 1:D:127:LEU:HD22 | 1:D:129:PRO:CD | 2.22 | 0.69 |
| 1:D:768:LYS:CD | 1:D:769:ASP:N | 2.55 | 0.69 |
| 1:D:768:LYS:C | 1:D:772:PRO:HD2 | 2.13 | 0.69 |
| 1:D:85:GLU:OE1 | 1:D:130:LEU:HD22 | 1.92 | 0.69 |
| 1:D:992:LEU:HD23 | 1:D:997:LEU:HD12 | 1.73 | 0.69 |
| 2:E:254:PHE:HB2 | 2:E:257:ARG:NH1 | 2.03 | 0.69 |
| 2:E:384:ALA:O | 2:E:414:TRP:N | 2.26 | 0.69 |
| 1:A:285:GLN:C | 1:A:1128:ARG:NH2 | 2.46 | 0.69 |
| 1:A:741:ASP:OD1 | 1:A:742:VAL:N | 2.25 | 0.69 |
| 1:A:805:HIS:C | 1:A:805:HIS:ND1 | 2.45 | 0.69 |
| 2:B:234:LYS:N | 2:B:234:LYS:HE2 | 2.07 | 0.69 |
| 2:C:435:MET:O | 2:C:436:SER:CB | 2.40 | 0.69 |
| 1:D:127:LEU:O | 1:D:130:LEU:HD21 | 1.93 | 0.69 |
| 1:D:648:PRO:CD | 1:D:649:TYR:H | 2.01 | 0.69 |
| 2:E:289:LEU:O | 2:E:299:LEU:HA | 1.92 | 0.69 |
| 2:E:391:PRO:HD2 | 2:E:395:LEU:HB2 | 1.73 | 0.69 |
| 2:F:314:MET:HB3 | 2:F:315:TYR:CD2 | 2.28 | 0.69 |
| 2:F:374:LEU:CD1 | 2:F:379:ALA:HA | 2.21 | 0.69 |
| 2:F:81:GLY:CA | 2:F:97:PRO:HB2 | 2.22 | 0.69 |
| 1:A:1006:ARG:HH22 | 1:A:1010:LEU:HD11 | 1.56 | 0.69 |
| 1:A:1193:VAL:CG2 | 1:A:1194:THR:N | 2.55 | 0.69 |
| 1:A:165:LYS:O | 1:A:167:PRO:HD3 | 1.92 | 0.69 |
| 1:A:213:VAL:HG13 | 1:A:221:TYR:HH | 1.53 | 0.69 |
| 1:A:352:SER:O | 1:A:358:LEU:CD2 | 2.40 | 0.69 |
| 1:A:363:ARG:HD2 | 1:A:406:VAL:CB | 2.16 | 0.69 |
| 1:A:559:LEU:HB3 | 1:A:560:PRO:CD | 2.22 | 0.69 |
| 1:A:926:SER:O | 1:A:927:ARG:CB | 2.41 | 0.69 |
| 1:A:963:GLU:O | 1:A:967:MET:HG3 | 1.93 | 0.69 |
| 2:B:99:PHE:CE1 | 2:B:343:ASP:OD1 | 2.46 | 0.69 |
| 2:C:241:TRP:CD1 | 2:C:243:THR:HG23 | 2.28 | 0.69 |
| 2:C:307:GLY:HA2 | 2:C:335:VAL:HG12 | 1.75 | 0.69 |
| 2:C:388:GLY:HA3 | 2:C:444:THR:HG22 | 1.73 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1047:ARG:O | 1:D:1050:LYS:N | 2.26 | 0.69 |
| 1:D:167:PRO:O | 1:D:169:TRP:N | 2.25 | 0.69 |
| 1:D:279:ARG:CB | 1:D:841:LEU:HB2 | 2.22 | 0.69 |
| 2:E:371:VAL:CG1 | 2:E:372:LEU:N | 2.55 | 0.69 |
| 1:A:451:THR:OG1 | 1:A:1202:ASN:ND2 | 2.26 | 0.69 |
| 1:A:183:GLU:OE1 | 1:A:184:ALA:HB2 | 1.93 | 0.69 |
| 1:A:992:LEU:HD13 | 1:A:993:ARG:H | 1.57 | 0.69 |
| 2:B:383:VAL:HG22 | 2:B:384:ALA:N | 2.07 | 0.69 |
| 2:C:357:THR:C | 2:C:359:ASN:H | 1.97 | 0.69 |
| 2:C:388:GLY:O | 2:C:395:LEU:HD13 | 1.92 | 0.69 |
| 2:C:81:GLY:HA3 | 2:C:97:PRO:CG | 2.23 | 0.69 |
| 1:D:1107:ASP:O | 1:D:1111:LEU:HD13 | 1.93 | 0.69 |
| 1:D:273:PHE:HA | 1:D:276:ALA:H | 1.58 | 0.69 |
| 1:D:606:THR:OG1 | 1:D:614:TYR:CZ | 2.46 | 0.69 |
| 1:D:641:GLU:O | 1:D:650:ARG:HD3 | 1.91 | 0.69 |
| 2:E:439:PHE:CZ | 2:E:478:TYR:CE1 | 2.81 | 0.69 |
| 2:F:207:GLY:HA3 | 2:F:239:LEU:HD11 | 1.75 | 0.69 |
| 1:A:107:LEU:HD12 | 1:A:112:LEU:HD13 | 1.74 | 0.69 |
| 1:A:853:ARG:NH2 | 1:A:1105:ALA:CB | 2.55 | 0.69 |
| 1:A:451:THR:C | 1:A:869:ARG:HH22 | 1.95 | 0.69 |
| 1:A:462:SER:OG | 1:A:463:LEU:N | 2.21 | 0.69 |
| 1:A:719:LEU:O | 1:A:722:ARG:HG3 | 1.93 | 0.69 |
| 1:A:827:ARG:HA | 1:A:831:TYR:CE1 | 2.28 | 0.69 |
| 1:A:951:TYR:HB3 | 1:A:955:TYR:HE1 | 1.58 | 0.69 |
| 2:C:341:ASP:O | 2:C:342:LEU:CD1 | 2.38 | 0.69 |
| 2:C:389:ARG:HG3 | 2:C:390:GLY:H | 1.57 | 0.69 |
| 1:D:872:SER:OG | 1:D:1200:PRO:CD | 2.40 | 0.69 |
| 1:D:483:PRO:O | 1:D:486:TRP:CB | 2.41 | 0.69 |
| 1:D:725:PRO:O | 1:D:726:LYS:HB2 | 1.92 | 0.69 |
| 1:D:742:VAL:HG13 | 1:D:743:ASP:N | 2.07 | 0.69 |
| 1:D:656:TYR:CB | 1:D:744:ILE:HG21 | 2.22 | 0.69 |
| 1:D:76:ILE:HB | 1:D:911:HIS:CE1 | 2.27 | 0.69 |
| 1:D:801:TRP:HD1 | 1:D:869:ARG:HH21 | 1.38 | 0.69 |
| 1:D:826:ILE:HB | 1:D:831:TYR:HE2 | 1.56 | 0.69 |
| 1:D:946:ALA:HA | 1:D:949:PHE:CD2 | 2.28 | 0.69 |
| 1:D:996:ARG:CZ | 1:D:996:ARG:H | 2.05 | 0.69 |
| 2:E:183:GLU:HG3 | 2:E:216:HIS:CD2 | 2.28 | 0.69 |
| 2:E:193:TYR:CD2 | 2:E:322:LEU:HD22 | 2.27 | 0.69 |
| 2:F:254:PHE:HA | 2:F:257:ARG:HH21 | 1.56 | 0.69 |
| 2:F:356:LEU:HD22 | 2:F:359:ASN:OD1 | 1.93 | 0.69 |
| 1:A:1024:ASP:O | 1:A:1026:ARG:HD2 | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1114:VAL:N | 1:A:1117:LYS:HZ2 | 1.90 | 0.69 |
| 1:A:192:GLU:CD | 1:A:193:ARG:N | 2.46 | 0.69 |
| 1:A:214:ALA:CA | 1:A:401:TRP:CZ2 | 2.75 | 0.69 |
| 1:A:373:PRO:HD2 | 1:A:374:ARG:HH11 | 1.58 | 0.69 |
| 1:A:363:ARG:CZ | 1:A:406:VAL:HA | 2.22 | 0.69 |
| 1:A:623:LEU:H | 1:A:623:LEU:HD23 | 1.58 | 0.69 |
| 1:A:850:ILE:HG12 | 1:A:1099:TRP:NE1 | 2.07 | 0.69 |
| 1:A:86:GLN:O | 1:A:87:ILE:HG13 | 1.92 | 0.69 |
| 2:C:303:LEU:C | 2:C:337:SER:CB | 2.60 | 0.69 |
| 2:B:199:LEU:HD23 | 2:C:77:HIS:CD2 | 2.27 | 0.69 |
| 1:D:1197:CYS:C | 1:D:1204:THR:HG1 | 1.95 | 0.69 |
| 1:D:1231:LEU:CG | 1:D:1232:GLU:H | 1.83 | 0.69 |
| 1:D:167:PRO:HD2 | 1:D:168:ALA:H | 1.55 | 0.69 |
| 1:D:307:PHE:HD1 | 1:D:307:PHE:H | 1.39 | 0.69 |
| 2:E:371:VAL:HG12 | 2:E:372:LEU:N | 2.07 | 0.69 |
| 2:E:450:ASN:HD22 | 2:E:452:LEU:HD21 | 1.57 | 0.69 |
| 2:F:114:TRP:NE1 | 2:F:259:ARG:NH2 | 2.40 | 0.69 |
| 2:E:419:GLU:HA | 2:F:203:ARG:HH22 | 1.54 | 0.69 |
| 2:F:272:ASN:HB3 | 2:F:292:ASN:HB2 | 1.73 | 0.69 |
| 2:F:344:ARG:HA | 2:F:347:LEU:HB2 | 1.73 | 0.69 |
| 2:F:344:ARG:HA | 2:F:347:LEU:HD13 | 1.75 | 0.69 |
| 2:F:355:GLN:O | 2:F:357:THR:N | 2.25 | 0.69 |
| 2:F:389:ARG:CZ | 2:F:390:GLY:HA3 | 2.23 | 0.69 |
| 1:A:853:ARG:NH2 | 1:A:1105:ALA:HB3 | 2.07 | 0.68 |
| 1:A:230:GLU:CD | 1:A:231:GLU:H | 1.91 | 0.68 |
| 1:A:420:HIS:ND1 | 1:A:421:PRO:HD2 | 2.08 | 0.68 |
| 1:A:453:GLU:O | 1:A:454:GLU:C | 2.31 | 0.68 |
| 1:A:559:LEU:HD23 | 1:A:560:PRO:HD2 | 1.74 | 0.68 |
| 1:A:601:LYS:NZ | 1:A:616:GLU:HG2 | 2.07 | 0.68 |
| 1:A:951:TYR:O | 1:A:954:ILE:HB | 1.93 | 0.68 |
| 2:B:115:TRP:CZ2 | 2:C:108:LYS:HD3 | 2.29 | 0.68 |
| 2:C:402:LEU:HG | 2:C:472:LYS:HZ3 | 1.58 | 0.68 |
| 2:C:443:VAL:CG1 | 2:C:447:THR:HG21 | 2.22 | 0.68 |
| 1:D:1019:TRP:HD1 | 1:D:1020:ILE:HG22 | 1.57 | 0.68 |
| 1:D:1232:GLU:CG | 1:D:1234:ARG:HB2 | 2.22 | 0.68 |
| 1:D:356:LEU:CD1 | 1:D:369:LEU:CD2 | 2.64 | 0.68 |
| 1:D:457:ARG:C | 1:D:460:LYS:HE3 | 2.12 | 0.68 |
| 1:D:496:LYS:HE3 | 1:D:571:GLY:HA2 | 1.73 | 0.68 |
| 1:D:595:GLN:O | 1:D:596:MET:C | 2.31 | 0.68 |
| 1:D:283:LEU:HG | 1:D:814:VAL:HG23 | 1.74 | 0.68 |
| 1:D:990:LYS:HG2 | 1:D:1000:GLU:HB2 | 1.73 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:456:ARG:NE | 2:E:463:LYS:HE3 | 2.07 | 0.68 |
| 2:E:82:SER:N | 2:E:85:GLN:HG3 | 2.04 | 0.68 |
| 1:A:1030:ARG:HD3 | 1:A:1091:GLU:OE1 | 1.91 | 0.68 |
| 1:A:1129:PHE:HD2 | 1:A:1138:ARG:O | 1.76 | 0.68 |
| 1:A:1223:ILE:O | 1:A:1227:THR:HG23 | 1.93 | 0.68 |
| 1:A:564:GLN:CA | 1:A:567:PRO:HD2 | 2.23 | 0.68 |
| 1:A:607:TRP:CH2 | 1:A:671:GLN:HA | 2.27 | 0.68 |
| 1:A:659:HIS:CB | 1:A:719:LEU:HD12 | 2.17 | 0.68 |
| 1:A:997:LEU:CD2 | 1:A:998:SER:N | 2.51 | 0.68 |
| 2:C:353:SER:HB2 | 2:C:373:LYS:O | 1.94 | 0.68 |
| 2:C:444:THR:H | 2:C:447:THR:HG23 | 1.58 | 0.68 |
| 1:D:312:TRP:HH2 | 1:D:346:ASP:O | 1.75 | 0.68 |
| 1:D:482:ASP:HB2 | 1:D:483:PRO:HD2 | 1.74 | 0.68 |
| 1:D:491:ASP:OD2 | 1:D:578:PRO:HB3 | 1.94 | 0.68 |
| 1:D:651:ALA:O | 1:D:655:LEU:HD23 | 1.93 | 0.68 |
| 1:D:656:TYR:CD1 | 1:D:743:ASP:HB2 | 2.28 | 0.68 |
| 1:D:767:ALA:HB3 | 1:D:771:LEU:HD22 | 1.75 | 0.68 |
| 1:D:887:VAL:N | 1:D:1146:ARG:NH1 | 2.39 | 0.68 |
| 2:F:244:PRO:CD | 2:F:247:THR:CG2 | 2.71 | 0.68 |
| 1:A:190:PRO:CB | 1:A:192:GLU:HG3 | 2.23 | 0.68 |
| 1:A:192:GLU:HB2 | 1:A:195:LEU:HD21 | 1.75 | 0.68 |
| 1:A:222:SER:CB | 1:A:223:TRP:HD1 | 2.02 | 0.68 |
| 1:A:307:PHE:HD1 | 1:A:307:PHE:H | 1.42 | 0.68 |
| 1:A:374:ARG:HH11 | 1:A:374:ARG:CG | 2.06 | 0.68 |
| 1:A:203:LEU:HD12 | 1:A:379:LYS:C | 2.13 | 0.68 |
| 1:A:476:GLY:HA3 | 1:A:711:ALA:HB1 | 1.76 | 0.68 |
| 1:A:734:HIS:HA | 1:A:752:LEU:HD11 | 1.76 | 0.68 |
| 2:B:217:PRO:O | 2:B:230:SER:O | 2.12 | 0.68 |
| 1:D:1027:LYS:HG3 | 1:D:1091:GLU:HA | 1.74 | 0.68 |
| 1:D:1202:ASN:O | 1:D:1205:GLY:N | 2.27 | 0.68 |
| 1:D:440:ASN:OD1 | 1:D:1210:TYR:O | 2.11 | 0.68 |
| 1:D:369:LEU:HB3 | 1:D:372:GLU:HG3 | 1.74 | 0.68 |
| 1:D:414:PHE:O | 1:D:417:ARG:HB2 | 1.94 | 0.68 |
| 1:D:424:LEU:N | 1:D:424:LEU:HD23 | 2.07 | 0.68 |
| 1:D:814:VAL:O | 1:D:838:GLY:HA3 | 1.94 | 0.68 |
| 1:D:856:GLU:HB2 | 1:D:860:LEU:H | 1.58 | 0.68 |
| 1:D:952:GLY:O | 1:D:954:ILE:O | 2.10 | 0.68 |
| 2:E:187:HIS:CA | 2:E:190:LEU:HD22 | 2.22 | 0.68 |
| 2:E:460:THR:O | 2:E:461:THR:HG22 | 1.93 | 0.68 |
| 2:F:203:ARG:HG2 | 2:F:325:ARG:NE | 2.08 | 0.68 |
| 2:F:81:GLY:HA3 | 2:F:97:PRO:CD | 2.23 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1199:THR:HA | 1:A:1200:PRO:O | 1.93 | 0.68 |
| 1:A:299:MET:CE | 1:A:353:VAL:HB | 2.24 | 0.68 |
| 1:A:297:MET:SD | 1:A:411:LEU:CB | 2.80 | 0.68 |
| 1:A:582:ASP:N | 1:A:583:PRO:CD | 2.56 | 0.68 |
| 1:A:630:ASN:ND2 | 1:A:632:ALA:H | 1.92 | 0.68 |
| 1:A:713:PRO:HA | 1:A:719:LEU:HD13 | 1.75 | 0.68 |
| 1:A:767:ALA:HB3 | 1:A:771:LEU:CD2 | 2.24 | 0.68 |
| 1:A:974:THR:CG2 | 1:A:975:GLN:N | 2.56 | 0.68 |
| 2:B:116:THR:HA | 2:B:120:VAL:CG2 | 2.24 | 0.68 |
| 2:B:417:TYR:C | 2:B:419:GLU:H | 1.97 | 0.68 |
| 2:C:239:LEU:HG | 2:C:336:LEU:HD13 | 1.75 | 0.68 |
| 2:C:357:THR:HA | 2:C:370:LYS:HZ1 | 1.55 | 0.68 |
| 1:D:1129:PHE:HB3 | 1:D:1139:TYR:HA | 1.75 | 0.68 |
| 1:D:880:ALA:CB | 1:D:1187:ARG:O | 2.39 | 0.68 |
| 1:D:1138:ARG:HH22 | 1:D:1191:LYS:HE2 | 1.57 | 0.68 |
| 1:D:131:TYR:HB3 | 1:D:138:HIS:CE1 | 2.29 | 0.68 |
| 1:D:167:PRO:CD | 1:D:168:ALA:N | 2.56 | 0.68 |
| 1:D:203:LEU:O | 1:D:203:LEU:HD23 | 1.93 | 0.68 |
| 1:D:659:HIS:NE2 | 1:D:719:LEU:HB2 | 2.08 | 0.68 |
| 2:E:318:ASN:O | 2:E:321:LYS:N | 2.18 | 0.68 |
| 2:E:443:VAL:CG2 | 2:E:453:ILE:HG21 | 2.20 | 0.68 |
| 2:F:78:PHE:CD1 | 2:F:102:LEU:HD22 | 2.29 | 0.68 |
| 1:A:167:PRO:HB2 | 1:A:177:ARG:CZ | 2.24 | 0.68 |
| 1:A:286:GLY:O | 1:A:287:SER:HB3 | 1.91 | 0.68 |
| 1:A:577:CYS:CB | 1:A:578:PRO:CD | 2.72 | 0.68 |
| 1:A:890:ASP:CG | 1:A:1191:LYS:NZ | 2.47 | 0.68 |
| 2:B:211:ILE:HG23 | 2:B:237:ALA:HB2 | 1.73 | 0.68 |
| 2:B:288:LYS:HG2 | 2:B:302:THR:HG22 | 1.74 | 0.68 |
| 1:D:131:TYR:HB3 | 1:D:138:HIS:HE1 | 1.58 | 0.68 |
| 1:D:307:PHE:HA | 1:D:310:SER:OG | 1.94 | 0.68 |
| 1:D:623:LEU:HD22 | 1:D:667:GLN:OE1 | 1.94 | 0.68 |
| 1:D:645:VAL:HG13 | 1:D:650:ARG:CG | 2.23 | 0.68 |
| 1:D:739:TYR:CD2 | 1:D:740:ASN:N | 2.62 | 0.68 |
| 1:D:770:PHE:HA | 1:D:773:LYS:HG3 | 1.76 | 0.68 |
| 1:D:275:ARG:NH1 | 1:D:843:GLN:NE2 | 2.40 | 0.68 |
| 2:E:377:CYS:HA | 2:E:380:PRO:HG2 | 1.74 | 0.68 |
| 2:E:411:ILE:HD12 | 2:E:411:ILE:N | 2.09 | 0.68 |
| 2:E:450:ASN:HB3 | 2:E:452:LEU:CD2 | 2.23 | 0.68 |
| 2:F:268:MET:N | 2:F:352:ASP:OD2 | 2.27 | 0.68 |
| 1:A:245:ILE:O | 1:A:248:GLU:CD | 2.32 | 0.68 |
| 1:A:498:LYS:O | 1:A:499:LYS:HB3 | 1.91 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:597:ARG:CB | 1:A:616:GLU:OE1 | 2.40 | 0.68 |
| 1:A:741:ASP:CG | 1:A:742:VAL:HG23 | 2.13 | 0.68 |
| 1:A:865:ALA:O | 1:A:868:ASP:OD2 | 2.12 | 0.68 |
| 1:A:884:TYR:N | 1:A:884:TYR:HD1 | 1.91 | 0.68 |
| 2:B:479:ILE:HG22 | 2:B:480:SER:N | 2.07 | 0.68 |
| 2:C:132:HIS:HA | 2:C:182:ARG:HG3 | 1.75 | 0.68 |
| 2:C:206:TYR:O | 2:C:241:TRP:CD1 | 2.47 | 0.68 |
| 2:C:471:LEU:HA | 2:C:474:PHE:CD2 | 2.28 | 0.68 |
| 1:D:347:TRP:HE1 | 1:D:349:ASP:CG | 1.96 | 0.68 |
| 1:D:736:ASN:HA | 1:D:750:PHE:CZ | 2.28 | 0.68 |
| 1:D:922:GLN:NE2 | 1:D:931:LEU:HD13 | 2.08 | 0.68 |
| 2:F:203:ARG:HB3 | 2:F:204:LEU:HD12 | 1.76 | 0.68 |
| 2:F:455:LEU:HA | 2:F:456:ARG:NH2 | 2.07 | 0.68 |
| 2:F:474:PHE:HA | 2:F:477:LYS:HD2 | 1.75 | 0.68 |
| 1:A:869:ARG:CA | 1:A:1201:SER:H | 2.07 | 0.68 |
| 1:A:605:LEU:C | 1:A:781:ALA:HB3 | 2.14 | 0.68 |
| 1:A:792:LEU:HD12 | 1:A:793:GLU:HG2 | 1.76 | 0.68 |
| 1:A:973:LEU:HB3 | 1:A:977:GLU:CB | 2.24 | 0.68 |
| 2:B:463:LYS:HD2 | 2:B:463:LYS:H | 1.58 | 0.68 |
| 2:B:469:SER:C | 2:B:471:LEU:N | 2.47 | 0.68 |
| 1:D:316:LYS:HG2 | 1:D:348:LEU:CG | 2.20 | 0.68 |
| 1:D:301:ILE:HD11 | 1:D:414:PHE:O | 1.94 | 0.68 |
| 1:D:492:LEU:HD22 | 1:D:495:PHE:CZ | 2.29 | 0.68 |
| 1:D:549:LEU:N | 1:D:551:LYS:HZ3 | 1.84 | 0.68 |
| 1:D:622:TYR:N | 1:D:747:CYS:O | 2.26 | 0.68 |
| 1:D:607:TRP:CD1 | 1:D:779:LEU:HA | 2.29 | 0.68 |
| 1:D:847:ALA:HA | 1:D:852:ARG:HB3 | 1.75 | 0.68 |
| 2:E:107:ARG:CG | 2:E:107:ARG:NH1 | 2.33 | 0.68 |
| 2:E:318:ASN:O | 2:E:320:SER:N | 2.27 | 0.68 |
| 2:E:400:GLN:HA | 2:E:403:PHE:HB3 | 1.76 | 0.68 |
| 2:F:314:MET:HB3 | 2:F:315:TYR:CE2 | 2.28 | 0.68 |
| 2:F:322:LEU:C | 2:F:322:LEU:HD22 | 2.13 | 0.68 |
| 1:A:1220:ILE:CD1 | 1:A:1220:ILE:N | 2.57 | 0.68 |
| 1:A:276:ALA:CA | 1:A:279:ARG:HB2 | 2.24 | 0.68 |
| 1:A:313:ILE:HA | 1:A:316:LYS:HE2 | 1.75 | 0.68 |
| 1:A:532:PRO:HB3 | 1:A:534:SER:HB3 | 1.76 | 0.68 |
| 1:A:569:HIS:CG | 1:A:570:PRO:HD2 | 2.29 | 0.68 |
| 1:A:739:TYR:C | 1:A:741:ASP:N | 2.45 | 0.68 |
| 1:A:916:PHE:CD1 | 1:A:919:MET:HB3 | 2.29 | 0.68 |
| 2:B:338:VAL:C | 2:B:339:ASN:HD22 | 1.97 | 0.68 |
| 2:C:384:ALA:HB3 | 2:C:440:THR:HG22 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1206:MET:HA | 2:F:253:ASP:OD2 | 1.94 | 0.68 |
| 1:D:79:LEU:HD23 | 1:D:83:LEU:CD1 | 2.22 | 0.68 |
| 1:D:914:THR:OG1 | 1:D:999:ASP:HB3 | 1.92 | 0.68 |
| 2:E:407:LEU:HA | 2:E:411:ILE:O | 1.93 | 0.68 |
| 2:F:259:ARG:NE | 2:F:339:ASN:HD21 | 1.91 | 0.68 |
| 2:F:442:LEU:H | 2:F:455:LEU:HD22 | 1.58 | 0.68 |
| 1:A:1026:ARG:CB | 1:A:1029:GLN:NE2 | 2.57 | 0.68 |
| 1:A:1165:ALA:HB2 | 1:A:1173:LEU:HG | 1.75 | 0.68 |
| 1:A:194:ALA:HA | 1:A:265:LEU:CB | 2.21 | 0.68 |
| 1:A:393:MET:HE3 | 1:A:396:CYS:SG | 2.33 | 0.68 |
| 2:C:222:LYS:O | 2:C:223:GLN:HB2 | 1.93 | 0.68 |
| 2:C:485:VAL:HG22 | 2:C:485:VAL:OXT | 1.94 | 0.68 |
| 1:D:1209:ARG:HH21 | 2:F:253:ASP:N | 1.92 | 0.68 |
| 1:D:147:SER:HB3 | 1:D:425:ALA:HB2 | 1.74 | 0.68 |
| 1:D:236:THR:OG1 | 1:D:237:SER:N | 2.27 | 0.68 |
| 1:D:241:PRO:O | 1:D:244:LEU:CG | 2.40 | 0.68 |
| 1:D:407:PHE:HD1 | 1:D:411:LEU:HD21 | 1.57 | 0.68 |
| 1:D:603:MET:HB3 | 1:D:605:LEU:HD21 | 1.76 | 0.68 |
| 1:D:901:VAL:HG23 | 1:D:902:LEU:N | 2.08 | 0.68 |
| 2:F:395:LEU:HB3 | 2:F:443:VAL:HG21 | 1.75 | 0.68 |
| 2:F:472:LYS:HA | 2:F:475:LEU:HD11 | 1.76 | 0.68 |
| 1:A:583:PRO:O | 1:A:585:TRP:N | 2.25 | 0.68 |
| 1:A:744:ILE:CG1 | 1:A:745:PRO:CD | 2.71 | 0.68 |
| 2:C:387:VAL:HA | 2:C:443:VAL:O | 1.93 | 0.68 |
| 2:C:456:ARG:HB2 | 2:C:463:LYS:CB | 2.24 | 0.68 |
| 2:C:72:ILE:HD12 | 2:C:76:ARG:HE | 1.57 | 0.68 |
| 1:D:1141:VAL:HG23 | 1:D:1146:ARG:HH21 | 1.58 | 0.68 |
| 1:D:371:LYS:HD3 | 1:D:392:LEU:CD2 | 2.23 | 0.68 |
| 1:D:499:LYS:HZ2 | 1:D:499:LYS:HB2 | 1.59 | 0.68 |
| 1:D:610:PHE:N | 1:D:611:PRO:CD | 2.51 | 0.68 |
| 1:D:660:CYS:HB2 | 1:D:745:PRO:CG | 2.23 | 0.68 |
| 1:D:824:ALA:CA | 1:D:827:ARG:HG3 | 2.24 | 0.68 |
| 1:D:831:TYR:HB2 | 1:D:837:TYR:OH | 1.93 | 0.68 |
| 1:D:427:MET:O | 1:D:846:THR:CG2 | 2.41 | 0.68 |
| 2:E:353:SER:CB | 2:E:372:LEU:HD11 | 2.23 | 0.68 |
| 2:E:431:LYS:HG3 | 2:E:432:TYR:HD1 | 1.59 | 0.68 |
| 2:F:474:PHE:C | 2:F:474:PHE:CD1 | 2.68 | 0.68 |
| 1:A:1005:VAL:CA | 1:A:1008:LEU:HD13 | 2.18 | 0.67 |
| 1:A:359:ALA:HB2 | 1:A:407:PHE:CE2 | 2.26 | 0.67 |
| 1:A:382:MET:SD | 1:A:385:ILE:CG2 | 2.82 | 0.67 |
| 1:A:76:ILE:CG1 | 1:A:911:HIS:NE2 | 2.57 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:395:LEU:HD11 | 2:B:443:VAL:HG12 | 1.76 | 0.67 |
| 2:B:133:HIS:NE2 | 2:C:231:ILE:CG2 | 2.57 | 0.67 |
| 2:C:306:LEU:O | 2:C:306:LEU:HD12 | 1.94 | 0.67 |
| 2:C:439:PHE:CD1 | 2:C:458:ARG:CG | 2.77 | 0.67 |
| 1:D:104:VAL:O | 1:D:108:GLN:HG3 | 1.93 | 0.67 |
| 1:D:127:LEU:O | 1:D:130:LEU:CD2 | 2.42 | 0.67 |
| 1:D:179:GLY:CA | 1:D:182:GLY:N | 2.57 | 0.67 |
| 1:D:312:TRP:CH2 | 1:D:346:ASP:O | 2.47 | 0.67 |
| 1:D:600:PRO:HA | 1:D:603:MET:HB2 | 1.77 | 0.67 |
| 1:D:726:LYS:O | 1:D:727:ASP:CB | 2.41 | 0.67 |
| 2:E:374:LEU:N | 2:E:458:ARG:NH2 | 2.42 | 0.67 |
| 2:F:393:LEU:HD23 | 2:F:396:ARG:HG2 | 1.76 | 0.67 |
| 1:A:1117:LYS:O | 1:A:1121:GLU:HG3 | 1.94 | 0.67 |
| 1:A:255:SER:HB2 | 1:A:257:THR:O | 1.94 | 0.67 |
| 1:A:363:ARG:HH11 | 1:A:406:VAL:HA | 1.58 | 0.67 |
| 1:A:472:GLN:HB3 | 2:C:461:THR:HG23 | 1.76 | 0.67 |
| 1:A:869:ARG:O | 1:A:872:SER:HB2 | 1.94 | 0.67 |
| 2:B:213:VAL:CA | 2:B:235:THR:O | 2.38 | 0.67 |
| 1:D:177:ARG:HG2 | 1:D:178:TYR:H | 1.58 | 0.67 |
| 1:D:316:LYS:CD | 1:D:348:LEU:HD23 | 2.24 | 0.67 |
| 1:D:642:SER:N | 1:D:645:VAL:HG21 | 2.08 | 0.67 |
| 1:D:791:ALA:C | 1:D:795:ASN:HD21 | 1.96 | 0.67 |
| 1:D:847:ALA:HA | 1:D:852:ARG:CA | 2.24 | 0.67 |
| 2:E:218:VAL:C | 2:E:230:SER:HG | 1.96 | 0.67 |
| 2:E:254:PHE:HA | 2:E:257:ARG:HE | 1.59 | 0.67 |
| 2:F:387:VAL:CG2 | 2:F:417:TYR:CA | 2.65 | 0.67 |
| 2:E:129:ASP:CG | 2:F:98:GLY:HA3 | 2.14 | 0.67 |
| 1:A:1043:VAL:HG22 | 1:A:1046:GLU:CB | 2.23 | 0.67 |
| 1:A:1047:ARG:CZ | 1:A:1050:LYS:HD2 | 2.24 | 0.67 |
| 1:A:955:TYR:CD2 | 1:A:1102:GLN:NE2 | 2.62 | 0.67 |
| 1:A:1236:GLN:H | 1:A:1236:GLN:HE21 | 1.40 | 0.67 |
| 1:A:202:CYS:HB2 | 1:A:204:ALA:H | 1.59 | 0.67 |
| 1:A:265:LEU:O | 1:A:265:LEU:HD12 | 1.94 | 0.67 |
| 1:A:276:ALA:O | 1:A:280:GLU:OE1 | 2.11 | 0.67 |
| 2:B:69:LEU:HD21 | 2:B:351:TYR:CZ | 2.30 | 0.67 |
| 1:D:119:PRO:C | 1:D:121:PRO:HD2 | 2.15 | 0.67 |
| 1:D:177:ARG:H | 1:D:218:SER:CB | 2.06 | 0.67 |
| 1:D:273:PHE:HA | 1:D:276:ALA:HB2 | 1.76 | 0.67 |
| 1:D:498:LYS:NZ | 1:D:521:PRO:HB3 | 2.10 | 0.67 |
| 1:D:636:THR:HG22 | 1:D:637:GLY:N | 2.10 | 0.67 |
| 1:D:770:PHE:CE1 | 1:D:968:GLN:HB3 | 2.29 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:E:270:PRO:O | 2:E:273:PHE:HD2 | 1.77 | 0.67 |
| 2:F:134:LYS:HB3 | 2:F:180:LYS:CE | 2.25 | 0.67 |
| 2:F:351:TYR:CD1 | 2:F:355:GLN:HG2 | 2.29 | 0.67 |
| 2:F:360:SER:CB | 2:F:364:LYS:HD2 | 2.24 | 0.67 |
| 2:F:383:VAL:HG22 | 2:F:384:ALA:N | 2.09 | 0.67 |
| 1:A:80:SER:CB | 1:A:125:LEU:HD21 | 2.24 | 0.67 |
| 1:A:500:ALA:HB1 | 1:A:520:ALA:CB | 2.24 | 0.67 |
| 1:A:873:GLU:OE1 | 1:A:875:LYS:HG3 | 1.94 | 0.67 |
| 2:B:217:PRO:C | 2:B:231:ILE:HA | 2.14 | 0.67 |
| 2:B:475:LEU:C | 2:B:479:ILE:HD13 | 2.15 | 0.67 |
| 2:C:389:ARG:CD | 2:C:390:GLY:H | 2.06 | 0.67 |
| 2:C:78:PHE:CD1 | 2:C:102:LEU:HD22 | 2.30 | 0.67 |
| 1:D:273:PHE:HA | 1:D:276:ALA:CB | 2.24 | 0.67 |
| 1:D:483:PRO:O | 1:D:486:TRP:N | 2.26 | 0.67 |
| 1:D:548:CYS:C | 1:D:551:LYS:CD | 2.54 | 0.67 |
| 1:D:515:ILE:CG1 | 1:D:568:GLY:O | 2.42 | 0.67 |
| 1:D:607:TRP:CB | 1:D:779:LEU:HD23 | 2.19 | 0.67 |
| 1:D:847:ALA:HA | 1:D:852:ARG:CB | 2.25 | 0.67 |
| 1:D:112:LEU:HD23 | 1:D:917:GLY:O | 1.94 | 0.67 |
| 2:E:129:ASP:OD2 | 2:F:98:GLY:HA3 | 1.94 | 0.67 |
| 2:E:272:ASN:HA | 2:E:292:ASN:HD22 | 1.55 | 0.67 |
| 1:A:278:ILE:HD13 | 1:A:291:PHE:CD1 | 2.28 | 0.67 |
| 1:A:503:VAL:HG21 | 1:A:521:PRO:HA | 1.74 | 0.67 |
| 1:A:564:GLN:CA | 1:A:564:GLN:HE21 | 2.08 | 0.67 |
| 1:A:711:ALA:O | 1:A:712:VAL:CG2 | 2.42 | 0.67 |
| 2:B:116:THR:O | 2:B:121:PHE:HD2 | 1.77 | 0.67 |
| 2:B:125:VAL:HG22 | 2:B:207:GLY:H | 1.57 | 0.67 |
| 2:B:336:LEU:HD21 | 2:B:338:VAL:CG2 | 2.19 | 0.67 |
| 2:B:426:GLU:N | 2:B:426:GLU:OE1 | 2.27 | 0.67 |
| 2:C:309:HIS:HB3 | 2:C:310:GLU:OE1 | 1.94 | 0.67 |
| 2:C:326:ASP:CG | 2:C:327:GLY:N | 2.46 | 0.67 |
| 1:D:1224:ILE:HD13 | 1:D:1224:ILE:C | 2.15 | 0.67 |
| 1:D:272:SER:HB3 | 1:D:843:GLN:NE2 | 2.10 | 0.67 |
| 1:D:512:LYS:HG2 | 1:D:570:PRO:HG3 | 1.77 | 0.67 |
| 1:D:792:LEU:HA | 1:D:795:ASN:ND2 | 2.09 | 0.67 |
| 1:D:801:TRP:HH2 | 1:D:805:HIS:ND1 | 1.93 | 0.67 |
| 1:D:995:TYR:CG | 1:D:995:TYR:O | 2.47 | 0.67 |
| 2:E:217:PRO:HA | 2:E:231:ILE:HG23 | 1.77 | 0.67 |
| 2:E:335:VAL:HG22 | 2:E:336:LEU:N | 2.10 | 0.67 |
| 2:F:208:LEU:CD1 | 2:F:240:VAL:CB | 2.62 | 0.67 |
| 2:F:213:VAL:HG23 | 2:F:235:THR:OG1 | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:314:MET:CE | 2:F:315:TYR:HE2 | 2.07 | 0.67 |
| 2:F:387:VAL:HA | 2:F:443:VAL:CG2 | 2.05 | 0.67 |
| 2:F:467:HIS:O | 2:F:471:LEU:HD11 | 1.93 | 0.67 |
| 1:A:1040:LYS:O | 1:A:1044:VAL:HB | 1.94 | 0.67 |
| 1:A:769:ASP:OD2 | 1:A:770:PHE:CD2 | 2.47 | 0.67 |
| 1:A:798:ILE:HD11 | 1:A:802:ARG:HE | 1.59 | 0.67 |
| 1:A:296:SER:CB | 1:A:846:THR:O | 2.43 | 0.67 |
| 2:B:343:ASP:HB3 | 2:B:344:ARG:NE | 2.08 | 0.67 |
| 2:B:69:LEU:HD12 | 2:B:70:LEU:N | 2.09 | 0.67 |
| 2:C:306:LEU:H | 2:C:335:VAL:HG11 | 1.56 | 0.67 |
| 1:D:1010:LEU:N | 1:D:1011:PRO:HD2 | 2.08 | 0.67 |
| 1:D:297:MET:SD | 1:D:411:LEU:HD13 | 2.35 | 0.67 |
| 1:D:439:GLN:HG2 | 1:D:835:GLY:HA3 | 1.76 | 0.67 |
| 1:D:461:LYS:HA | 1:D:464:MET:CE | 2.24 | 0.67 |
| 1:D:591:LEU:HD12 | 1:D:591:LEU:O | 1.94 | 0.67 |
| 1:D:613:HIS:ND1 | 1:D:717:LEU:HD22 | 2.09 | 0.67 |
| 2:E:266:PHE:O | 2:E:349:TYR:HE1 | 1.77 | 0.67 |
| 2:F:127:PRO:HD2 | 2:F:128:VAL:H | 1.56 | 0.67 |
| 2:F:456:ARG:HG2 | 2:F:457:SER:N | 2.10 | 0.67 |
| 1:A:1030:ARG:CD | 1:A:1040:LYS:NZ | 2.58 | 0.67 |
| 1:A:169:TRP:O | 1:A:170:ALA:CB | 2.43 | 0.67 |
| 1:A:414:PHE:HA | 1:A:417:ARG:HB2 | 1.75 | 0.67 |
| 1:A:720:THR:HG23 | 1:A:721:ALA:N | 2.08 | 0.67 |
| 2:B:343:ASP:CB | 2:B:344:ARG:HE | 2.07 | 0.67 |
| 1:D:1006:ARG:NH2 | 1:D:1017:GLY:HA3 | 2.09 | 0.67 |
| 1:D:516:GLU:HA | 1:D:565:HIS:HE1 | 1.57 | 0.67 |
| 1:D:904:ASP:CG | 1:D:915:ALA:HB3 | 2.15 | 0.67 |
| 2:E:105:GLU:O | 2:E:108:LYS:HG2 | 1.94 | 0.67 |
| 2:E:244:PRO:HG3 | 2:E:326:ASP:OD2 | 1.95 | 0.67 |
| 2:F:372:LEU:HD21 | 2:F:435:MET:O | 1.95 | 0.67 |
| 1:A:245:ILE:CD1 | 1:A:246:PRO:HD3 | 2.24 | 0.67 |
| 1:A:308:GLN:HB3 | 1:A:1090:GLU:HA | 1.76 | 0.67 |
| 1:A:386:ARG:HA | 1:A:389:PHE:HB3 | 1.76 | 0.67 |
| 1:A:473:LEU:HD23 | 1:A:473:LEU:N | 2.09 | 0.67 |
| 1:A:904:ASP:CB | 1:A:910:MET:O | 2.42 | 0.67 |
| 2:C:193:TYR:HB2 | 2:C:242:PHE:CE2 | 2.29 | 0.67 |
| 1:D:206:GLY:CA | 1:D:245:ILE:HG22 | 2.24 | 0.67 |
| 1:D:550:GLN:N | 1:D:551:LYS:HE3 | 2.10 | 0.67 |
| 1:D:652:ILE:O | 1:D:656:TYR:HD2 | 1.76 | 0.67 |
| 1:D:660:CYS:SG | 1:D:661:LEU:N | 2.68 | 0.67 |
| 2:E:448:LEU:O | 2:E:450:ASN:N | 2.27 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:240:VAL:O | 2:F:336:LEU:HD13 | 1.95 | 0.67 |
| 2:F:344:ARG:CA | 2:F:347:LEU:HD13 | 2.25 | 0.67 |
| 2:F:454:HIS:NE2 | 2:F:472:LYS:HD3 | 2.09 | 0.67 |
| 2:F:79:LEU:HA | 2:F:99:PHE:HA | 1.77 | 0.67 |
| 1:A:1046:GLU:OE1 | 1:A:1049:TRP:CB | 2.43 | 0.67 |
| 1:A:276:ALA:HA | 1:A:279:ARG:CB | 2.24 | 0.67 |
| 1:A:439:GLN:NE2 | 1:A:837:TYR:HE2 | 1.92 | 0.67 |
| 1:A:941:ILE:HG23 | 1:A:942:SER:N | 2.10 | 0.67 |
| 1:A:973:LEU:HB3 | 1:A:977:GLU:HB2 | 1.76 | 0.67 |
| 2:B:323:HIS:HB2 | 2:B:332:VAL:HA | 1.73 | 0.67 |
| 2:B:93:SER:C | 2:B:95:CYS:H | 1.98 | 0.67 |
| 2:C:239:LEU:H | 2:C:338:VAL:CG1 | 2.03 | 0.67 |
| 2:C:455:LEU:HB3 | 2:C:456:ARG:CZ | 2.25 | 0.67 |
| 1:D:1029:GLN:HE21 | 1:D:1030:ARG:HH21 | 1.43 | 0.67 |
| 1:D:285:GLN:HE22 | 1:D:1128:ARG:CG | 2.07 | 0.67 |
| 1:D:1154:GLN:O | 1:D:1157:ASN:HB2 | 1.94 | 0.67 |
| 1:D:245:ILE:HG13 | 1:D:246:PRO:HD3 | 1.75 | 0.67 |
| 1:D:401:TRP:HD1 | 1:D:404:HIS:CD2 | 2.13 | 0.67 |
| 1:D:647:CYS:SG | 1:D:648:PRO:HD2 | 2.35 | 0.67 |
| 1:D:853:ARG:NH1 | 1:D:1105:ALA:HB3 | 2.09 | 0.67 |
| 2:E:257:ARG:O | 2:E:261:GLN:HG3 | 1.95 | 0.67 |
| 2:E:370:LYS:HG3 | 2:E:434:GLU:OE2 | 1.95 | 0.67 |
| 2:F:211:ILE:HG23 | 2:F:236:GLU:O | 1.95 | 0.67 |
| 2:F:471:LEU:CA | 2:F:474:PHE:HD2 | 2.08 | 0.67 |
| 1:A:996:ARG:HH11 | 1:A:1000:GLU:HB3 | 1.57 | 0.67 |
| 1:A:426:GLY:HA2 | 1:A:1117:LYS:NZ | 2.10 | 0.67 |
| 1:A:297:MET:O | 1:A:300:ALA:HB3 | 1.95 | 0.67 |
| 1:A:953:ARG:HD3 | 1:A:986:TYR:CE2 | 2.30 | 0.67 |
| 1:D:364:VAL:O | 1:D:364:VAL:CG1 | 2.43 | 0.67 |
| 1:D:466:LEU:HD13 | 1:D:466:LEU:N | 2.10 | 0.67 |
| 1:D:847:ALA:CA | 1:D:852:ARG:HA | 2.24 | 0.67 |
| 1:D:902:LEU:HD11 | 1:D:1168:LEU:HD22 | 1.75 | 0.67 |
| 2:E:445:GLU:OE2 | 2:E:446:THR:N | 2.26 | 0.67 |
| 2:F:277:ASP:CG | 2:F:287:ASN:HB3 | 2.15 | 0.67 |
| 2:F:300:ILE:HG23 | 2:F:342:LEU:HD11 | 1.75 | 0.67 |
| 2:F:368:HIS:O | 2:F:368:HIS:ND1 | 2.28 | 0.67 |
| 2:F:391:PRO:HD2 | 2:F:394:GLU:HG2 | 1.77 | 0.67 |
| 1:A:1000:GLU:O | 1:A:1004:LEU:HB2 | 1.95 | 0.66 |
| 1:A:1131:ILE:HG23 | 1:A:1132:SER:N | 2.07 | 0.66 |
| 1:A:1165:ALA:CB | 1:A:1173:LEU:HG | 2.25 | 0.66 |
| 1:A:270:ASN:C | 1:A:271:VAL:HG23 | 2.16 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:660:CYS:HB2 | 1:A:745:PRO:CG | 2.25 | 0.66 |
| 1:A:859:TRP:HZ3 | 1:A:878:VAL:HG13 | 1.60 | 0.66 |
| 1:A:875:LYS:O | 1:A:878:VAL:CG2 | 2.39 | 0.66 |
| 1:A:893:SER:HB2 | 1:A:896:LEU:CD2 | 2.25 | 0.66 |
| 1:A:996:ARG:HD2 | 1:A:1000:GLU:O | 1.94 | 0.66 |
| 2:B:101:PRO:N | 2:C:128:VAL:HG21 | 2.10 | 0.66 |
| 2:B:183:GLU:O | 2:B:214:CYS:SG | 2.53 | 0.66 |
| 2:C:129:ASP:OD1 | 2:C:131:LEU:CD2 | 2.43 | 0.66 |
| 2:C:204:LEU:HD21 | 2:C:206:TYR:CG | 2.31 | 0.66 |
| 2:C:305:ASN:HA | 2:C:335:VAL:HG11 | 1.76 | 0.66 |
| 1:D:194:ALA:CB | 1:D:265:LEU:HB2 | 2.25 | 0.66 |
| 1:D:249:VAL:CG2 | 1:D:250:PRO:CD | 2.73 | 0.66 |
| 1:D:259:ARG:HA | 1:D:259:ARG:NE | 2.05 | 0.66 |
| 1:D:504:LYS:O | 1:D:504:LYS:HG3 | 1.95 | 0.66 |
| 1:D:564:GLN:C | 1:D:566:LEU:O | 2.32 | 0.66 |
| 2:E:410:GLY:C | 2:E:411:ILE:HD12 | 2.15 | 0.66 |
| 2:F:241:TRP:CD1 | 2:F:243:THR:CG2 | 2.78 | 0.66 |
| 1:A:110:HIS:O | 1:A:112:LEU:HD12 | 1.94 | 0.66 |
| 1:A:253:ALA:HB2 | 1:A:280:GLU:C | 2.15 | 0.66 |
| 1:A:612:LEU:HD21 | 1:A:614:TYR:O | 1.94 | 0.66 |
| 1:A:633:LYS:HD2 | 1:A:634:LEU:N | 2.11 | 0.66 |
| 2:C:209:ALA:CB | 2:C:238:SER:O | 2.42 | 0.66 |
| 2:C:236:GLU:HA | 2:C:341:ASP:CG | 2.16 | 0.66 |
| 2:C:353:SER:HB2 | 2:C:373:LYS:H | 1.59 | 0.66 |
| 1:D:1009:ASN:C | 1:D:1010:LEU:HG | 2.13 | 0.66 |
| 1:D:1015:THR:OG1 | 1:D:1022:LEU:HD23 | 1.94 | 0.66 |
| 1:D:270:ASN:HA | 1:D:294:THR:OG1 | 1.95 | 0.66 |
| 1:D:270:ASN:CA | 1:D:294:THR:CG2 | 2.71 | 0.66 |
| 1:D:298:HIS:CD2 | 1:D:411:LEU:HD23 | 2.29 | 0.66 |
| 1:D:417:ARG:C | 1:D:418:CYS:SG | 2.74 | 0.66 |
| 1:D:822:PRO:O | 1:D:826:ILE:HD13 | 1.94 | 0.66 |
| 1:D:923:GLY:C | 1:D:931:LEU:HD11 | 2.15 | 0.66 |
| 2:E:394:GLU:O | 2:E:397:GLN:HB2 | 1.94 | 0.66 |
| 2:E:72:ILE:HD11 | 2:E:370:LYS:CE | 2.25 | 0.66 |
| 2:F:298:GLU:OE1 | 2:F:344:ARG:NH2 | 2.28 | 0.66 |
| 1:A:1016:GLU:OE2 | 1:A:1022:LEU:CD2 | 2.42 | 0.66 |
| 1:A:1037:GLN:C | 1:A:1039:LYS:N | 2.46 | 0.66 |
| 1:A:1113:LEU:HB2 | 1:A:1117:LYS:HZ2 | 1.61 | 0.66 |
| 1:A:1129:PHE:CD2 | 1:A:1138:ARG:O | 2.48 | 0.66 |
| 1:A:241:PRO:CA | 1:A:244:LEU:HB2 | 2.23 | 0.66 |
| 1:A:355:SER:HA | 1:A:407:PHE:HE1 | 1.61 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:609:GLY:H | 1:A:610:PHE:HD2 | 1.44 | 0.66 |
| 1:A:74:LEU:C | 1:A:76:ILE:N | 2.42 | 0.66 |
| 1:A:756:ASP:HB3 | 1:A:1057:MET:CG | 2.12 | 0.66 |
| 2:B:113:GLU:O | 2:B:262:TRP:HZ2 | 1.78 | 0.66 |
| 2:C:245:PRO:HG2 | 2:C:246:ARG:HD3 | 1.77 | 0.66 |
| 2:C:342:LEU:CB | 2:C:344:ARG:HD3 | 2.25 | 0.66 |
| 2:C:358:GLU:HA | 2:C:361:PHE:HB2 | 1.78 | 0.66 |
| 2:C:403:PHE:HD1 | 2:C:417:TYR:OH | 1.78 | 0.66 |
| 1:D:224:CYS:C | 1:D:228:LEU:HD23 | 2.15 | 0.66 |
| 1:D:269:HIS:CE1 | 1:D:291:PHE:CA | 2.78 | 0.66 |
| 1:D:307:PHE:O | 1:D:311:LEU:HD12 | 1.96 | 0.66 |
| 2:E:76:ARG:HE | 2:E:431:LYS:HE3 | 1.60 | 0.66 |
| 2:F:125:VAL:CG2 | 2:F:126:PHE:N | 2.55 | 0.66 |
| 2:F:303:LEU:CB | 2:F:337:SER:OG | 2.43 | 0.66 |
| 2:F:314:MET:HE3 | 2:F:315:TYR:HE2 | 1.59 | 0.66 |
| 2:F:367:LEU:O | 2:F:369:ARG:HD2 | 1.95 | 0.66 |
| 1:A:402:ALA:O | 1:A:406:VAL:N | 2.22 | 0.66 |
| 2:B:260:LEU:O | 2:B:264:ARG:CG | 2.43 | 0.66 |
| 2:B:67:GLU:HB3 | 2:B:70:LEU:HD13 | 1.75 | 0.66 |
| 2:C:372:LEU:HD12 | 2:C:373:LYS:N | 2.11 | 0.66 |
| 1:A:552:LEU:HD22 | 2:C:448:LEU:CD2 | 2.25 | 0.66 |
| 1:D:1049:TRP:C | 1:D:1052:GLY:H | 1.99 | 0.66 |
| 1:D:140:ARG:HH11 | 1:D:140:ARG:CG | 2.08 | 0.66 |
| 1:D:768:LYS:O | 1:D:772:PRO:HD2 | 1.95 | 0.66 |
| 1:D:949:PHE:O | 1:D:953:ARG:N | 2.28 | 0.66 |
| 1:D:1209:ARG:HG3 | 2:F:249:ASN:CB | 2.26 | 0.66 |
| 1:D:1208:ARG:NH2 | 2:F:285:LYS:CD | 2.50 | 0.66 |
| 2:F:325:ARG:HG3 | 2:F:325:ARG:NH1 | 1.99 | 0.66 |
| 1:A:1019:TRP:O | 1:A:1020:ILE:HG22 | 1.94 | 0.66 |
| 1:A:1131:ILE:HG21 | 1:A:1138:ARG:H | 1.55 | 0.66 |
| 1:A:213:VAL:O | 1:A:401:TRP:CZ2 | 2.48 | 0.66 |
| 1:A:515:ILE:CG2 | 1:A:565:HIS:HA | 2.15 | 0.66 |
| 1:A:744:ILE:HG12 | 1:A:745:PRO:CD | 2.24 | 0.66 |
| 1:A:962:ALA:CB | 1:A:986:TYR:OH | 2.39 | 0.66 |
| 2:C:129:ASP:O | 2:C:130:ALA:HB3 | 1.94 | 0.66 |
| 2:C:208:LEU:CD1 | 2:C:240:VAL:CB | 2.68 | 0.66 |
| 2:C:335:VAL:CG2 | 2:C:336:LEU:N | 2.57 | 0.66 |
| 2:C:435:MET:SD | 2:C:435:MET:O | 2.53 | 0.66 |
| 2:C:454:HIS:CA | 2:C:468:ILE:HD12 | 2.23 | 0.66 |
| 1:D:857:PRO:O | 1:D:1062:GLU:OE2 | 2.13 | 0.66 |
| 1:D:271:VAL:HA | 1:D:293:ASP:OD2 | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:307:PHE:CD1 | 1:D:307:PHE:N | 2.63 | 0.66 |
| 1:D:408:GLN:O | 1:D:411:LEU:HD12 | 1.95 | 0.66 |
| 1:D:550:GLN:H | 1:D:551:LYS:NZ | 1.92 | 0.66 |
| 1:D:914:THR:OG1 | 1:D:999:ASP:CG | 2.34 | 0.66 |
| 1:D:923:GLY:CA | 1:D:931:LEU:HD11 | 2.26 | 0.66 |
| 2:E:109:ASN:HD22 | 2:E:378:LEU:C | 1.99 | 0.66 |
| 2:F:209:ALA:HB2 | 2:F:239:LEU:HA | 1.76 | 0.66 |
| 2:F:445:GLU:C | 2:F:447:THR:N | 2.43 | 0.66 |
| 1:A:308:GLN:HB3 | 1:A:1090:GLU:CB | 2.25 | 0.66 |
| 1:A:559:LEU:HD23 | 1:A:560:PRO:CD | 2.26 | 0.66 |
| 2:B:323:HIS:HA | 2:B:333:PRO:CD | 2.25 | 0.66 |
| 2:C:288:LYS:HB2 | 2:C:290:TYR:OH | 1.96 | 0.66 |
| 1:D:240:SER:HB2 | 1:D:241:PRO:HD3 | 1.77 | 0.66 |
| 1:D:374:ARG:HD3 | 1:D:392:LEU:CD2 | 2.23 | 0.66 |
| 1:D:552:LEU:O | 2:F:452:LEU:HD21 | 1.96 | 0.66 |
| 2:E:402:LEU:O | 2:E:406:LEU:HD23 | 1.94 | 0.66 |
| 2:E:132:HIS:HB2 | 2:F:233:GLU:CD | 2.16 | 0.66 |
| 2:F:353:SER:HB2 | 2:F:373:LYS:N | 2.08 | 0.66 |
| 2:F:368:HIS:NE2 | 2:F:370:LYS:CD | 2.58 | 0.66 |
| 2:F:81:GLY:HA3 | 2:F:97:PRO:CG | 2.25 | 0.66 |
| 1:A:515:ILE:N | 1:A:515:ILE:HD12 | 2.11 | 0.66 |
| 1:A:597:ARG:O | 1:A:598:VAL:HB | 1.96 | 0.66 |
| 1:A:652:ILE:O | 1:A:655:LEU:HG | 1.95 | 0.66 |
| 1:A:436:PRO:HD2 | 1:A:879:GLN:CD | 2.15 | 0.66 |
| 2:B:235:THR:H | 2:B:343:ASP:HB2 | 1.60 | 0.66 |
| 2:B:425:LEU:HD23 | 2:B:425:LEU:O | 1.96 | 0.66 |
| 1:D:1175:GLN:O | 1:D:1177:VAL:N | 2.28 | 0.66 |
| 1:D:418:CYS:N | 1:D:419:PRO:HD3 | 2.10 | 0.66 |
| 1:D:577:CYS:C | 1:D:579:ARG:N | 2.36 | 0.66 |
| 1:D:870:VAL:HG13 | 1:D:871:GLY:N | 2.10 | 0.66 |
| 2:E:108:LYS:NZ | 2:E:108:LYS:HB2 | 2.11 | 0.66 |
| 2:F:242:PHE:HB3 | 2:F:333:PRO:CB | 2.18 | 0.66 |
| 1:D:1209:ARG:NH2 | 2:F:253:ASP:CA | 2.50 | 0.66 |
| 2:F:344:ARG:CA | 2:F:347:LEU:HD22 | 2.25 | 0.66 |
| 2:F:413:VAL:HG12 | 2:F:414:TRP:N | 2.10 | 0.66 |
| 2:F:469:SER:O | 2:F:472:LYS:HB2 | 1.95 | 0.66 |
| 1:A:1002:GLU:O | 1:A:1006:ARG:N | 2.26 | 0.66 |
| 1:A:717:LEU:O | 1:A:721:ALA:CB | 2.44 | 0.66 |
| 1:A:769:ASP:O | 1:A:772:PRO:HD2 | 1.96 | 0.66 |
| 1:A:439:GLN:HG3 | 1:A:836:LEU:H | 1.59 | 0.66 |
| 1:A:858:THR:HB | 1:A:859:TRP:CD1 | 2.31 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:204:LEU:HD22 | 2:B:205:PRO:HB3 | 1.77 | 0.66 |
| 2:B:323:HIS:CB | 2:B:332:VAL:CA | 2.71 | 0.66 |
| 2:C:302:THR:C | 2:C:303:LEU:HD12 | 2.16 | 0.66 |
| 2:C:395:LEU:CD1 | 2:C:444:THR:HA | 2.25 | 0.66 |
| 1:D:1165:ALA:CB | 1:D:1173:LEU:CD1 | 2.72 | 0.66 |
| 1:D:176:THR:N | 1:D:185:VAL:CG1 | 2.59 | 0.66 |
| 1:D:386:ARG:HA | 1:D:389:PHE:CD2 | 2.31 | 0.66 |
| 1:D:657:ARG:HA | 1:D:660:CYS:HB3 | 1.77 | 0.66 |
| 1:D:771:LEU:HD12 | 1:D:771:LEU:N | 2.11 | 0.66 |
| 1:D:802:ARG:CG | 1:D:803:ASN:OD1 | 2.44 | 0.66 |
| 1:D:826:ILE:HG12 | 1:D:827:ARG:N | 2.10 | 0.66 |
| 1:D:87:ILE:HG22 | 1:D:88:PHE:H | 1.61 | 0.66 |
| 2:E:424:SER:C | 2:E:428:LEU:HD11 | 2.16 | 0.66 |
| 2:E:380:PRO:HG3 | 2:E:438:LEU:HD13 | 1.77 | 0.66 |
| 2:E:475:LEU:HB3 | 2:E:479:ILE:HD11 | 1.78 | 0.66 |
| 2:F:415:PRO:HB3 | 2:F:417:TYR:HE2 | 1.57 | 0.66 |
| 1:A:1006:ARG:O | 1:A:1010:LEU:HD12 | 1.95 | 0.66 |
| 1:A:1007:GLU:O | 1:A:1011:PRO:CD | 2.44 | 0.66 |
| 1:A:355:SER:O | 1:A:358:LEU:HG | 1.96 | 0.66 |
| 1:A:522:GLY:O | 1:A:524:PRO:HD3 | 1.95 | 0.66 |
| 2:C:439:PHE:HD1 | 2:C:458:ARG:CG | 2.07 | 0.66 |
| 1:D:652:ILE:CA | 1:D:655:LEU:HG | 2.18 | 0.66 |
| 2:F:306:LEU:HD11 | 2:F:310:GLU:OE1 | 1.96 | 0.66 |
| 1:A:1047:ARG:NH1 | 1:A:1050:LYS:HB2 | 2.11 | 0.66 |
| 1:A:885:THR:C | 1:A:1146:ARG:HE | 1.99 | 0.66 |
| 1:A:166:PRO:HG3 | 1:A:398:GLN:OE1 | 1.96 | 0.66 |
| 1:A:192:GLU:OE1 | 1:A:265:LEU:HD23 | 1.96 | 0.66 |
| 1:A:271:VAL:HG21 | 1:A:295:MET:HE3 | 1.77 | 0.66 |
| 1:A:298:HIS:HE2 | 1:A:351:SER:C | 2.00 | 0.66 |
| 1:A:346:ASP:OD2 | 1:A:1040:LYS:HD2 | 1.97 | 0.66 |
| 1:A:522:GLY:C | 1:A:524:PRO:HD3 | 2.16 | 0.66 |
| 1:A:732:TYR:CD1 | 1:A:755:LYS:NZ | 2.62 | 0.66 |
| 1:A:830:ASP:C | 1:A:831:TYR:HD1 | 2.00 | 0.66 |
| 1:A:989:THR:CA | 1:A:998:SER:OG | 2.44 | 0.66 |
| 2:B:453:ILE:H | 2:B:453:ILE:HD13 | 1.60 | 0.66 |
| 2:B:70:LEU:HD22 | 2:B:88:ARG:NH1 | 2.05 | 0.66 |
| 2:B:74:GLN:O | 2:B:77:HIS:N | 2.29 | 0.66 |
| 2:B:231:ILE:CD1 | 2:C:135:PRO:HG3 | 2.25 | 0.66 |
| 1:D:194:ALA:CA | 1:D:265:LEU:HB2 | 2.25 | 0.66 |
| 1:D:457:ARG:HA | 1:D:460:LYS:CD | 2.26 | 0.66 |
| 1:D:580:LEU:HD21 | 1:D:593:SER:OG | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:601:LYS:HD2 | 1:D:616:GLU:CG | 2.26 | 0.66 |
| 1:D:658:LYS:HE2 | 1:D:713:PRO:HB2 | 1.76 | 0.66 |
| 1:D:719:LEU:HD12 | 1:D:720:THR:OG1 | 1.95 | 0.66 |
| 1:D:736:ASN:HB3 | 1:D:748:TRP:O | 1.96 | 0.66 |
| 1:D:737:GLY:N | 1:D:750:PHE:CE1 | 2.64 | 0.66 |
| 1:D:798:ILE:CG2 | 1:D:869:ARG:NH2 | 2.56 | 0.66 |
| 1:D:873:GLU:HB3 | 1:D:1200:PRO:HD2 | 1.78 | 0.66 |
| 2:F:317:GLY:CA | 2:F:320:SER:CB | 2.72 | 0.66 |
| 1:A:1207:GLU:CA | 1:A:1210:TYR:HD1 | 2.09 | 0.65 |
| 1:A:432:VAL:HG12 | 1:A:432:VAL:O | 1.95 | 0.65 |
| 1:A:606:THR:H | 1:A:613:HIS:HA | 1.60 | 0.65 |
| 1:A:659:HIS:ND1 | 1:A:716:PRO:HA | 2.11 | 0.65 |
| 1:A:768:LYS:HG2 | 1:A:769:ASP:H | 1.59 | 0.65 |
| 1:A:861:THR:HG22 | 1:A:861:THR:O | 1.96 | 0.65 |
| 1:A:884:TYR:N | 1:A:884:TYR:CD1 | 2.65 | 0.65 |
| 1:A:905:ALA:N | 1:A:910:MET:HA | 2.11 | 0.65 |
| 1:D:1015:THR:HG23 | 1:D:1026:ARG:CB | 2.25 | 0.65 |
| 1:D:1131:ILE:CD1 | 1:D:1138:ARG:HB2 | 2.27 | 0.65 |
| 1:D:1165:ALA:HB2 | 1:D:1173:LEU:CD1 | 2.14 | 0.65 |
| 1:D:175:TRP:HB2 | 1:D:185:VAL:HG22 | 1.78 | 0.65 |
| 1:D:208:CYS:SG | 1:D:244:LEU:CD1 | 2.84 | 0.65 |
| 1:D:292:LEU:HD23 | 1:D:297:MET:CE | 2.26 | 0.65 |
| 1:D:307:PHE:HD1 | 1:D:307:PHE:N | 1.93 | 0.65 |
| 1:D:481:GLU:O | 1:D:482:ASP:CG | 2.34 | 0.65 |
| 1:D:485:LEU:O | 1:D:489:GLU:HG3 | 1.96 | 0.65 |
| 1:D:504:LYS:O | 1:D:504:LYS:CG | 2.44 | 0.65 |
| 1:D:608:ASP:OD1 | 1:D:611:PRO:N | 2.29 | 0.65 |
| 1:D:616:GLU:O | 1:D:725:PRO:CD | 2.37 | 0.65 |
| 1:D:618:HIS:CB | 1:D:725:PRO:HG2 | 2.25 | 0.65 |
| 1:D:664:GLY:HA2 | 1:D:667:GLN:HG3 | 1.77 | 0.65 |
| 2:E:263:TRP:CZ3 | 2:E:300:ILE:HD12 | 2.31 | 0.65 |
| 2:E:79:LEU:C | 2:E:100:GLY:HA3 | 2.17 | 0.65 |
| 2:F:347:LEU:HA | 2:F:350:LEU:HD11 | 1.76 | 0.65 |
| 1:A:271:VAL:CG2 | 1:A:295:MET:HE3 | 2.27 | 0.65 |
| 1:A:309:ARG:HH12 | 1:A:352:SER:HA | 1.61 | 0.65 |
| 1:A:601:LYS:NZ | 1:A:721:ALA:O | 2.28 | 0.65 |
| 1:A:616:GLU:CD | 1:A:724:GLY:H | 2.00 | 0.65 |
| 1:A:588:GLY:CA | 1:A:806:LYS:NZ | 2.59 | 0.65 |
| 1:A:879:GLN:CA | 1:A:879:GLN:HE21 | 2.08 | 0.65 |
| 2:B:122:ARG:HD3 | 2:B:124:GLN:NE2 | 2.11 | 0.65 |
| 2:B:215:PHE:HE2 | 2:B:233:GLU:HG2 | 1.60 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:407:LEU:HD21 | 2:C:120:VAL:CA | 2.14 | 0.65 |
| 2:B:74:GLN:HB2 | 2:B:77:HIS:HD2 | 1.62 | 0.65 |
| 2:C:406:LEU:HA | 2:C:409:ASN:HD22 | 1.57 | 0.65 |
| 2:C:447:THR:HG22 | 2:C:455:LEU:HD11 | 1.77 | 0.65 |
| 2:C:80:SER:OG | 2:C:99:PHE:O | 2.12 | 0.65 |
| 1:D:1131:ILE:HD11 | 1:D:1138:ARG:HB2 | 1.78 | 0.65 |
| 1:D:1138:ARG:HG2 | 1:D:1138:ARG:NH1 | 2.07 | 0.65 |
| 1:D:78:MET:HE3 | 1:D:121:PRO:HB2 | 1.77 | 0.65 |
| 1:D:641:GLU:O | 1:D:645:VAL:HG21 | 1.96 | 0.65 |
| 1:D:711:ALA:C | 1:D:713:PRO:HD3 | 2.16 | 0.65 |
| 1:D:275:ARG:CZ | 1:D:843:GLN:HG2 | 2.26 | 0.65 |
| 1:D:900:ALA:C | 1:D:915:ALA:HB1 | 2.16 | 0.65 |
| 1:D:923:GLY:O | 1:D:927:ARG:O | 2.14 | 0.65 |
| 1:D:948:ILE:HG21 | 1:D:1071:ARG:CB | 2.25 | 0.65 |
| 2:E:101:PRO:HD3 | 2:F:128:VAL:HG21 | 1.78 | 0.65 |
| 2:E:437:ILE:O | 2:E:458:ARG:HD3 | 1.95 | 0.65 |
| 2:F:336:LEU:HD23 | 2:F:337:SER:C | 2.16 | 0.65 |
| 2:F:69:LEU:HD23 | 2:F:351:TYR:CE1 | 2.29 | 0.65 |
| 2:F:395:LEU:HD23 | 2:F:448:LEU:HD11 | 1.77 | 0.65 |
| 1:A:303:GLY:O | 1:A:1025:LEU:CD1 | 2.44 | 0.65 |
| 1:A:190:PRO:HB3 | 1:A:192:GLU:HG3 | 1.78 | 0.65 |
| 1:A:253:ALA:O | 1:A:254:SER:HB3 | 1.95 | 0.65 |
| 1:A:298:HIS:NE2 | 1:A:358:LEU:HD22 | 2.11 | 0.65 |
| 1:A:474:LEU:CD1 | 1:A:474:LEU:N | 2.59 | 0.65 |
| 1:A:601:LYS:HD2 | 1:A:616:GLU:HB3 | 1.78 | 0.65 |
| 1:A:612:LEU:HD23 | 1:A:620:TRP:CB | 2.26 | 0.65 |
| 1:A:664:GLY:HA2 | 1:A:667:GLN:HE21 | 1.61 | 0.65 |
| 1:A:898:ILE:CG1 | 1:A:899:ALA:N | 2.59 | 0.65 |
| 2:B:289:LEU:HB3 | 2:B:300:ILE:CG1 | 2.27 | 0.65 |
| 2:B:303:LEU:HD12 | 2:B:303:LEU:N | 2.11 | 0.65 |
| 2:C:204:LEU:HG | 2:C:206:TYR:HB3 | 1.77 | 0.65 |
| 2:C:270:PRO:HA | 2:C:273:PHE:CD2 | 2.32 | 0.65 |
| 2:C:423:SER:HB2 | 2:C:427:GLN:OE1 | 1.96 | 0.65 |
| 2:C:439:PHE:HB3 | 2:C:458:ARG:HB2 | 1.78 | 0.65 |
| 1:D:1008:LEU:O | 1:D:1011:PRO:HD2 | 1.96 | 0.65 |
| 1:D:1141:VAL:HG23 | 1:D:1146:ARG:NH2 | 2.10 | 0.65 |
| 1:D:297:MET:CG | 1:D:411:LEU:HD22 | 2.21 | 0.65 |
| 1:D:798:ILE:HG22 | 1:D:869:ARG:NH1 | 2.10 | 0.65 |
| 1:D:80:SER:HB2 | 1:D:125:LEU:CB | 2.27 | 0.65 |
| 1:D:999:ASP:O | 1:D:1001:GLY:N | 2.30 | 0.65 |
| 1:A:1026:ARG:HB3 | 1:A:1029:GLN:NE2 | 2.10 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1200:PRO:C | 1:A:1202:ASN:N | 2.42 | 0.65 |
| 1:A:213:VAL:HG21 | 1:A:397:ALA:HA | 1.78 | 0.65 |
| 1:A:498:LYS:HE2 | 1:A:499:LYS:N | 2.08 | 0.65 |
| 1:A:612:LEU:CD2 | 1:A:621:GLY:N | 2.50 | 0.65 |
| 2:B:229:LYS:N | 2:B:229:LYS:HD2 | 2.10 | 0.65 |
| 2:B:269:SER:O | 2:B:271:SER:N | 2.27 | 0.65 |
| 2:C:209:ALA:HB2 | 2:C:239:LEU:HA | 1.77 | 0.65 |
| 2:C:353:SER:CB | 2:C:373:LYS:O | 2.44 | 0.65 |
| 1:A:553:LYS:HD2 | 2:C:468:ILE:HG22 | 1.79 | 0.65 |
| 1:D:1048:ALA:O | 1:D:1052:GLY:N | 2.29 | 0.65 |
| 1:D:267:VAL:O | 1:D:269:HIS:CE1 | 2.49 | 0.65 |
| 1:D:458:GLU:N | 1:D:460:LYS:HZ2 | 1.94 | 0.65 |
| 1:D:461:LYS:HA | 1:D:464:MET:HE3 | 1.78 | 0.65 |
| 1:D:798:ILE:HA | 1:D:869:ARG:NH2 | 2.12 | 0.65 |
| 2:E:130:ALA:N | 2:E:210:GLN:HE22 | 1.94 | 0.65 |
| 2:E:400:GLN:O | 2:E:403:PHE:N | 2.30 | 0.65 |
| 2:F:197:LEU:HD11 | 2:F:322:LEU:CD2 | 2.27 | 0.65 |
| 2:F:294:PRO:HG3 | 2:F:355:GLN:NE2 | 2.11 | 0.65 |
| 2:F:342:LEU:CB | 2:F:344:ARG:HB2 | 2.27 | 0.65 |
| 1:A:1060:LYS:CD | 1:A:1073:PRO:HB2 | 2.25 | 0.65 |
| 1:A:1133:ILE:HD13 | 1:A:1134:HIS:HB2 | 1.78 | 0.65 |
| 1:A:1164:PHE:HD2 | 1:A:1168:LEU:HD11 | 1.60 | 0.65 |
| 1:A:556:THR:CG2 | 2:C:452:LEU:CB | 2.75 | 0.65 |
| 1:A:601:LYS:HE2 | 1:A:616:GLU:OE2 | 1.96 | 0.65 |
| 1:A:624:VAL:O | 1:A:745:PRO:O | 2.15 | 0.65 |
| 1:A:87:ILE:CG2 | 1:A:1166:TYR:OH | 2.44 | 0.65 |
| 2:C:200:VAL:HG12 | 2:C:200:VAL:O | 1.95 | 0.65 |
| 2:C:387:VAL:HG12 | 2:C:443:VAL:HB | 1.79 | 0.65 |
| 1:D:955:TYR:HB3 | 1:D:1098:ASN:CG | 2.16 | 0.65 |
| 1:D:275:ARG:HH21 | 1:D:842:PRO:CA | 2.09 | 0.65 |
| 1:D:279:ARG:HB3 | 1:D:841:LEU:CB | 2.24 | 0.65 |
| 1:D:308:GLN:NE2 | 1:D:1027:LYS:NZ | 2.44 | 0.65 |
| 1:D:407:PHE:CD1 | 1:D:407:PHE:C | 2.70 | 0.65 |
| 1:D:721:ALA:O | 1:D:722:ARG:HB2 | 1.96 | 0.65 |
| 1:D:732:TYR:HD2 | 1:D:732:TYR:N | 1.92 | 0.65 |
| 1:D:783:PRO:HG2 | 1:D:784:GLY:H | 1.61 | 0.65 |
| 2:E:283:GLY:HA3 | 2:E:306:LEU:CA | 2.24 | 0.65 |
| 2:E:323:HIS:O | 2:E:324:GLY:C | 2.34 | 0.65 |
| 2:E:417:TYR:CD1 | 2:E:418:LEU:HG | 2.31 | 0.65 |
| 2:F:431:LYS:HZ1 | 2:F:435:MET:HG2 | 1.60 | 0.65 |
| 1:A:136:ASP:O | 1:A:140:ARG:HG2 | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:211:LEU:HG | 1:A:221:TYR:CB | 2.26 | 0.65 |
| 1:A:305:SER:HB2 | 1:A:308:GLN:HG3 | 1.77 | 0.65 |
| 1:A:660:CYS:SG | 1:A:745:PRO:CG | 2.83 | 0.65 |
| 1:A:862:ALA:HB1 | 1:A:875:LYS:HE3 | 1.79 | 0.65 |
| 2:B:306:LEU:O | 2:B:308:ASP:N | 2.29 | 0.65 |
| 2:C:204:LEU:CD2 | 2:C:206:TYR:CG | 2.80 | 0.65 |
| 1:D:177:ARG:HE | 1:D:216:SER:H | 1.43 | 0.65 |
| 1:D:203:LEU:O | 1:D:204:ALA:C | 2.35 | 0.65 |
| 1:D:313:ILE:HG13 | 1:D:314:ALA:H | 1.62 | 0.65 |
| 1:D:371:LYS:HE2 | 1:D:396:CYS:SG | 2.37 | 0.65 |
| 1:D:546:ARG:C | 1:D:551:LYS:NZ | 2.49 | 0.65 |
| 1:D:668:LEU:O | 1:D:671:GLN:CB | 2.35 | 0.65 |
| 1:D:741:ASP:O | 1:D:742:VAL:HB | 1.95 | 0.65 |
| 1:D:768:LYS:CA | 1:D:772:PRO:HG3 | 2.26 | 0.65 |
| 1:D:780:GLN:OE1 | 1:D:780:GLN:CA | 2.45 | 0.65 |
| 1:D:776:ASP:CB | 1:D:796:LYS:HZ3 | 2.10 | 0.65 |
| 1:D:798:ILE:N | 1:D:869:ARG:NH1 | 2.45 | 0.65 |
| 1:D:929:THR:O | 1:D:933:SER:HB3 | 1.96 | 0.65 |
| 1:D:983:GLN:HA | 1:D:983:GLN:HE21 | 1.62 | 0.65 |
| 2:E:372:LEU:O | 2:E:458:ARG:HD2 | 1.96 | 0.65 |
| 1:A:392:LEU:O | 1:A:395:TYR:N | 2.24 | 0.65 |
| 1:A:479:TYR:O | 1:A:480:LYS:CG | 2.40 | 0.65 |
| 1:A:966:LEU:HD12 | 1:A:967:MET:N | 2.12 | 0.65 |
| 1:A:784:GLY:HA3 | 2:C:363:ARG:HG2 | 1.78 | 0.65 |
| 1:D:876:ALA:CA | 1:D:1189:LEU:HB2 | 2.23 | 0.65 |
| 1:D:177:ARG:HB3 | 1:D:218:SER:CB | 2.22 | 0.65 |
| 1:D:175:TRP:CZ2 | 1:D:183:GLU:HG3 | 2.31 | 0.65 |
| 1:D:301:ILE:O | 1:D:1024:ASP:HB2 | 1.97 | 0.65 |
| 1:D:406:VAL:HG22 | 1:D:407:PHE:N | 2.10 | 0.65 |
| 1:D:913:CYS:O | 1:D:917:GLY:CA | 2.45 | 0.65 |
| 1:D:996:ARG:N | 1:D:996:ARG:HD3 | 2.10 | 0.65 |
| 2:E:200:VAL:O | 2:F:418:LEU:HD21 | 1.96 | 0.65 |
| 2:F:270:PRO:HA | 2:F:273:PHE:CD2 | 2.32 | 0.65 |
| 2:F:375:HIS:HB3 | 2:F:378:LEU:HD22 | 1.77 | 0.65 |
| 1:A:907:PHE:CZ | 1:A:1001:GLY:N | 2.65 | 0.65 |
| 1:A:1133:ILE:CG2 | 1:A:1136:GLU:HB2 | 2.26 | 0.65 |
| 1:A:1236:GLN:N | 1:A:1236:GLN:NE2 | 2.41 | 0.65 |
| 1:A:301:ILE:HD13 | 1:A:414:PHE:CB | 2.27 | 0.65 |
| 1:A:417:ARG:NH1 | 1:A:417:ARG:HG2 | 2.10 | 0.65 |
| 1:A:577:CYS:SG | 1:A:578:PRO:HD3 | 2.37 | 0.65 |
| 1:A:851:THR:CG2 | 1:A:853:ARG:HB2 | 2.27 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:215:PHE:CE2 | 2:B:233:GLU:HG2 | 2.32 | 0.65 |
| 2:B:67:GLU:CB | 2:B:70:LEU:HB2 | 2.24 | 0.65 |
| 1:D:550:GLN:N | 1:D:551:LYS:HZ2 | 1.95 | 0.65 |
| 1:D:576:LEU:CG | 1:D:577:CYS:N | 2.58 | 0.65 |
| 1:D:804:ALA:HB1 | 1:D:808:ILE:HD11 | 1.78 | 0.65 |
| 1:D:957:ALA:HB3 | 1:D:961:PHE:CE1 | 2.32 | 0.65 |
| 2:E:437:ILE:HG22 | 2:E:439:PHE:N | 2.12 | 0.65 |
| 2:F:311:LEU:HA | 2:F:314:MET:HB2 | 1.78 | 0.65 |
| 2:F:385:LEU:O | 2:F:416:GLY:CA | 2.43 | 0.65 |
| 1:A:1108:TYR:HA | 1:A:1164:PHE:HZ | 1.61 | 0.65 |
| 1:A:1190:ARG:CZ | 1:A:1197:CYS:CB | 2.70 | 0.65 |
| 1:A:196:VAL:CG1 | 1:A:269:HIS:CD2 | 2.78 | 0.65 |
| 1:A:271:VAL:C | 1:A:275:ARG:HD3 | 2.18 | 0.65 |
| 1:A:813:VAL:HG11 | 1:A:815:TRP:CZ2 | 2.32 | 0.65 |
| 1:A:823:ARG:C | 1:A:825:VAL:N | 2.49 | 0.65 |
| 1:A:848:GLY:O | 1:A:849:THR:HB | 1.96 | 0.65 |
| 2:B:217:PRO:HB2 | 2:B:231:ILE:HG22 | 1.79 | 0.65 |
| 2:B:309:HIS:ND1 | 2:B:309:HIS:N | 2.43 | 0.65 |
| 2:C:309:HIS:HA | 2:C:312:LEU:HD12 | 1.78 | 0.65 |
| 2:C:403:PHE:HD2 | 2:C:403:PHE:C | 2.00 | 0.65 |
| 2:C:439:PHE:CB | 2:C:457:SER:O | 2.44 | 0.65 |
| 2:C:474:PHE:C | 2:C:474:PHE:CD1 | 2.70 | 0.65 |
| 1:D:944:GLU:CD | 1:D:1071:ARG:NH1 | 2.51 | 0.65 |
| 1:D:113:TRP:HA | 1:D:116:PRO:HG2 | 1.77 | 0.65 |
| 1:D:256:PRO:HB3 | 1:D:281:GLN:CB | 2.26 | 0.65 |
| 1:D:460:LYS:CA | 1:D:460:LYS:HE2 | 2.19 | 0.65 |
| 1:D:502:LYS:HG2 | 1:D:506:GLU:OE1 | 1.97 | 0.65 |
| 1:D:616:GLU:C | 1:D:617:ARG:HG3 | 2.16 | 0.65 |
| 1:D:618:HIS:HA | 1:D:762:VAL:HG21 | 1.78 | 0.65 |
| 1:D:612:LEU:HG | 1:D:622:TYR:N | 2.10 | 0.65 |
| 2:E:240:VAL:HG12 | 2:E:242:PHE:CE2 | 2.31 | 0.65 |
| 2:F:290:TYR:HA | 2:F:298:GLU:O | 1.97 | 0.65 |
| 2:F:445:GLU:C | 2:F:447:THR:H | 1.98 | 0.65 |
| 1:A:1209:ARG:HH22 | 2:C:256:LEU:CD2 | 2.10 | 0.65 |
| 1:A:608:ASP:C | 1:A:620:TRP:CH2 | 2.71 | 0.65 |
| 2:B:114:TRP:O | 2:B:117:SER:HB3 | 1.97 | 0.65 |
| 2:B:293:PHE:HB2 | 2:B:297:LYS:HA | 1.79 | 0.65 |
| 2:B:324:GLY:HA3 | 2:B:325:ARG:NH2 | 2.12 | 0.65 |
| 2:C:305:ASN:CA | 2:C:335:VAL:HG11 | 2.27 | 0.65 |
| 2:C:464:GLU:OE2 | 2:C:466:MET:HG2 | 1.97 | 0.65 |
| 1:D:1136:GLU:OE2 | 1:D:1191:LYS:HE3 | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:719:LEU:CG | 1:D:720:THR:H | 2.09 | 0.65 |
| 1:D:897:TRP:CZ2 | 1:D:1173:LEU:HD22 | 2.32 | 0.65 |
| 1:D:112:LEU:HD23 | 1:D:920:THR:HB | 1.78 | 0.65 |
| 2:E:194:VAL:HG13 | 2:E:195:ASN:H | 1.59 | 0.65 |
| 2:F:242:PHE:HA | 2:F:334:CYS:O | 1.96 | 0.65 |
| 2:F:309:HIS:CA | 2:F:312:LEU:HD12 | 2.25 | 0.65 |
| 1:A:1122:GLU:C | 1:A:1123:PHE:CD1 | 2.70 | 0.64 |
| 1:A:1232:GLU:OE2 | 1:A:1234:ARG:NH2 | 2.30 | 0.64 |
| 1:A:228:LEU:HD23 | 1:A:229:VAL:H | 1.62 | 0.64 |
| 1:A:417:ARG:HH11 | 1:A:417:ARG:CG | 2.10 | 0.64 |
| 1:A:418:CYS:N | 1:A:419:PRO:CD | 2.60 | 0.64 |
| 1:A:493:GLN:O | 1:A:494:GLU:CG | 2.42 | 0.64 |
| 1:A:553:LYS:O | 1:A:556:THR:HB | 1.97 | 0.64 |
| 1:A:612:LEU:HD23 | 1:A:620:TRP:CA | 2.28 | 0.64 |
| 1:A:612:LEU:HD23 | 1:A:620:TRP:HA | 1.79 | 0.64 |
| 2:B:396:ARG:HG3 | 2:B:417:TYR:CB | 2.25 | 0.64 |
| 2:C:129:ASP:OD1 | 2:C:131:LEU:CD1 | 2.44 | 0.64 |
| 2:C:431:LYS:CA | 2:C:434:GLU:OE1 | 2.38 | 0.64 |
| 2:C:473:ASP:CA | 2:C:476:ILE:HG23 | 2.24 | 0.64 |
| 1:D:404:HIS:O | 1:D:408:GLN:N | 2.29 | 0.64 |
| 1:D:462:SER:O | 1:D:466:LEU:HD22 | 1.97 | 0.64 |
| 1:D:481:GLU:O | 1:D:482:ASP:OD1 | 2.15 | 0.64 |
| 1:D:608:ASP:O | 1:D:610:PHE:N | 2.30 | 0.64 |
| 1:D:658:LYS:HE3 | 1:D:713:PRO:CG | 2.27 | 0.64 |
| 1:D:770:PHE:O | 1:D:774:MET:CG | 2.45 | 0.64 |
| 1:D:854:ALA:O | 1:D:855:VAL:HG22 | 1.96 | 0.64 |
| 2:E:205:PRO:CG | 2:E:241:TRP:HE1 | 2.10 | 0.64 |
| 2:E:418:LEU:HD13 | 2:F:122:ARG:HE | 1.62 | 0.64 |
| 2:F:238:SER:HA | 2:F:338:VAL:CG1 | 2.24 | 0.64 |
| 1:A:907:PHE:CE1 | 1:A:1001:GLY:HA3 | 2.31 | 0.64 |
| 1:A:1145:ASP:CA | 1:A:1148:ARG:HB2 | 2.28 | 0.64 |
| 1:A:1153:LEU:HD13 | 1:A:1157:ASN:ND2 | 2.13 | 0.64 |
| 1:A:444:TYR:CE2 | 1:A:874:LEU:HA | 2.32 | 0.64 |
| 1:A:645:VAL:O | 1:A:646:VAL:CG1 | 2.38 | 0.64 |
| 1:A:744:ILE:HB | 1:A:745:PRO:CD | 2.24 | 0.64 |
| 1:A:849:THR:HG22 | 1:A:851:THR:N | 2.08 | 0.64 |
| 1:A:907:PHE:HZ | 1:A:1001:GLY:H | 1.45 | 0.64 |
| 2:B:341:ASP:O | 2:B:344:ARG:HD2 | 1.97 | 0.64 |
| 2:B:99:PHE:HE1 | 2:B:343:ASP:OD1 | 1.81 | 0.64 |
| 2:C:242:PHE:HB3 | 2:C:333:PRO:CB | 2.21 | 0.64 |
| 2:C:371:VAL:HG23 | 2:C:433:ASP:HB3 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:1014:ARG:CD | 1:D:1026:ARG:HG3 | 2.27 | 0.64 |
| 1:D:142:LEU:HD22 | 1:D:1118:TRP:CD1 | 2.33 | 0.64 |
| 1:D:1141:VAL:HG21 | 1:D:1149:ALA:CB | 2.27 | 0.64 |
| 1:D:278:ILE:CD1 | 1:D:291:PHE:HD1 | 2.10 | 0.64 |
| 1:D:301:ILE:O | 1:D:1024:ASP:OD1 | 2.15 | 0.64 |
| 1:D:408:GLN:HA | 1:D:411:LEU:HD11 | 1.78 | 0.64 |
| 1:D:591:LEU:CD1 | 1:D:594:LEU:CG | 2.70 | 0.64 |
| 1:D:732:TYR:HB3 | 1:D:755:LYS:NZ | 2.12 | 0.64 |
| 2:E:239:LEU:HD23 | 2:E:338:VAL:CG2 | 2.26 | 0.64 |
| 2:E:261:GLN:O | 2:E:265:LYS:HB2 | 1.97 | 0.64 |
| 2:E:451:GLY:C | 2:E:452:LEU:HD22 | 2.17 | 0.64 |
| 1:A:1033:ALA:O | 1:A:1034:ARG:HB2 | 1.97 | 0.64 |
| 1:A:1131:ILE:HG21 | 1:A:1137:VAL:HA | 1.75 | 0.64 |
| 1:A:1190:ARG:HD3 | 1:A:1197:CYS:SG | 2.38 | 0.64 |
| 1:A:301:ILE:HD13 | 1:A:414:PHE:HB2 | 1.79 | 0.64 |
| 1:A:813:VAL:CG2 | 1:A:814:VAL:H | 2.10 | 0.64 |
| 1:A:898:ILE:HD11 | 1:A:1101:VAL:CG1 | 2.27 | 0.64 |
| 2:B:311:LEU:CD1 | 2:B:322:LEU:HD13 | 2.27 | 0.64 |
| 2:C:205:PRO:O | 2:C:241:TRP:NE1 | 2.27 | 0.64 |
| 2:C:357:THR:O | 2:C:358:GLU:CG | 2.44 | 0.64 |
| 1:A:472:GLN:CG | 2:C:460:THR:CA | 2.67 | 0.64 |
| 1:D:1026:ARG:CD | 1:D:1026:ARG:N | 2.60 | 0.64 |
| 1:D:608:ASP:HA | 1:D:620:TRP:CZ3 | 2.33 | 0.64 |
| 2:E:253:ASP:O | 2:E:256:LEU:HB3 | 1.96 | 0.64 |
| 2:F:240:VAL:C | 2:F:336:LEU:HB3 | 2.18 | 0.64 |
| 2:F:237:ALA:O | 2:F:339:ASN:O | 2.16 | 0.64 |
| 1:D:472:GLN:HG3 | 2:F:460:THR:OG1 | 1.97 | 0.64 |
| 1:A:213:VAL:HG11 | 1:A:397:ALA:HB1 | 1.80 | 0.64 |
| 1:A:282:TYR:OH | 1:A:432:VAL:HG22 | 1.97 | 0.64 |
| 1:A:484:TRP:CE3 | 1:A:484:TRP:HA | 2.32 | 0.64 |
| 1:A:729:GLN:HB2 | 1:A:731:SER:OG | 1.98 | 0.64 |
| 1:A:886:LEU:HD22 | 1:A:1140:LEU:HG | 1.78 | 0.64 |
| 1:A:755:LYS:HD3 | 1:A:964:ARG:HH11 | 1.58 | 0.64 |
| 2:B:396:ARG:HH11 | 2:B:417:TYR:HD2 | 1.39 | 0.64 |
| 2:B:374:LEU:N | 2:B:458:ARG:NH2 | 2.38 | 0.64 |
| 2:C:228:VAL:HG23 | 2:C:228:VAL:O | 1.98 | 0.64 |
| 2:C:386:ASP:O | 2:C:387:VAL:HG13 | 1.96 | 0.64 |
| 1:D:309:ARG:O | 1:D:313:ILE:N | 2.25 | 0.64 |
| 1:D:302:SER:CB | 1:D:351:SER:CB | 2.73 | 0.64 |
| 1:D:653:GLU:O | 1:D:656:TYR:HB2 | 1.97 | 0.64 |
| 1:D:618:HIS:HB2 | 1:D:725:PRO:HG2 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:101:PRO:N | 2:F:128:VAL:HG21 | 2.12 | 0.64 |
| 2:E:288:LYS:HB3 | 2:E:299:LEU:HD12 | 1.79 | 0.64 |
| 2:F:446:THR:O | 2:F:450:ASN:N | 2.30 | 0.64 |
| 1:A:1043:VAL:HG13 | 1:A:1046:GLU:CB | 2.10 | 0.64 |
| 1:A:1129:PHE:HB3 | 1:A:1139:TYR:HA | 1.80 | 0.64 |
| 1:A:113:TRP:HA | 1:A:116:PRO:HD3 | 1.79 | 0.64 |
| 1:A:1188:CYS:O | 1:A:1189:LEU:HD22 | 1.97 | 0.64 |
| 1:A:163:PRO:CB | 1:A:164:PRO:CD | 2.75 | 0.64 |
| 1:A:276:ALA:C | 1:A:279:ARG:H | 2.01 | 0.64 |
| 1:A:274:ASP:C | 1:A:276:ALA:N | 2.48 | 0.64 |
| 1:A:608:ASP:HB3 | 1:A:779:LEU:HB2 | 1.78 | 0.64 |
| 1:A:812:MET:C | 1:A:813:VAL:HG12 | 2.18 | 0.64 |
| 1:A:880:ALA:H | 1:A:881:PRO:HD3 | 1.61 | 0.64 |
| 2:B:114:TRP:NE1 | 2:B:259:ARG:NE | 2.45 | 0.64 |
| 2:B:389:ARG:HB2 | 2:B:445:GLU:H | 1.62 | 0.64 |
| 2:C:194:VAL:O | 2:C:197:LEU:HB3 | 1.97 | 0.64 |
| 2:C:241:TRP:HZ3 | 2:C:255:TRP:CE2 | 2.16 | 0.64 |
| 2:C:263:TRP:HZ2 | 2:C:301:GLU:OE2 | 1.81 | 0.64 |
| 2:C:317:GLY:CA | 2:C:320:SER:CB | 2.74 | 0.64 |
| 1:A:553:LYS:HD3 | 2:C:468:ILE:HG21 | 1.80 | 0.64 |
| 2:C:475:LEU:HA | 2:C:478:TYR:HB2 | 1.78 | 0.64 |
| 1:D:1067:SER:HB2 | 1:D:1071:ARG:HB3 | 1.79 | 0.64 |
| 1:D:270:ASN:N | 1:D:274:ASP:OD1 | 2.31 | 0.64 |
| 1:D:298:HIS:CE1 | 1:D:362:LEU:HD11 | 2.33 | 0.64 |
| 1:D:282:TYR:CE2 | 1:D:432:VAL:HG13 | 2.32 | 0.64 |
| 2:E:133:HIS:CE1 | 2:F:231:ILE:HG22 | 2.32 | 0.64 |
| 2:E:301:GLU:HG2 | 2:E:303:LEU:HD11 | 1.78 | 0.64 |
| 2:E:324:GLY:N | 2:E:331:VAL:O | 2.30 | 0.64 |
| 2:F:194:VAL:O | 2:F:197:LEU:HD22 | 1.98 | 0.64 |
| 2:F:273:PHE:CE1 | 2:F:291:TYR:HD1 | 2.15 | 0.64 |
| 2:F:301:GLU:HG2 | 2:F:339:ASN:HB3 | 1.78 | 0.64 |
| 2:F:74:GLN:HG3 | 2:F:75:ARG:N | 2.10 | 0.64 |
| 1:A:597:ARG:HB3 | 1:A:616:GLU:OE1 | 1.98 | 0.64 |
| 1:A:937:THR:O | 1:A:940:GLY:N | 2.30 | 0.64 |
| 2:B:423:SER:OG | 2:B:428:LEU:HD22 | 1.97 | 0.64 |
| 2:C:190:LEU:HB2 | 2:C:314:MET:HE1 | 1.79 | 0.64 |
| 2:C:204:LEU:CG | 2:C:206:TYR:HB3 | 2.27 | 0.64 |
| 2:C:243:THR:O | 2:C:334:CYS:SG | 2.56 | 0.64 |
| 1:D:1204:THR:O | 1:D:1205:GLY:C | 2.36 | 0.64 |
| 1:D:142:LEU:O | 1:D:146:GLN:HG2 | 1.97 | 0.64 |
| 1:D:196:VAL:HG12 | 1:D:268:GLY:H | 1.62 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:265:LEU:CD2 | 1:D:267:VAL:HG13 | 2.27 | 0.64 |
| 1:D:455:LEU:HD12 | 1:D:869:ARG:CZ | 2.27 | 0.64 |
| 2:E:200:VAL:CG1 | 2:F:418:LEU:CD2 | 2.76 | 0.64 |
| 2:E:386:ASP:OD2 | 2:E:442:LEU:HA | 1.97 | 0.64 |
| 2:E:437:ILE:HG21 | 2:E:440:THR:OG1 | 1.98 | 0.64 |
| 2:E:475:LEU:O | 2:E:479:ILE:N | 2.31 | 0.64 |
| 2:F:375:HIS:N | 2:F:378:LEU:HD22 | 2.06 | 0.64 |
| 2:F:416:GLY:CA | 2:F:419:GLU:HB3 | 2.28 | 0.64 |
| 2:F:442:LEU:CA | 2:F:455:LEU:HD22 | 2.27 | 0.64 |
| 2:F:82:SER:O | 2:F:83:LYS:HG3 | 1.97 | 0.64 |
| 1:A:604:ALA:CB | 1:A:717:LEU:HD11 | 2.27 | 0.64 |
| 1:A:624:VAL:C | 1:A:745:PRO:O | 2.36 | 0.64 |
| 1:A:829:PRO:HB3 | 1:A:882:PRO:C | 2.17 | 0.64 |
| 1:A:913:CYS:O | 1:A:914:THR:C | 2.35 | 0.64 |
| 2:C:262:TRP:O | 2:C:265:LYS:HB3 | 1.97 | 0.64 |
| 2:C:425:LEU:HD13 | 2:C:442:LEU:HD11 | 1.79 | 0.64 |
| 2:C:455:LEU:C | 2:C:456:ARG:NE | 2.51 | 0.64 |
| 1:D:1027:LYS:CB | 1:D:1091:GLU:HA | 2.27 | 0.64 |
| 1:D:1227:THR:O | 1:D:1227:THR:OG1 | 2.10 | 0.64 |
| 1:D:223:TRP:N | 1:D:223:TRP:CD1 | 2.65 | 0.64 |
| 1:D:288:ARG:NH1 | 1:D:288:ARG:HG3 | 2.13 | 0.64 |
| 1:D:597:ARG:HB3 | 1:D:616:GLU:OE2 | 1.97 | 0.64 |
| 1:D:80:SER:O | 1:D:83:LEU:HD13 | 1.97 | 0.64 |
| 1:D:826:ILE:HG12 | 1:D:827:ARG:H | 1.62 | 0.64 |
| 1:D:948:ILE:HD12 | 1:D:1071:ARG:HB3 | 1.79 | 0.64 |
| 2:F:317:GLY:HA2 | 2:F:320:SER:CB | 2.24 | 0.64 |
| 2:F:384:ALA:HB2 | 2:F:437:ILE:HD12 | 1.77 | 0.64 |
| 2:F:474:PHE:HA | 2:F:477:LYS:HD3 | 1.77 | 0.64 |
| 2:F:376:PRO:HG3 | 2:F:482:ALA:HB1 | 1.79 | 0.64 |
| 1:A:1140:LEU:HD23 | 1:A:1141:VAL:N | 2.12 | 0.64 |
| 1:A:83:LEU:O | 1:A:85:GLU:N | 2.30 | 0.64 |
| 2:C:200:VAL:CG1 | 2:C:204:LEU:HB2 | 2.28 | 0.64 |
| 2:C:351:TYR:O | 2:C:355:GLN:N | 2.24 | 0.64 |
| 2:C:354:PHE:CE1 | 2:C:370:LYS:HB3 | 2.32 | 0.64 |
| 2:C:396:ARG:NH1 | 2:C:397:GLN:CA | 2.60 | 0.64 |
| 2:C:395:LEU:HD21 | 2:C:443:VAL:HB | 1.80 | 0.64 |
| 1:D:1019:TRP:HD1 | 1:D:1020:ILE:N | 1.94 | 0.64 |
| 1:D:1131:ILE:O | 1:D:1137:VAL:HA | 1.98 | 0.64 |
| 1:D:885:THR:O | 1:D:1140:LEU:HD23 | 1.98 | 0.64 |
| 1:D:1207:GLU:OE2 | 1:D:1210:TYR:HE2 | 1.80 | 0.64 |
| 1:D:204:ALA:O | 1:D:205:GLU:HG2 | 1.98 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:271:VAL:HA | 1:D:293:ASP:CG | 2.18 | 0.64 |
| 1:D:586:THR:H | 1:D:587:PRO:HD3 | 1.63 | 0.64 |
| 1:D:592:LEU:CA | 1:D:595:GLN:HG3 | 2.19 | 0.64 |
| 1:D:608:ASP:OD2 | 1:D:612:LEU:HB2 | 1.97 | 0.64 |
| 1:D:73:PRO:HG3 | 1:D:90:GLN:CG | 2.24 | 0.64 |
| 1:D:76:ILE:CB | 1:D:911:HIS:NE2 | 2.61 | 0.64 |
| 1:D:873:GLU:HB3 | 1:D:1200:PRO:HD3 | 1.78 | 0.64 |
| 1:D:914:THR:OG1 | 1:D:999:ASP:CB | 2.46 | 0.64 |
| 1:D:917:GLY:O | 1:D:920:THR:CA | 2.46 | 0.64 |
| 2:F:120:VAL:CG2 | 2:F:121:PHE:N | 2.61 | 0.64 |
| 2:F:456:ARG:HB2 | 2:F:463:LYS:HA | 1.79 | 0.64 |
| 1:A:996:ARG:CZ | 1:A:1003:TRP:HB3 | 2.28 | 0.64 |
| 1:A:192:GLU:C | 1:A:193:ARG:CG | 2.66 | 0.64 |
| 1:A:807:ARG:O | 1:A:810:SER:OG | 2.15 | 0.64 |
| 2:C:238:SER:HA | 2:C:338:VAL:HB | 1.80 | 0.64 |
| 2:C:356:LEU:CD1 | 2:C:359:ASN:HD21 | 2.10 | 0.64 |
| 2:C:456:ARG:HG2 | 2:C:457:SER:N | 2.11 | 0.64 |
| 2:C:454:HIS:CB | 2:C:466:MET:HB2 | 2.26 | 0.64 |
| 1:D:999:ASP:C | 1:D:1001:GLY:H | 2.01 | 0.64 |
| 1:D:116:PRO:HB3 | 1:D:921:LEU:HD11 | 1.78 | 0.64 |
| 1:D:179:GLY:C | 1:D:181:GLU:H | 1.86 | 0.64 |
| 1:D:247:LEU:O | 1:D:248:GLU:CB | 2.44 | 0.64 |
| 1:D:255:SER:HG | 1:D:258:GLN:H | 1.41 | 0.64 |
| 1:D:438:ASN:O | 1:D:441:TRP:CB | 2.45 | 0.64 |
| 1:D:550:GLN:H | 1:D:551:LYS:HZ2 | 1.46 | 0.64 |
| 1:D:633:LYS:CB | 1:D:638:THR:CG2 | 2.76 | 0.64 |
| 2:E:369:ARG:HA | 2:E:430:SER:CB | 2.28 | 0.64 |
| 2:F:241:TRP:CB | 2:F:336:LEU:CB | 2.71 | 0.64 |
| 2:F:403:PHE:O | 2:F:407:LEU:N | 2.28 | 0.64 |
| 2:F:455:LEU:C | 2:F:456:ARG:NE | 2.51 | 0.64 |
| 2:F:468:ILE:HG13 | 2:F:472:LYS:HE3 | 1.79 | 0.64 |
| 1:A:890:ASP:OD1 | 1:A:1136:GLU:HG3 | 1.98 | 0.64 |
| 1:A:528:GLU:OE2 | 1:A:528:GLU:HA | 1.97 | 0.64 |
| 1:A:542:ASP:O | 1:A:546:ARG:N | 2.24 | 0.64 |
| 1:A:606:THR:HG23 | 1:A:613:HIS:H | 1.59 | 0.64 |
| 1:A:648:PRO:O | 1:A:652:ILE:N | 2.28 | 0.64 |
| 1:A:813:VAL:HG23 | 1:A:814:VAL:H | 1.63 | 0.64 |
| 1:A:823:ARG:C | 1:A:825:VAL:H | 2.00 | 0.64 |
| 2:C:253:ASP:O | 2:C:257:ARG:HD2 | 1.98 | 0.64 |
| 2:C:343:ASP:C | 2:C:347:LEU:CD1 | 2.64 | 0.64 |
| 2:C:417:TYR:H | 2:C:417:TYR:HD2 | 0.82 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:474:PHE:HA | 2:C:477:LYS:HD2 | 1.79 | 0.64 |
| 1:D:259:ARG:CA | 1:D:259:ARG:CZ | 2.62 | 0.64 |
| 1:D:556:THR:CA | 1:D:559:LEU:HD23 | 2.21 | 0.64 |
| 1:D:767:ALA:HB3 | 1:D:771:LEU:HB2 | 1.80 | 0.64 |
| 1:D:865:ALA:HB2 | 1:D:872:SER:O | 1.98 | 0.64 |
| 2:E:254:PHE:CB | 2:E:257:ARG:HH11 | 2.08 | 0.64 |
| 2:E:259:ARG:NH1 | 2:E:263:TRP:HE1 | 1.95 | 0.64 |
| 2:F:246:ARG:O | 2:F:247:THR:C | 2.36 | 0.64 |
| 1:A:1040:LYS:CB | 1:A:1044:VAL:HG11 | 2.28 | 0.63 |
| 1:A:192:GLU:HB2 | 1:A:195:LEU:CD2 | 2.29 | 0.63 |
| 1:A:275:ARG:HH21 | 1:A:845:VAL:CA | 2.04 | 0.63 |
| 1:A:624:VAL:CG1 | 1:A:747:CYS:SG | 2.86 | 0.63 |
| 1:A:652:ILE:HA | 1:A:655:LEU:CG | 2.27 | 0.63 |
| 1:A:878:VAL:HG12 | 1:A:879:GLN:NE2 | 2.13 | 0.63 |
| 2:C:203:ARG:N | 2:C:325:ARG:HD3 | 2.13 | 0.63 |
| 2:C:240:VAL:C | 2:C:336:LEU:HB3 | 2.18 | 0.63 |
| 1:D:1116:MET:HE2 | 1:D:1116:MET:HA | 1.80 | 0.63 |
| 1:D:1126:ASP:N | 1:D:1126:ASP:OD1 | 2.30 | 0.63 |
| 1:D:1131:ILE:HD13 | 1:D:1131:ILE:N | 2.11 | 0.63 |
| 1:D:1155:ILE:O | 1:D:1158:LEU:HG | 1.97 | 0.63 |
| 1:D:307:PHE:CD2 | 1:D:1048:ALA:O | 2.51 | 0.63 |
| 1:D:349:ASP:O | 1:D:351:SER:N | 2.31 | 0.63 |
| 1:D:895:GLU:O | 1:D:898:ILE:HG12 | 1.98 | 0.63 |
| 2:E:270:PRO:HA | 2:E:273:PHE:HE2 | 1.59 | 0.63 |
| 2:F:126:PHE:HA | 2:F:209:ALA:C | 2.18 | 0.63 |
| 2:F:308:ASP:OD1 | 2:F:332:VAL:O | 2.16 | 0.63 |
| 2:F:323:HIS:O | 2:F:333:PRO:HD3 | 1.98 | 0.63 |
| 1:A:1210:TYR:CD1 | 1:A:1213:PRO:HG2 | 2.31 | 0.63 |
| 1:A:271:VAL:CG1 | 1:A:272:SER:H | 1.83 | 0.63 |
| 1:A:509:THR:HB | 1:A:513:LEU:HD21 | 1.80 | 0.63 |
| 1:A:556:THR:CG2 | 2:C:452:LEU:HB2 | 2.28 | 0.63 |
| 1:A:591:LEU:HD12 | 1:A:594:LEU:CG | 2.28 | 0.63 |
| 1:A:769:ASP:CG | 1:A:770:PHE:H | 2.01 | 0.63 |
| 1:A:275:ARG:HH22 | 1:A:845:VAL:HA | 1.60 | 0.63 |
| 1:A:944:GLU:CA | 1:A:947:LYS:HE3 | 2.28 | 0.63 |
| 2:B:116:THR:HG22 | 2:B:121:PHE:CE2 | 2.34 | 0.63 |
| 2:B:313:HIS:CD2 | 2:B:314:MET:N | 2.66 | 0.63 |
| 2:C:268:MET:N | 2:C:352:ASP:OD2 | 2.27 | 0.63 |
| 1:D:1026:ARG:CZ | 1:D:1029:GLN:OE1 | 2.46 | 0.63 |
| 1:D:101:ARG:O | 1:D:105:GLU:HG3 | 1.97 | 0.63 |
| 1:D:869:ARG:N | 1:D:1200:PRO:HB2 | 2.08 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:131:TYR:HB2 | 1:D:138:HIS:ND1 | 2.13 | 0.63 |
| 1:D:551:LYS:CE | 1:D:551:LYS:H | 2.10 | 0.63 |
| 1:D:576:LEU:CD1 | 1:D:577:CYS:H | 2.12 | 0.63 |
| 1:D:632:ALA:CB | 1:D:657:ARG:HD2 | 2.28 | 0.63 |
| 1:D:282:TYR:HB2 | 1:D:841:LEU:HD12 | 1.80 | 0.63 |
| 1:D:918:TRP:C | 1:D:920:THR:H | 1.98 | 0.63 |
| 2:E:268:MET:CE | 2:E:373:LYS:HD3 | 2.28 | 0.63 |
| 2:F:300:ILE:HG22 | 2:F:301:GLU:H | 1.62 | 0.63 |
| 2:F:351:TYR:HD1 | 2:F:355:GLN:HG2 | 1.62 | 0.63 |
| 2:F:432:TYR:CG | 2:F:437:ILE:HD11 | 2.32 | 0.63 |
| 2:F:88:ARG:HB2 | 2:F:88:ARG:NH1 | 2.13 | 0.63 |
| 1:A:363:ARG:O | 1:A:364:LEU:HD12 | 1.98 | 0.63 |
| 1:A:433:SER:HB2 | 1:A:1129:PHE:CE1 | 2.33 | 0.63 |
| 1:A:539:PHE:O | 1:A:540:GLN:CB | 2.45 | 0.63 |
| 1:A:586:THR:N | 1:A:587:PRO:HD2 | 2.14 | 0.63 |
| 1:A:652:ILE:O | 1:A:655:LEU:CD1 | 2.46 | 0.63 |
| 1:A:657:ARG:HA | 1:A:660:CYS:HB3 | 1.79 | 0.63 |
| 1:A:868:ASP:O | 1:A:869:ARG:CB | 2.46 | 0.63 |
| 2:B:231:ILE:HD11 | 2:C:135:PRO:CG | 2.29 | 0.63 |
| 2:B:261:GLN:O | 2:B:265:LYS:N | 2.30 | 0.63 |
| 2:C:347:LEU:C | 2:C:350:LEU:HD11 | 2.18 | 0.63 |
| 2:C:387:VAL:HG12 | 2:C:395:LEU:HD22 | 1.80 | 0.63 |
| 2:C:88:ARG:NH1 | 2:C:88:ARG:HB2 | 2.14 | 0.63 |
| 1:D:308:GLN:CD | 1:D:1027:LYS:NZ | 2.51 | 0.63 |
| 1:D:1064:ILE:O | 1:D:1064:ILE:HG23 | 1.97 | 0.63 |
| 1:D:113:TRP:CZ3 | 1:D:116:PRO:HD2 | 2.34 | 0.63 |
| 1:D:1197:CYS:O | 1:D:1199:THR:O | 2.17 | 0.63 |
| 1:D:131:TYR:HB2 | 1:D:138:HIS:CE1 | 2.32 | 0.63 |
| 1:D:371:LYS:HG3 | 1:D:396:CYS:HB2 | 1.80 | 0.63 |
| 1:D:425:ALA:O | 1:D:428:LEU:HD13 | 1.97 | 0.63 |
| 1:D:275:ARG:NH2 | 1:D:842:PRO:HB3 | 2.09 | 0.63 |
| 1:D:967:MET:HA | 1:D:967:MET:CE | 2.27 | 0.63 |
| 2:E:132:HIS:HB2 | 2:F:233:GLU:OE2 | 1.98 | 0.63 |
| 2:E:121:PHE:HA | 2:F:407:LEU:HD11 | 1.80 | 0.63 |
| 2:F:454:HIS:HB2 | 2:F:466:MET:CB | 2.28 | 0.63 |
| 1:A:238:GLN:O | 1:A:242:ALA:HB2 | 1.97 | 0.63 |
| 1:A:436:PRO:CD | 1:A:879:GLN:NE2 | 2.60 | 0.63 |
| 1:A:539:PHE:CE2 | 1:A:540:GLN:HG2 | 2.34 | 0.63 |
| 1:A:893:SER:C | 1:A:895:GLU:N | 2.48 | 0.63 |
| 1:A:919:MET:O | 1:A:920:THR:O | 2.15 | 0.63 |
| 1:A:996:ARG:HB2 | 1:A:1004:LEU:CD2 | 2.26 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:269:SER:C | 2:B:271:SER:H | 2.02 | 0.63 |
| 2:B:374:LEU:N | 2:B:458:ARG:HH22 | 1.90 | 0.63 |
| 2:B:481:SER:HA | 2:B:484:ASN:OD1 | 1.98 | 0.63 |
| 2:C:241:TRP:CB | 2:C:336:LEU:CB | 2.75 | 0.63 |
| 2:C:240:VAL:CA | 2:C:336:LEU:HB3 | 2.28 | 0.63 |
| 1:D:293:ASP:CB | 1:D:296:SER:HB2 | 2.28 | 0.63 |
| 1:D:283:LEU:HA | 1:D:434:TYR:HE1 | 1.61 | 0.63 |
| 1:D:499:LYS:HB2 | 1:D:499:LYS:NZ | 2.13 | 0.63 |
| 1:D:516:GLU:O | 1:D:517:GLY:O | 2.16 | 0.63 |
| 1:D:576:LEU:C | 1:D:577:CYS:O | 2.34 | 0.63 |
| 1:D:612:LEU:HD11 | 1:D:622:TYR:CD2 | 2.33 | 0.63 |
| 1:D:788:GLY:O | 1:D:791:ALA:HB3 | 1.98 | 0.63 |
| 1:D:856:GLU:HG3 | 1:D:860:LEU:HG | 1.81 | 0.63 |
| 1:D:876:ALA:HA | 1:D:1189:LEU:CB | 2.25 | 0.63 |
| 2:E:200:VAL:CG1 | 2:F:418:LEU:HD23 | 2.29 | 0.63 |
| 1:A:1006:ARG:CA | 1:A:1006:ARG:HH11 | 2.12 | 0.63 |
| 1:A:1030:ARG:CZ | 1:A:1040:LYS:HG2 | 2.29 | 0.63 |
| 1:A:1112:MET:HB2 | 1:A:1113:LEU:HD23 | 1.81 | 0.63 |
| 1:A:114:GLY:C | 1:A:116:PRO:HD2 | 2.18 | 0.63 |
| 1:A:890:ASP:OD2 | 1:A:1191:LYS:NZ | 2.30 | 0.63 |
| 1:A:260:ASP:N | 1:A:264:GLN:NE2 | 2.46 | 0.63 |
| 1:A:570:PRO:CB | 1:A:572:TRP:CZ3 | 2.81 | 0.63 |
| 1:A:81:ARG:NH1 | 1:A:126:ARG:HA | 2.12 | 0.63 |
| 1:A:879:GLN:HA | 1:A:879:GLN:HE21 | 1.63 | 0.63 |
| 1:A:885:THR:O | 1:A:1140:LEU:HD23 | 1.98 | 0.63 |
| 2:B:270:PRO:HB3 | 2:B:273:PHE:CE2 | 2.33 | 0.63 |
| 2:C:389:ARG:NE | 2:C:390:GLY:H | 1.94 | 0.63 |
| 1:D:1060:LYS:HA | 1:D:1060:LYS:HE3 | 1.81 | 0.63 |
| 1:D:1133:ILE:O | 1:D:1136:GLU:N | 2.27 | 0.63 |
| 1:D:495:PHE:HB2 | 1:D:573:TYR:HE1 | 1.64 | 0.63 |
| 1:D:658:LYS:O | 1:D:662:GLU:HG2 | 1.98 | 0.63 |
| 1:D:659:HIS:CD2 | 1:D:719:LEU:CB | 2.82 | 0.63 |
| 2:E:375:HIS:ND1 | 2:E:376:PRO:HA | 2.13 | 0.63 |
| 2:F:263:TRP:CZ2 | 2:F:301:GLU:OE2 | 2.51 | 0.63 |
| 2:F:363:ARG:HB3 | 2:F:363:ARG:CZ | 2.29 | 0.63 |
| 2:F:360:SER:HB3 | 2:F:364:LYS:CD | 2.28 | 0.63 |
| 2:F:442:LEU:HB2 | 2:F:455:LEU:CD2 | 2.28 | 0.63 |
| 2:F:449:GLU:C | 2:F:451:GLY:N | 2.43 | 0.63 |
| 2:F:470:LYS:HE3 | 2:F:471:LEU:HD21 | 1.79 | 0.63 |
| 1:A:301:ILE:HG23 | 1:A:302:SER:N | 2.13 | 0.63 |
| 1:A:412:PRO:HG2 | 1:A:413:LEU:N | 2.11 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:503:VAL:HG21 | 1:A:521:PRO:CA | 2.28 | 0.63 |
| 1:A:658:LYS:HB2 | 1:A:713:PRO:O | 1.99 | 0.63 |
| 1:A:898:ILE:HG12 | 1:A:899:ALA:N | 2.14 | 0.63 |
| 1:A:914:THR:CA | 1:A:918:TRP:HB3 | 2.23 | 0.63 |
| 2:C:338:VAL:O | 2:C:339:ASN:C | 2.34 | 0.63 |
| 2:C:425:LEU:HD11 | 2:C:429:TYR:CE2 | 2.34 | 0.63 |
| 1:D:136:ASP:OD2 | 1:D:1167:LYS:HE3 | 1.99 | 0.63 |
| 1:D:196:VAL:HG21 | 1:D:215:ILE:CD1 | 2.26 | 0.63 |
| 1:D:221:TYR:O | 1:D:222:SER:OG | 2.13 | 0.63 |
| 1:D:350:ILE:C | 1:D:352:SER:N | 2.48 | 0.63 |
| 1:D:283:LEU:HA | 1:D:434:TYR:CE1 | 2.33 | 0.63 |
| 1:D:601:LYS:HG2 | 1:D:721:ALA:HA | 1.80 | 0.63 |
| 2:F:375:HIS:HB3 | 2:F:378:LEU:HD13 | 1.80 | 0.63 |
| 2:F:474:PHE:HE1 | 2:F:478:TYR:CD2 | 2.15 | 0.63 |
| 1:A:1006:ARG:CA | 1:A:1006:ARG:NH1 | 2.58 | 0.63 |
| 1:A:1131:ILE:HG23 | 1:A:1137:VAL:HG13 | 1.80 | 0.63 |
| 1:A:1190:ARG:NE | 1:A:1197:CYS:HB2 | 2.12 | 0.63 |
| 1:A:545:ALA:HA | 1:A:548:CYS:SG | 2.38 | 0.63 |
| 1:A:559:LEU:CB | 1:A:560:PRO:CD | 2.77 | 0.63 |
| 1:A:831:TYR:HD1 | 1:A:831:TYR:N | 1.97 | 0.63 |
| 1:A:83:LEU:CD2 | 1:A:89:GLY:HA2 | 2.28 | 0.63 |
| 1:A:974:THR:HG22 | 1:A:975:GLN:N | 2.14 | 0.63 |
| 2:B:381:ILE:HD13 | 2:B:437:ILE:HG23 | 1.79 | 0.63 |
| 2:B:78:PHE:HD1 | 2:B:78:PHE:O | 1.82 | 0.63 |
| 2:C:127:PRO:CD | 2:C:128:VAL:N | 2.60 | 0.63 |
| 2:C:472:LYS:HA | 2:C:475:LEU:CD1 | 2.28 | 0.63 |
| 1:D:1000:GLU:O | 1:D:1003:TRP:N | 2.32 | 0.63 |
| 1:D:175:TRP:HB2 | 1:D:185:VAL:CG1 | 2.27 | 0.63 |
| 1:D:439:GLN:HG2 | 1:D:835:GLY:HA2 | 1.79 | 0.63 |
| 1:D:457:ARG:CA | 1:D:460:LYS:HD2 | 2.27 | 0.63 |
| 1:D:576:LEU:CD2 | 1:D:579:ARG:HE | 2.11 | 0.63 |
| 2:E:380:PRO:O | 2:E:382:LYS:CD | 2.47 | 0.63 |
| 2:E:390:GLY:N | 2:E:395:LEU:CG | 2.54 | 0.63 |
| 2:E:75:ARG:NH1 | 2:E:434:GLU:OE2 | 2.32 | 0.63 |
| 2:F:203:ARG:NE | 2:F:204:LEU:CD1 | 2.62 | 0.63 |
| 2:F:303:LEU:HA | 2:F:337:SER:CB | 2.29 | 0.63 |
| 2:F:347:LEU:C | 2:F:350:LEU:CD1 | 2.67 | 0.63 |
| 2:F:387:VAL:CG1 | 2:F:399:CYS:HB2 | 2.29 | 0.63 |
| 1:A:1157:ASN:O | 1:A:1161:ARG:HD2 | 1.99 | 0.63 |
| 1:A:224:CYS:O | 1:A:227:ARG:HB3 | 1.98 | 0.63 |
| 1:A:612:LEU:HB2 | 1:A:621:GLY:O | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:127:PRO:HB2 | 2:C:104:VAL:CG1 | 2.24 | 0.63 |
| 2:C:406:LEU:HA | 2:C:409:ASN:HD21 | 1.63 | 0.63 |
| 1:D:1007:GLU:O | 1:D:1011:PRO:CD | 2.45 | 0.63 |
| 1:D:1190:ARG:HH11 | 1:D:1195:MET:HE3 | 1.62 | 0.63 |
| 1:D:294:THR:O | 1:D:298:HIS:HB2 | 1.98 | 0.63 |
| 1:D:386:ARG:O | 1:D:389:PHE:CG | 2.51 | 0.63 |
| 1:D:420:HIS:HD2 | 1:D:1020:ILE:CD1 | 1.92 | 0.63 |
| 1:D:544:MET:O | 1:D:548:CYS:HB3 | 1.99 | 0.63 |
| 1:D:598:VAL:O | 1:D:600:PRO:N | 2.32 | 0.63 |
| 1:D:760:CYS:O | 1:D:761:ASN:C | 2.36 | 0.63 |
| 1:D:770:PHE:CZ | 1:D:968:GLN:O | 2.52 | 0.63 |
| 1:D:948:ILE:HG21 | 1:D:1071:ARG:HB3 | 1.81 | 0.63 |
| 2:F:215:PHE:N | 2:F:215:PHE:CD1 | 2.65 | 0.63 |
| 2:F:239:LEU:N | 2:F:338:VAL:CG2 | 2.61 | 0.63 |
| 2:F:193:TYR:OH | 2:F:333:PRO:HG3 | 1.99 | 0.63 |
| 2:F:353:SER:CB | 2:F:373:LYS:O | 2.45 | 0.63 |
| 1:A:490:TRP:HA | 1:A:580:LEU:HB2 | 1.80 | 0.63 |
| 1:A:630:ASN:ND2 | 1:A:632:ALA:N | 2.47 | 0.63 |
| 1:A:634:LEU:HG | 1:A:635:PRO:HA | 1.80 | 0.63 |
| 1:A:955:TYR:HB3 | 1:A:1098:ASN:OD1 | 1.98 | 0.63 |
| 2:B:234:LYS:HG2 | 2:B:341:ASP:OD2 | 1.99 | 0.63 |
| 2:B:461:THR:CG2 | 2:B:463:LYS:HZ2 | 2.12 | 0.63 |
| 2:C:235:THR:O | 2:C:341:ASP:OD1 | 2.16 | 0.63 |
| 2:C:342:LEU:CD2 | 2:C:345:GLY:N | 2.54 | 0.63 |
| 2:C:402:LEU:C | 2:C:406:LEU:HD22 | 2.19 | 0.63 |
| 1:D:1044:VAL:O | 1:D:1047:ARG:CG | 2.47 | 0.63 |
| 1:D:1028:VAL:CG2 | 1:D:1096:ARG:NH1 | 2.61 | 0.63 |
| 1:D:1171:ASN:O | 1:D:1172:ASP:CB | 2.47 | 0.63 |
| 1:D:164:PRO:CD | 1:D:165:LYS:H | 2.10 | 0.63 |
| 1:D:316:LYS:CE | 1:D:348:LEU:HD23 | 2.28 | 0.63 |
| 1:D:375:GLU:CD | 1:D:379:LYS:HB3 | 2.18 | 0.63 |
| 1:D:454:GLU:HA | 1:D:457:ARG:HG3 | 1.81 | 0.63 |
| 1:D:561:LYS:O | 1:D:562:ARG:HB2 | 1.97 | 0.63 |
| 1:D:715:GLN:HG2 | 1:D:717:LEU:CG | 2.29 | 0.63 |
| 1:D:728:THR:HG22 | 1:D:729:GLN:H | 1.64 | 0.63 |
| 1:D:957:ALA:HB2 | 1:D:1094:THR:OG1 | 1.99 | 0.63 |
| 1:A:539:PHE:CD2 | 1:A:540:GLN:HG2 | 2.34 | 0.62 |
| 1:A:754:HIS:O | 1:A:758:ASN:N | 2.32 | 0.62 |
| 1:A:812:MET:HG3 | 1:A:813:VAL:H | 1.64 | 0.62 |
| 1:A:913:CYS:HB2 | 1:A:999:ASP:OD1 | 1.99 | 0.62 |
| 2:B:342:LEU:C | 2:B:342:LEU:HD13 | 2.20 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:77:HIS:HB2 | 2:C:195:ASN:OD1 | 1.99 | 0.62 |
| 2:C:322:LEU:C | 2:C:322:LEU:HD22 | 2.19 | 0.62 |
| 2:C:342:LEU:CG | 2:C:344:ARG:HB2 | 2.29 | 0.62 |
| 1:D:1058:PHE:CE2 | 1:D:1059:ASN:HB3 | 2.33 | 0.62 |
| 1:D:359:VAL:CG2 | 1:D:406:VAL:HG21 | 2.29 | 0.62 |
| 1:D:584:ALA:C | 1:D:585:TRP:CE3 | 2.72 | 0.62 |
| 1:D:612:LEU:CD2 | 1:D:622:TYR:CE1 | 2.79 | 0.62 |
| 1:D:549:LEU:CD1 | 2:F:401:GLY:HA3 | 2.26 | 0.62 |
| 1:A:1207:GLU:C | 1:A:1210:TYR:CD1 | 2.72 | 0.62 |
| 1:A:157:LEU:HD11 | 1:A:195:LEU:CA | 2.29 | 0.62 |
| 1:A:385:ILE:HA | 1:A:388:ASN:ND2 | 2.14 | 0.62 |
| 1:A:652:ILE:CA | 1:A:655:LEU:HG | 2.29 | 0.62 |
| 1:A:734:HIS:CA | 1:A:752:LEU:HD11 | 2.29 | 0.62 |
| 1:A:786:ALA:HB1 | 1:A:790:ARG:CZ | 2.28 | 0.62 |
| 1:A:792:LEU:CD1 | 1:A:793:GLU:HG2 | 2.29 | 0.62 |
| 1:A:448:ALA:CB | 1:A:870:VAL:CG1 | 2.77 | 0.62 |
| 2:B:125:VAL:HG13 | 2:B:207:GLY:C | 2.19 | 0.62 |
| 2:B:261:GLN:HA | 2:B:264:ARG:CG | 2.29 | 0.62 |
| 2:B:231:ILE:HG13 | 2:C:135:PRO:HG3 | 1.79 | 0.62 |
| 1:D:1208:ARG:HG3 | 1:D:1209:ARG:N | 2.12 | 0.62 |
| 1:D:134:ASN:CB | 1:D:137:GLN:HB2 | 2.29 | 0.62 |
| 1:D:177:ARG:O | 1:D:178:TYR:C | 2.37 | 0.62 |
| 1:D:213:VAL:CG1 | 1:D:401:TRP:CZ2 | 2.81 | 0.62 |
| 1:D:251:THR:OG1 | 1:D:254:SER:CA | 2.43 | 0.62 |
| 1:D:917:GLY:O | 1:D:920:THR:CB | 2.46 | 0.62 |
| 2:E:199:LEU:HG | 2:E:200:VAL:CG2 | 2.29 | 0.62 |
| 2:F:403:PHE:CD2 | 2:F:403:PHE:C | 2.72 | 0.62 |
| 1:A:885:THR:C | 1:A:1146:ARG:NE | 2.53 | 0.62 |
| 1:A:1124:ALA:CB | 1:A:1148:ARG:NH1 | 2.59 | 0.62 |
| 1:A:223:TRP:O | 1:A:227:ARG:CB | 2.47 | 0.62 |
| 1:A:226:GLN:CD | 1:A:226:GLN:O | 2.37 | 0.62 |
| 1:A:228:LEU:N | 1:A:228:LEU:HD22 | 2.15 | 0.62 |
| 1:A:203:LEU:HD13 | 1:A:379:LYS:O | 1.99 | 0.62 |
| 1:A:392:LEU:HD22 | 1:A:393:MET:HE3 | 1.80 | 0.62 |
| 1:A:655:LEU:HD13 | 1:A:719:LEU:O | 1.98 | 0.62 |
| 1:A:656:TYR:CE1 | 1:A:744:ILE:HD12 | 2.34 | 0.62 |
| 2:B:396:ARG:HD2 | 2:B:417:TYR:CB | 2.25 | 0.62 |
| 2:C:128:VAL:CG1 | 2:C:192:HIS:CD2 | 2.82 | 0.62 |
| 2:C:215:PHE:N | 2:C:215:PHE:CD1 | 2.67 | 0.62 |
| 2:C:399:CYS:SG | 2:C:400:GLN:N | 2.72 | 0.62 |
| 1:D:1117:LYS:O | 1:D:1121:GLU:HG2 | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:1236:GLN:CB | 1:D:1237:PRO:HD3 | 2.29 | 0.62 |
| 1:D:197:PHE:HB2 | 1:D:277:HIS:HE1 | 1.64 | 0.62 |
| 1:D:210:THR:HG23 | 1:D:224:CYS:CB | 2.23 | 0.62 |
| 1:D:389:PHE:HA | 1:D:393:MET:HG2 | 1.77 | 0.62 |
| 1:D:459:MET:CB | 1:D:460:LYS:HZ1 | 2.12 | 0.62 |
| 1:D:456:GLN:C | 1:D:460:LYS:HZ2 | 1.97 | 0.62 |
| 1:D:608:ASP:CA | 1:D:620:TRP:CZ3 | 2.82 | 0.62 |
| 1:D:627:ARG:O | 1:D:628:ARG:HB3 | 1.98 | 0.62 |
| 1:D:648:PRO:O | 1:D:652:ILE:HG13 | 1.99 | 0.62 |
| 1:D:743:ASP:HB2 | 1:D:744:ILE:HD13 | 1.80 | 0.62 |
| 1:D:452:TYR:HB3 | 1:D:801:TRP:CD1 | 2.33 | 0.62 |
| 1:D:282:TYR:HB2 | 1:D:841:LEU:CD1 | 2.29 | 0.62 |
| 2:F:124:GLN:O | 2:F:125:VAL:HG12 | 2.00 | 0.62 |
| 2:E:233:GLU:OE1 | 2:F:131:LEU:HD12 | 1.98 | 0.62 |
| 2:F:277:ASP:OD2 | 2:F:285:LYS:HD2 | 1.99 | 0.62 |
| 2:F:307:GLY:HA2 | 2:F:335:VAL:H | 1.64 | 0.62 |
| 2:F:343:ASP:O | 2:F:347:LEU:HD13 | 2.00 | 0.62 |
| 2:E:201:ASN:OD1 | 2:F:422:GLN:CB | 2.47 | 0.62 |
| 1:A:1149:ALA:O | 1:A:1152:ALA:HB3 | 2.00 | 0.62 |
| 1:A:365:TYR:C | 1:A:367:GLY:N | 2.52 | 0.62 |
| 1:A:756:ASP:OD1 | 1:A:770:PHE:CZ | 2.53 | 0.62 |
| 1:A:795:ASN:HD22 | 1:A:796:LYS:N | 1.97 | 0.62 |
| 1:A:80:SER:N | 1:A:83:LEU:CD1 | 2.55 | 0.62 |
| 1:A:869:ARG:CG | 1:A:870:VAL:HG23 | 2.28 | 0.62 |
| 2:B:131:LEU:HD22 | 2:C:233:GLU:OE2 | 1.99 | 0.62 |
| 2:B:322:LEU:O | 2:B:323:HIS:O | 2.17 | 0.62 |
| 2:C:209:ALA:CB | 2:C:239:LEU:HA | 2.29 | 0.62 |
| 2:C:395:LEU:CD2 | 2:C:443:VAL:O | 2.47 | 0.62 |
| 1:D:1133:ILE:HG22 | 1:D:1134:HIS:CD2 | 2.35 | 0.62 |
| 1:D:1133:ILE:O | 1:D:1134:HIS:C | 2.37 | 0.62 |
| 1:D:1200:PRO:HG2 | 1:D:1203:PRO:CG | 2.25 | 0.62 |
| 1:D:434:TYR:CG | 1:D:435:LEU:N | 2.67 | 0.62 |
| 1:D:614:TYR:HA | 1:D:620:TRP:HA | 1.81 | 0.62 |
| 1:D:748:TRP:CZ3 | 1:D:750:PHE:HE2 | 2.17 | 0.62 |
| 2:E:233:GLU:O | 2:E:234:LYS:HG3 | 2.00 | 0.62 |
| 2:E:475:LEU:O | 2:E:478:TYR:N | 2.31 | 0.62 |
| 2:F:372:LEU:HD23 | 2:F:434:GLU:O | 1.99 | 0.62 |
| 2:F:403:PHE:HD2 | 2:F:403:PHE:C | 2.03 | 0.62 |
| 1:A:1145:ASP:HB3 | 1:A:1148:ARG:NH2 | 2.14 | 0.62 |
| 1:A:145:LYS:O | 1:A:149:PRO:CD | 2.47 | 0.62 |
| 1:A:607:TRP:CA | 1:A:610:PHE:O | 2.40 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:767:ALA:O | 1:A:768:LYS:O | 2.18 | 0.62 |
| 1:A:851:THR:HG22 | 1:A:853:ARG:HB2 | 1.80 | 0.62 |
| 2:B:236:GLU:HA | 2:B:342:LEU:H | 1.63 | 0.62 |
| 2:B:474:PHE:O | 2:B:475:LEU:HB2 | 1.97 | 0.62 |
| 2:C:114:TRP:HE1 | 2:C:259:ARG:NH1 | 1.97 | 0.62 |
| 2:C:114:TRP:HE1 | 2:C:259:ARG:NH2 | 1.95 | 0.62 |
| 2:C:126:PHE:HA | 2:C:209:ALA:C | 2.19 | 0.62 |
| 2:C:264:ARG:HA | 2:C:270:PRO:CB | 2.28 | 0.62 |
| 1:D:80:SER:HB2 | 1:D:125:LEU:CG | 2.29 | 0.62 |
| 1:D:257:THR:OG1 | 1:D:287:SER:HB2 | 1.98 | 0.62 |
| 1:D:282:TYR:CE2 | 1:D:432:VAL:HG22 | 2.29 | 0.62 |
| 1:D:509:THR:HB | 1:D:512:LYS:CB | 2.18 | 0.62 |
| 1:D:633:LYS:HB2 | 1:D:638:THR:CG2 | 2.29 | 0.62 |
| 1:D:771:LEU:O | 1:D:774:MET:HB2 | 1.99 | 0.62 |
| 1:D:300:ALA:CB | 1:D:847:ALA:HB1 | 2.13 | 0.62 |
| 2:E:91:LEU:HB3 | 2:E:347:LEU:HD11 | 1.81 | 0.62 |
| 2:E:380:PRO:N | 2:E:438:LEU:CD1 | 2.62 | 0.62 |
| 2:F:114:TRP:NE1 | 2:F:259:ARG:CZ | 2.56 | 0.62 |
| 2:F:346:MET:HE1 | 2:F:347:LEU:HD12 | 1.81 | 0.62 |
| 2:F:68:ALA:O | 2:F:72:ILE:HG12 | 2.00 | 0.62 |
| 1:A:1155:ILE:HA | 1:A:1158:LEU:CD1 | 2.29 | 0.62 |
| 1:A:215:ILE:CG2 | 1:A:216:SER:N | 2.51 | 0.62 |
| 1:A:157:LEU:HD21 | 1:A:216:SER:OG | 1.99 | 0.62 |
| 1:A:241:PRO:O | 1:A:244:LEU:HB2 | 1.99 | 0.62 |
| 1:A:376:LEU:C | 1:A:378:VAL:H | 2.02 | 0.62 |
| 1:A:382:MET:O | 1:A:383:LYS:HB2 | 2.00 | 0.62 |
| 1:A:559:LEU:CD2 | 2:C:451:GLY:O | 2.47 | 0.62 |
| 1:A:801:TRP:HZ3 | 1:A:808:ILE:HD12 | 1.62 | 0.62 |
| 1:A:931:LEU:HD23 | 1:A:931:LEU:C | 2.19 | 0.62 |
| 1:A:990:LYS:HD3 | 1:A:1000:GLU:OE2 | 1.99 | 0.62 |
| 1:A:992:LEU:CD2 | 1:A:997:LEU:HD12 | 2.16 | 0.62 |
| 2:B:103:GLY:O | 2:B:106:LEU:HB3 | 1.99 | 0.62 |
| 2:C:431:LYS:NZ | 2:C:435:MET:CG | 2.61 | 0.62 |
| 1:D:1014:ARG:HB3 | 1:D:1014:ARG:HH11 | 1.65 | 0.62 |
| 1:D:1145:ASP:HA | 1:D:1148:ARG:NE | 2.14 | 0.62 |
| 1:D:1157:ASN:OD1 | 1:D:1161:ARG:CZ | 2.47 | 0.62 |
| 1:D:1193:VAL:O | 1:D:1195:MET:HE2 | 2.00 | 0.62 |
| 1:D:1200:PRO:CD | 1:D:1203:PRO:HG2 | 2.28 | 0.62 |
| 1:D:282:TYR:O | 1:D:434:TYR:CD1 | 2.52 | 0.62 |
| 1:D:350:ILE:N | 1:D:350:ILE:HD12 | 2.09 | 0.62 |
| 1:D:631:LEU:HD23 | 1:D:631:LEU:N | 2.15 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:649:TYR:HD2 | 1:D:652:ILE:CG2 | 2.12 | 0.62 |
| 1:D:656:TYR:CB | 1:D:744:ILE:HD12 | 2.28 | 0.62 |
| 1:D:922:GLN:HE21 | 1:D:931:LEU:HD13 | 1.64 | 0.62 |
| 1:D:944:GLU:HG2 | 1:D:1071:ARG:NH1 | 2.14 | 0.62 |
| 1:D:546:ARG:CZ | 2:F:404:ASN:HB3 | 2.30 | 0.62 |
| 2:F:428:LEU:O | 2:F:429:TYR:C | 2.37 | 0.62 |
| 1:A:197:PHE:CD1 | 1:A:213:VAL:O | 2.53 | 0.62 |
| 1:A:241:PRO:HA | 1:A:244:LEU:HG | 1.79 | 0.62 |
| 1:A:297:MET:HE1 | 1:A:415:LEU:HD21 | 1.80 | 0.62 |
| 1:A:452:TYR:CD2 | 1:A:453:GLU:HG2 | 2.35 | 0.62 |
| 1:A:482:ASP:HB2 | 1:A:483:PRO:HD3 | 1.80 | 0.62 |
| 1:A:732:TYR:HD1 | 1:A:755:LYS:HZ3 | 1.44 | 0.62 |
| 1:A:898:ILE:HG12 | 1:A:899:ALA:H | 1.64 | 0.62 |
| 2:B:259:ARG:O | 2:B:262:TRP:N | 2.33 | 0.62 |
| 2:B:324:GLY:HA2 | 2:B:325:ARG:NH2 | 2.13 | 0.62 |
| 2:B:407:LEU:CD2 | 2:C:120:VAL:HA | 2.14 | 0.62 |
| 2:C:208:LEU:HD11 | 2:C:240:VAL:CB | 2.28 | 0.62 |
| 1:D:1163:MET:HG3 | 1:D:1164:PHE:N | 2.13 | 0.62 |
| 1:D:265:LEU:HD21 | 1:D:267:VAL:CG1 | 2.29 | 0.62 |
| 1:D:290:ARG:HB3 | 1:D:428:LEU:HB3 | 1.81 | 0.62 |
| 1:D:359:VAL:HG22 | 1:D:406:VAL:HG21 | 1.82 | 0.62 |
| 1:D:515:ILE:HG23 | 1:D:565:HIS:O | 1.98 | 0.62 |
| 1:D:496:LYS:HE3 | 1:D:571:GLY:HA3 | 1.81 | 0.62 |
| 1:D:575:LYS:CE | 1:D:581:ASP:O | 2.47 | 0.62 |
| 1:D:744:ILE:CG1 | 1:D:745:PRO:CD | 2.77 | 0.62 |
| 2:E:106:LEU:CA | 2:E:109:ASN:OD1 | 2.47 | 0.62 |
| 2:E:112:ALA:O | 2:E:115:TRP:N | 2.33 | 0.62 |
| 2:E:297:LYS:O | 2:E:298:GLU:HB2 | 1.99 | 0.62 |
| 2:F:193:TYR:CD1 | 2:F:193:TYR:C | 2.72 | 0.62 |
| 2:F:425:LEU:HD11 | 2:F:429:TYR:CE2 | 2.35 | 0.62 |
| 1:A:1153:LEU:CD1 | 1:A:1157:ASN:HD21 | 2.13 | 0.62 |
| 1:A:1200:PRO:CB | 1:A:1202:ASN:O | 2.46 | 0.62 |
| 1:A:256:PRO:HB3 | 1:A:280:GLU:O | 1.99 | 0.62 |
| 1:A:624:VAL:CG2 | 1:A:624:VAL:O | 2.48 | 0.62 |
| 2:B:247:THR:O | 2:B:251:TRP:HB2 | 2.00 | 0.62 |
| 2:B:396:ARG:NH1 | 2:B:417:TYR:HD2 | 1.93 | 0.62 |
| 1:D:1190:ARG:NH1 | 1:D:1195:MET:CE | 2.62 | 0.62 |
| 1:D:200:GLU:CB | 1:D:211:LEU:HD13 | 2.30 | 0.62 |
| 1:D:214:ALA:HB2 | 1:D:219:ALA:HB3 | 1.81 | 0.62 |
| 1:D:229:VAL:HG12 | 1:D:382:MET:O | 2.00 | 0.62 |
| 1:D:366:GLY:N | 1:D:367:PRO:CD | 2.61 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:429:GLU:HA | 1:D:429:GLU:OE1 | 1.99 | 0.62 |
| 1:D:608:ASP:CB | 1:D:620:TRP:CE3 | 2.78 | 0.62 |
| 1:D:823:ARG:O | 1:D:827:ARG:N | 2.18 | 0.62 |
| 1:D:964:ARG:O | 1:D:968:GLN:HG2 | 1.99 | 0.62 |
| 2:E:131:LEU:C | 2:E:182:ARG:HH21 | 2.03 | 0.62 |
| 2:E:249:ASN:HA | 2:E:252:LEU:HB2 | 1.80 | 0.62 |
| 2:F:336:LEU:CD2 | 2:F:336:LEU:C | 2.68 | 0.62 |
| 1:A:1068:ASP:O | 1:A:1069:ILE:HG22 | 1.99 | 0.62 |
| 1:A:669:MET:O | 1:A:673:ALA:CA | 2.48 | 0.62 |
| 2:C:384:ALA:CB | 2:C:437:ILE:HD12 | 2.29 | 0.62 |
| 1:D:175:TRP:HA | 1:D:185:VAL:HG21 | 1.81 | 0.62 |
| 1:D:345:TRP:CA | 1:D:1040:LYS:HZ2 | 2.13 | 0.62 |
| 1:D:295:MET:HE2 | 1:D:354:ASN:HA | 1.80 | 0.62 |
| 1:D:74:LEU:HD13 | 1:D:76:ILE:O | 2.00 | 0.62 |
| 1:D:860:LEU:HD22 | 1:D:1132:SER:O | 2.00 | 0.62 |
| 1:D:877:MET:CE | 1:D:1207:GLU:HB2 | 2.30 | 0.62 |
| 1:D:973:LEU:N | 1:D:973:LEU:HD23 | 2.14 | 0.62 |
| 2:E:205:PRO:HB3 | 2:E:242:PHE:O | 1.99 | 0.62 |
| 2:F:241:TRP:CG | 2:F:243:THR:HG23 | 2.34 | 0.62 |
| 1:A:175:TRP:HB2 | 1:A:184:ALA:O | 2.00 | 0.62 |
| 1:A:394:GLN:O | 1:A:397:ALA:HB3 | 2.00 | 0.62 |
| 1:A:400:VAL:CG1 | 1:A:404:HIS:NE2 | 2.63 | 0.62 |
| 1:A:623:LEU:O | 1:A:625:PRO:HD2 | 2.00 | 0.62 |
| 1:A:960:PRO:HD2 | 1:A:961:PHE:CE1 | 2.35 | 0.62 |
| 2:C:335:VAL:HG22 | 2:C:336:LEU:N | 2.15 | 0.62 |
| 2:C:403:PHE:CD2 | 2:C:403:PHE:C | 2.73 | 0.62 |
| 1:D:1027:LYS:CB | 1:D:1096:ARG:HE | 2.12 | 0.62 |
| 1:D:1044:VAL:O | 1:D:1047:ARG:HG3 | 1.99 | 0.62 |
| 1:D:1060:LYS:HD2 | 1:D:1060:LYS:N | 2.15 | 0.62 |
| 1:D:193:ARG:HD2 | 1:D:263:GLU:CD | 2.20 | 0.62 |
| 1:D:215:ILE:O | 1:D:215:ILE:HG22 | 1.99 | 0.62 |
| 1:D:242:ALA:HB1 | 1:D:245:ILE:HD13 | 1.82 | 0.62 |
| 1:D:719:LEU:CD1 | 1:D:720:THR:N | 2.62 | 0.62 |
| 1:D:597:ARG:HD3 | 1:D:724:GLY:O | 1.99 | 0.62 |
| 1:D:735:GLY:CA | 1:D:749:PHE:HA | 2.30 | 0.62 |
| 1:D:739:TYR:O | 1:D:741:ASP:N | 2.33 | 0.62 |
| 1:D:767:ALA:O | 1:D:768:LYS:HB3 | 2.00 | 0.62 |
| 1:D:868:ASP:C | 1:D:869:ARG:HG3 | 2.20 | 0.62 |
| 2:F:240:VAL:HA | 2:F:336:LEU:HB3 | 1.82 | 0.62 |
| 2:F:371:VAL:HG23 | 2:F:433:ASP:HB3 | 1.82 | 0.62 |
| 1:A:1068:ASP:HA | 1:A:1071:ARG:HD3 | 1.80 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1155:ILE:O | 1:A:1159:LEU:HG | 1.99 | 0.61 |
| 1:A:273:PHE:CA | 1:A:276:ALA:CB | 2.74 | 0.61 |
| 1:A:299:MET:HE1 | 1:A:353:VAL:HB | 1.82 | 0.61 |
| 1:A:385:ILE:HA | 1:A:388:ASN:HD22 | 1.65 | 0.61 |
| 1:A:624:VAL:H | 1:A:746:GLY:HA2 | 1.64 | 0.61 |
| 1:A:771:LEU:HD22 | 1:A:771:LEU:N | 2.09 | 0.61 |
| 1:A:893:SER:CB | 1:A:896:LEU:HD23 | 2.29 | 0.61 |
| 2:B:419:GLU:CB | 2:C:203:ARG:NH2 | 2.59 | 0.61 |
| 1:D:1010:LEU:O | 1:D:1028:VAL:HG21 | 1.99 | 0.61 |
| 1:D:145:LYS:HB2 | 1:D:1118:TRP:CH2 | 2.34 | 0.61 |
| 1:D:213:VAL:CG2 | 1:D:401:TRP:CZ2 | 2.82 | 0.61 |
| 1:D:279:ARG:NH1 | 1:D:433:SER:O | 2.32 | 0.61 |
| 1:D:470:ALA:O | 1:D:474:LEU:CD1 | 2.47 | 0.61 |
| 1:D:738:PRO:O | 1:D:740:ASN:ND2 | 2.33 | 0.61 |
| 1:D:656:TYR:CE1 | 1:D:743:ASP:CB | 2.83 | 0.61 |
| 1:D:891:VAL:HG13 | 1:D:1135:ASP:CB | 2.16 | 0.61 |
| 1:D:938:THR:O | 1:D:939:VAL:CB | 2.47 | 0.61 |
| 1:D:948:ILE:O | 1:D:951:TYR:HB2 | 2.00 | 0.61 |
| 2:E:203:ARG:HH21 | 2:E:203:ARG:HG3 | 1.64 | 0.61 |
| 2:E:110:LEU:HA | 2:E:378:LEU:CD2 | 2.30 | 0.61 |
| 2:E:406:LEU:HG | 2:E:413:VAL:CG2 | 2.29 | 0.61 |
| 2:E:69:LEU:N | 2:E:69:LEU:HD12 | 2.14 | 0.61 |
| 2:F:290:TYR:CD1 | 2:F:299:LEU:HA | 2.35 | 0.61 |
| 2:F:314:MET:HE3 | 2:F:315:TYR:CE2 | 2.35 | 0.61 |
| 2:F:400:GLN:HE21 | 2:F:404:ASN:CG | 2.03 | 0.61 |
| 2:F:385:LEU:HD21 | 2:F:402:LEU:HD23 | 1.81 | 0.61 |
| 1:A:169:TRP:O | 1:A:170:ALA:HB3 | 1.99 | 0.61 |
| 1:A:434:TYR:C | 1:A:435:LEU:HG | 2.20 | 0.61 |
| 1:A:630:ASN:C | 1:A:631:LEU:HD23 | 2.20 | 0.61 |
| 1:A:945:HIS:HA | 1:A:948:ILE:HD11 | 1.82 | 0.61 |
| 2:B:113:GLU:C | 2:B:262:TRP:HZ2 | 2.04 | 0.61 |
| 2:B:400:GLN:HE22 | 2:B:417:TYR:HB3 | 1.65 | 0.61 |
| 2:C:416:GLY:CA | 2:C:419:GLU:HB3 | 2.30 | 0.61 |
| 2:C:395:LEU:HD13 | 2:C:444:THR:HA | 1.80 | 0.61 |
| 1:D:1131:ILE:CD1 | 1:D:1138:ARG:N | 2.33 | 0.61 |
| 1:D:1187:ARG:HD2 | 1:D:1212:ILE:HD11 | 1.81 | 0.61 |
| 1:D:869:ARG:CA | 1:D:1200:PRO:HB2 | 2.30 | 0.61 |
| 1:D:1200:PRO:HG2 | 1:D:1200:PRO:O | 2.00 | 0.61 |
| 1:D:1232:GLU:HG3 | 1:D:1234:ARG:HB2 | 1.80 | 0.61 |
| 1:D:252:GLY:O | 1:D:253:ALA:HB3 | 2.00 | 0.61 |
| 1:D:453:GLU:O | 1:D:456:GLN:N | 2.32 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:499:LYS:O | 1:D:499:LYS:HE3 | 2.00 | 0.61 |
| 1:D:576:LEU:HD23 | 1:D:579:ARG:HE | 1.64 | 0.61 |
| 1:D:81:ARG:CZ | 1:D:81:ARG:HB2 | 2.30 | 0.61 |
| 1:D:827:ARG:O | 1:D:829:PRO:CD | 2.30 | 0.61 |
| 1:D:831:TYR:O | 1:D:831:TYR:HD1 | 1.83 | 0.61 |
| 1:D:902:LEU:O | 1:D:905:ALA:HB3 | 1.99 | 0.61 |
| 2:E:407:LEU:C | 2:E:409:ASN:H | 2.04 | 0.61 |
| 2:F:466:MET:CA | 2:F:471:LEU:HD22 | 2.31 | 0.61 |
| 1:A:1030:ARG:HE | 1:A:1040:LYS:HE3 | 1.64 | 0.61 |
| 1:A:158:LEU:O | 1:A:409:GLN:NE2 | 2.29 | 0.61 |
| 1:A:308:GLN:HB3 | 1:A:1090:GLU:HG3 | 1.83 | 0.61 |
| 1:A:719:LEU:HD23 | 1:A:719:LEU:H | 1.64 | 0.61 |
| 1:A:743:ASP:CB | 1:A:744:ILE:HD13 | 2.30 | 0.61 |
| 2:B:116:THR:HA | 2:B:120:VAL:HG23 | 1.82 | 0.61 |
| 2:B:378:LEU:HD12 | 2:B:378:LEU:N | 2.16 | 0.61 |
| 2:B:106:LEU:HB2 | 2:B:380:PRO:HG3 | 1.81 | 0.61 |
| 2:C:120:VAL:CG2 | 2:C:121:PHE:N | 2.63 | 0.61 |
| 2:C:342:LEU:HB2 | 2:C:344:ARG:HG3 | 1.82 | 0.61 |
| 2:C:414:TRP:O | 2:C:415:PRO:O | 2.19 | 0.61 |
| 2:C:443:VAL:C | 2:C:447:THR:HG21 | 2.21 | 0.61 |
| 1:D:1027:LYS:HB3 | 1:D:1091:GLU:HA | 1.83 | 0.61 |
| 1:D:543:VAL:O | 1:D:547:ALA:HB3 | 2.00 | 0.61 |
| 1:D:598:VAL:HA | 1:D:601:LYS:CD | 2.30 | 0.61 |
| 1:D:733:HIS:ND1 | 1:D:750:PHE:HD1 | 1.98 | 0.61 |
| 2:E:123:GLU:HB3 | 2:F:403:PHE:CE1 | 2.36 | 0.61 |
| 2:F:243:THR:O | 2:F:334:CYS:CB | 2.48 | 0.61 |
| 2:F:306:LEU:HD21 | 2:F:310:GLU:HG2 | 1.81 | 0.61 |
| 2:F:310:GLU:O | 2:F:314:MET:N | 2.30 | 0.61 |
| 2:F:342:LEU:CD2 | 2:F:345:GLY:N | 2.55 | 0.61 |
| 2:F:455:LEU:O | 2:F:465:MET:HA | 1.99 | 0.61 |
| 1:A:1002:GLU:O | 1:A:1005:VAL:CG2 | 2.44 | 0.61 |
| 1:A:1048:ALA:HB3 | 1:A:1092:PHE:HE1 | 1.65 | 0.61 |
| 1:A:372:GLU:OE2 | 1:A:399:ASP:OD2 | 2.17 | 0.61 |
| 1:A:660:CYS:HB2 | 1:A:745:PRO:HG3 | 1.83 | 0.61 |
| 1:A:769:ASP:CG | 1:A:770:PHE:N | 2.52 | 0.61 |
| 2:B:294:PRO:HG2 | 2:B:295:TRP:H | 1.66 | 0.61 |
| 2:B:93:SER:OG | 2:B:95:CYS:HB2 | 2.01 | 0.61 |
| 2:C:367:LEU:O | 2:C:369:ARG:CD | 2.47 | 0.61 |
| 1:D:1207:GLU:O | 1:D:1208:ARG:C | 2.39 | 0.61 |
| 1:D:161:GLN:O | 1:D:163:PRO:HD3 | 2.00 | 0.61 |
| 1:D:270:ASN:HA | 1:D:294:THR:CB | 2.31 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:383:LYS:O | 1:D:386:ARG:CG | 2.46 | 0.61 |
| 1:D:486:TRP:HE1 | 1:D:722:ARG:HG3 | 1.65 | 0.61 |
| 1:D:666:GLN:O | 1:D:669:MET:O | 2.17 | 0.61 |
| 1:D:742:VAL:HB | 1:D:748:TRP:CZ3 | 2.35 | 0.61 |
| 1:D:795:ASN:HA | 1:D:798:ILE:HD11 | 1.80 | 0.61 |
| 1:D:283:LEU:HG | 1:D:814:VAL:CG2 | 2.30 | 0.61 |
| 1:D:977:GLU:HA | 1:D:980:GLU:HG3 | 1.81 | 0.61 |
| 2:E:189:ALA:HB1 | 2:E:240:VAL:HG11 | 1.82 | 0.61 |
| 2:F:241:TRP:H | 2:F:336:LEU:CB | 2.11 | 0.61 |
| 1:A:1030:ARG:CD | 1:A:1040:LYS:HZ1 | 2.14 | 0.61 |
| 1:A:228:LEU:CD2 | 1:A:229:VAL:N | 2.55 | 0.61 |
| 1:A:477:GLU:HG2 | 1:A:482:ASP:OD1 | 2.00 | 0.61 |
| 1:A:503:VAL:CG2 | 1:A:520:ALA:O | 2.45 | 0.61 |
| 1:A:656:TYR:C | 1:A:659:HIS:HB3 | 2.21 | 0.61 |
| 1:A:815:TRP:HE3 | 1:A:838:GLY:H | 1.47 | 0.61 |
| 1:A:886:LEU:H | 1:A:1146:ARG:NH2 | 1.96 | 0.61 |
| 2:B:106:LEU:O | 2:B:109:ASN:HB3 | 2.00 | 0.61 |
| 2:B:238:SER:HA | 2:B:339:ASN:ND2 | 2.14 | 0.61 |
| 2:B:311:LEU:O | 2:B:313:HIS:N | 2.33 | 0.61 |
| 2:C:402:LEU:HG | 2:C:472:LYS:HZ1 | 1.63 | 0.61 |
| 2:C:431:LYS:HE2 | 2:C:435:MET:HB2 | 1.83 | 0.61 |
| 1:D:1210:TYR:C | 1:D:1210:TYR:CD1 | 2.74 | 0.61 |
| 1:D:176:THR:OG1 | 1:D:218:SER:HB2 | 2.00 | 0.61 |
| 1:D:307:PHE:HD2 | 1:D:1048:ALA:O | 1.82 | 0.61 |
| 1:D:359:VAL:O | 1:D:359:VAL:CG1 | 2.46 | 0.61 |
| 1:D:792:LEU:CA | 1:D:795:ASN:ND2 | 2.64 | 0.61 |
| 1:D:996:ARG:HD3 | 1:D:996:ARG:H | 1.60 | 0.61 |
| 2:E:189:ALA:CB | 2:E:240:VAL:HG21 | 2.30 | 0.61 |
| 2:E:303:LEU:HA | 2:E:337:SER:O | 2.00 | 0.61 |
| 2:F:243:THR:HB | 2:F:247:THR:HG1 | 1.66 | 0.61 |
| 2:F:439:PHE:HD1 | 2:F:458:ARG:CG | 2.13 | 0.61 |
| 1:A:1002:GLU:HG3 | 1:A:1003:TRP:HE3 | 1.65 | 0.61 |
| 1:A:1055:SER:O | 1:A:1059:ASN:OD1 | 2.19 | 0.61 |
| 1:A:169:TRP:HZ3 | 1:A:391:ASP:CA | 2.11 | 0.61 |
| 1:A:225:SER:HG | 1:A:386:ARG:HB2 | 1.64 | 0.61 |
| 1:A:572:TRP:O | 1:A:573:TYR:C | 2.36 | 0.61 |
| 1:A:894:GLN:O | 1:A:898:ILE:HG23 | 2.00 | 0.61 |
| 2:B:281:GLU:HG3 | 2:B:282:GLU:HG2 | 1.82 | 0.61 |
| 2:B:342:LEU:HD13 | 2:B:342:LEU:O | 2.00 | 0.61 |
| 2:C:307:GLY:C | 2:C:308:ASP:OD2 | 2.39 | 0.61 |
| 2:C:78:PHE:HZ | 2:C:346:MET:CE | 2.14 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:447:THR:O | 2:C:448:LEU:C | 2.38 | 0.61 |
| 1:D:1025:LEU:CD2 | 1:D:1025:LEU:O | 2.49 | 0.61 |
| 1:D:1031:GLU:CD | 1:D:1096:ARG:HH22 | 2.03 | 0.61 |
| 1:D:380:GLY:O | 1:D:385:ILE:HD12 | 2.00 | 0.61 |
| 1:D:595:GLN:O | 1:D:597:ARG:N | 2.33 | 0.61 |
| 1:D:626:GLY:HA3 | 1:D:628:ARG:O | 2.00 | 0.61 |
| 1:D:938:THR:O | 1:D:939:VAL:HB | 2.00 | 0.61 |
| 2:E:478:TYR:CD1 | 2:E:478:TYR:O | 2.54 | 0.61 |
| 2:E:90:SER:HA | 2:E:93:SER:HB2 | 1.81 | 0.61 |
| 2:F:132:HIS:ND1 | 2:F:132:HIS:N | 2.42 | 0.61 |
| 2:F:255:TRP:O | 2:F:256:LEU:C | 2.39 | 0.61 |
| 1:A:1113:LEU:HB3 | 1:A:1117:LYS:CE | 2.29 | 0.61 |
| 1:A:169:TRP:CZ3 | 1:A:391:ASP:CA | 2.80 | 0.61 |
| 1:A:241:PRO:C | 1:A:244:LEU:H | 2.04 | 0.61 |
| 1:A:259:ARG:HG3 | 1:A:261:TRP:CD1 | 2.35 | 0.61 |
| 1:A:196:VAL:C | 1:A:401:TRP:HH2 | 2.04 | 0.61 |
| 1:A:473:LEU:N | 1:A:473:LEU:CD2 | 2.62 | 0.61 |
| 1:A:70:ARG:CB | 1:A:81:ARG:HB3 | 2.20 | 0.61 |
| 1:A:893:SER:CA | 1:A:896:LEU:HD23 | 2.30 | 0.61 |
| 2:C:131:LEU:O | 2:C:133:HIS:HB2 | 2.01 | 0.61 |
| 2:C:244:PRO:N | 2:C:247:THR:CG2 | 2.63 | 0.61 |
| 2:C:387:VAL:CG1 | 2:C:399:CYS:CB | 2.78 | 0.61 |
| 2:C:394:GLU:O | 2:C:397:GLN:HB3 | 2.01 | 0.61 |
| 1:D:1210:TYR:CG | 1:D:1211:GLY:N | 2.68 | 0.61 |
| 1:D:1187:ARG:CD | 1:D:1212:ILE:HD11 | 2.29 | 0.61 |
| 1:D:1183:VAL:O | 1:D:1217:ALA:HA | 2.00 | 0.61 |
| 1:D:275:ARG:HB2 | 1:D:843:GLN:CA | 2.30 | 0.61 |
| 1:D:353:VAL:HG23 | 1:D:354:ASN:N | 2.15 | 0.61 |
| 1:D:369:LEU:HD13 | 1:D:372:GLU:HB3 | 1.82 | 0.61 |
| 1:D:434:TYR:O | 1:D:435:LEU:CG | 2.47 | 0.61 |
| 1:D:866:ARG:HB3 | 1:D:867:PRO:CD | 2.24 | 0.61 |
| 2:F:301:GLU:OE1 | 2:F:339:ASN:ND2 | 2.33 | 0.61 |
| 2:F:309:HIS:HA | 2:F:312:LEU:CD1 | 2.23 | 0.61 |
| 2:F:306:LEU:HD21 | 2:F:310:GLU:OE1 | 2.01 | 0.61 |
| 2:F:81:GLY:HA3 | 2:F:97:PRO:CB | 2.31 | 0.61 |
| 1:A:1026:ARG:CB | 1:A:1029:GLN:CD | 2.66 | 0.61 |
| 1:A:1189:LEU:HD22 | 1:A:1189:LEU:N | 2.16 | 0.61 |
| 1:A:199:VAL:CG2 | 1:A:277:HIS:HB2 | 2.31 | 0.61 |
| 1:A:275:ARG:HH22 | 1:A:844:VAL:C | 2.03 | 0.61 |
| 1:A:928:GLY:O | 1:A:931:LEU:HB3 | 2.00 | 0.61 |
| 2:B:258:HIS:CG | 2:B:259:ARG:N | 2.66 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:124:GLN:O | 2:C:125:VAL:HG12 | 2.01 | 0.61 |
| 2:C:208:LEU:CD2 | 2:C:242:PHE:CD2 | 2.84 | 0.61 |
| 2:C:282:GLU:C | 2:C:284:ARG:H | 2.04 | 0.61 |
| 2:C:298:GLU:OE1 | 2:C:344:ARG:NH2 | 2.33 | 0.61 |
| 1:D:1056:GLU:HB3 | 1:D:1057:MET:CE | 2.31 | 0.61 |
| 1:D:1055:SER:O | 1:D:1059:ASN:ND2 | 2.34 | 0.61 |
| 1:D:1210:TYR:HH | 1:D:1212:ILE:HB | 1.64 | 0.61 |
| 1:D:185:VAL:HB | 1:D:186:PRO:HD2 | 1.83 | 0.61 |
| 1:D:190:PRO:HG3 | 1:D:219:ALA:HB2 | 1.81 | 0.61 |
| 1:D:313:ILE:HG13 | 1:D:314:ALA:N | 2.16 | 0.61 |
| 1:D:367:PRO:HG2 | 1:D:368:PRO:HD3 | 1.82 | 0.61 |
| 1:D:632:ALA:HB1 | 1:D:657:ARG:HD2 | 1.83 | 0.61 |
| 2:E:217:PRO:HA | 2:E:231:ILE:HA | 1.82 | 0.61 |
| 2:E:456:ARG:CG | 2:E:457:SER:N | 2.64 | 0.61 |
| 2:E:456:ARG:CB | 2:E:463:LYS:HG2 | 2.17 | 0.61 |
| 2:F:442:LEU:O | 2:F:455:LEU:CD2 | 2.48 | 0.61 |
| 1:A:1072:THR:N | 1:A:1073:PRO:HD2 | 2.15 | 0.61 |
| 1:A:1236:GLN:N | 1:A:1236:GLN:HE21 | 1.97 | 0.61 |
| 1:A:392:LEU:HD23 | 1:A:392:LEU:C | 2.22 | 0.61 |
| 1:A:410:GLN:O | 1:A:414:PHE:HD2 | 1.83 | 0.61 |
| 1:A:420:HIS:O | 1:A:424:LEU:HG | 2.01 | 0.61 |
| 1:A:653:GLU:HA | 1:A:656:TYR:CE2 | 2.35 | 0.61 |
| 1:A:73:PRO:HB2 | 1:A:90:GLN:HB3 | 1.83 | 0.61 |
| 2:B:125:VAL:HG12 | 2:B:126:PHE:N | 2.15 | 0.61 |
| 2:B:127:PRO:O | 2:C:104:VAL:HG21 | 2.01 | 0.61 |
| 2:B:236:GLU:CD | 2:B:341:ASP:HB3 | 2.21 | 0.61 |
| 2:C:402:LEU:O | 2:C:406:LEU:HD13 | 2.00 | 0.61 |
| 1:D:1221:TYR:O | 1:D:1222:GLN:C | 2.36 | 0.61 |
| 1:D:289:MET:SD | 1:D:291:PHE:CZ | 2.94 | 0.61 |
| 1:D:412:PRO:HG2 | 1:D:413:LEU:H | 1.66 | 0.61 |
| 1:D:420:HIS:O | 1:D:424:LEU:HG | 2.01 | 0.61 |
| 1:D:428:LEU:CD1 | 1:D:428:LEU:N | 2.46 | 0.61 |
| 1:D:500:ALA:HB2 | 1:D:521:PRO:CG | 2.31 | 0.61 |
| 1:D:548:CYS:H | 1:D:551:LYS:HZ3 | 1.45 | 0.61 |
| 1:D:494:GLU:HA | 1:D:573:TYR:H | 1.66 | 0.61 |
| 1:D:612:LEU:HD12 | 1:D:612:LEU:H | 1.62 | 0.61 |
| 1:D:801:TRP:CG | 1:D:802:ARG:N | 2.69 | 0.61 |
| 2:F:241:TRP:H | 2:F:336:LEU:HB3 | 1.65 | 0.61 |
| 2:F:456:ARG:CG | 2:F:457:SER:N | 2.63 | 0.61 |
| 1:A:1204:THR:CG2 | 1:A:1204:THR:O | 2.37 | 0.61 |
| 1:A:259:ARG:CA | 1:A:259:ARG:NE | 2.60 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:261:TRP:O | 1:A:262:GLN:HB2 | 2.00 | 0.61 |
| 1:A:195:LEU:HG | 1:A:265:LEU:CD2 | 2.31 | 0.61 |
| 1:A:411:LEU:N | 1:A:412:PRO:HD2 | 2.16 | 0.61 |
| 1:A:441:TRP:CZ3 | 1:A:445:LEU:HD12 | 2.36 | 0.61 |
| 1:A:553:LYS:HD2 | 2:C:468:ILE:CG2 | 2.31 | 0.61 |
| 1:A:813:VAL:CG1 | 1:A:815:TRP:CZ2 | 2.84 | 0.61 |
| 1:A:81:ARG:HH11 | 1:A:81:ARG:HG3 | 1.66 | 0.61 |
| 2:B:466:MET:HG2 | 2:B:467:HIS:N | 2.15 | 0.61 |
| 2:C:200:VAL:CB | 2:C:204:LEU:HD22 | 2.31 | 0.61 |
| 2:C:407:LEU:HD13 | 2:C:408:GLU:OE2 | 2.01 | 0.61 |
| 2:C:395:LEU:CD2 | 2:C:443:VAL:HG12 | 2.28 | 0.61 |
| 1:D:1030:ARG:C | 1:D:1032:THR:H | 2.04 | 0.61 |
| 1:D:275:ARG:HB2 | 1:D:843:GLN:HB3 | 0.75 | 0.61 |
| 1:D:293:ASP:HB3 | 1:D:296:SER:HB2 | 1.83 | 0.61 |
| 1:D:371:LYS:HG3 | 1:D:396:CYS:CB | 2.31 | 0.61 |
| 1:D:402:ALA:O | 1:D:406:VAL:HG13 | 2.00 | 0.61 |
| 1:D:618:HIS:CB | 1:D:725:PRO:CG | 2.77 | 0.61 |
| 1:D:914:THR:HG21 | 1:D:999:ASP:CB | 2.30 | 0.61 |
| 1:D:966:LEU:CD2 | 1:D:970:ASN:ND2 | 2.64 | 0.61 |
| 2:E:417:TYR:HD1 | 2:E:418:LEU:HG | 1.66 | 0.61 |
| 2:E:456:ARG:HD3 | 2:E:463:LYS:CG | 2.29 | 0.61 |
| 2:F:425:LEU:HD21 | 2:F:429:TYR:OH | 2.00 | 0.61 |
| 2:F:449:GLU:C | 2:F:449:GLU:CD | 2.59 | 0.61 |
| 1:A:1060:LYS:NZ | 1:A:1073:PRO:HB2 | 2.16 | 0.60 |
| 1:A:210:THR:O | 1:A:211:LEU:CB | 2.38 | 0.60 |
| 1:A:257:THR:HA | 1:A:258:GLN:OE1 | 2.01 | 0.60 |
| 1:A:411:LEU:N | 1:A:412:PRO:CD | 2.64 | 0.60 |
| 1:A:851:THR:HG22 | 1:A:853:ARG:N | 2.13 | 0.60 |
| 1:A:887:VAL:N | 1:A:1146:ARG:NH1 | 2.48 | 0.60 |
| 1:A:950:ASN:O | 1:A:951:TYR:C | 2.39 | 0.60 |
| 1:A:96:GLY:O | 1:A:100:VAL:HG23 | 2.01 | 0.60 |
| 2:C:307:GLY:HA2 | 2:C:335:VAL:H | 1.66 | 0.60 |
| 2:C:317:GLY:C | 2:C:319:VAL:N | 2.47 | 0.60 |
| 2:C:368:HIS:NE2 | 2:C:370:LYS:HD2 | 2.16 | 0.60 |
| 2:C:387:VAL:CG2 | 2:C:417:TYR:HA | 2.31 | 0.60 |
| 1:D:1031:GLU:CD | 1:D:1096:ARG:NH2 | 2.54 | 0.60 |
| 1:D:1107:ASP:O | 1:D:1110:HIS:HB2 | 2.01 | 0.60 |
| 1:D:1113:LEU:O | 1:D:1116:MET:HB2 | 2.01 | 0.60 |
| 1:D:1190:ARG:CD | 1:D:1195:MET:HE3 | 2.26 | 0.60 |
| 1:D:1221:TYR:O | 1:D:1224:ILE:N | 2.34 | 0.60 |
| 1:D:140:ARG:HH11 | 1:D:140:ARG:HG3 | 1.65 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:239:LEU:N | 1:D:239:LEU:HD23 | 2.16 | 0.60 |
| 1:D:603:MET:O | 1:D:605:LEU:N | 2.34 | 0.60 |
| 1:D:909:GLY:O | 1:D:912:GLY:HA2 | 2.00 | 0.60 |
| 2:E:375:HIS:NE2 | 2:E:376:PRO:HB3 | 2.16 | 0.60 |
| 2:F:303:LEU:HG | 2:F:337:SER:OG | 2.01 | 0.60 |
| 2:F:197:LEU:CD1 | 2:F:322:LEU:HD21 | 2.31 | 0.60 |
| 2:F:326:ASP:CG | 2:F:329:LYS:HB2 | 2.22 | 0.60 |
| 2:F:403:PHE:HE1 | 2:F:415:PRO:HG3 | 1.60 | 0.60 |
| 2:F:395:LEU:CB | 2:F:443:VAL:HG21 | 2.30 | 0.60 |
| 1:A:1019:TRP:CZ2 | 1:A:1111:LEU:HD21 | 2.36 | 0.60 |
| 1:A:1128:ARG:CG | 1:A:1129:PHE:N | 2.43 | 0.60 |
| 1:A:1231:LEU:HD12 | 1:A:1235:SER:HB2 | 1.83 | 0.60 |
| 1:A:174:GLY:O | 1:A:175:TRP:CD2 | 2.54 | 0.60 |
| 1:A:254:SER:O | 1:A:255:SER:CB | 2.49 | 0.60 |
| 1:A:313:ILE:HA | 1:A:316:LYS:HG2 | 1.84 | 0.60 |
| 1:A:434:TYR:O | 1:A:1129:PHE:CE1 | 2.54 | 0.60 |
| 1:A:513:LEU:CB | 1:A:568:GLY:CA | 2.56 | 0.60 |
| 1:A:582:ASP:O | 1:A:583:PRO:C | 2.39 | 0.60 |
| 1:A:739:TYR:C | 1:A:741:ASP:O | 2.39 | 0.60 |
| 2:B:122:ARG:HB3 | 2:B:122:ARG:NH1 | 2.16 | 0.60 |
| 2:B:182:ARG:HB3 | 2:B:215:PHE:CD1 | 2.36 | 0.60 |
| 2:C:114:TRP:NE1 | 2:C:259:ARG:NH1 | 2.49 | 0.60 |
| 2:C:272:ASN:HA | 2:C:292:ASN:ND2 | 2.15 | 0.60 |
| 2:C:387:VAL:HG12 | 2:C:395:LEU:HD23 | 1.81 | 0.60 |
| 1:D:1006:ARG:HH21 | 1:D:1017:GLY:HA3 | 1.64 | 0.60 |
| 1:D:1014:ARG:C | 1:D:1014:ARG:HD2 | 2.21 | 0.60 |
| 1:D:1198:LYS:HA | 1:D:1204:THR:HB | 1.83 | 0.60 |
| 1:D:129:PRO:O | 1:D:131:TYR:CZ | 2.54 | 0.60 |
| 1:D:273:PHE:O | 1:D:277:HIS:HD2 | 1.84 | 0.60 |
| 1:D:347:TRP:NE1 | 1:D:349:ASP:OD2 | 2.33 | 0.60 |
| 1:D:790:ARG:O | 1:D:794:ILE:HG12 | 2.01 | 0.60 |
| 2:E:385:LEU:CD1 | 2:E:441:VAL:HB | 2.31 | 0.60 |
| 2:E:447:THR:HG23 | 2:E:452:LEU:N | 2.16 | 0.60 |
| 1:A:866:ARG:CG | 1:A:1069:ILE:CG2 | 2.75 | 0.60 |
| 1:A:1093:MET:O | 1:A:1097:VAL:HG23 | 2.01 | 0.60 |
| 1:A:352:SER:C | 1:A:358:LEU:HD21 | 2.22 | 0.60 |
| 1:A:816:LEU:HD12 | 1:A:837:TYR:O | 2.00 | 0.60 |
| 1:A:918:TRP:C | 1:A:920:THR:N | 2.52 | 0.60 |
| 1:A:932:HIS:O | 1:A:935:THR:HB | 2.01 | 0.60 |
| 1:A:964:ARG:HD2 | 1:A:1053:THR:HG21 | 1.82 | 0.60 |
| 2:B:437:ILE:HG22 | 2:B:438:LEU:N | 2.15 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:239:LEU:O | 2:C:338:VAL:HG13 | 2.01 | 0.60 |
| 2:C:338:VAL:O | 2:C:338:VAL:HG23 | 2.01 | 0.60 |
| 1:D:891:VAL:CG1 | 1:D:1135:ASP:CB | 2.76 | 0.60 |
| 1:D:368:PRO:CB | 1:D:369:LEU:HD23 | 2.31 | 0.60 |
| 2:E:214:CYS:SG | 2:E:236:GLU:HB3 | 2.41 | 0.60 |
| 2:F:254:PHE:N | 2:F:257:ARG:NH2 | 2.48 | 0.60 |
| 1:A:1133:ILE:HD13 | 1:A:1133:ILE:C | 2.21 | 0.60 |
| 1:A:213:VAL:HG22 | 1:A:221:TYR:CE2 | 2.36 | 0.60 |
| 1:A:301:ILE:CG2 | 1:A:302:SER:N | 2.64 | 0.60 |
| 1:A:878:VAL:C | 1:A:879:GLN:NE2 | 2.54 | 0.60 |
| 2:B:244:PRO:O | 2:B:248:SER:CB | 2.45 | 0.60 |
| 2:B:260:LEU:O | 2:B:264:ARG:CD | 2.49 | 0.60 |
| 2:B:440:THR:O | 2:B:441:VAL:HG13 | 2.01 | 0.60 |
| 2:C:110:LEU:O | 2:C:111:ALA:C | 2.40 | 0.60 |
| 2:C:144:ALA:O | 2:C:145:PHE:HB2 | 2.01 | 0.60 |
| 2:C:204:LEU:HD11 | 2:C:206:TYR:HB3 | 1.81 | 0.60 |
| 2:C:336:LEU:CD2 | 2:C:337:SER:O | 2.50 | 0.60 |
| 2:C:342:LEU:O | 2:C:342:LEU:CD2 | 2.48 | 0.60 |
| 2:C:421:MET:HE2 | 2:C:422:GLN:CB | 2.30 | 0.60 |
| 1:D:1155:ILE:CA | 1:D:1158:LEU:HD21 | 2.27 | 0.60 |
| 1:D:224:CYS:O | 1:D:227:ARG:N | 2.35 | 0.60 |
| 2:E:319:VAL:HG13 | 2:E:320:SER:N | 2.16 | 0.60 |
| 2:F:200:VAL:O | 2:F:201:ASN:HB2 | 2.01 | 0.60 |
| 1:D:1209:ARG:HH12 | 2:F:252:LEU:HD13 | 1.64 | 0.60 |
| 2:F:254:PHE:O | 2:F:257:ARG:HB2 | 2.01 | 0.60 |
| 1:A:1019:TRP:CD1 | 1:A:1020:ILE:HG22 | 2.36 | 0.60 |
| 1:A:1028:VAL:O | 1:A:1031:GLU:O | 2.18 | 0.60 |
| 1:A:448:ALA:CA | 1:A:870:VAL:CG1 | 2.80 | 0.60 |
| 1:A:572:TRP:HE3 | 1:A:572:TRP:HA | 1.66 | 0.60 |
| 1:A:606:THR:HG23 | 1:A:613:HIS:CA | 2.29 | 0.60 |
| 1:A:869:ARG:O | 1:A:872:SER:CB | 2.48 | 0.60 |
| 2:B:304:TRP:HB2 | 2:B:337:SER:HB3 | 1.83 | 0.60 |
| 2:B:400:GLN:NE2 | 2:B:417:TYR:HB3 | 2.16 | 0.60 |
| 2:C:305:ASN:C | 2:C:335:VAL:HG11 | 2.21 | 0.60 |
| 2:C:344:ARG:CA | 2:C:347:LEU:HD13 | 2.31 | 0.60 |
| 2:C:372:LEU:CD1 | 2:C:374:LEU:HG | 2.32 | 0.60 |
| 2:C:456:ARG:HE | 2:C:456:ARG:N | 1.99 | 0.60 |
| 2:C:471:LEU:CA | 2:C:474:PHE:HD2 | 2.15 | 0.60 |
| 1:D:219:ALA:O | 1:D:220:TRP:CB | 2.44 | 0.60 |
| 1:D:242:ALA:O | 1:D:245:ILE:HG12 | 2.02 | 0.60 |
| 1:D:267:VAL:O | 1:D:269:HIS:NE2 | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:436:PRO:HA | 1:D:839:ALA:HB2 | 1.84 | 0.60 |
| 1:D:842:PRO:O | 1:D:844:VAL:HG22 | 2.01 | 0.60 |
| 2:E:214:CYS:SG | 2:E:236:GLU:CD | 2.79 | 0.60 |
| 2:F:206:TYR:N | 2:F:206:TYR:CD2 | 2.69 | 0.60 |
| 1:A:1118:TRP:CE3 | 1:A:1118:TRP:HA | 2.36 | 0.60 |
| 2:B:217:PRO:O | 2:B:231:ILE:HA | 2.02 | 0.60 |
| 2:B:231:ILE:N | 2:B:231:ILE:HD13 | 2.15 | 0.60 |
| 2:B:431:LYS:O | 2:B:435:MET:N | 2.32 | 0.60 |
| 2:C:121:PHE:O | 2:C:123:GLU:N | 2.35 | 0.60 |
| 2:C:187:HIS:HA | 2:C:190:LEU:HD12 | 1.84 | 0.60 |
| 2:C:389:ARG:CG | 2:C:390:GLY:N | 2.65 | 0.60 |
| 1:D:301:ILE:O | 1:D:1024:ASP:CG | 2.39 | 0.60 |
| 1:D:944:GLU:HG2 | 1:D:1071:ARG:CZ | 2.31 | 0.60 |
| 1:D:1144:GLU:O | 1:D:1145:ASP:HB2 | 2.01 | 0.60 |
| 1:D:1232:GLU:HB2 | 1:D:1234:ARG:HB2 | 1.84 | 0.60 |
| 1:D:194:ALA:O | 1:D:195:LEU:HG | 2.02 | 0.60 |
| 1:D:316:LYS:HD2 | 1:D:348:LEU:HD23 | 1.83 | 0.60 |
| 1:D:359:VAL:O | 1:D:360:HIS:C | 2.37 | 0.60 |
| 1:D:371:LYS:HD3 | 1:D:392:LEU:HD21 | 1.81 | 0.60 |
| 1:D:379:LYS:O | 1:D:379:LYS:HD3 | 2.00 | 0.60 |
| 1:D:414:PHE:C | 1:D:417:ARG:HB2 | 2.21 | 0.60 |
| 1:D:491:ASP:O | 1:D:492:LEU:O | 2.20 | 0.60 |
| 1:D:666:GLN:HG2 | 1:D:669:MET:CE | 2.31 | 0.60 |
| 1:D:718:ALA:O | 1:D:722:ARG:CD | 2.48 | 0.60 |
| 1:D:86:GLN:C | 1:D:87:ILE:HG12 | 2.21 | 0.60 |
| 2:E:325:ARG:HG2 | 2:E:330:ASN:CA | 2.27 | 0.60 |
| 2:E:437:ILE:CD1 | 2:E:437:ILE:N | 2.64 | 0.60 |
| 2:E:443:VAL:HA | 2:E:453:ILE:HG22 | 1.84 | 0.60 |
| 2:E:93:SER:O | 2:E:95:CYS:N | 2.34 | 0.60 |
| 2:F:311:LEU:O | 2:F:314:MET:HB2 | 2.01 | 0.60 |
| 2:F:340:GLY:O | 2:F:341:ASP:O | 2.18 | 0.60 |
| 2:F:386:ASP:HB3 | 2:F:442:LEU:CD2 | 2.26 | 0.60 |
| 2:F:430:SER:OG | 2:F:431:LYS:N | 2.34 | 0.60 |
| 2:F:461:THR:OG1 | 2:F:461:THR:O | 2.20 | 0.60 |
| 2:F:94:GLY:HA2 | 2:F:96:HIS:ND1 | 2.16 | 0.60 |
| 1:A:1069:ILE:HG22 | 1:A:1070:PRO:CD | 2.28 | 0.60 |
| 1:A:136:ASP:OD1 | 1:A:137:GLN:N | 2.34 | 0.60 |
| 1:A:216:SER:O | 1:A:217:PRO:O | 2.19 | 0.60 |
| 1:A:271:VAL:O | 1:A:275:ARG:HD3 | 2.01 | 0.60 |
| 1:A:386:ARG:HB2 | 1:A:390:GLN:HE22 | 1.67 | 0.60 |
| 1:A:400:VAL:HG12 | 1:A:404:HIS:CD2 | 2.35 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:570:PRO:HB2 | 1:A:572:TRP:CE3 | 2.37 | 0.60 |
| 1:A:844:VAL:HG13 | 1:A:844:VAL:O | 2.02 | 0.60 |
| 1:A:811:GLN:NE2 | 1:A:859:TRP:HZ2 | 1.99 | 0.60 |
| 1:A:451:THR:HB | 1:A:869:ARG:NH2 | 2.17 | 0.60 |
| 1:A:894:GLN:O | 1:A:898:ILE:CG2 | 2.50 | 0.60 |
| 2:B:116:THR:HA | 2:B:120:VAL:HB | 1.84 | 0.60 |
| 2:B:447:THR:HA | 2:B:450:ASN:OD1 | 2.02 | 0.60 |
| 2:C:402:LEU:HB3 | 2:C:406:LEU:HD21 | 1.84 | 0.60 |
| 1:D:1029:GLN:HE21 | 1:D:1030:ARG:NH2 | 1.97 | 0.60 |
| 1:D:214:ALA:N | 1:D:401:TRP:CH2 | 2.69 | 0.60 |
| 1:D:251:THR:O | 1:D:254:SER:C | 2.39 | 0.60 |
| 1:D:350:ILE:HG23 | 1:D:352:SER:CB | 2.20 | 0.60 |
| 1:D:422:VAL:HG11 | 1:D:1111:LEU:CD1 | 2.31 | 0.60 |
| 1:D:597:ARG:HB3 | 1:D:616:GLU:CD | 2.22 | 0.60 |
| 1:D:618:HIS:HB3 | 1:D:725:PRO:HB2 | 1.83 | 0.60 |
| 1:D:427:MET:O | 1:D:846:THR:HG21 | 2.01 | 0.60 |
| 1:D:894:GLN:O | 1:D:898:ILE:HG23 | 2.02 | 0.60 |
| 1:D:961:PHE:HD1 | 1:D:961:PHE:H | 1.48 | 0.60 |
| 2:E:199:LEU:HD22 | 2:F:77:HIS:CD2 | 2.35 | 0.60 |
| 2:E:94:GLY:N | 2:E:234:LYS:HE2 | 2.16 | 0.60 |
| 2:E:371:VAL:CG1 | 2:E:372:LEU:H | 2.14 | 0.60 |
| 2:E:385:LEU:O | 2:E:440:THR:HG23 | 2.01 | 0.60 |
| 2:F:260:LEU:O | 2:F:264:ARG:HG3 | 2.02 | 0.60 |
| 1:A:1120:PHE:O | 1:A:1125:ILE:HD13 | 2.02 | 0.60 |
| 1:A:177:ARG:HB2 | 1:A:183:GLU:HB3 | 1.83 | 0.60 |
| 1:A:177:ARG:CB | 1:A:183:GLU:HB3 | 2.32 | 0.60 |
| 1:A:188:ALA:O | 1:A:189:ILE:HG12 | 2.01 | 0.60 |
| 1:A:232:ARG:HB3 | 1:A:239:LEU:CD2 | 2.08 | 0.60 |
| 1:A:297:MET:CE | 1:A:411:LEU:HD22 | 2.32 | 0.60 |
| 1:A:572:TRP:CE3 | 1:A:572:TRP:HA | 2.37 | 0.60 |
| 1:A:655:LEU:HB2 | 1:A:719:LEU:CB | 2.26 | 0.60 |
| 1:A:655:LEU:HD22 | 1:A:722:ARG:CZ | 2.32 | 0.60 |
| 1:A:823:ARG:O | 1:A:824:ALA:HB3 | 2.02 | 0.60 |
| 2:C:395:LEU:HD22 | 2:C:443:VAL:O | 2.01 | 0.60 |
| 1:D:1065:ALA:O | 1:D:1067:SER:N | 2.35 | 0.60 |
| 1:D:1027:LYS:HB2 | 1:D:1096:ARG:NE | 2.17 | 0.60 |
| 1:D:136:ASP:O | 1:D:140:ARG:HD3 | 2.02 | 0.60 |
| 1:D:656:TYR:O | 1:D:744:ILE:HG13 | 2.02 | 0.60 |
| 1:D:954:ILE:HG22 | 1:D:955:TYR:CD2 | 2.37 | 0.60 |
| 2:E:187:HIS:O | 2:E:190:LEU:HB2 | 2.01 | 0.60 |
| 2:F:134:LYS:CB | 2:F:180:LYS:HE2 | 2.32 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:447:THR:O | 2:F:452:LEU:CA | 2.46 | 0.60 |
| 1:A:1016:GLU:HB2 | 1:A:1020:ILE:HA | 1.84 | 0.60 |
| 1:A:256:PRO:CD | 1:A:257:THR:N | 2.61 | 0.60 |
| 1:A:353:VAL:O | 1:A:354:ASN:HB3 | 2.02 | 0.60 |
| 1:A:228:LEU:HD11 | 1:A:386:ARG:CB | 2.31 | 0.60 |
| 1:A:410:GLN:C | 1:A:412:PRO:HD2 | 2.22 | 0.60 |
| 1:A:481:GLU:O | 1:A:484:TRP:HB2 | 2.02 | 0.60 |
| 1:A:573:TYR:C | 1:A:574:ARG:HG3 | 2.22 | 0.60 |
| 1:A:612:LEU:CD2 | 1:A:620:TRP:CA | 2.78 | 0.60 |
| 1:A:766:PHE:O | 1:A:767:ALA:C | 2.40 | 0.60 |
| 1:A:891:VAL:HA | 1:A:1180:PHE:CE1 | 2.27 | 0.60 |
| 2:B:208:LEU:HD21 | 2:B:240:VAL:HB | 1.84 | 0.60 |
| 2:B:259:ARG:C | 2:B:261:GLN:N | 2.51 | 0.60 |
| 2:C:290:TYR:CD1 | 2:C:299:LEU:HA | 2.36 | 0.60 |
| 2:C:309:HIS:HA | 2:C:312:LEU:CD1 | 2.32 | 0.60 |
| 1:D:1006:ARG:CA | 1:D:1006:ARG:NH1 | 2.39 | 0.60 |
| 1:D:173:GLU:O | 1:D:175:TRP:N | 2.34 | 0.60 |
| 1:D:273:PHE:O | 1:D:277:HIS:CD2 | 2.54 | 0.60 |
| 1:D:457:ARG:CA | 1:D:460:LYS:HZ2 | 2.15 | 0.60 |
| 1:D:620:TRP:CE2 | 1:D:751:LYS:HB2 | 2.37 | 0.60 |
| 1:D:656:TYR:HD1 | 1:D:743:ASP:HB2 | 1.65 | 0.60 |
| 1:D:815:TRP:CE3 | 1:D:836:LEU:HB3 | 2.36 | 0.60 |
| 1:D:883:GLY:HA2 | 1:D:1143:GLU:OE1 | 2.02 | 0.60 |
| 2:E:119:VAL:O | 2:E:123:GLU:HA | 2.00 | 0.60 |
| 2:E:189:ALA:CB | 2:E:240:VAL:HG11 | 2.32 | 0.60 |
| 2:E:388:GLY:CA | 2:E:395:LEU:HD11 | 2.32 | 0.60 |
| 2:E:393:LEU:O | 2:E:396:ARG:HG3 | 2.02 | 0.60 |
| 2:F:267:ALA:O | 2:F:270:PRO:HD3 | 2.01 | 0.60 |
| 1:A:156:LEU:HD23 | 1:A:156:LEU:N | 2.16 | 0.60 |
| 1:A:225:SER:OG | 1:A:386:ARG:CB | 2.47 | 0.60 |
| 1:A:348:LEU:C | 1:A:350:ILE:H | 1.99 | 0.60 |
| 1:A:389:PHE:HD1 | 1:A:390:GLN:NE2 | 2.00 | 0.60 |
| 1:A:592:LEU:O | 1:A:596:MET:HG2 | 2.02 | 0.60 |
| 1:A:612:LEU:CD2 | 1:A:614:TYR:H | 2.14 | 0.60 |
| 1:A:616:GLU:O | 1:A:617:ARG:HB2 | 2.01 | 0.60 |
| 1:A:659:HIS:NE2 | 1:A:720:THR:HG22 | 2.17 | 0.60 |
| 1:A:812:MET:HE3 | 1:A:813:VAL:HG13 | 1.83 | 0.60 |
| 1:A:844:VAL:HA | 1:A:856:GLU:HG3 | 1.82 | 0.60 |
| 2:B:265:LYS:CD | 2:B:349:TYR:OH | 2.50 | 0.60 |
| 2:B:412:SER:O | 2:B:413:VAL:CG2 | 2.48 | 0.60 |
| 2:B:463:LYS:H | 2:B:463:LYS:CD | 2.15 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:204:LEU:CD1 | 2:C:206:TYR:HB3 | 2.31 | 0.60 |
| 1:D:85:GLU:OE1 | 1:D:130:LEU:HD13 | 2.01 | 0.60 |
| 2:E:193:TYR:O | 2:E:197:LEU:CB | 2.50 | 0.60 |
| 1:A:1058:PHE:O | 1:A:1060:LYS:N | 2.35 | 0.59 |
| 1:A:1165:ALA:HB2 | 1:A:1173:LEU:CG | 2.32 | 0.59 |
| 1:A:1210:TYR:HE1 | 1:A:1213:PRO:CG | 2.09 | 0.59 |
| 1:A:184:ALA:C | 1:A:186:PRO:HD3 | 2.23 | 0.59 |
| 1:A:204:ALA:C | 1:A:206:GLY:H | 2.04 | 0.59 |
| 1:A:215:ILE:HB | 1:A:401:TRP:CZ3 | 2.37 | 0.59 |
| 1:A:476:GLY:HA2 | 1:A:711:ALA:HB1 | 1.84 | 0.59 |
| 1:A:515:ILE:H | 1:A:515:ILE:HD12 | 1.66 | 0.59 |
| 1:A:769:ASP:C | 1:A:772:PRO:HD2 | 2.22 | 0.59 |
| 2:B:213:VAL:HA | 2:B:235:THR:C | 2.22 | 0.59 |
| 2:C:336:LEU:HD23 | 2:C:337:SER:C | 2.21 | 0.59 |
| 2:C:235:THR:O | 2:C:341:ASP:CG | 2.41 | 0.59 |
| 2:C:342:LEU:HD21 | 2:C:345:GLY:H | 1.65 | 0.59 |
| 2:C:354:PHE:O | 2:C:355:GLN:C | 2.40 | 0.59 |
| 2:C:372:LEU:HD11 | 2:C:436:SER:OG | 2.00 | 0.59 |
| 2:C:388:GLY:N | 2:C:443:VAL:O | 2.32 | 0.59 |
| 2:C:456:ARG:HB2 | 2:C:463:LYS:O | 2.02 | 0.59 |
| 1:D:1002:GLU:CG | 1:D:1003:TRP:N | 2.64 | 0.59 |
| 1:D:853:ARG:HH12 | 1:D:1102:GLN:HA | 1.67 | 0.59 |
| 1:D:1116:MET:HG2 | 1:D:1156:THR:HG21 | 1.84 | 0.59 |
| 1:D:407:PHE:CD1 | 1:D:408:GLN:N | 2.70 | 0.59 |
| 1:D:444:TYR:OH | 1:D:1206:MET:CB | 2.49 | 0.59 |
| 1:D:549:LEU:HD23 | 1:D:552:LEU:HD12 | 1.84 | 0.59 |
| 1:D:665:LYS:C | 1:D:669:MET:HG2 | 2.22 | 0.59 |
| 1:D:815:TRP:CZ3 | 1:D:836:LEU:HB3 | 2.36 | 0.59 |
| 1:D:807:ARG:CB | 1:D:858:THR:HG23 | 2.31 | 0.59 |
| 2:E:262:TRP:O | 2:E:265:LYS:CB | 2.46 | 0.59 |
| 2:E:380:PRO:HA | 2:E:438:LEU:HD12 | 1.84 | 0.59 |
| 2:E:444:THR:OG1 | 2:E:446:THR:CG2 | 2.49 | 0.59 |
| 2:E:455:LEU:HD23 | 2:E:455:LEU:N | 2.16 | 0.59 |
| 2:E:86:LEU:HB2 | 2:E:91:LEU:CD2 | 2.31 | 0.59 |
| 2:F:306:LEU:C | 2:F:335:VAL:HB | 2.22 | 0.59 |
| 2:F:342:LEU:CG | 2:F:344:ARG:HB2 | 2.31 | 0.59 |
| 2:F:352:ASP:N | 2:F:355:GLN:HB2 | 2.17 | 0.59 |
| 2:F:266:PHE:HB3 | 2:F:378:LEU:HD11 | 1.83 | 0.59 |
| 2:F:395:LEU:CD2 | 2:F:448:LEU:HD11 | 2.32 | 0.59 |
| 1:A:1119:LEU:HD23 | 1:A:1122:GLU:HG3 | 1.85 | 0.59 |
| 1:A:1112:MET:HA | 1:A:1156:THR:HG23 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:309:ARG:O | 1:A:313:ILE:N | 2.34 | 0.59 |
| 1:A:198:ASP:CB | 1:A:400:VAL:HG11 | 2.32 | 0.59 |
| 1:A:371:LYS:HZ3 | 1:A:400:VAL:HG23 | 1.66 | 0.59 |
| 1:A:435:LEU:HD12 | 1:A:842:PRO:HD3 | 1.83 | 0.59 |
| 1:A:488:LEU:N | 1:A:488:LEU:HD23 | 2.17 | 0.59 |
| 1:A:556:THR:HG22 | 2:C:467:HIS:NE2 | 2.17 | 0.59 |
| 1:A:570:PRO:HB2 | 1:A:572:TRP:CZ3 | 2.37 | 0.59 |
| 1:A:845:VAL:HG11 | 1:A:848:GLY:HA3 | 1.84 | 0.59 |
| 1:A:887:VAL:HG22 | 1:A:1146:ARG:NH1 | 2.14 | 0.59 |
| 1:A:948:ILE:HG13 | 1:A:949:PHE:HD2 | 1.66 | 0.59 |
| 1:D:1010:LEU:N | 1:D:1011:PRO:CD | 2.65 | 0.59 |
| 1:D:1204:THR:O | 1:D:1207:GLU:N | 2.35 | 0.59 |
| 1:D:184:ALA:O | 1:D:185:VAL:HG12 | 2.02 | 0.59 |
| 1:D:309:ARG:C | 1:D:313:ILE:HG23 | 2.22 | 0.59 |
| 1:D:389:PHE:CA | 1:D:393:MET:CG | 2.72 | 0.59 |
| 1:D:504:LYS:CB | 1:D:523:ASP:O | 2.47 | 0.59 |
| 1:D:752:LEU:HB3 | 1:D:753:PRO:HB3 | 1.83 | 0.59 |
| 1:D:992:LEU:HB3 | 1:D:996:ARG:CD | 2.32 | 0.59 |
| 2:E:104:VAL:HG21 | 2:F:128:VAL:CA | 2.32 | 0.59 |
| 2:F:346:MET:SD | 2:F:346:MET:C | 2.81 | 0.59 |
| 2:F:387:VAL:HG13 | 2:F:399:CYS:HB2 | 1.83 | 0.59 |
| 2:F:446:THR:CB | 2:F:450:ASN:H | 2.15 | 0.59 |
| 2:F:472:LYS:O | 2:F:475:LEU:HG | 2.02 | 0.59 |
| 1:A:1153:LEU:CD1 | 1:A:1157:ASN:ND2 | 2.65 | 0.59 |
| 1:A:1190:ARG:NH2 | 1:A:1197:CYS:HB2 | 2.18 | 0.59 |
| 1:A:245:ILE:O | 1:A:248:GLU:HG2 | 2.02 | 0.59 |
| 1:A:665:LYS:HG2 | 1:A:666:GLN:H | 1.66 | 0.59 |
| 1:A:275:ARG:HG2 | 1:A:843:GLN:CB | 2.32 | 0.59 |
| 2:B:440:THR:O | 2:B:455:LEU:HB2 | 2.02 | 0.59 |
| 2:B:79:LEU:CA | 2:B:100:GLY:HA3 | 2.33 | 0.59 |
| 2:C:208:LEU:CD2 | 2:C:242:PHE:CE2 | 2.84 | 0.59 |
| 2:C:456:ARG:CB | 2:C:463:LYS:O | 2.50 | 0.59 |
| 1:D:1190:ARG:NE | 1:D:1195:MET:HG2 | 2.17 | 0.59 |
| 1:D:1207:GLU:OE2 | 1:D:1210:TYR:CE2 | 2.54 | 0.59 |
| 1:D:285:GLN:NE2 | 1:D:1128:ARG:CG | 2.61 | 0.59 |
| 1:D:257:THR:OG1 | 1:D:287:SER:CB | 2.50 | 0.59 |
| 1:D:798:ILE:HG22 | 1:D:869:ARG:HH12 | 1.61 | 0.59 |
| 2:E:380:PRO:O | 2:E:382:LYS:HD2 | 2.02 | 0.59 |
| 2:E:442:LEU:C | 2:E:442:LEU:HD13 | 2.23 | 0.59 |
| 2:E:447:THR:HG21 | 2:E:453:ILE:CG2 | 2.24 | 0.59 |
| 2:F:186:LEU:O | 2:F:189:ALA:HB3 | 2.01 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:264:ARG:HA | 2:F:270:PRO:HB3 | 1.84 | 0.59 |
| 1:A:115:GLN:O | 1:A:118:VAL:HG13 | 2.02 | 0.59 |
| 1:A:1232:GLU:HG3 | 1:A:1234:ARG:NE | 2.17 | 0.59 |
| 1:A:275:ARG:NH2 | 1:A:844:VAL:C | 2.55 | 0.59 |
| 1:A:869:ARG:O | 1:A:872:SER:N | 2.30 | 0.59 |
| 2:B:246:ARG:C | 2:B:248:SER:H | 2.06 | 0.59 |
| 2:B:344:ARG:N | 2:B:344:ARG:CD | 2.65 | 0.59 |
| 2:B:372:LEU:O | 2:B:458:ARG:HD2 | 2.01 | 0.59 |
| 2:B:83:LYS:N | 2:B:83:LYS:HD2 | 2.15 | 0.59 |
| 2:C:310:GLU:OE1 | 2:C:310:GLU:N | 2.36 | 0.59 |
| 2:C:239:LEU:HG | 2:C:336:LEU:CD1 | 2.33 | 0.59 |
| 2:C:353:SER:OG | 2:C:354:PHE:N | 2.33 | 0.59 |
| 1:D:113:TRP:CE3 | 1:D:116:PRO:HG2 | 2.36 | 0.59 |
| 1:D:1193:VAL:CG2 | 1:D:1194:THR:N | 2.36 | 0.59 |
| 1:D:192:GLU:OE1 | 1:D:193:ARG:NH1 | 2.35 | 0.59 |
| 1:D:247:LEU:CA | 1:D:815:TRP:CD1 | 2.84 | 0.59 |
| 1:D:808:ILE:HG21 | 1:D:874:LEU:HD23 | 1.83 | 0.59 |
| 1:D:887:VAL:H | 1:D:1146:ARG:NH2 | 1.98 | 0.59 |
| 1:D:930:ASP:C | 1:D:930:ASP:OD2 | 2.40 | 0.59 |
| 1:D:97:GLU:O | 1:D:101:ARG:HG3 | 2.02 | 0.59 |
| 2:F:78:PHE:C | 2:F:100:GLY:H | 2.06 | 0.59 |
| 2:E:101:PRO:CG | 2:F:128:VAL:HG21 | 2.32 | 0.59 |
| 2:F:193:TYR:HB2 | 2:F:242:PHE:CZ | 2.38 | 0.59 |
| 2:F:343:ASP:C | 2:F:347:LEU:CD1 | 2.70 | 0.59 |
| 1:A:1006:ARG:NH2 | 1:A:1010:LEU:CD1 | 2.57 | 0.59 |
| 1:A:1200:PRO:HB2 | 1:A:1203:PRO:CD | 2.32 | 0.59 |
| 1:A:608:ASP:CA | 1:A:779:LEU:HD22 | 2.32 | 0.59 |
| 2:B:132:HIS:HA | 2:B:182:ARG:NE | 2.17 | 0.59 |
| 2:B:413:VAL:HG12 | 2:B:414:TRP:H | 1.66 | 0.59 |
| 2:C:454:HIS:HD2 | 2:C:472:LYS:HE3 | 1.68 | 0.59 |
| 2:C:69:LEU:HD23 | 2:C:351:TYR:CD1 | 2.37 | 0.59 |
| 1:D:1015:THR:CG2 | 1:D:1026:ARG:CB | 2.80 | 0.59 |
| 1:D:866:ARG:NE | 1:D:1069:ILE:HB | 2.17 | 0.59 |
| 1:D:1198:LYS:N | 1:D:1204:THR:HG21 | 2.18 | 0.59 |
| 1:D:127:LEU:HD23 | 1:D:128:PRO:CD | 2.32 | 0.59 |
| 1:D:182:GLY:O | 1:D:183:GLU:HB2 | 2.03 | 0.59 |
| 1:D:289:MET:HE2 | 1:D:290:ARG:H | 1.68 | 0.59 |
| 1:D:416:GLU:C | 1:D:418:CYS:H | 2.03 | 0.59 |
| 1:D:458:GLU:N | 1:D:460:LYS:NZ | 2.50 | 0.59 |
| 1:D:586:THR:N | 1:D:587:PRO:HD3 | 2.16 | 0.59 |
| 1:D:770:PHE:HZ | 1:D:968:GLN:O | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:793:GLU:O | 1:D:797:MET:HG3 | 2.02 | 0.59 |
| 1:D:822:PRO:O | 1:D:825:VAL:HB | 2.03 | 0.59 |
| 1:D:938:THR:O | 1:D:939:VAL:HG23 | 2.03 | 0.59 |
| 2:E:127:PRO:HG2 | 2:F:101:PRO:CA | 2.33 | 0.59 |
| 2:E:211:ILE:HD13 | 2:E:211:ILE:N | 2.18 | 0.59 |
| 2:E:456:ARG:HD2 | 2:E:461:THR:C | 2.23 | 0.59 |
| 2:F:446:THR:C | 2:F:449:GLU:H | 2.06 | 0.59 |
| 1:A:1131:ILE:CG2 | 1:A:1138:ARG:N | 2.57 | 0.59 |
| 1:A:1219:ASP:O | 1:A:1223:ILE:HG22 | 2.02 | 0.59 |
| 1:A:974:THR:CG2 | 1:A:975:GLN:H | 2.16 | 0.59 |
| 2:B:69:LEU:HD13 | 2:B:73:CYS:SG | 2.43 | 0.59 |
| 2:C:206:TYR:O | 2:C:241:TRP:HA | 2.02 | 0.59 |
| 2:C:307:GLY:CA | 2:C:335:VAL:HG12 | 2.32 | 0.59 |
| 2:C:197:LEU:HD11 | 2:C:322:LEU:CD2 | 2.32 | 0.59 |
| 2:C:341:ASP:OD1 | 2:C:342:LEU:N | 2.30 | 0.59 |
| 1:D:1069:ILE:HG12 | 1:D:1070:PRO:CD | 2.32 | 0.59 |
| 1:D:1175:GLN:HG3 | 1:D:1176:SER:N | 2.16 | 0.59 |
| 1:D:872:SER:OG | 1:D:1200:PRO:N | 2.35 | 0.59 |
| 1:D:873:GLU:OE1 | 1:D:1203:PRO:CG | 2.50 | 0.59 |
| 1:D:359:VAL:C | 1:D:361:ARG:N | 2.49 | 0.59 |
| 1:D:403:THR:HA | 1:D:406:VAL:HG13 | 1.85 | 0.59 |
| 1:D:76:ILE:CA | 1:D:911:HIS:NE2 | 2.66 | 0.59 |
| 2:E:193:TYR:HE2 | 2:E:322:LEU:HD22 | 1.66 | 0.59 |
| 2:E:447:THR:HG23 | 2:E:452:LEU:H | 1.68 | 0.59 |
| 2:E:78:PHE:CD2 | 2:E:102:LEU:CD1 | 2.85 | 0.59 |
| 1:D:472:GLN:HB3 | 2:F:460:THR:C | 2.23 | 0.59 |
| 1:A:851:THR:OG1 | 1:A:1102:GLN:HB3 | 2.02 | 0.59 |
| 1:A:868:ASP:CG | 1:A:1199:THR:HG21 | 2.23 | 0.59 |
| 1:A:175:TRP:CD1 | 1:A:176:THR:N | 2.71 | 0.59 |
| 1:A:365:TYR:CD2 | 1:A:365:TYR:N | 2.70 | 0.59 |
| 1:A:634:LEU:HD12 | 1:A:638:THR:CG2 | 2.33 | 0.59 |
| 1:A:776:ASP:C | 1:A:776:ASP:OD1 | 2.41 | 0.59 |
| 1:A:83:LEU:O | 1:A:84:HIS:C | 2.41 | 0.59 |
| 2:B:204:LEU:CG | 2:B:325:ARG:HH21 | 2.05 | 0.59 |
| 2:B:82:SER:HB3 | 2:B:85:GLN:HG2 | 1.85 | 0.59 |
| 1:D:1015:THR:CG2 | 1:D:1026:ARG:HB2 | 2.32 | 0.59 |
| 1:D:306:SER:CB | 1:D:1058:PHE:CE2 | 2.86 | 0.59 |
| 1:D:875:LYS:HG3 | 1:D:1189:LEU:O | 2.01 | 0.59 |
| 1:D:1148:ARG:CZ | 1:D:1231:LEU:HD22 | 2.33 | 0.59 |
| 1:D:167:PRO:CD | 1:D:168:ALA:H | 2.16 | 0.59 |
| 1:D:245:ILE:CG1 | 1:D:246:PRO:HD3 | 2.33 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:312:TRP:CA | 1:D:316:LYS:HD3 | 2.32 | 0.59 |
| 1:D:479:TYR:HD1 | 1:D:480:LYS:HG3 | 1.65 | 0.59 |
| 1:D:509:THR:HG21 | 1:D:512:LYS:HD3 | 1.85 | 0.59 |
| 1:D:769:ASP:O | 1:D:773:LYS:HG2 | 2.02 | 0.59 |
| 1:D:775:GLU:CG | 1:D:780:GLN:HG3 | 2.20 | 0.59 |
| 1:D:795:ASN:N | 1:D:795:ASN:ND2 | 2.34 | 0.59 |
| 2:E:106:LEU:O | 2:E:109:ASN:OD1 | 2.20 | 0.59 |
| 2:E:205:PRO:HG2 | 2:E:241:TRP:HE1 | 1.67 | 0.59 |
| 2:E:282:GLU:HG3 | 2:E:309:HIS:CE1 | 2.37 | 0.59 |
| 2:E:466:MET:HG2 | 2:E:467:HIS:H | 1.67 | 0.59 |
| 2:E:475:LEU:HB3 | 2:E:479:ILE:CD1 | 2.33 | 0.59 |
| 2:F:251:TRP:HE3 | 2:F:251:TRP:HA | 1.66 | 0.59 |
| 2:F:306:LEU:HD21 | 2:F:310:GLU:CG | 2.33 | 0.59 |
| 2:F:343:ASP:HB2 | 2:F:347:LEU:HD11 | 1.83 | 0.59 |
| 2:F:428:LEU:HB3 | 2:F:432:TYR:CE1 | 2.38 | 0.59 |
| 2:F:432:TYR:CB | 2:F:437:ILE:HD11 | 2.31 | 0.59 |
| 2:F:67:GLU:O | 2:F:71:GLU:N | 2.33 | 0.59 |
| 1:A:996:ARG:CD | 1:A:1000:GLU:O | 2.51 | 0.59 |
| 1:A:1003:TRP:HA | 1:A:1006:ARG:HB2 | 1.85 | 0.59 |
| 1:A:1231:LEU:HD12 | 1:A:1235:SER:CB | 2.33 | 0.59 |
| 1:A:154:ALA:O | 1:A:158:LEU:HD13 | 2.02 | 0.59 |
| 1:A:213:VAL:HG12 | 1:A:401:TRP:CE2 | 2.36 | 0.59 |
| 1:A:282:TYR:CZ | 1:A:291:PHE:CE1 | 2.91 | 0.59 |
| 1:A:460:LYS:O | 1:A:464:MET:N | 2.36 | 0.59 |
| 1:A:605:LEU:HB2 | 1:A:614:TYR:CD1 | 2.38 | 0.59 |
| 1:A:601:LYS:HZ1 | 1:A:721:ALA:C | 2.05 | 0.59 |
| 1:A:728:THR:CG2 | 1:A:729:GLN:H | 2.03 | 0.59 |
| 1:A:875:LYS:O | 1:A:1189:LEU:HB2 | 2.02 | 0.59 |
| 2:B:106:LEU:O | 2:B:110:LEU:N | 2.32 | 0.59 |
| 2:C:344:ARG:CA | 2:C:347:LEU:HB2 | 2.25 | 0.59 |
| 2:C:393:LEU:HA | 2:C:396:ARG:HG3 | 1.85 | 0.59 |
| 1:D:176:THR:HG23 | 1:D:177:ARG:N | 2.16 | 0.59 |
| 1:D:279:ARG:CZ | 1:D:433:SER:O | 2.51 | 0.59 |
| 1:D:460:LYS:O | 1:D:461:LYS:C | 2.38 | 0.59 |
| 1:D:646:VAL:HG12 | 1:D:647:CYS:N | 2.18 | 0.59 |
| 1:D:742:VAL:CG2 | 1:D:748:TRP:CE3 | 2.86 | 0.59 |
| 1:D:868:ASP:OD1 | 1:D:1199:THR:HG21 | 2.03 | 0.59 |
| 1:D:898:ILE:CG1 | 1:D:899:ALA:N | 2.66 | 0.59 |
| 2:F:208:LEU:O | 2:F:208:LEU:CD1 | 2.48 | 0.59 |
| 2:F:208:LEU:HD11 | 2:F:240:VAL:C | 2.23 | 0.59 |
| 1:D:472:GLN:CG | 2:F:460:THR:OG1 | 2.51 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1060:LYS:HE2 | 1:A:1064:ILE:HG23 | 1.85 | 0.59 |
| 1:A:1113:LEU:HB2 | 1:A:1117:LYS:NZ | 2.18 | 0.59 |
| 1:A:157:LEU:HD21 | 1:A:194:ALA:O | 2.03 | 0.59 |
| 1:A:245:ILE:HG13 | 1:A:246:PRO:CD | 2.22 | 0.59 |
| 1:A:560:PRO:HB2 | 2:C:452:LEU:HD21 | 1.85 | 0.59 |
| 1:A:464:MET:SD | 1:A:579:ARG:HB2 | 2.43 | 0.59 |
| 1:A:617:ARG:HB3 | 1:A:763:GLY:O | 2.03 | 0.59 |
| 1:A:604:ALA:CB | 1:A:717:LEU:CD1 | 2.80 | 0.59 |
| 2:B:411:ILE:HD12 | 2:B:411:ILE:N | 2.18 | 0.59 |
| 2:B:87:SER:C | 2:B:89:ASP:H | 2.06 | 0.59 |
| 2:C:466:MET:CA | 2:C:471:LEU:HD22 | 2.33 | 0.59 |
| 1:D:1008:LEU:HD22 | 1:D:1008:LEU:C | 2.22 | 0.59 |
| 1:D:1057:MET:HB3 | 1:D:1064:ILE:CD1 | 2.26 | 0.59 |
| 1:D:1069:ILE:CB | 1:D:1070:PRO:CD | 2.77 | 0.59 |
| 1:D:1109:LEU:HD21 | 1:D:1137:VAL:HG21 | 1.85 | 0.59 |
| 1:D:86:GLN:HE21 | 1:D:132:GLY:HA3 | 1.68 | 0.59 |
| 1:D:312:TRP:CE3 | 1:D:316:LYS:HD2 | 2.38 | 0.59 |
| 1:D:348:LEU:HD21 | 1:D:350:ILE:CG1 | 2.23 | 0.59 |
| 1:D:597:ARG:NH1 | 1:D:725:PRO:N | 2.51 | 0.59 |
| 1:D:907:PHE:HE2 | 1:D:913:CYS:HG | 1.50 | 0.59 |
| 1:D:973:LEU:HB3 | 1:D:977:GLU:OE1 | 2.01 | 0.59 |
| 1:D:993:ARG:C | 1:D:996:ARG:CD | 2.70 | 0.59 |
| 2:E:199:LEU:CG | 2:E:200:VAL:N | 2.65 | 0.59 |
| 2:E:218:VAL:HB | 2:E:230:SER:OG | 2.02 | 0.59 |
| 2:E:247:THR:HB | 2:E:251:TRP:NE1 | 2.18 | 0.59 |
| 2:E:379:ALA:HB3 | 2:E:438:LEU:HD21 | 1.85 | 0.59 |
| 2:E:76:ARG:CG | 2:E:435:MET:SD | 2.90 | 0.59 |
| 2:F:442:LEU:O | 2:F:455:LEU:CD1 | 2.50 | 0.59 |
| 1:A:1147:TYR:O | 1:A:1150:ALA:HB3 | 2.03 | 0.59 |
| 1:A:868:ASP:CB | 1:A:1199:THR:HB | 2.33 | 0.59 |
| 1:A:1179:PHE:O | 1:A:1220:ILE:HD11 | 2.03 | 0.59 |
| 1:A:173:GLU:OE2 | 1:A:223:TRP:CZ2 | 2.47 | 0.59 |
| 1:A:509:THR:CB | 1:A:513:LEU:HD21 | 2.33 | 0.59 |
| 1:A:853:ARG:NH1 | 1:A:1102:GLN:O | 2.36 | 0.59 |
| 1:A:896:LEU:HD21 | 1:A:951:TYR:CE2 | 2.38 | 0.59 |
| 2:B:182:ARG:HB3 | 2:B:215:PHE:HD1 | 1.67 | 0.59 |
| 2:C:229:LYS:O | 2:C:230:SER:HB2 | 2.02 | 0.59 |
| 2:C:114:TRP:NE1 | 2:C:259:ARG:NH2 | 2.51 | 0.59 |
| 2:C:361:PHE:HD2 | 2:C:362:THR:HG23 | 1.66 | 0.59 |
| 2:C:67:GLU:O | 2:C:71:GLU:HB3 | 2.02 | 0.59 |
| 2:C:81:GLY:HA3 | 2:C:97:PRO:CD | 2.33 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:1165:ALA:HB3 | 1:D:1166:TYR:CD1 | 2.37 | 0.59 |
| 1:D:877:MET:HE1 | 1:D:1203:PRO:C | 2.22 | 0.59 |
| 1:D:297:MET:HG3 | 1:D:415:LEU:CD1 | 2.32 | 0.59 |
| 1:D:482:ASP:CB | 1:D:483:PRO:HD2 | 2.32 | 0.59 |
| 1:D:502:LYS:CG | 1:D:506:GLU:HB3 | 2.33 | 0.59 |
| 1:D:516:GLU:HG2 | 1:D:565:HIS:NE2 | 2.17 | 0.59 |
| 1:D:514:PRO:O | 1:D:568:GLY:HA3 | 2.03 | 0.59 |
| 1:D:742:VAL:CG1 | 1:D:743:ASP:N | 2.65 | 0.59 |
| 1:D:795:ASN:C | 1:D:798:ILE:HG12 | 2.22 | 0.59 |
| 2:F:304:TRP:N | 2:F:337:SER:CB | 2.52 | 0.59 |
| 2:F:371:VAL:HG23 | 2:F:433:ASP:CA | 2.32 | 0.59 |
| 2:F:382:LYS:O | 2:F:438:LEU:HB2 | 2.02 | 0.59 |
| 1:A:1015:THR:C | 1:A:1016:GLU:OE2 | 2.41 | 0.58 |
| 1:A:426:GLY:HA2 | 1:A:1117:LYS:HZ1 | 1.66 | 0.58 |
| 1:A:201:VAL:HG13 | 1:A:206:GLY:O | 2.03 | 0.58 |
| 1:A:245:ILE:O | 1:A:248:GLU:CG | 2.51 | 0.58 |
| 1:A:371:LYS:HD3 | 1:A:396:CYS:CA | 2.21 | 0.58 |
| 1:A:750:PHE:N | 1:A:750:PHE:CD1 | 2.71 | 0.58 |
| 1:A:937:THR:HA | 1:A:940:GLY:HA2 | 1.84 | 0.58 |
| 1:A:996:ARG:NH1 | 1:A:1003:TRP:HB3 | 2.17 | 0.58 |
| 2:B:122:ARG:O | 2:B:124:GLN:N | 2.30 | 0.58 |
| 2:B:203:ARG:HH11 | 2:B:206:TYR:HB3 | 1.68 | 0.58 |
| 2:B:385:LEU:CB | 2:B:441:VAL:HG23 | 2.32 | 0.58 |
| 2:C:128:VAL:CG1 | 2:C:192:HIS:HD2 | 2.16 | 0.58 |
| 2:C:344:ARG:CG | 2:C:347:LEU:HD22 | 2.33 | 0.58 |
| 2:C:351:TYR:HD1 | 2:C:355:GLN:HA | 1.67 | 0.58 |
| 2:C:394:GLU:C | 2:C:397:GLN:HB3 | 2.23 | 0.58 |
| 2:C:484:ASN:C | 2:C:485:VAL:HG13 | 2.23 | 0.58 |
| 2:C:74:GLN:HG3 | 2:C:75:ARG:N | 2.17 | 0.58 |
| 2:C:81:GLY:HA3 | 2:C:97:PRO:HD2 | 1.84 | 0.58 |
| 1:D:1056:GLU:HB3 | 1:D:1057:MET:HE3 | 1.83 | 0.58 |
| 1:D:1188:CYS:SG | 1:D:1189:LEU:N | 2.75 | 0.58 |
| 1:D:291:PHE:O | 1:D:293:ASP:N | 2.36 | 0.58 |
| 1:D:213:VAL:HG13 | 1:D:401:TRP:NE1 | 2.17 | 0.58 |
| 1:D:439:GLN:NE2 | 1:D:837:TYR:HE2 | 2.01 | 0.58 |
| 1:D:474:LEU:CD1 | 1:D:474:LEU:N | 2.65 | 0.58 |
| 1:D:498:LYS:HZ3 | 1:D:521:PRO:HB3 | 1.68 | 0.58 |
| 1:D:567:PRO:O | 1:D:569:HIS:N | 2.36 | 0.58 |
| 1:D:620:TRP:CD1 | 1:D:620:TRP:N | 2.69 | 0.58 |
| 1:D:967:MET:CE | 1:D:978:ALA:HB2 | 2.33 | 0.58 |
| 1:D:981:LYS:O | 1:D:985:MET:HG3 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:380:PRO:C | 2:E:382:LYS:N | 2.55 | 0.58 |
| 2:F:131:LEU:O | 2:F:133:HIS:HB2 | 2.03 | 0.58 |
| 2:F:239:LEU:H | 2:F:338:VAL:CB | 2.14 | 0.58 |
| 2:F:294:PRO:HD2 | 2:F:295:TRP:CZ3 | 2.38 | 0.58 |
| 2:F:475:LEU:HA | 2:F:478:TYR:HB2 | 1.85 | 0.58 |
| 1:A:886:LEU:C | 1:A:1146:ARG:CZ | 2.72 | 0.58 |
| 1:A:445:LEU:O | 1:A:449:GLN:HG3 | 2.03 | 0.58 |
| 1:A:526:ASP:OD2 | 1:A:527:GLN:N | 2.36 | 0.58 |
| 1:A:627:ARG:O | 1:A:627:ARG:HG3 | 2.03 | 0.58 |
| 1:A:655:LEU:O | 1:A:659:HIS:CB | 2.48 | 0.58 |
| 1:A:80:SER:OG | 1:A:81:ARG:N | 2.35 | 0.58 |
| 1:A:296:SER:CB | 1:A:847:ALA:HB3 | 2.30 | 0.58 |
| 1:A:877:MET:HE2 | 1:A:877:MET:O | 2.03 | 0.58 |
| 1:A:76:ILE:CB | 1:A:911:HIS:CE1 | 2.82 | 0.58 |
| 2:B:269:SER:CB | 2:B:352:ASP:OD1 | 2.51 | 0.58 |
| 2:C:287:ASN:O | 2:C:302:THR:O | 2.21 | 0.58 |
| 2:C:403:PHE:HD1 | 2:C:417:TYR:HH | 1.48 | 0.58 |
| 2:C:452:LEU:HD12 | 2:C:453:ILE:CG1 | 2.33 | 0.58 |
| 1:D:1067:SER:HB3 | 1:D:1073:PRO:HG2 | 1.85 | 0.58 |
| 1:D:1196:ASP:OD2 | 1:D:1204:THR:HG21 | 2.03 | 0.58 |
| 1:D:177:ARG:HG2 | 1:D:218:SER:OG | 2.03 | 0.58 |
| 1:D:371:LYS:HZ1 | 1:D:396:CYS:HB2 | 1.66 | 0.58 |
| 1:D:456:GLN:O | 1:D:460:LYS:HD3 | 2.03 | 0.58 |
| 1:D:607:TRP:O | 1:D:611:PRO:O | 2.21 | 0.58 |
| 1:D:737:GLY:N | 1:D:750:PHE:HZ | 1.94 | 0.58 |
| 1:D:802:ARG:HG3 | 1:D:803:ASN:OD1 | 2.02 | 0.58 |
| 1:D:247:LEU:CA | 1:D:815:TRP:HD1 | 2.16 | 0.58 |
| 1:D:829:PRO:HG3 | 1:D:831:TYR:CZ | 2.38 | 0.58 |
| 2:E:79:LEU:CA | 2:E:100:GLY:N | 2.65 | 0.58 |
| 2:E:369:ARG:CA | 2:E:430:SER:HB3 | 2.33 | 0.58 |
| 2:F:254:PHE:CE2 | 2:F:255:TRP:CE2 | 2.90 | 0.58 |
| 2:F:396:ARG:HD2 | 2:F:396:ARG:C | 2.23 | 0.58 |
| 2:F:455:LEU:HB3 | 2:F:456:ARG:HE | 1.66 | 0.58 |
| 1:A:1046:GLU:OE1 | 1:A:1046:GLU:HA | 2.03 | 0.58 |
| 1:A:167:PRO:O | 1:A:168:ALA:C | 2.42 | 0.58 |
| 1:A:371:LYS:HZ1 | 1:A:400:VAL:HG23 | 1.65 | 0.58 |
| 1:A:297:MET:HE3 | 1:A:411:LEU:HD13 | 1.84 | 0.58 |
| 1:A:579:ARG:HH11 | 1:A:579:ARG:HG2 | 1.68 | 0.58 |
| 1:A:606:THR:N | 1:A:613:HIS:O | 2.36 | 0.58 |
| 1:A:752:LEU:HB3 | 1:A:753:PRO:CA | 2.33 | 0.58 |
| 1:A:976:GLN:O | 1:A:979:ALA:HB3 | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:133:HIS:CE1 | 2:C:231:ILE:CG2 | 2.86 | 0.58 |
| 2:B:445:GLU:C | 2:B:447:THR:H | 2.05 | 0.58 |
| 2:C:201:ASN:C | 2:C:203:ARG:N | 2.56 | 0.58 |
| 2:C:354:PHE:HE1 | 2:C:370:LYS:CB | 2.16 | 0.58 |
| 2:C:398:VAL:CA | 2:C:401:GLY:H | 2.15 | 0.58 |
| 2:C:405:GLU:OE1 | 2:C:406:LEU:HD12 | 2.03 | 0.58 |
| 1:D:1069:ILE:CG2 | 1:D:1070:PRO:CD | 2.61 | 0.58 |
| 1:D:1141:VAL:HG11 | 1:D:1146:ARG:HA | 1.86 | 0.58 |
| 1:D:1151:LEU:CD2 | 1:D:1223:ILE:HD11 | 2.33 | 0.58 |
| 1:D:131:TYR:CB | 1:D:138:HIS:HE1 | 2.13 | 0.58 |
| 1:D:375:GLU:O | 1:D:378:VAL:N | 2.34 | 0.58 |
| 1:D:617:ARG:O | 1:D:762:VAL:CG2 | 2.49 | 0.58 |
| 1:D:801:TRP:O | 1:D:804:ALA:N | 2.36 | 0.58 |
| 1:D:91:GLY:O | 1:D:92:GLY:C | 2.42 | 0.58 |
| 2:E:102:LEU:C | 2:E:102:LEU:CD1 | 2.71 | 0.58 |
| 2:E:123:GLU:HB3 | 2:F:403:PHE:CZ | 2.39 | 0.58 |
| 2:E:239:LEU:CD2 | 2:E:338:VAL:HG21 | 2.34 | 0.58 |
| 2:E:390:GLY:H | 2:E:395:LEU:HG | 1.64 | 0.58 |
| 2:F:130:ALA:HB1 | 2:F:182:ARG:NH1 | 2.17 | 0.58 |
| 2:F:241:TRP:HZ3 | 2:F:255:TRP:CZ2 | 2.21 | 0.58 |
| 2:F:368:HIS:CE1 | 2:F:370:LYS:HD2 | 2.37 | 0.58 |
| 2:F:388:GLY:O | 2:F:444:THR:HA | 2.03 | 0.58 |
| 2:F:456:ARG:HE | 2:F:456:ARG:N | 2.00 | 0.58 |
| 2:F:466:MET:CE | 2:F:471:LEU:HB3 | 2.33 | 0.58 |
| 1:A:1014:ARG:O | 1:A:1015:THR:HG23 | 2.03 | 0.58 |
| 1:A:1020:ILE:CG1 | 1:A:1021:SER:N | 2.66 | 0.58 |
| 1:A:1123:PHE:C | 1:A:1125:ILE:N | 2.56 | 0.58 |
| 1:A:1209:ARG:HH12 | 2:C:256:LEU:CB | 2.16 | 0.58 |
| 1:A:291:PHE:O | 1:A:292:LEU:HB2 | 2.04 | 0.58 |
| 1:A:312:TRP:O | 1:A:316:LYS:HB3 | 2.03 | 0.58 |
| 1:A:374:ARG:NE | 1:A:392:LEU:CD1 | 2.62 | 0.58 |
| 1:A:385:ILE:HG23 | 1:A:386:ARG:N | 2.17 | 0.58 |
| 1:A:443:ARG:O | 1:A:447:GLU:HG3 | 2.02 | 0.58 |
| 1:A:616:GLU:HG3 | 1:A:724:GLY:O | 2.03 | 0.58 |
| 1:A:744:ILE:CB | 1:A:745:PRO:CD | 2.74 | 0.58 |
| 1:A:74:LEU:C | 1:A:76:ILE:H | 2.05 | 0.58 |
| 1:A:79:LEU:CB | 1:A:89:GLY:HA2 | 2.28 | 0.58 |
| 1:A:929:THR:HG23 | 1:A:947:LYS:HD3 | 1.85 | 0.58 |
| 1:A:958:GLY:CA | 1:A:986:TYR:CE2 | 2.86 | 0.58 |
| 2:B:248:SER:O | 2:B:252:LEU:HD13 | 2.03 | 0.58 |
| 2:C:383:VAL:HG22 | 2:C:384:ALA:N | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:435:MET:HE2 | 2:C:435:MET:CA | 2.23 | 0.58 |
| 2:C:448:LEU:HA | 2:C:451:GLY:HA2 | 1.83 | 0.58 |
| 2:C:59:ALA:HA | 2:C:62:SER:OG | 2.02 | 0.58 |
| 1:D:1138:ARG:NH2 | 1:D:1191:LYS:NZ | 2.51 | 0.58 |
| 1:D:259:ARG:O | 1:D:260:ASP:OD2 | 2.21 | 0.58 |
| 1:D:401:TRP:CD1 | 1:D:404:HIS:HD2 | 2.21 | 0.58 |
| 1:D:597:ARG:CA | 1:D:616:GLU:OE1 | 2.51 | 0.58 |
| 1:D:728:THR:HG23 | 1:D:741:ASP:OD2 | 2.04 | 0.58 |
| 1:D:868:ASP:O | 1:D:869:ARG:HB2 | 2.02 | 0.58 |
| 1:D:916:PHE:O | 1:D:916:PHE:HD1 | 1.86 | 0.58 |
| 1:D:995:TYR:CE1 | 1:D:1004:LEU:CB | 2.62 | 0.58 |
| 2:E:130:ALA:HB2 | 2:E:210:GLN:NE2 | 2.19 | 0.58 |
| 2:E:72:ILE:HD11 | 2:E:370:LYS:HE2 | 1.85 | 0.58 |
| 2:E:88:ARG:H | 2:E:88:ARG:HD3 | 1.66 | 0.58 |
| 2:F:208:LEU:CD2 | 2:F:242:PHE:CD2 | 2.87 | 0.58 |
| 2:F:400:GLN:NE2 | 2:F:404:ASN:CG | 2.56 | 0.58 |
| 1:A:228:LEU:C | 1:A:228:LEU:CD2 | 2.69 | 0.58 |
| 1:A:316:LYS:HZ2 | 1:A:350:ILE:CG2 | 2.17 | 0.58 |
| 1:A:376:LEU:C | 1:A:378:VAL:N | 2.56 | 0.58 |
| 1:A:572:TRP:HB2 | 2:C:477:LYS:HE2 | 1.85 | 0.58 |
| 1:A:732:TYR:CE1 | 1:A:755:LYS:HG2 | 2.38 | 0.58 |
| 1:A:660:CYS:CB | 1:A:745:PRO:HG3 | 2.33 | 0.58 |
| 2:B:309:HIS:HB3 | 2:B:312:LEU:HD23 | 1.78 | 0.58 |
| 2:B:385:LEU:HB3 | 2:B:441:VAL:CG2 | 2.33 | 0.58 |
| 2:C:146:ARG:CB | 2:C:228:VAL:HG11 | 2.33 | 0.58 |
| 2:C:456:ARG:HB2 | 2:C:463:LYS:HB3 | 1.84 | 0.58 |
| 2:C:88:ARG:HG2 | 2:C:89:ASP:N | 2.17 | 0.58 |
| 1:D:1068:ASP:O | 1:D:1069:ILE:O | 2.21 | 0.58 |
| 1:D:249:VAL:CG2 | 1:D:251:THR:HG22 | 2.33 | 0.58 |
| 1:D:223:TRP:CZ3 | 1:D:250:PRO:HB2 | 2.38 | 0.58 |
| 1:D:449:GLN:O | 1:D:452:TYR:CD2 | 2.56 | 0.58 |
| 2:E:429:TYR:O | 2:E:431:LYS:O | 2.20 | 0.58 |
| 2:F:274:SER:OG | 2:F:275:SER:N | 2.35 | 0.58 |
| 2:F:241:TRP:HB2 | 2:F:336:LEU:HB2 | 1.82 | 0.58 |
| 2:F:414:TRP:O | 2:F:414:TRP:CG | 2.56 | 0.58 |
| 1:A:1131:ILE:HG12 | 1:A:1133:ILE:H | 1.68 | 0.58 |
| 1:A:886:LEU:N | 1:A:1146:ARG:CZ | 2.67 | 0.58 |
| 1:A:1154:GLN:NE2 | 1:A:1220:ILE:HG13 | 2.19 | 0.58 |
| 1:A:77:GLN:HB2 | 1:A:1174:PRO:CB | 2.34 | 0.58 |
| 1:A:257:THR:OG1 | 1:A:258:GLN:N | 2.35 | 0.58 |
| 1:A:197:PHE:HB3 | 1:A:277:HIS:CD2 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:296:SER:HB2 | 1:A:846:THR:O | 2.02 | 0.58 |
| 1:A:214:ALA:HA | 1:A:401:TRP:HZ2 | 1.62 | 0.58 |
| 1:A:588:GLY:HA3 | 1:A:806:LYS:NZ | 2.18 | 0.58 |
| 1:A:930:ASP:CA | 1:A:933:SER:HB3 | 2.31 | 0.58 |
| 1:A:948:ILE:HG13 | 1:A:949:PHE:CD2 | 2.38 | 0.58 |
| 2:B:451:GLY:C | 2:B:452:LEU:HD22 | 2.24 | 0.58 |
| 2:B:133:HIS:NE2 | 2:C:231:ILE:HG22 | 2.19 | 0.58 |
| 2:C:452:LEU:CD1 | 2:C:453:ILE:H | 2.16 | 0.58 |
| 1:D:857:PRO:C | 1:D:1062:GLU:OE2 | 2.42 | 0.58 |
| 1:D:265:LEU:HG | 1:D:266:VAL:C | 2.24 | 0.58 |
| 1:D:381:THR:HG23 | 1:D:382:MET:N | 2.19 | 0.58 |
| 1:D:401:TRP:O | 1:D:405:GLU:HG2 | 2.03 | 0.58 |
| 1:D:415:LEU:C | 1:D:417:ARG:N | 2.57 | 0.58 |
| 1:D:472:GLN:O | 2:F:461:THR:HG21 | 2.03 | 0.58 |
| 1:D:652:ILE:HG22 | 1:D:656:TYR:HE2 | 1.67 | 0.58 |
| 1:D:272:SER:CB | 1:D:843:GLN:CD | 2.68 | 0.58 |
| 1:D:948:ILE:CG2 | 1:D:1071:ARG:CB | 2.80 | 0.58 |
| 2:E:278:CYS:O | 2:E:286:GLY:O | 2.20 | 0.58 |
| 2:E:377:CYS:C | 2:E:380:PRO:CD | 2.67 | 0.58 |
| 2:E:379:ALA:C | 2:E:438:LEU:HD11 | 2.24 | 0.58 |
| 2:E:425:LEU:N | 2:E:428:LEU:HD11 | 2.17 | 0.58 |
| 1:A:1006:ARG:CZ | 1:A:1010:LEU:CD1 | 2.81 | 0.58 |
| 1:A:190:PRO:C | 1:A:192:GLU:HG3 | 2.24 | 0.58 |
| 1:A:220:TRP:NE1 | 1:A:221:TYR:CD1 | 2.72 | 0.58 |
| 1:A:232:ARG:HD2 | 1:A:239:LEU:HD23 | 1.86 | 0.58 |
| 1:A:605:LEU:H | 1:A:717:LEU:HD21 | 1.69 | 0.58 |
| 1:A:637:GLY:O | 1:A:641:GLU:HG2 | 2.03 | 0.58 |
| 1:A:659:HIS:HD2 | 1:A:720:THR:HB | 1.68 | 0.58 |
| 1:A:739:TYR:O | 1:A:740:ASN:HB3 | 2.02 | 0.58 |
| 1:A:622:TYR:N | 1:A:747:CYS:O | 2.37 | 0.58 |
| 1:A:884:TYR:HB3 | 1:A:1140:LEU:HD21 | 1.84 | 0.58 |
| 1:A:914:THR:O | 1:A:915:ALA:HB3 | 2.04 | 0.58 |
| 2:B:396:ARG:HD2 | 2:B:418:LEU:N | 2.19 | 0.58 |
| 2:B:417:TYR:C | 2:B:419:GLU:N | 2.54 | 0.58 |
| 2:C:423:SER:CB | 2:C:428:LEU:HD21 | 2.33 | 0.58 |
| 2:C:484:ASN:C | 2:C:485:VAL:CG1 | 2.72 | 0.58 |
| 2:C:68:ALA:O | 2:C:72:ILE:HG12 | 2.04 | 0.58 |
| 1:D:872:SER:HG | 1:D:1200:PRO:N | 2.02 | 0.58 |
| 1:D:357:ALA:O | 1:D:358:GLU:C | 2.40 | 0.58 |
| 1:D:464:MET:O | 1:D:467:ALA:HB3 | 2.03 | 0.58 |
| 1:D:601:LYS:HZ1 | 1:D:722:ARG:H | 1.51 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:744:ILE:HB | 1:D:745:PRO:CD | 2.34 | 0.58 |
| 1:D:823:ARG:NH1 | 1:D:824:ALA:HB2 | 2.18 | 0.58 |
| 1:D:279:ARG:CB | 1:D:841:LEU:CB | 2.82 | 0.58 |
| 1:D:273:PHE:N | 1:D:843:GLN:OE1 | 2.37 | 0.58 |
| 2:E:229:LYS:HG2 | 2:E:231:ILE:HG13 | 1.84 | 0.58 |
| 2:E:456:ARG:HG2 | 2:E:457:SER:N | 2.16 | 0.58 |
| 2:E:104:VAL:HG21 | 2:F:128:VAL:HA | 1.84 | 0.58 |
| 2:F:323:HIS:C | 2:F:331:VAL:O | 2.41 | 0.58 |
| 2:F:435:MET:CA | 2:F:435:MET:HE2 | 2.26 | 0.58 |
| 1:A:110:HIS:O | 1:A:112:LEU:CD1 | 2.51 | 0.58 |
| 1:A:296:SER:HB3 | 1:A:846:THR:O | 2.03 | 0.58 |
| 1:A:389:PHE:HD2 | 1:A:393:MET:HG2 | 1.68 | 0.58 |
| 1:A:392:LEU:CD2 | 1:A:393:MET:HE3 | 2.33 | 0.58 |
| 1:A:588:GLY:CA | 1:A:806:LYS:HZ1 | 2.16 | 0.58 |
| 1:A:623:LEU:O | 1:A:625:PRO:CD | 2.52 | 0.58 |
| 1:A:76:ILE:CG1 | 1:A:77:GLN:HG3 | 2.22 | 0.58 |
| 1:A:788:GLY:HA2 | 1:A:791:ALA:HB3 | 1.86 | 0.58 |
| 2:B:323:HIS:CB | 2:B:331:VAL:O | 2.52 | 0.58 |
| 2:B:475:LEU:O | 2:B:479:ILE:HD13 | 2.04 | 0.58 |
| 2:C:444:THR:N | 2:C:447:THR:CG2 | 2.67 | 0.58 |
| 2:C:454:HIS:CB | 2:C:468:ILE:HD12 | 2.33 | 0.58 |
| 1:D:252:GLY:O | 1:D:253:ALA:CB | 2.49 | 0.58 |
| 1:D:312:TRP:O | 1:D:316:LYS:HD3 | 2.04 | 0.58 |
| 1:D:371:LYS:O | 1:D:372:GLU:HB2 | 2.03 | 0.58 |
| 1:D:441:TRP:NE1 | 1:D:880:ALA:N | 2.47 | 0.58 |
| 1:D:670:PRO:CG | 1:D:673:ALA:HB2 | 2.20 | 0.58 |
| 1:D:798:ILE:CG2 | 1:D:869:ARG:CZ | 2.80 | 0.58 |
| 1:D:900:ALA:C | 1:D:915:ALA:CB | 2.71 | 0.58 |
| 1:D:949:PHE:CD1 | 1:D:950:ASN:N | 2.72 | 0.58 |
| 1:D:972:ARG:C | 1:D:974:THR:N | 2.55 | 0.58 |
| 2:E:104:VAL:HG21 | 2:F:128:VAL:C | 2.24 | 0.58 |
| 2:F:342:LEU:N | 2:F:342:LEU:HD22 | 2.19 | 0.58 |
| 2:F:458:ARG:HH11 | 2:F:458:ARG:HG3 | 1.69 | 0.58 |
| 2:F:474:PHE:CE2 | 2:F:475:LEU:HD23 | 2.39 | 0.58 |
| 1:A:129:PRO:C | 1:A:130:LEU:HD12 | 2.24 | 0.58 |
| 1:A:230:GLU:OE1 | 1:A:231:GLU:N | 2.23 | 0.58 |
| 1:A:386:ARG:CZ | 1:A:387:GLU:HG2 | 2.34 | 0.58 |
| 1:A:389:PHE:CD2 | 1:A:393:MET:HG2 | 2.39 | 0.58 |
| 1:A:618:HIS:HB2 | 1:A:725:PRO:CD | 2.34 | 0.58 |
| 1:A:630:ASN:HD21 | 1:A:632:ALA:HB2 | 1.68 | 0.58 |
| 1:A:726:LYS:HD3 | 1:A:727:ASP:OD2 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:134:LYS:CB | 2:C:180:LYS:CE | 2.81 | 0.58 |
| 2:C:344:ARG:HA | 2:C:347:LEU:HD13 | 1.86 | 0.58 |
| 2:C:395:LEU:HD11 | 2:C:447:THR:OG1 | 2.03 | 0.58 |
| 1:D:1207:GLU:CA | 1:D:1210:TYR:CD2 | 2.79 | 0.58 |
| 1:D:169:TRP:O | 1:D:169:TRP:CD1 | 2.57 | 0.58 |
| 1:D:195:LEU:H | 1:D:265:LEU:HD13 | 1.68 | 0.58 |
| 1:D:203:LEU:N | 1:D:380:GLY:CA | 2.52 | 0.58 |
| 1:D:549:LEU:N | 1:D:551:LYS:HD3 | 2.17 | 0.58 |
| 1:D:742:VAL:HG21 | 1:D:748:TRP:CE3 | 2.38 | 0.58 |
| 1:D:770:PHE:HA | 1:D:773:LYS:CG | 2.34 | 0.58 |
| 1:D:891:VAL:CG2 | 1:D:1135:ASP:HA | 2.34 | 0.58 |
| 1:D:993:ARG:O | 1:D:996:ARG:CD | 2.52 | 0.58 |
| 2:E:215:PHE:HB2 | 2:E:232:GLY:O | 2.04 | 0.58 |
| 2:E:270:PRO:HA | 2:E:273:PHE:HD2 | 1.66 | 0.58 |
| 2:E:326:ASP:H | 2:E:331:VAL:CG1 | 2.16 | 0.58 |
| 2:F:214:CYS:SG | 2:F:236:GLU:HG2 | 2.43 | 0.58 |
| 2:F:253:ASP:HB3 | 2:F:257:ARG:CZ | 2.34 | 0.58 |
| 2:F:197:LEU:HD11 | 2:F:322:LEU:HD21 | 1.85 | 0.58 |
| 2:F:241:TRP:HB2 | 2:F:336:LEU:CB | 2.33 | 0.58 |
| 2:F:442:LEU:O | 2:F:455:LEU:HD21 | 2.04 | 0.58 |
| 1:A:1027:LYS:CB | 1:A:1092:PHE:HD2 | 2.09 | 0.58 |
| 1:A:1236:GLN:CB | 1:A:1237:PRO:HD3 | 2.22 | 0.58 |
| 1:A:167:PRO:HB2 | 1:A:177:ARG:NE | 2.19 | 0.58 |
| 1:A:253:ALA:HB2 | 1:A:280:GLU:CA | 2.34 | 0.58 |
| 1:A:276:ALA:C | 1:A:279:ARG:HB2 | 2.24 | 0.58 |
| 1:A:316:LYS:NZ | 1:A:350:ILE:HG13 | 2.18 | 0.58 |
| 1:A:392:LEU:HD21 | 1:A:395:TYR:HB2 | 1.86 | 0.58 |
| 1:A:448:ALA:O | 1:A:870:VAL:CG1 | 2.51 | 0.58 |
| 1:A:534:SER:OG | 1:A:535:GLU:N | 2.37 | 0.58 |
| 1:A:620:TRP:N | 1:A:620:TRP:CD1 | 2.70 | 0.58 |
| 1:A:775:GLU:HB3 | 1:A:796:LYS:HD2 | 1.84 | 0.58 |
| 1:A:900:ALA:HA | 1:A:915:ALA:HB1 | 1.83 | 0.58 |
| 1:A:900:ALA:HA | 1:A:915:ALA:HB2 | 1.84 | 0.58 |
| 2:B:217:PRO:HA | 2:B:232:GLY:H | 1.69 | 0.58 |
| 2:B:93:SER:C | 2:B:95:CYS:N | 2.56 | 0.58 |
| 1:D:1116:MET:HE3 | 1:D:1153:LEU:CA | 2.28 | 0.58 |
| 1:D:145:LYS:CB | 1:D:1118:TRP:CH2 | 2.86 | 0.58 |
| 1:D:371:LYS:HG3 | 1:D:396:CYS:N | 2.18 | 0.58 |
| 1:D:490:TRP:HZ2 | 1:D:598:VAL:HB | 1.66 | 0.58 |
| 1:D:652:ILE:O | 1:D:653:GLU:C | 2.42 | 0.58 |
| 1:D:727:ASP:OD2 | 1:D:727:ASP:C | 2.42 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:218:VAL:N | 2:E:231:ILE:HA | 2.19 | 0.58 |
| 2:E:389:ARG:NH2 | 2:E:390:GLY:O | 2.37 | 0.58 |
| 2:E:396:ARG:HA | 2:E:399:CYS:SG | 2.44 | 0.58 |
| 2:E:403:PHE:CZ | 2:E:407:LEU:HD11 | 2.39 | 0.58 |
| 2:E:422:GLN:C | 2:E:424:SER:N | 2.57 | 0.58 |
| 2:F:240:VAL:C | 2:F:336:LEU:HD13 | 2.23 | 0.58 |
| 2:F:421:MET:HG3 | 2:F:422:GLN:N | 2.18 | 0.58 |
| 2:F:439:PHE:CD1 | 2:F:458:ARG:HG3 | 2.39 | 0.58 |
| 1:A:1131:ILE:HG12 | 1:A:1137:VAL:HA | 1.86 | 0.57 |
| 1:A:1207:GLU:CA | 1:A:1210:TYR:CD1 | 2.87 | 0.57 |
| 1:A:214:ALA:N | 1:A:401:TRP:HZ2 | 2.02 | 0.57 |
| 1:A:576:LEU:HD23 | 2:C:481:SER:HG | 1.68 | 0.57 |
| 1:A:808:ILE:O | 1:A:811:GLN:CD | 2.42 | 0.57 |
| 1:A:847:ALA:HA | 1:A:852:ARG:HB3 | 1.86 | 0.57 |
| 2:B:260:LEU:O | 2:B:264:ARG:HG3 | 2.03 | 0.57 |
| 2:B:323:HIS:CE1 | 2:B:330:ASN:HB2 | 2.38 | 0.57 |
| 2:B:104:VAL:CG2 | 2:C:128:VAL:O | 2.52 | 0.57 |
| 2:C:193:TYR:HB2 | 2:C:242:PHE:CZ | 2.38 | 0.57 |
| 2:C:185:LEU:HG | 2:C:214:CYS:SG | 2.44 | 0.57 |
| 2:C:294:PRO:HD2 | 2:C:295:TRP:CZ3 | 2.39 | 0.57 |
| 2:C:413:VAL:HG12 | 2:C:414:TRP:N | 2.18 | 0.57 |
| 1:D:1124:ALA:CB | 1:D:1148:ARG:NH1 | 2.61 | 0.57 |
| 1:D:86:GLN:HG3 | 1:D:132:GLY:O | 2.04 | 0.57 |
| 1:D:176:THR:H | 1:D:185:VAL:CG1 | 2.17 | 0.57 |
| 1:D:347:TRP:NE1 | 1:D:349:ASP:CG | 2.57 | 0.57 |
| 1:D:815:TRP:CE3 | 1:D:838:GLY:N | 2.67 | 0.57 |
| 2:E:322:LEU:C | 2:E:324:GLY:N | 2.55 | 0.57 |
| 2:E:404:ASN:O | 2:E:406:LEU:N | 2.37 | 0.57 |
| 2:E:94:GLY:O | 2:E:96:HIS:CD2 | 2.57 | 0.57 |
| 2:F:308:ASP:OD2 | 2:F:308:ASP:N | 2.36 | 0.57 |
| 2:F:354:PHE:O | 2:F:355:GLN:C | 2.42 | 0.57 |
| 1:A:996:ARG:HH12 | 1:A:1003:TRP:C | 2.08 | 0.57 |
| 1:A:1019:TRP:HZ2 | 1:A:1111:LEU:HD21 | 1.67 | 0.57 |
| 1:A:243:ASP:C | 1:A:246:PRO:HD2 | 2.24 | 0.57 |
| 1:A:712:VAL:N | 1:A:713:PRO:HD3 | 2.20 | 0.57 |
| 2:B:208:LEU:CD2 | 2:B:240:VAL:HB | 2.33 | 0.57 |
| 2:B:472:LYS:HG3 | 2:B:473:ASP:H | 1.68 | 0.57 |
| 2:C:206:TYR:CZ | 2:C:208:LEU:HD23 | 2.39 | 0.57 |
| 2:C:255:TRP:O | 2:C:256:LEU:C | 2.41 | 0.57 |
| 2:C:278:CYS:SG | 2:C:279:GLN:N | 2.77 | 0.57 |
| 2:C:299:LEU:CD2 | 2:C:299:LEU:N | 2.64 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:363:ARG:NH1 | 2:C:363:ARG:CA | 2.64 | 0.57 |
| 2:C:389:ARG:CZ | 2:C:390:GLY:N | 2.67 | 0.57 |
| 2:C:452:LEU:CD1 | 2:C:453:ILE:N | 2.65 | 0.57 |
| 2:C:454:HIS:HA | 2:C:468:ILE:CD1 | 2.27 | 0.57 |
| 1:D:1131:ILE:CG1 | 1:D:1138:ARG:H | 2.15 | 0.57 |
| 1:D:1166:TYR:C | 1:D:1169:GLY:H | 2.06 | 0.57 |
| 1:D:1151:LEU:CD1 | 1:D:1227:THR:OG1 | 2.51 | 0.57 |
| 1:D:1236:GLN:HB2 | 1:D:1237:PRO:HD2 | 1.86 | 0.57 |
| 1:D:371:LYS:CE | 1:D:396:CYS:HB2 | 2.34 | 0.57 |
| 1:D:459:MET:N | 1:D:460:LYS:CE | 2.67 | 0.57 |
| 1:D:484:TRP:CD1 | 1:D:484:TRP:C | 2.77 | 0.57 |
| 1:D:580:LEU:O | 1:D:580:LEU:HD12 | 2.04 | 0.57 |
| 1:D:607:TRP:HD1 | 1:D:779:LEU:CA | 2.17 | 0.57 |
| 1:D:726:LYS:O | 1:D:726:LYS:HD3 | 2.03 | 0.57 |
| 1:D:900:ALA:CA | 1:D:915:ALA:CB | 2.81 | 0.57 |
| 2:E:255:TRP:HE3 | 2:E:255:TRP:HA | 1.67 | 0.57 |
| 2:E:430:SER:C | 2:E:433:ASP:HB3 | 2.25 | 0.57 |
| 2:F:216:HIS:O | 2:F:231:ILE:HD13 | 2.03 | 0.57 |
| 2:F:92:LEU:HD21 | 2:F:344:ARG:HE | 1.69 | 0.57 |
| 2:F:78:PHE:HZ | 2:F:346:MET:HE2 | 1.68 | 0.57 |
| 1:A:1183:VAL:O | 1:A:1217:ALA:HB1 | 2.03 | 0.57 |
| 1:A:272:SER:HA | 1:A:275:ARG:HD3 | 1.86 | 0.57 |
| 1:A:274:ASP:C | 1:A:277:HIS:H | 2.08 | 0.57 |
| 1:A:389:PHE:CD1 | 1:A:390:GLN:NE2 | 2.72 | 0.57 |
| 1:A:403:THR:OG1 | 1:A:404:HIS:N | 2.37 | 0.57 |
| 1:A:421:PRO:HG2 | 1:A:422:VAL:N | 2.19 | 0.57 |
| 1:A:608:ASP:HB3 | 1:A:779:LEU:CB | 2.34 | 0.57 |
| 1:A:634:LEU:HD12 | 1:A:638:THR:HG21 | 1.85 | 0.57 |
| 1:A:79:LEU:HB3 | 1:A:89:GLY:CA | 2.30 | 0.57 |
| 1:A:943:ARG:O | 1:A:947:LYS:HG3 | 2.04 | 0.57 |
| 2:B:67:GLU:CB | 2:B:70:LEU:HD13 | 2.35 | 0.57 |
| 2:C:352:ASP:C | 2:C:352:ASP:OD1 | 2.41 | 0.57 |
| 2:C:352:ASP:O | 2:C:356:LEU:HG | 2.04 | 0.57 |
| 2:C:395:LEU:O | 2:C:395:LEU:HD23 | 2.04 | 0.57 |
| 2:C:78:PHE:O | 2:C:99:PHE:HB3 | 2.03 | 0.57 |
| 1:D:1091:GLU:O | 1:D:1096:ARG:NH2 | 2.35 | 0.57 |
| 1:D:1171:ASN:O | 1:D:1172:ASP:HB2 | 2.02 | 0.57 |
| 1:D:157:LEU:HG | 1:D:194:ALA:HB1 | 1.84 | 0.57 |
| 1:D:175:TRP:CB | 1:D:185:VAL:HG13 | 2.33 | 0.57 |
| 1:D:357:ALA:C | 1:D:359:VAL:N | 2.54 | 0.57 |
| 1:D:442:GLU:OE2 | 1:D:442:GLU:CA | 2.50 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:613:HIS:ND1 | 1:D:717:LEU:CD2 | 2.67 | 0.57 |
| 1:D:959:GLN:O | 1:D:982:ALA:HB1 | 2.04 | 0.57 |
| 2:E:184:ASN:O | 2:E:184:ASN:OD1 | 2.21 | 0.57 |
| 2:F:132:HIS:HA | 2:F:182:ARG:HG3 | 1.86 | 0.57 |
| 2:F:311:LEU:HD22 | 2:F:311:LEU:N | 2.18 | 0.57 |
| 2:F:359:ASN:O | 2:F:360:SER:HB2 | 2.04 | 0.57 |
| 2:F:472:LYS:HA | 2:F:475:LEU:CD1 | 2.34 | 0.57 |
| 1:A:1030:ARG:NH2 | 1:A:1040:LYS:HG2 | 2.19 | 0.57 |
| 1:A:1054:GLU:O | 1:A:1058:PHE:HD2 | 1.86 | 0.57 |
| 1:A:612:LEU:O | 1:A:613:HIS:ND1 | 2.37 | 0.57 |
| 2:B:104:VAL:O | 2:B:105:GLU:C | 2.41 | 0.57 |
| 2:B:213:VAL:HG23 | 2:B:235:THR:HA | 1.86 | 0.57 |
| 2:C:198:ASP:OD1 | 2:C:198:ASP:C | 2.42 | 0.57 |
| 2:C:336:LEU:C | 2:C:336:LEU:CD2 | 2.72 | 0.57 |
| 1:D:138:HIS:HA | 1:D:141:LEU:HD13 | 1.84 | 0.57 |
| 1:D:145:LYS:CB | 1:D:1118:TRP:HH2 | 2.17 | 0.57 |
| 1:D:400:VAL:C | 1:D:403:THR:HG23 | 2.24 | 0.57 |
| 1:D:792:LEU:O | 1:D:795:ASN:N | 2.37 | 0.57 |
| 1:D:801:TRP:HH2 | 1:D:805:HIS:CE1 | 2.22 | 0.57 |
| 2:E:122:ARG:N | 2:E:122:ARG:HD2 | 2.20 | 0.57 |
| 2:E:247:THR:HG22 | 2:E:250:GLN:NE2 | 2.13 | 0.57 |
| 2:F:347:LEU:O | 2:F:350:LEU:CD1 | 2.52 | 0.57 |
| 1:A:1043:VAL:C | 1:A:1045:ALA:N | 2.48 | 0.57 |
| 1:A:211:LEU:HD12 | 1:A:222:SER:H | 1.67 | 0.57 |
| 1:A:376:LEU:HD12 | 1:A:379:LYS:HB3 | 1.85 | 0.57 |
| 1:A:498:LYS:CE | 1:A:499:LYS:H | 2.12 | 0.57 |
| 1:A:619:GLY:HA3 | 1:A:750:PHE:HA | 1.86 | 0.57 |
| 1:A:775:GLU:CA | 1:A:780:GLN:HG3 | 2.20 | 0.57 |
| 1:A:207:THR:HG21 | 1:A:812:MET:HB3 | 1.85 | 0.57 |
| 1:A:928:GLY:O | 1:A:931:LEU:N | 2.35 | 0.57 |
| 2:B:450:ASN:HB2 | 2:B:452:LEU:HD23 | 1.85 | 0.57 |
| 2:B:67:GLU:HB3 | 2:B:70:LEU:CB | 2.29 | 0.57 |
| 2:C:115:TRP:O | 2:C:119:VAL:HG23 | 2.05 | 0.57 |
| 2:C:471:LEU:CA | 2:C:474:PHE:HB3 | 2.30 | 0.57 |
| 1:D:1175:GLN:C | 1:D:1177:VAL:N | 2.58 | 0.57 |
| 1:D:382:MET:O | 1:D:385:ILE:HG22 | 2.04 | 0.57 |
| 1:D:417:ARG:HG2 | 1:D:417:ARG:NH1 | 2.19 | 0.57 |
| 1:D:458:GLU:C | 1:D:460:LYS:HE3 | 2.24 | 0.57 |
| 1:D:652:ILE:O | 1:D:655:LEU:N | 2.37 | 0.57 |
| 1:D:668:LEU:H | 1:D:668:LEU:HD23 | 1.70 | 0.57 |
| 1:D:831:TYR:CB | 1:D:837:TYR:OH | 2.52 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:966:LEU:C | 1:D:970:ASN:HD22 | 2.07 | 0.57 |
| 2:E:288:LYS:HB2 | 2:E:290:TYR:OH | 2.05 | 0.57 |
| 2:F:114:TRP:CB | 2:F:262:TRP:CZ2 | 2.87 | 0.57 |
| 2:F:326:ASP:OD2 | 2:F:327:GLY:N | 2.35 | 0.57 |
| 2:F:342:LEU:HD23 | 2:F:345:GLY:N | 2.09 | 0.57 |
| 1:A:1069:ILE:N | 1:A:1070:PRO:HD3 | 2.20 | 0.57 |
| 1:A:1125:ILE:HD12 | 1:A:1125:ILE:O | 2.04 | 0.57 |
| 1:A:1141:VAL:HG11 | 1:A:1145:ASP:O | 2.05 | 0.57 |
| 1:A:886:LEU:C | 1:A:1146:ARG:NH2 | 2.58 | 0.57 |
| 1:A:130:LEU:HG | 1:A:131:TYR:CE1 | 2.39 | 0.57 |
| 1:A:262:GLN:OE1 | 1:A:262:GLN:HA | 2.02 | 0.57 |
| 1:A:275:ARG:O | 1:A:278:ILE:C | 2.42 | 0.57 |
| 1:A:373:PRO:HD2 | 1:A:374:ARG:NH1 | 2.19 | 0.57 |
| 1:A:408:GLN:O | 1:A:411:LEU:HG | 2.03 | 0.57 |
| 2:B:113:GLU:C | 2:B:262:TRP:CZ2 | 2.78 | 0.57 |
| 2:B:309:HIS:CB | 2:B:312:LEU:HD22 | 2.18 | 0.57 |
| 2:B:398:VAL:O | 2:B:402:LEU:HG | 2.05 | 0.57 |
| 2:C:254:PHE:HA | 2:C:257:ARG:HD2 | 1.86 | 0.57 |
| 2:C:372:LEU:CD2 | 2:C:436:SER:HB2 | 2.35 | 0.57 |
| 2:C:82:SER:O | 2:C:83:LYS:CB | 2.53 | 0.57 |
| 1:D:1032:THR:O | 1:D:1032:THR:HG23 | 2.04 | 0.57 |
| 1:D:1196:ASP:C | 1:D:1196:ASP:OD2 | 2.41 | 0.57 |
| 1:D:272:SER:HA | 1:D:843:GLN:CB | 2.35 | 0.57 |
| 1:D:369:LEU:O | 1:D:371:LYS:N | 2.37 | 0.57 |
| 1:D:851:THR:HG22 | 1:D:851:THR:O | 2.03 | 0.57 |
| 2:E:300:ILE:HG13 | 2:E:301:GLU:N | 2.20 | 0.57 |
| 2:E:234:LYS:HA | 2:E:343:ASP:OD2 | 2.05 | 0.57 |
| 2:F:200:VAL:HG12 | 2:F:200:VAL:O | 2.04 | 0.57 |
| 2:F:416:GLY:HA2 | 2:F:419:GLU:CB | 2.34 | 0.57 |
| 2:F:425:LEU:HD13 | 2:F:442:LEU:HD11 | 1.86 | 0.57 |
| 2:F:441:VAL:HG23 | 2:F:441:VAL:O | 2.05 | 0.57 |
| 2:F:74:GLN:NE2 | 2:F:75:ARG:HH21 | 2.01 | 0.57 |
| 1:A:1020:ILE:HG13 | 1:A:1021:SER:N | 2.19 | 0.57 |
| 1:A:1205:GLY:HA3 | 1:A:1209:ARG:NE | 2.20 | 0.57 |
| 1:A:120:LEU:N | 1:A:120:LEU:HD22 | 2.18 | 0.57 |
| 1:A:1231:LEU:CD1 | 1:A:1236:GLN:HE22 | 2.15 | 0.57 |
| 1:A:203:LEU:CA | 1:A:205:GLU:H | 2.16 | 0.57 |
| 1:A:267:VAL:HG23 | 1:A:291:PHE:CE2 | 2.40 | 0.57 |
| 1:A:582:ASP:CB | 1:A:592:LEU:HD22 | 2.35 | 0.57 |
| 1:A:613:HIS:O | 1:A:614:TYR:HB2 | 2.03 | 0.57 |
| 1:A:620:TRP:C | 1:A:748:TRP:CB | 2.73 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:876:ALA:O | 1:A:877:MET:C | 2.43 | 0.57 |
| 2:B:206:TYR:CZ | 2:B:242:PHE:HZ | 2.22 | 0.57 |
| 2:B:325:ARG:N | 2:B:325:ARG:NE | 2.53 | 0.57 |
| 2:B:372:LEU:O | 2:B:436:SER:HA | 2.05 | 0.57 |
| 2:C:94:GLY:HA2 | 2:C:96:HIS:ND1 | 2.19 | 0.57 |
| 1:D:961:PHE:CZ | 1:D:1049:TRP:CE3 | 2.92 | 0.57 |
| 1:D:1090:GLU:O | 1:D:1090:GLU:HG3 | 2.04 | 0.57 |
| 1:D:392:LEU:HD23 | 1:D:392:LEU:O | 2.04 | 0.57 |
| 1:D:580:LEU:HD11 | 1:D:593:SER:CB | 2.35 | 0.57 |
| 1:D:628:ARG:O | 1:D:630:ASN:N | 2.33 | 0.57 |
| 1:D:719:LEU:CG | 1:D:720:THR:N | 2.65 | 0.57 |
| 1:D:770:PHE:HE1 | 1:D:968:GLN:CB | 2.18 | 0.57 |
| 2:E:108:LYS:HZ2 | 2:E:108:LYS:HB2 | 1.70 | 0.57 |
| 2:E:122:ARG:O | 2:E:125:VAL:HG23 | 2.05 | 0.57 |
| 2:E:123:GLU:HG2 | 2:F:415:PRO:CG | 2.33 | 0.57 |
| 2:E:200:VAL:HG13 | 2:F:418:LEU:HD23 | 1.86 | 0.57 |
| 2:E:215:PHE:CB | 2:E:233:GLU:HA | 2.35 | 0.57 |
| 2:E:243:THR:OG1 | 2:E:244:PRO:HD2 | 2.05 | 0.57 |
| 2:E:441:VAL:CG1 | 2:E:442:LEU:H | 2.17 | 0.57 |
| 2:E:460:THR:O | 2:E:461:THR:CG2 | 2.53 | 0.57 |
| 1:A:1017:GLY:O | 1:A:1019:TRP:N | 2.37 | 0.57 |
| 1:A:1191:LYS:O | 1:A:1192:GLU:CB | 2.51 | 0.57 |
| 1:A:192:GLU:CB | 1:A:217:PRO:CG | 2.77 | 0.57 |
| 1:A:197:PHE:HA | 1:A:213:VAL:O | 2.04 | 0.57 |
| 1:A:290:ARG:C | 1:A:291:PHE:CD2 | 2.78 | 0.57 |
| 1:A:299:MET:HG3 | 1:A:848:GLY:HA2 | 1.86 | 0.57 |
| 1:A:560:PRO:O | 1:A:561:LYS:HD3 | 2.05 | 0.57 |
| 1:A:770:PHE:HB2 | 1:A:771:LEU:HD22 | 1.86 | 0.57 |
| 2:C:145:PHE:O | 2:C:146:ARG:HG3 | 2.05 | 0.57 |
| 2:C:204:LEU:HD21 | 2:C:206:TYR:CD1 | 2.39 | 0.57 |
| 2:C:342:LEU:N | 2:C:342:LEU:HD22 | 2.20 | 0.57 |
| 1:D:274:ASP:OD2 | 1:D:293:ASP:CA | 2.47 | 0.57 |
| 1:D:406:VAL:CG2 | 1:D:407:PHE:N | 2.67 | 0.57 |
| 1:D:548:CYS:N | 1:D:551:LYS:NZ | 2.50 | 0.57 |
| 1:D:645:VAL:C | 1:D:646:VAL:HG23 | 2.25 | 0.57 |
| 1:D:711:ALA:O | 1:D:713:PRO:HD3 | 2.05 | 0.57 |
| 2:E:311:LEU:HD22 | 2:E:312:LEU:HD12 | 1.86 | 0.57 |
| 2:E:436:SER:O | 2:E:437:ILE:HD12 | 2.04 | 0.57 |
| 2:F:300:ILE:CG2 | 2:F:342:LEU:HD11 | 2.34 | 0.57 |
| 2:F:317:GLY:HA3 | 2:F:320:SER:CB | 2.33 | 0.57 |
| 1:A:192:GLU:O | 1:A:193:ARG:CG | 2.52 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:235:TRP:O | 1:A:235:TRP:HD1 | 1.88 | 0.57 |
| 1:A:407:PHE:O | 1:A:411:LEU:N | 2.38 | 0.57 |
| 1:A:515:ILE:CG1 | 1:A:568:GLY:O | 2.53 | 0.57 |
| 1:A:616:GLU:O | 1:A:617:ARG:CB | 2.52 | 0.57 |
| 1:A:618:HIS:HB2 | 1:A:725:PRO:HD2 | 1.87 | 0.57 |
| 1:A:949:PHE:N | 1:A:949:PHE:CD2 | 2.73 | 0.57 |
| 2:B:417:TYR:O | 2:C:203:ARG:NH1 | 2.38 | 0.57 |
| 2:C:243:THR:O | 2:C:334:CYS:CB | 2.52 | 0.57 |
| 2:C:398:VAL:C | 2:C:401:GLY:H | 2.07 | 0.57 |
| 1:D:1016:GLU:HG3 | 1:D:1022:LEU:HD21 | 1.87 | 0.57 |
| 1:D:1072:THR:N | 1:D:1073:PRO:CD | 2.66 | 0.57 |
| 1:D:1134:HIS:O | 1:D:1135:ASP:CB | 2.48 | 0.57 |
| 1:D:224:CYS:SG | 1:D:228:LEU:CD2 | 2.93 | 0.57 |
| 1:D:206:GLY:HA2 | 1:D:245:ILE:HG21 | 1.87 | 0.57 |
| 1:D:539:PHE:O | 1:D:540:GLN:CB | 2.53 | 0.57 |
| 2:E:387:VAL:HG12 | 2:E:416:GLY:N | 2.20 | 0.57 |
| 2:E:426:GLU:HA | 2:E:429:TYR:HB3 | 1.86 | 0.57 |
| 2:E:432:TYR:CD2 | 2:E:437:ILE:HG12 | 2.35 | 0.57 |
| 2:E:448:LEU:CD2 | 2:E:449:GLU:N | 2.67 | 0.57 |
| 2:E:442:LEU:O | 2:E:453:ILE:HB | 2.04 | 0.57 |
| 2:E:93:SER:C | 2:E:95:CYS:N | 2.54 | 0.57 |
| 1:A:956:GLY:O | 1:A:1094:THR:HA | 2.05 | 0.57 |
| 1:A:1208:ARG:H | 1:A:1210:TYR:N | 2.02 | 0.57 |
| 1:A:276:ALA:HA | 1:A:279:ARG:CG | 2.35 | 0.57 |
| 1:A:608:ASP:OD1 | 1:A:779:LEU:O | 2.22 | 0.57 |
| 1:A:655:LEU:CD1 | 1:A:719:LEU:C | 2.72 | 0.57 |
| 1:A:866:ARG:CB | 1:A:1069:ILE:HG21 | 2.35 | 0.57 |
| 2:C:351:TYR:C | 2:C:355:GLN:CB | 2.60 | 0.57 |
| 2:C:417:TYR:N | 2:C:417:TYR:CD2 | 2.40 | 0.57 |
| 1:D:136:ASP:OD2 | 1:D:1167:LYS:CE | 2.53 | 0.57 |
| 1:D:1231:LEU:O | 1:D:1232:GLU:HG2 | 2.05 | 0.57 |
| 1:D:211:LEU:HA | 1:D:221:TYR:CD1 | 2.40 | 0.57 |
| 1:D:597:ARG:NH1 | 1:D:724:GLY:C | 2.57 | 0.57 |
| 1:D:730:PRO:HB3 | 1:D:761:ASN:HA | 1.86 | 0.57 |
| 2:E:384:ALA:C | 2:E:414:TRP:HB3 | 2.26 | 0.57 |
| 2:E:481:SER:O | 2:E:484:ASN:HB2 | 2.04 | 0.57 |
| 2:F:406:LEU:CA | 2:F:409:ASN:ND2 | 2.56 | 0.57 |
| 2:F:82:SER:O | 2:F:83:LYS:CG | 2.52 | 0.57 |
| 2:F:88:ARG:HG2 | 2:F:89:ASP:N | 2.20 | 0.57 |
| 1:A:1113:LEU:CB | 1:A:1117:LYS:HE3 | 2.34 | 0.56 |
| 1:A:1154:GLN:O | 1:A:1158:LEU:HG | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:249:VAL:HG21 | 1:A:817:PRO:HG3 | 1.87 | 0.56 |
| 1:A:472:GLN:N | 1:A:472:GLN:OE1 | 2.38 | 0.56 |
| 1:A:504:LYS:HD3 | 1:A:523:ASP:CB | 2.34 | 0.56 |
| 1:A:516:GLU:O | 1:A:517:GLY:O | 2.21 | 0.56 |
| 1:A:869:ARG:N | 1:A:1201:SER:H | 2.03 | 0.56 |
| 2:B:262:TRP:O | 2:B:265:LYS:N | 2.38 | 0.56 |
| 2:C:115:TRP:CZ3 | 2:C:210:GLN:HA | 2.40 | 0.56 |
| 2:C:125:VAL:CG2 | 2:C:126:PHE:N | 2.61 | 0.56 |
| 2:C:144:ALA:O | 2:C:145:PHE:CB | 2.53 | 0.56 |
| 2:C:344:ARG:HG2 | 2:C:347:LEU:HD22 | 1.86 | 0.56 |
| 2:C:406:LEU:O | 2:C:407:LEU:C | 2.43 | 0.56 |
| 2:C:413:VAL:C | 2:C:415:PRO:HD2 | 2.24 | 0.56 |
| 2:C:446:THR:OG1 | 2:C:455:LEU:CD2 | 2.51 | 0.56 |
| 1:D:1002:GLU:O | 1:D:1005:VAL:N | 2.37 | 0.56 |
| 1:D:1219:ASP:OD2 | 1:D:1222:GLN:NE2 | 2.37 | 0.56 |
| 1:D:211:LEU:HG | 1:D:221:TYR:HE1 | 1.70 | 0.56 |
| 1:D:275:ARG:O | 1:D:279:ARG:N | 2.36 | 0.56 |
| 1:D:363:TYR:O | 1:D:364:VAL:HB | 2.05 | 0.56 |
| 1:D:550:GLN:HB2 | 1:D:551:LYS:HE3 | 1.86 | 0.56 |
| 1:D:293:ASP:OD1 | 1:D:845:VAL:HG13 | 2.04 | 0.56 |
| 1:D:914:THR:HA | 1:D:918:TRP:HB2 | 1.85 | 0.56 |
| 1:D:99:ALA:O | 1:D:100:VAL:C | 2.43 | 0.56 |
| 2:E:431:LYS:HG3 | 2:E:432:TYR:N | 2.20 | 0.56 |
| 1:A:80:SER:OG | 1:A:125:LEU:CG | 2.53 | 0.56 |
| 1:A:258:GLN:OE1 | 1:A:258:GLN:N | 2.38 | 0.56 |
| 1:A:474:LEU:N | 1:A:474:LEU:HD13 | 2.20 | 0.56 |
| 1:A:80:SER:HG | 1:A:125:LEU:HD11 | 1.70 | 0.56 |
| 1:A:435:LEU:O | 1:A:839:ALA:HB1 | 2.06 | 0.56 |
| 2:B:461:THR:HG23 | 2:B:463:LYS:HZ2 | 1.70 | 0.56 |
| 2:C:202:LYS:O | 2:C:325:ARG:HG2 | 2.05 | 0.56 |
| 2:C:365:LYS:HB3 | 2:C:367:LEU:HD21 | 1.88 | 0.56 |
| 1:D:948:ILE:HD13 | 1:D:1071:ARG:HD2 | 1.87 | 0.56 |
| 1:D:891:VAL:HG21 | 1:D:1135:ASP:HA | 1.87 | 0.56 |
| 1:D:1198:LYS:N | 1:D:1204:THR:OG1 | 2.38 | 0.56 |
| 1:D:132:GLY:N | 1:D:138:HIS:CE1 | 2.73 | 0.56 |
| 1:D:282:TYR:HD2 | 1:D:432:VAL:HG13 | 1.67 | 0.56 |
| 1:D:407:PHE:HD1 | 1:D:411:LEU:CD2 | 2.19 | 0.56 |
| 1:D:513:LEU:O | 1:D:568:GLY:HA2 | 2.05 | 0.56 |
| 1:D:652:ILE:HG22 | 1:D:656:TYR:CE2 | 2.40 | 0.56 |
| 1:D:767:ALA:C | 1:D:768:LYS:O | 2.36 | 0.56 |
| 2:E:241:TRP:CZ3 | 2:E:255:TRP:HZ2 | 2.23 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:395:LEU:O | 2:E:399:CYS:SG | 2.64 | 0.56 |
| 2:E:432:TYR:HB3 | 2:E:437:ILE:HD11 | 1.82 | 0.56 |
| 2:E:445:GLU:OE2 | 2:E:445:GLU:N | 2.38 | 0.56 |
| 2:F:127:PRO:CG | 2:F:128:VAL:N | 2.67 | 0.56 |
| 2:F:395:LEU:HB3 | 2:F:443:VAL:HG23 | 1.86 | 0.56 |
| 2:F:403:PHE:HD1 | 2:F:417:TYR:OH | 1.82 | 0.56 |
| 2:F:265:LYS:HE2 | 2:F:485:VAL:HG22 | 1.86 | 0.56 |
| 1:A:1060:LYS:CD | 1:A:1073:PRO:CB | 2.76 | 0.56 |
| 1:A:196:VAL:CG1 | 1:A:401:TRP:HZ3 | 2.18 | 0.56 |
| 1:A:232:ARG:HD2 | 1:A:239:LEU:CD2 | 2.34 | 0.56 |
| 1:A:293:ASP:HB2 | 1:A:296:SER:HB3 | 1.85 | 0.56 |
| 1:A:371:LYS:HG3 | 1:A:372:GLU:N | 2.19 | 0.56 |
| 1:A:608:ASP:O | 1:A:620:TRP:CZ2 | 2.58 | 0.56 |
| 1:A:730:PRO:HB3 | 1:A:761:ASN:HA | 1.88 | 0.56 |
| 1:A:620:TRP:C | 1:A:748:TRP:HB3 | 2.24 | 0.56 |
| 1:A:867:PRO:CG | 1:A:1067:SER:OG | 2.53 | 0.56 |
| 1:A:913:CYS:C | 1:A:918:TRP:N | 2.58 | 0.56 |
| 1:A:938:THR:O | 1:A:939:VAL:HG23 | 2.05 | 0.56 |
| 2:B:88:ARG:HA | 2:B:91:LEU:HD12 | 1.86 | 0.56 |
| 2:C:204:LEU:HG | 2:C:206:TYR:CB | 2.36 | 0.56 |
| 2:C:393:LEU:HA | 2:C:396:ARG:CG | 2.34 | 0.56 |
| 2:C:414:TRP:CG | 2:C:414:TRP:O | 2.57 | 0.56 |
| 2:C:386:ASP:CB | 2:C:442:LEU:HD23 | 2.25 | 0.56 |
| 2:C:444:THR:O | 2:C:446:THR:N | 2.38 | 0.56 |
| 1:D:1027:LYS:CG | 1:D:1091:GLU:HA | 2.35 | 0.56 |
| 1:D:556:THR:HG23 | 2:F:451:GLY:O | 2.04 | 0.56 |
| 1:D:559:LEU:HD12 | 1:D:560:PRO:CD | 2.33 | 0.56 |
| 1:D:496:LYS:CE | 1:D:571:GLY:HA2 | 2.36 | 0.56 |
| 1:D:757:GLY:O | 1:D:758:ASN:HB2 | 2.05 | 0.56 |
| 1:D:850:ILE:HG12 | 1:D:851:THR:N | 2.20 | 0.56 |
| 1:D:992:LEU:C | 1:D:996:ARG:HD2 | 2.24 | 0.56 |
| 2:E:214:CYS:N | 2:E:234:LYS:O | 2.32 | 0.56 |
| 1:A:1040:LYS:HB3 | 1:A:1044:VAL:HG12 | 1.86 | 0.56 |
| 1:A:1172:ASP:O | 1:A:1173:LEU:HG | 2.05 | 0.56 |
| 1:A:1212:ILE:HD12 | 1:A:1212:ILE:N | 2.19 | 0.56 |
| 1:A:176:THR:OG1 | 1:A:177:ARG:N | 2.35 | 0.56 |
| 1:A:411:LEU:HD12 | 1:A:412:PRO:CD | 2.35 | 0.56 |
| 1:A:482:ASP:CB | 1:A:483:PRO:CD | 2.83 | 0.56 |
| 1:A:877:MET:HA | 1:A:877:MET:CE | 2.36 | 0.56 |
| 1:A:905:ALA:HA | 1:A:910:MET:HB3 | 1.86 | 0.56 |
| 1:A:981:LYS:O | 1:A:985:MET:HG3 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:417:TYR:O | 2:B:418:LEU:HB3 | 2.06 | 0.56 |
| 2:B:78:PHE:CD1 | 2:B:78:PHE:O | 2.58 | 0.56 |
| 2:C:234:LYS:HZ1 | 2:C:344:ARG:HD2 | 1.65 | 0.56 |
| 1:D:1202:ASN:O | 1:D:1203:PRO:O | 2.24 | 0.56 |
| 1:D:297:MET:HG3 | 1:D:415:LEU:HD11 | 1.87 | 0.56 |
| 1:D:418:CYS:N | 1:D:419:PRO:CD | 2.68 | 0.56 |
| 1:D:656:TYR:CD1 | 1:D:743:ASP:CB | 2.89 | 0.56 |
| 1:D:813:VAL:HB | 1:D:840:ILE:CG1 | 2.31 | 0.56 |
| 1:D:873:GLU:OE1 | 1:D:1203:PRO:HG3 | 2.05 | 0.56 |
| 1:D:112:LEU:HD21 | 1:D:917:GLY:O | 2.06 | 0.56 |
| 1:D:919:MET:C | 1:D:920:THR:O | 2.43 | 0.56 |
| 1:D:970:ASN:C | 1:D:971:HIS:ND1 | 2.59 | 0.56 |
| 2:E:431:LYS:CD | 2:E:432:TYR:H | 2.17 | 0.56 |
| 2:F:221:THR:HG22 | 2:F:222:LYS:N | 2.20 | 0.56 |
| 2:F:311:LEU:HD22 | 2:F:311:LEU:H | 1.71 | 0.56 |
| 2:F:298:GLU:HG3 | 2:F:344:ARG:HH21 | 1.70 | 0.56 |
| 2:F:350:LEU:HD12 | 2:F:351:TYR:H | 1.71 | 0.56 |
| 2:F:354:PHE:CE1 | 2:F:370:LYS:HB3 | 2.38 | 0.56 |
| 2:F:466:MET:CB | 2:F:471:LEU:CD2 | 2.70 | 0.56 |
| 1:A:1047:ARG:HA | 1:A:1047:ARG:CZ | 2.34 | 0.56 |
| 1:A:196:VAL:HG13 | 1:A:269:HIS:NE2 | 2.21 | 0.56 |
| 1:A:197:PHE:H | 1:A:269:HIS:CD2 | 2.20 | 0.56 |
| 1:A:602:LEU:O | 1:A:603:MET:C | 2.41 | 0.56 |
| 1:A:721:ALA:O | 1:A:722:ARG:C | 2.42 | 0.56 |
| 1:A:870:VAL:C | 1:A:872:SER:H | 2.09 | 0.56 |
| 1:A:886:LEU:H | 1:A:1146:ARG:HH21 | 1.50 | 0.56 |
| 2:B:311:LEU:HD12 | 2:B:312:LEU:H | 1.68 | 0.56 |
| 2:C:308:ASP:OD2 | 2:C:334:CYS:SG | 2.62 | 0.56 |
| 2:C:350:LEU:O | 2:C:353:SER:OG | 2.22 | 0.56 |
| 2:C:431:LYS:O | 2:C:434:GLU:HB2 | 2.05 | 0.56 |
| 1:D:1133:ILE:HD13 | 1:D:1133:ILE:N | 2.19 | 0.56 |
| 1:D:1202:ASN:O | 1:D:1205:GLY:CA | 2.53 | 0.56 |
| 1:D:1200:PRO:HD2 | 1:D:1203:PRO:HG2 | 1.88 | 0.56 |
| 1:D:253:ALA:HB2 | 1:D:280:GLU:HB2 | 1.88 | 0.56 |
| 1:D:278:ILE:HD13 | 1:D:291:PHE:CD1 | 2.37 | 0.56 |
| 1:D:278:ILE:HG21 | 1:D:431:GLY:O | 2.04 | 0.56 |
| 1:D:559:LEU:CG | 1:D:560:PRO:CD | 2.82 | 0.56 |
| 1:D:76:ILE:HB | 1:D:911:HIS:NE2 | 2.19 | 0.56 |
| 1:D:901:VAL:HA | 1:D:904:ASP:OD2 | 2.06 | 0.56 |
| 2:F:308:ASP:CG | 2:F:334:CYS:HA | 2.26 | 0.56 |
| 2:F:483:LYS:C | 2:F:483:LYS:HE2 | 2.25 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:82:SER:O | 2:F:83:LYS:CB | 2.52 | 0.56 |
| 1:A:1027:LYS:HD3 | 1:A:1092:PHE:HE2 | 1.71 | 0.56 |
| 1:A:1143:GLU:O | 1:A:1146:ARG:HB2 | 2.05 | 0.56 |
| 1:A:1212:ILE:N | 1:A:1212:ILE:CD1 | 2.68 | 0.56 |
| 1:A:196:VAL:HG11 | 1:A:404:HIS:CG | 2.41 | 0.56 |
| 1:A:354:ASN:O | 1:A:355:SER:CB | 2.54 | 0.56 |
| 1:A:386:ARG:CB | 1:A:390:GLN:HE22 | 2.19 | 0.56 |
| 1:A:437:VAL:HG12 | 1:A:438:ASN:N | 2.20 | 0.56 |
| 1:A:585:TRP:N | 1:A:585:TRP:HE3 | 2.02 | 0.56 |
| 1:A:821:LEU:O | 1:A:821:LEU:HG | 2.05 | 0.56 |
| 2:C:241:TRP:HB2 | 2:C:336:LEU:HB2 | 1.85 | 0.56 |
| 2:C:416:GLY:C | 2:C:419:GLU:HB3 | 2.25 | 0.56 |
| 2:C:426:GLU:OE2 | 2:C:429:TYR:HD1 | 1.87 | 0.56 |
| 2:C:371:VAL:HG23 | 2:C:433:ASP:CA | 2.35 | 0.56 |
| 1:D:1092:PHE:O | 1:D:1096:ARG:CZ | 2.54 | 0.56 |
| 1:D:1154:GLN:O | 1:D:1158:LEU:HD23 | 2.05 | 0.56 |
| 1:D:171:TRP:O | 1:D:172:ALA:CB | 2.44 | 0.56 |
| 1:D:193:ARG:HA | 1:D:193:ARG:HH11 | 1.68 | 0.56 |
| 1:D:245:ILE:CG1 | 1:D:246:PRO:CD | 2.77 | 0.56 |
| 1:D:251:THR:O | 1:D:255:SER:N | 2.39 | 0.56 |
| 1:D:463:LEU:CA | 1:D:466:LEU:HD22 | 2.35 | 0.56 |
| 1:D:486:TRP:HZ2 | 1:D:722:ARG:N | 2.03 | 0.56 |
| 1:D:490:TRP:O | 1:D:580:LEU:HA | 2.06 | 0.56 |
| 1:D:641:GLU:O | 1:D:645:VAL:CG2 | 2.54 | 0.56 |
| 1:D:648:PRO:CD | 1:D:649:TYR:N | 2.68 | 0.56 |
| 1:D:770:PHE:HE1 | 1:D:968:GLN:HB3 | 1.67 | 0.56 |
| 1:D:74:LEU:HD13 | 1:D:77:GLN:HA | 1.86 | 0.56 |
| 1:D:788:GLY:O | 1:D:792:LEU:HD13 | 2.04 | 0.56 |
| 1:D:892:ASP:HA | 1:D:1135:ASP:OD2 | 2.05 | 0.56 |
| 1:D:97:GLU:O | 1:D:101:ARG:CG | 2.53 | 0.56 |
| 2:F:115:TRP:NE1 | 2:F:119:VAL:HG21 | 2.21 | 0.56 |
| 2:F:265:LYS:HG3 | 2:F:485:VAL:HG21 | 1.88 | 0.56 |
| 2:F:387:VAL:CG1 | 2:F:443:VAL:CG2 | 2.83 | 0.56 |
| 1:A:278:ILE:HD13 | 1:A:291:PHE:HD1 | 1.71 | 0.56 |
| 1:A:520:ALA:HB3 | 1:A:521:PRO:HD3 | 1.87 | 0.56 |
| 1:A:597:ARG:O | 1:A:598:VAL:CB | 2.54 | 0.56 |
| 1:A:598:VAL:HA | 1:A:601:LYS:HD2 | 1.87 | 0.56 |
| 1:A:616:GLU:HG3 | 1:A:724:GLY:C | 2.25 | 0.56 |
| 1:A:732:TYR:CE1 | 1:A:755:LYS:CA | 2.88 | 0.56 |
| 1:A:83:LEU:C | 1:A:87:ILE:O | 2.44 | 0.56 |
| 1:A:870:VAL:O | 1:A:872:SER:N | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:269:SER:O | 2:B:272:ASN:ND2 | 2.38 | 0.56 |
| 2:B:385:LEU:HD23 | 2:B:385:LEU:N | 2.20 | 0.56 |
| 2:B:430:SER:O | 2:B:433:ASP:HB2 | 2.05 | 0.56 |
| 2:B:67:GLU:HG2 | 2:B:69:LEU:HG | 1.88 | 0.56 |
| 2:B:72:ILE:CG1 | 2:B:73:CYS:N | 2.67 | 0.56 |
| 2:C:185:LEU:HD21 | 2:C:214:CYS:SG | 2.45 | 0.56 |
| 2:C:286:GLY:HA3 | 2:C:304:TRP:HA | 1.88 | 0.56 |
| 2:C:303:LEU:CA | 2:C:337:SER:CB | 2.81 | 0.56 |
| 2:C:432:TYR:CD1 | 2:C:440:THR:HG21 | 2.41 | 0.56 |
| 2:C:454:HIS:CD2 | 2:C:472:LYS:HE3 | 2.40 | 0.56 |
| 1:D:1025:LEU:HD13 | 1:D:1027:LYS:CE | 2.30 | 0.56 |
| 1:D:1129:PHE:CB | 1:D:1139:TYR:HA | 2.35 | 0.56 |
| 1:D:242:ALA:C | 1:D:245:ILE:HG12 | 2.26 | 0.56 |
| 1:D:257:THR:C | 1:D:258:GLN:HG3 | 2.26 | 0.56 |
| 1:D:194:ALA:HB1 | 1:D:265:LEU:HD12 | 1.85 | 0.56 |
| 1:D:269:HIS:C | 1:D:274:ASP:OD1 | 2.44 | 0.56 |
| 1:D:289:MET:SD | 1:D:291:PHE:CE2 | 2.99 | 0.56 |
| 1:D:412:PRO:HG2 | 1:D:413:LEU:N | 2.21 | 0.56 |
| 1:D:580:LEU:CD1 | 1:D:593:SER:OG | 2.47 | 0.56 |
| 1:D:914:THR:C | 1:D:918:TRP:HB3 | 2.19 | 0.56 |
| 2:E:128:VAL:O | 2:E:210:GLN:NE2 | 2.39 | 0.56 |
| 2:E:283:GLY:HA3 | 2:E:306:LEU:CD2 | 2.35 | 0.56 |
| 2:F:204:LEU:N | 2:F:204:LEU:HD12 | 2.21 | 0.56 |
| 2:F:403:PHE:CE2 | 2:F:407:LEU:HB2 | 2.41 | 0.56 |
| 1:A:107:LEU:CB | 1:A:113:TRP:CD1 | 2.84 | 0.56 |
| 1:A:1019:TRP:CZ3 | 1:A:1164:PHE:HA | 2.39 | 0.56 |
| 1:A:278:ILE:CD1 | 1:A:291:PHE:CD1 | 2.88 | 0.56 |
| 1:A:392:LEU:HD23 | 1:A:392:LEU:O | 2.05 | 0.56 |
| 1:A:656:TYR:CB | 1:A:720:THR:OG1 | 2.51 | 0.56 |
| 1:A:754:HIS:ND1 | 1:A:760:CYS:O | 2.39 | 0.56 |
| 1:A:798:ILE:CD1 | 1:A:802:ARG:HE | 2.19 | 0.56 |
| 1:A:440:ASN:CB | 1:A:877:MET:SD | 2.92 | 0.56 |
| 2:C:285:LYS:HZ1 | 2:C:285:LYS:HB2 | 1.71 | 0.56 |
| 1:A:576:LEU:CD2 | 2:C:481:SER:OG | 2.51 | 0.56 |
| 1:D:1069:ILE:O | 1:D:1071:ARG:NH1 | 2.39 | 0.56 |
| 1:D:1108:TYR:HE1 | 1:D:1160:THR:HG22 | 1.71 | 0.56 |
| 1:D:196:VAL:HG12 | 1:D:268:GLY:CA | 2.36 | 0.56 |
| 1:D:369:LEU:HB3 | 1:D:372:GLU:CB | 2.35 | 0.56 |
| 1:D:369:LEU:HB3 | 1:D:372:GLU:HB2 | 1.86 | 0.56 |
| 1:D:576:LEU:HD11 | 1:D:577:CYS:SG | 2.46 | 0.56 |
| 1:D:660:CYS:SG | 1:D:745:PRO:HG3 | 2.45 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:666:GLN:CA | 1:D:669:MET:O | 2.54 | 0.56 |
| 1:D:795:ASN:CA | 1:D:798:ILE:HG12 | 2.35 | 0.56 |
| 1:D:797:MET:O | 1:D:869:ARG:HD3 | 2.05 | 0.56 |
| 1:D:797:MET:CA | 1:D:869:ARG:HD3 | 2.35 | 0.56 |
| 1:D:916:PHE:CE2 | 1:D:1174:PRO:HG2 | 2.40 | 0.56 |
| 2:E:133:HIS:NE2 | 2:F:231:ILE:HG22 | 2.20 | 0.56 |
| 2:E:263:TRP:O | 2:E:265:LYS:N | 2.38 | 0.56 |
| 2:F:236:GLU:CB | 2:F:341:ASP:HB3 | 2.36 | 0.56 |
| 2:F:375:HIS:ND1 | 2:F:376:PRO:HD2 | 2.20 | 0.56 |
| 2:F:390:GLY:HA2 | 2:F:392:THR:N | 2.20 | 0.56 |
| 2:F:76:ARG:CZ | 2:F:434:GLU:OE1 | 2.54 | 0.56 |
| 2:F:483:LYS:O | 2:F:485:VAL:CG1 | 2.54 | 0.56 |
| 2:F:78:PHE:HB2 | 2:F:102:LEU:HD22 | 1.87 | 0.56 |
| 1:A:1091:GLU:O | 1:A:1092:PHE:HB2 | 2.06 | 0.56 |
| 1:A:1093:MET:O | 1:A:1094:THR:C | 2.44 | 0.56 |
| 1:A:1108:TYR:HA | 1:A:1164:PHE:CZ | 2.41 | 0.56 |
| 1:A:253:ALA:O | 1:A:254:SER:CB | 2.54 | 0.56 |
| 1:A:277:HIS:O | 1:A:281:GLN:HG3 | 2.06 | 0.56 |
| 1:A:301:ILE:CD1 | 1:A:414:PHE:HB3 | 2.36 | 0.56 |
| 1:A:734:HIS:N | 1:A:752:LEU:HD11 | 2.21 | 0.56 |
| 1:A:823:ARG:CG | 1:A:823:ARG:O | 2.53 | 0.56 |
| 1:A:279:ARG:NH1 | 1:A:841:LEU:O | 2.39 | 0.56 |
| 1:A:897:TRP:NE1 | 1:A:901:VAL:CG1 | 2.64 | 0.56 |
| 2:B:132:HIS:CG | 2:B:182:ARG:NH2 | 2.73 | 0.56 |
| 2:C:432:TYR:CB | 2:C:437:ILE:HD11 | 2.35 | 0.56 |
| 1:D:1116:MET:O | 1:D:1120:PHE:HD1 | 1.88 | 0.56 |
| 1:D:223:TRP:CZ3 | 1:D:250:PRO:CB | 2.88 | 0.56 |
| 1:D:255:SER:CB | 1:D:256:PRO:C | 2.73 | 0.56 |
| 1:D:270:ASN:OD1 | 1:D:404:HIS:CE1 | 2.59 | 0.56 |
| 1:D:213:VAL:CG2 | 1:D:397:ALA:HB1 | 2.26 | 0.56 |
| 1:D:410:GLN:HA | 1:D:410:GLN:OE1 | 2.06 | 0.56 |
| 1:D:457:ARG:HH22 | 2:F:485:VAL:CG2 | 2.15 | 0.56 |
| 1:D:458:GLU:CA | 1:D:461:LYS:HD3 | 2.19 | 0.56 |
| 1:D:951:TYR:O | 1:D:954:ILE:HB | 2.05 | 0.56 |
| 2:E:193:TYR:HE2 | 2:E:322:LEU:HB3 | 1.70 | 0.56 |
| 2:E:478:TYR:O | 2:E:482:ALA:HB2 | 2.05 | 0.56 |
| 2:E:86:LEU:HB2 | 2:E:91:LEU:HD22 | 1.88 | 0.56 |
| 2:F:415:PRO:CB | 2:F:417:TYR:HE2 | 2.18 | 0.56 |
| 2:F:454:HIS:CA | 2:F:468:ILE:HD12 | 2.20 | 0.56 |
| 2:F:473:ASP:O | 2:F:477:LYS:HG3 | 2.06 | 0.56 |
| 1:A:1232:GLU:HG3 | 1:A:1234:ARG:HG2 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:253:ALA:CB | 1:A:280:GLU:C | 2.73 | 0.56 |
| 1:A:656:TYR:HB3 | 1:A:720:THR:HG1 | 1.68 | 0.56 |
| 1:A:817:PRO:HG2 | 1:A:818:ARG:H | 1.71 | 0.56 |
| 1:A:955:TYR:HB3 | 1:A:1098:ASN:ND2 | 2.20 | 0.56 |
| 2:B:213:VAL:HA | 2:B:235:THR:HA | 1.88 | 0.56 |
| 2:B:79:LEU:HA | 2:B:100:GLY:H | 1.71 | 0.56 |
| 2:C:194:VAL:O | 2:C:197:LEU:CD2 | 2.54 | 0.56 |
| 2:C:241:TRP:HB2 | 2:C:336:LEU:CB | 2.36 | 0.56 |
| 2:C:254:PHE:HA | 2:C:257:ARG:CD | 2.36 | 0.56 |
| 2:C:268:MET:HB2 | 2:C:352:ASP:OD1 | 2.06 | 0.56 |
| 2:C:270:PRO:HA | 2:C:273:PHE:CE2 | 2.41 | 0.56 |
| 2:C:325:ARG:HH11 | 2:C:325:ARG:CG | 2.07 | 0.56 |
| 2:C:347:LEU:C | 2:C:350:LEU:CD1 | 2.74 | 0.56 |
| 2:C:356:LEU:HD13 | 2:C:359:ASN:HD21 | 1.70 | 0.56 |
| 2:C:371:VAL:HG23 | 2:C:433:ASP:C | 2.27 | 0.56 |
| 1:D:1163:MET:HE1 | 1:D:1167:LYS:HE3 | 1.88 | 0.56 |
| 1:D:1231:LEU:C | 1:D:1232:GLU:HG2 | 2.25 | 0.56 |
| 1:D:196:VAL:CG2 | 1:D:215:ILE:CD1 | 2.83 | 0.56 |
| 1:D:270:ASN:CA | 1:D:294:THR:HG23 | 2.29 | 0.56 |
| 1:D:437:VAL:HA | 1:D:441:TRP:CD1 | 2.38 | 0.56 |
| 1:D:539:PHE:O | 1:D:540:GLN:CG | 2.54 | 0.56 |
| 1:D:546:ARG:O | 1:D:550:GLN:NE2 | 2.39 | 0.56 |
| 1:D:652:ILE:CG1 | 1:D:655:LEU:HG | 2.36 | 0.56 |
| 1:D:721:ALA:O | 1:D:722:ARG:CB | 2.53 | 0.56 |
| 2:F:270:PRO:HA | 2:F:273:PHE:CE2 | 2.41 | 0.56 |
| 1:A:1095:SER:O | 1:A:1099:TRP:HE3 | 1.89 | 0.56 |
| 1:A:1109:LEU:O | 1:A:1113:LEU:HG | 2.05 | 0.56 |
| 1:A:215:ILE:HB | 1:A:401:TRP:CE3 | 2.41 | 0.56 |
| 1:A:434:TYR:CE2 | 1:A:1128:ARG:HD2 | 2.40 | 0.56 |
| 1:A:441:TRP:CZ3 | 1:A:445:LEU:CD1 | 2.89 | 0.56 |
| 1:A:612:LEU:HD22 | 1:A:620:TRP:HA | 1.88 | 0.56 |
| 1:A:249:VAL:CG2 | 1:A:815:TRP:O | 2.52 | 0.56 |
| 1:A:885:THR:OG1 | 1:A:1146:ARG:NE | 2.39 | 0.56 |
| 2:C:347:LEU:O | 2:C:350:LEU:CD1 | 2.54 | 0.56 |
| 1:D:430:MET:CE | 1:D:1132:SER:HB3 | 2.35 | 0.56 |
| 1:D:1154:GLN:HG2 | 1:D:1179:PHE:CE2 | 2.40 | 0.56 |
| 1:D:189:ILE:HG12 | 1:D:190:PRO:HD2 | 1.88 | 0.56 |
| 1:D:443:ARG:NH1 | 1:D:443:ARG:HG2 | 2.19 | 0.56 |
| 1:D:515:ILE:HG23 | 1:D:565:HIS:C | 2.25 | 0.56 |
| 1:D:753:PRO:HG3 | 1:D:770:PHE:CG | 2.41 | 0.56 |
| 2:E:247:THR:O | 2:E:250:GLN:HB3 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:322:LEU:C | 2:E:324:GLY:H | 2.07 | 0.56 |
| 2:F:134:LYS:CB | 2:F:180:LYS:CE | 2.83 | 0.56 |
| 2:F:423:SER:CB | 2:F:428:LEU:HD21 | 2.36 | 0.56 |
| 1:A:1013:ASP:OD1 | 1:A:1014:ARG:N | 2.36 | 0.55 |
| 1:A:1038:TRP:CE3 | 1:A:1041:TRP:HA | 2.40 | 0.55 |
| 1:A:392:LEU:HG | 1:A:395:TYR:CB | 2.35 | 0.55 |
| 1:A:475:SER:O | 1:A:711:ALA:HA | 2.06 | 0.55 |
| 2:C:285:LYS:NZ | 2:C:285:LYS:HB2 | 2.21 | 0.55 |
| 2:C:397:GLN:C | 2:C:399:CYS:H | 2.10 | 0.55 |
| 2:C:403:PHE:CE2 | 2:C:407:LEU:HB2 | 2.41 | 0.55 |
| 2:C:473:ASP:C | 2:C:476:ILE:HG23 | 2.26 | 0.55 |
| 1:D:196:VAL:HG12 | 1:D:268:GLY:N | 2.21 | 0.55 |
| 1:D:278:ILE:HA | 1:D:282:TYR:CE1 | 2.41 | 0.55 |
| 1:D:253:ALA:N | 1:D:280:GLU:OE1 | 2.39 | 0.55 |
| 1:D:282:TYR:HE2 | 1:D:432:VAL:CG2 | 2.14 | 0.55 |
| 1:D:278:ILE:HA | 1:D:291:PHE:CE1 | 2.41 | 0.55 |
| 1:D:400:VAL:O | 1:D:403:THR:HG23 | 2.07 | 0.55 |
| 1:D:449:GLN:CA | 1:D:452:TYR:CE2 | 2.87 | 0.55 |
| 1:D:466:LEU:H | 1:D:466:LEU:HD13 | 1.70 | 0.55 |
| 1:D:479:TYR:CE1 | 1:D:480:LYS:HE2 | 2.41 | 0.55 |
| 1:D:550:GLN:N | 1:D:551:LYS:NZ | 2.53 | 0.55 |
| 1:D:247:LEU:N | 1:D:815:TRP:CD1 | 2.74 | 0.55 |
| 1:D:88:PHE:HB2 | 1:D:91:GLY:HA3 | 1.88 | 0.55 |
| 2:E:259:ARG:NH2 | 2:E:263:TRP:HE1 | 2.04 | 0.55 |
| 2:E:69:LEU:H | 2:E:69:LEU:CD1 | 2.18 | 0.55 |
| 2:F:234:LYS:NZ | 2:F:344:ARG:CD | 2.63 | 0.55 |
| 2:F:303:LEU:CG | 2:F:337:SER:OG | 2.54 | 0.55 |
| 2:F:305:ASN:C | 2:F:307:GLY:H | 2.09 | 0.55 |
| 2:F:389:ARG:CG | 2:F:390:GLY:N | 2.69 | 0.55 |
| 1:A:1189:LEU:CD2 | 1:A:1189:LEU:N | 2.69 | 0.55 |
| 1:A:370:PRO:O | 1:A:371:LYS:CG | 2.52 | 0.55 |
| 1:A:421:PRO:HG2 | 1:A:422:VAL:H | 1.71 | 0.55 |
| 1:A:487:ASP:O | 1:A:491:ASP:CG | 2.45 | 0.55 |
| 1:A:667:GLN:HG3 | 1:A:668:LEU:N | 2.20 | 0.55 |
| 2:B:233:GLU:OE2 | 2:C:133:HIS:ND1 | 2.35 | 0.55 |
| 2:B:263:TRP:O | 2:B:265:LYS:HG2 | 2.05 | 0.55 |
| 2:B:341:ASP:OD1 | 2:B:344:ARG:HD3 | 2.07 | 0.55 |
| 2:C:221:THR:CG2 | 2:C:222:LYS:N | 2.69 | 0.55 |
| 2:C:339:ASN:O | 2:C:340:GLY:O | 2.25 | 0.55 |
| 1:D:1001:GLY:C | 1:D:1004:LEU:HB2 | 2.27 | 0.55 |
| 1:D:1031:GLU:OE2 | 1:D:1092:PHE:CD2 | 2.59 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1108:TYR:CE1 | 1:D:1160:THR:HG22 | 2.40 | 0.55 |
| 1:D:877:MET:HE1 | 1:D:1203:PRO:O | 2.06 | 0.55 |
| 1:D:173:GLU:OE2 | 1:D:223:TRP:CD1 | 2.59 | 0.55 |
| 1:D:177:ARG:HH21 | 1:D:216:SER:HA | 1.70 | 0.55 |
| 1:D:656:TYR:CE1 | 1:D:743:ASP:CG | 2.78 | 0.55 |
| 1:D:659:HIS:CE1 | 1:D:719:LEU:HD22 | 2.39 | 0.55 |
| 1:D:615:SER:C | 1:D:725:PRO:HG3 | 2.26 | 0.55 |
| 1:D:744:ILE:N | 1:D:744:ILE:HD13 | 2.21 | 0.55 |
| 1:D:753:PRO:HD3 | 1:D:770:PHE:CD2 | 2.41 | 0.55 |
| 1:D:854:ALA:C | 1:D:855:VAL:CG2 | 2.74 | 0.55 |
| 1:D:885:THR:O | 1:D:886:LEU:HD23 | 2.06 | 0.55 |
| 1:D:987:ALA:O | 1:D:988:ALA:C | 2.43 | 0.55 |
| 2:E:186:LEU:C | 2:E:190:LEU:HD13 | 2.25 | 0.55 |
| 2:E:199:LEU:HD12 | 2:E:200:VAL:H | 1.71 | 0.55 |
| 2:E:315:TYR:HD1 | 2:E:316:PRO:HD2 | 1.71 | 0.55 |
| 2:E:456:ARG:HG3 | 2:E:462:MET:N | 2.21 | 0.55 |
| 2:F:358:GLU:O | 2:F:360:SER:N | 2.39 | 0.55 |
| 1:A:1016:GLU:CB | 1:A:1020:ILE:HA | 2.36 | 0.55 |
| 1:A:1060:LYS:CE | 1:A:1073:PRO:HB2 | 2.36 | 0.55 |
| 1:A:1171:ASN:N | 1:A:1171:ASN:OD1 | 2.38 | 0.55 |
| 1:A:221:TYR:OH | 1:A:397:ALA:CB | 2.54 | 0.55 |
| 1:A:665:LYS:O | 1:A:669:MET:HG2 | 2.06 | 0.55 |
| 1:A:77:GLN:OE1 | 1:A:1174:PRO:HB3 | 2.06 | 0.55 |
| 1:A:938:THR:O | 1:A:939:VAL:CB | 2.54 | 0.55 |
| 1:A:932:HIS:CB | 1:A:947:LYS:HG2 | 2.34 | 0.55 |
| 2:B:453:ILE:CG2 | 2:B:468:ILE:HD12 | 2.33 | 0.55 |
| 2:C:116:THR:O | 2:C:120:VAL:HG13 | 2.06 | 0.55 |
| 2:C:221:THR:HG22 | 2:C:222:LYS:N | 2.21 | 0.55 |
| 2:C:205:PRO:C | 2:C:241:TRP:HE1 | 2.08 | 0.55 |
| 2:C:245:PRO:C | 2:C:248:SER:HB2 | 2.24 | 0.55 |
| 2:C:301:GLU:OE1 | 2:C:339:ASN:ND2 | 2.38 | 0.55 |
| 2:C:308:ASP:N | 2:C:308:ASP:OD2 | 2.39 | 0.55 |
| 2:C:351:TYR:CD1 | 2:C:355:GLN:HG2 | 2.42 | 0.55 |
| 1:D:857:PRO:CA | 1:D:1062:GLU:OE2 | 2.55 | 0.55 |
| 1:D:233:TYR:O | 1:D:234:SER:CB | 2.51 | 0.55 |
| 1:D:421:PRO:HG2 | 1:D:422:VAL:H | 1.71 | 0.55 |
| 1:D:575:LYS:CD | 1:D:581:ASP:O | 2.55 | 0.55 |
| 1:D:727:ASP:O | 1:D:728:THR:CB | 2.54 | 0.55 |
| 1:D:735:GLY:HA2 | 1:D:749:PHE:HA | 1.89 | 0.55 |
| 2:E:204:LEU:HD22 | 2:E:242:PHE:O | 2.05 | 0.55 |
| 2:E:415:PRO:HB2 | 2:E:417:TYR:CE2 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:F:115:TRP:NE1 | 2:F:119:VAL:CG2 | 2.70 | 0.55 |
| 2:F:144:ALA:O | 2:F:145:PHE:HB2 | 2.06 | 0.55 |
| 2:F:238:SER:C | 2:F:338:VAL:HG11 | 2.26 | 0.55 |
| 2:F:406:LEU:CD1 | 2:F:406:LEU:N | 2.69 | 0.55 |
| 1:A:106:HIS:C | 1:A:107:LEU:HD22 | 2.26 | 0.55 |
| 1:A:203:LEU:CD1 | 1:A:379:LYS:O | 2.54 | 0.55 |
| 1:A:196:VAL:HG11 | 1:A:404:HIS:HB3 | 1.89 | 0.55 |
| 1:A:444:TYR:HE2 | 1:A:874:LEU:HA | 1.71 | 0.55 |
| 1:A:586:THR:N | 1:A:587:PRO:CD | 2.70 | 0.55 |
| 1:A:739:TYR:HA | 1:A:741:ASP:O | 2.06 | 0.55 |
| 1:A:936:ALA:HB2 | 1:A:946:ALA:CB | 2.35 | 0.55 |
| 2:B:123:GLU:CB | 2:C:403:PHE:HZ | 2.20 | 0.55 |
| 2:C:192:HIS:C | 2:C:196:CYS:HG | 2.09 | 0.55 |
| 2:C:291:TYR:OH | 2:C:352:ASP:N | 2.38 | 0.55 |
| 2:C:402:LEU:HB3 | 2:C:406:LEU:CD2 | 2.34 | 0.55 |
| 1:D:1069:ILE:HG23 | 1:D:1070:PRO:CG | 2.37 | 0.55 |
| 1:D:1113:LEU:HB3 | 1:D:1117:LYS:HE3 | 1.88 | 0.55 |
| 1:D:886:LEU:HD22 | 1:D:1140:LEU:HG | 1.88 | 0.55 |
| 1:D:1207:GLU:HA | 1:D:1210:TYR:HD2 | 1.55 | 0.55 |
| 1:D:213:VAL:HG13 | 1:D:401:TRP:HZ2 | 1.68 | 0.55 |
| 1:D:251:THR:C | 1:D:254:SER:H | 2.08 | 0.55 |
| 1:D:455:LEU:HD13 | 1:D:869:ARG:NH1 | 2.22 | 0.55 |
| 1:D:509:THR:C | 1:D:510:ALA:O | 2.38 | 0.55 |
| 2:E:378:LEU:CD1 | 2:E:378:LEU:N | 2.69 | 0.55 |
| 2:F:344:ARG:HA | 2:F:347:LEU:CG | 2.36 | 0.55 |
| 2:F:346:MET:O | 2:F:350:LEU:CD1 | 2.55 | 0.55 |
| 2:F:88:ARG:HH11 | 2:F:88:ARG:HB2 | 1.70 | 0.55 |
| 1:A:1008:LEU:HD22 | 1:A:1009:ASN:N | 2.22 | 0.55 |
| 1:A:1009:ASN:C | 1:A:1010:LEU:HG | 2.25 | 0.55 |
| 1:A:1026:ARG:HG2 | 1:A:1029:GLN:NE2 | 2.21 | 0.55 |
| 1:A:1069:ILE:N | 1:A:1070:PRO:CD | 2.69 | 0.55 |
| 1:A:430:MET:HA | 1:A:1130:CYS:HB2 | 1.89 | 0.55 |
| 1:A:1165:ALA:HB2 | 1:A:1173:LEU:CD1 | 2.37 | 0.55 |
| 1:A:127:LEU:CD2 | 1:A:129:PRO:HD3 | 2.34 | 0.55 |
| 1:A:283:LEU:HD13 | 1:A:283:LEU:C | 2.26 | 0.55 |
| 1:A:386:ARG:HG2 | 1:A:387:GLU:N | 2.21 | 0.55 |
| 1:A:411:LEU:O | 1:A:415:LEU:HD13 | 2.05 | 0.55 |
| 1:A:416:GLU:O | 1:A:419:PRO:HD3 | 2.06 | 0.55 |
| 1:A:442:GLU:OE1 | 1:A:815:TRP:CZ2 | 2.60 | 0.55 |
| 1:A:469:ASP:O | 1:A:473:LEU:HD23 | 2.07 | 0.55 |
| 2:B:102:LEU:CD1 | 2:B:102:LEU:H | 2.17 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:439:PHE:O | 2:B:440:THR:OG1 | 2.21 | 0.55 |
| 2:B:452:LEU:HD22 | 2:B:452:LEU:N | 2.21 | 0.55 |
| 2:C:290:TYR:CE1 | 2:C:299:LEU:HD22 | 2.42 | 0.55 |
| 2:C:351:TYR:O | 2:C:353:SER:N | 2.38 | 0.55 |
| 2:C:354:PHE:C | 2:C:356:LEU:N | 2.53 | 0.55 |
| 1:D:1188:CYS:O | 1:D:1189:LEU:HD13 | 2.06 | 0.55 |
| 1:D:1190:ARG:HH11 | 1:D:1195:MET:CE | 2.17 | 0.55 |
| 1:D:242:ALA:C | 1:D:246:PRO:HD3 | 2.27 | 0.55 |
| 1:D:733:HIS:CE1 | 1:D:750:PHE:CD1 | 2.95 | 0.55 |
| 1:D:795:ASN:O | 1:D:798:ILE:CG1 | 2.53 | 0.55 |
| 1:D:802:ARG:HG2 | 1:D:803:ASN:OD1 | 2.07 | 0.55 |
| 1:D:279:ARG:HH11 | 1:D:841:LEU:CB | 2.19 | 0.55 |
| 1:D:951:TYR:O | 1:D:955:TYR:CD1 | 2.60 | 0.55 |
| 1:D:967:MET:SD | 1:D:978:ALA:HB2 | 2.47 | 0.55 |
| 2:F:180:LYS:O | 2:F:181:LEU:HD23 | 2.06 | 0.55 |
| 2:F:300:ILE:HG23 | 2:F:342:LEU:CD1 | 2.36 | 0.55 |
| 2:F:300:ILE:CG2 | 2:F:301:GLU:H | 2.19 | 0.55 |
| 2:F:397:GLN:HG2 | 2:F:398:VAL:N | 2.22 | 0.55 |
| 2:F:403:PHE:O | 2:F:406:LEU:HB2 | 2.06 | 0.55 |
| 2:E:120:VAL:O | 2:F:407:LEU:HG | 2.07 | 0.55 |
| 1:A:1005:VAL:CA | 1:A:1008:LEU:CD1 | 2.67 | 0.55 |
| 1:A:1068:ASP:O | 1:A:1070:PRO:HD3 | 2.07 | 0.55 |
| 1:A:1091:GLU:O | 1:A:1092:PHE:CB | 2.54 | 0.55 |
| 1:A:1224:ILE:HD11 | 1:A:1229:GLY:H | 1.71 | 0.55 |
| 1:A:414:PHE:O | 1:A:417:ARG:CB | 2.54 | 0.55 |
| 1:A:439:GLN:HG2 | 1:A:836:LEU:N | 2.22 | 0.55 |
| 1:A:658:LYS:O | 1:A:662:GLU:CG | 2.53 | 0.55 |
| 1:A:786:ALA:CB | 1:A:790:ARG:NH1 | 2.67 | 0.55 |
| 1:A:916:PHE:O | 1:A:920:THR:HA | 2.05 | 0.55 |
| 2:C:233:GLU:O | 2:C:234:LYS:HG2 | 2.06 | 0.55 |
| 2:C:243:THR:HB | 2:C:247:THR:OG1 | 2.07 | 0.55 |
| 2:C:342:LEU:O | 2:C:342:LEU:HD22 | 2.06 | 0.55 |
| 2:C:415:PRO:HA | 2:C:417:TYR:HE2 | 1.72 | 0.55 |
| 1:D:1006:ARG:CZ | 1:D:1006:ARG:HA | 2.31 | 0.55 |
| 1:D:312:TRP:CZ3 | 1:D:348:LEU:HB2 | 2.40 | 0.55 |
| 1:D:607:TRP:NE1 | 1:D:780:GLN:O | 2.40 | 0.55 |
| 1:D:77:GLN:O | 1:D:78:MET:CB | 2.53 | 0.55 |
| 1:D:903:GLY:HA2 | 1:D:1002:GLU:HB2 | 1.86 | 0.55 |
| 2:E:77:HIS:CB | 2:E:101:PRO:HD2 | 2.33 | 0.55 |
| 2:E:109:ASN:O | 2:E:378:LEU:HG | 2.06 | 0.55 |
| 2:E:211:ILE:HA | 2:E:237:ALA:HA | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:284:ARG:O | 2:E:285:LYS:CB | 2.53 | 0.55 |
| 2:E:335:VAL:CG2 | 2:E:336:LEU:N | 2.70 | 0.55 |
| 2:F:290:TYR:CE1 | 2:F:299:LEU:HD22 | 2.40 | 0.55 |
| 2:F:311:LEU:O | 2:F:315:TYR:N | 2.32 | 0.55 |
| 2:F:322:LEU:HD22 | 2:F:323:HIS:C | 2.27 | 0.55 |
| 2:F:341:ASP:O | 2:F:342:LEU:CD1 | 2.50 | 0.55 |
| 1:A:1008:LEU:CD2 | 1:A:1008:LEU:C | 2.74 | 0.55 |
| 1:A:1013:ASP:CG | 1:A:1014:ARG:H | 2.09 | 0.55 |
| 1:A:1017:GLY:C | 1:A:1019:TRP:H | 2.09 | 0.55 |
| 1:A:1030:ARG:HD3 | 1:A:1091:GLU:CD | 2.27 | 0.55 |
| 1:A:312:TRP:CZ2 | 1:A:346:ASP:C | 2.80 | 0.55 |
| 1:A:221:TYR:OH | 1:A:397:ALA:HB1 | 2.07 | 0.55 |
| 1:A:897:TRP:O | 1:A:897:TRP:CD1 | 2.59 | 0.55 |
| 1:A:931:LEU:HA | 1:A:934:LYS:HE3 | 1.87 | 0.55 |
| 2:C:390:GLY:HA2 | 2:C:392:THR:N | 2.21 | 0.55 |
| 2:C:444:THR:N | 2:C:447:THR:HG23 | 2.20 | 0.55 |
| 1:D:1060:LYS:CE | 1:D:1060:LYS:HA | 2.36 | 0.55 |
| 1:D:77:GLN:O | 1:D:78:MET:HB2 | 2.07 | 0.55 |
| 1:D:892:ASP:OD2 | 1:D:893:SER:N | 2.40 | 0.55 |
| 1:D:903:GLY:O | 1:D:906:HIS:N | 2.40 | 0.55 |
| 2:E:119:VAL:HA | 2:E:125:VAL:HB | 1.87 | 0.55 |
| 2:E:201:ASN:CG | 2:F:422:GLN:HB2 | 2.26 | 0.55 |
| 2:E:114:TRP:NE1 | 2:E:259:ARG:NH2 | 2.49 | 0.55 |
| 2:E:266:PHE:CD1 | 2:E:376:PRO:HG3 | 2.42 | 0.55 |
| 2:E:338:VAL:O | 2:E:338:VAL:HG12 | 2.06 | 0.55 |
| 2:E:418:LEU:CD2 | 2:F:122:ARG:NH2 | 2.67 | 0.55 |
| 1:D:1209:ARG:CG | 2:F:249:ASN:HB3 | 2.32 | 0.55 |
| 2:F:312:LEU:O | 2:F:313:HIS:C | 2.44 | 0.55 |
| 2:F:407:LEU:HD23 | 2:F:407:LEU:C | 2.26 | 0.55 |
| 2:F:426:GLU:OE2 | 2:F:429:TYR:HD1 | 1.89 | 0.55 |
| 2:F:469:SER:C | 2:F:471:LEU:HD12 | 2.27 | 0.55 |
| 1:A:1129:PHE:CE2 | 1:A:1131:ILE:HB | 2.42 | 0.55 |
| 1:A:1131:ILE:HG13 | 1:A:1133:ILE:HG22 | 1.88 | 0.55 |
| 1:A:125:LEU:HD23 | 1:A:125:LEU:N | 2.00 | 0.55 |
| 1:A:267:VAL:CG1 | 1:A:269:HIS:CE1 | 2.90 | 0.55 |
| 1:A:379:LYS:HD3 | 1:A:379:LYS:H | 1.70 | 0.55 |
| 1:A:823:ARG:HB3 | 1:A:825:VAL:CG2 | 2.13 | 0.55 |
| 1:A:851:THR:C | 1:A:852:ARG:HG3 | 2.27 | 0.55 |
| 1:A:859:TRP:N | 1:A:859:TRP:CD1 | 2.73 | 0.55 |
| 2:C:245:PRO:O | 2:C:248:SER:CB | 2.45 | 0.55 |
| 2:C:243:THR:HB | 2:C:247:THR:CG2 | 2.37 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:236:GLU:CA | 2:C:341:ASP:CB | 2.69 | 0.55 |
| 1:A:784:GLY:CA | 2:C:362:THR:O | 2.55 | 0.55 |
| 2:C:432:TYR:HB3 | 2:C:437:ILE:HD11 | 1.88 | 0.55 |
| 1:D:1028:VAL:HG12 | 1:D:1028:VAL:O | 2.07 | 0.55 |
| 1:D:121:PRO:C | 1:D:122:ASP:OD2 | 2.44 | 0.55 |
| 1:D:1221:TYR:CA | 1:D:1224:ILE:HG22 | 2.33 | 0.55 |
| 1:D:192:GLU:HG3 | 1:D:195:LEU:HD12 | 1.89 | 0.55 |
| 1:D:211:LEU:HG | 1:D:221:TYR:CE1 | 2.42 | 0.55 |
| 1:D:259:ARG:CG | 1:D:261:TRP:HD1 | 2.17 | 0.55 |
| 1:D:271:VAL:N | 1:D:294:THR:OG1 | 2.39 | 0.55 |
| 1:D:407:PHE:CG | 1:D:408:GLN:N | 2.75 | 0.55 |
| 1:D:591:LEU:HD11 | 1:D:594:LEU:CG | 2.20 | 0.55 |
| 1:D:598:VAL:HA | 1:D:601:LYS:HD3 | 1.89 | 0.55 |
| 1:D:776:ASP:OD1 | 1:D:777:GLY:N | 2.39 | 0.55 |
| 1:D:916:PHE:O | 1:D:920:THR:HA | 2.04 | 0.55 |
| 1:D:954:ILE:HG22 | 1:D:955:TYR:CG | 2.42 | 0.55 |
| 1:D:995:TYR:N | 1:D:996:ARG:NH1 | 2.50 | 0.55 |
| 2:E:239:LEU:HB3 | 2:E:338:VAL:HB | 1.89 | 0.55 |
| 2:E:244:PRO:O | 2:E:248:SER:N | 2.40 | 0.55 |
| 2:E:301:GLU:HG2 | 2:E:303:LEU:CD1 | 2.36 | 0.55 |
| 2:F:112:ALA:O | 2:F:116:THR:HG22 | 2.06 | 0.55 |
| 2:F:244:PRO:N | 2:F:247:THR:CG2 | 2.70 | 0.55 |
| 2:F:358:GLU:HG2 | 2:F:359:ASN:N | 2.22 | 0.55 |
| 2:F:431:LYS:NZ | 2:F:435:MET:CG | 2.70 | 0.55 |
| 2:F:78:PHE:CD2 | 2:F:79:LEU:HD22 | 2.41 | 0.55 |
| 1:A:1209:ARG:HH22 | 2:C:256:LEU:CG | 2.20 | 0.55 |
| 1:A:433:SER:HB2 | 1:A:1129:PHE:HE1 | 1.72 | 0.55 |
| 1:A:460:LYS:O | 1:A:463:LEU:HB3 | 2.07 | 0.55 |
| 1:A:616:GLU:CG | 1:A:724:GLY:CA | 2.84 | 0.55 |
| 1:A:735:GLY:C | 1:A:736:ASN:CG | 2.66 | 0.55 |
| 1:A:825:VAL:O | 1:A:829:PRO:CG | 2.55 | 0.55 |
| 2:B:378:LEU:O | 2:B:379:ALA:C | 2.46 | 0.55 |
| 2:B:432:TYR:HA | 2:B:437:ILE:CD1 | 2.37 | 0.55 |
| 2:C:241:TRP:HE3 | 2:C:255:TRP:HE1 | 1.52 | 0.55 |
| 2:C:393:LEU:HD23 | 2:C:396:ARG:CG | 2.26 | 0.55 |
| 2:C:398:VAL:C | 2:C:401:GLY:N | 2.60 | 0.55 |
| 2:C:441:VAL:O | 2:C:441:VAL:HG23 | 2.07 | 0.55 |
| 2:C:72:ILE:O | 2:C:75:ARG:O | 2.25 | 0.55 |
| 1:D:1165:ALA:C | 1:D:1166:TYR:CD1 | 2.77 | 0.55 |
| 1:D:1163:MET:CE | 1:D:1167:LYS:HG2 | 2.37 | 0.55 |
| 1:D:1138:ARG:HH21 | 1:D:1191:LYS:HZ3 | 1.55 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:278:ILE:HD13 | 1:D:282:TYR:OH | 2.07 | 0.55 |
| 1:D:550:GLN:OE1 | 1:D:551:LYS:CE | 2.54 | 0.55 |
| 1:D:576:LEU:HG | 1:D:579:ARG:HE | 1.70 | 0.55 |
| 1:D:769:ASP:O | 1:D:773:LYS:NZ | 2.29 | 0.55 |
| 1:D:867:PRO:O | 1:D:868:ASP:CB | 2.55 | 0.55 |
| 1:D:874:LEU:O | 1:D:878:VAL:CG2 | 2.41 | 0.55 |
| 1:D:951:TYR:O | 1:D:955:TYR:CE1 | 2.59 | 0.55 |
| 2:E:431:LYS:CA | 2:E:434:GLU:HG2 | 2.34 | 0.55 |
| 2:F:243:THR:C | 2:F:334:CYS:HB2 | 2.26 | 0.55 |
| 2:F:351:TYR:C | 2:F:355:GLN:CB | 2.64 | 0.55 |
| 1:A:996:ARG:NH1 | 1:A:1003:TRP:C | 2.60 | 0.55 |
| 1:A:955:TYR:HD2 | 1:A:1102:GLN:HE22 | 1.52 | 0.55 |
| 1:A:430:MET:O | 1:A:1130:CYS:SG | 2.64 | 0.55 |
| 1:A:267:VAL:CG1 | 1:A:269:HIS:HE1 | 2.20 | 0.55 |
| 1:A:358:LEU:HD12 | 1:A:407:PHE:CE1 | 2.42 | 0.55 |
| 1:A:572:TRP:O | 1:A:574:ARG:N | 2.40 | 0.55 |
| 1:A:613:HIS:CG | 1:A:717:LEU:HG | 2.41 | 0.55 |
| 1:A:732:TYR:CD1 | 1:A:755:LYS:HG2 | 2.42 | 0.55 |
| 1:A:610:PHE:CE1 | 1:A:972:ARG:NH2 | 2.75 | 0.55 |
| 2:B:78:PHE:CD2 | 2:B:102:LEU:HD22 | 2.42 | 0.55 |
| 2:B:182:ARG:O | 2:B:182:ARG:HG2 | 2.06 | 0.55 |
| 2:B:348:ALA:C | 2:B:350:LEU:N | 2.61 | 0.55 |
| 2:B:388:GLY:O | 2:B:444:THR:HA | 2.07 | 0.55 |
| 2:B:69:LEU:O | 2:B:73:CYS:SG | 2.64 | 0.55 |
| 2:C:208:LEU:CD1 | 2:C:208:LEU:O | 2.54 | 0.55 |
| 2:C:244:PRO:N | 2:C:247:THR:HG21 | 2.22 | 0.55 |
| 2:C:344:ARG:O | 2:C:347:LEU:HB2 | 2.07 | 0.55 |
| 2:C:387:VAL:HG11 | 2:C:395:LEU:O | 2.07 | 0.55 |
| 2:C:387:VAL:CG1 | 2:C:399:CYS:HB2 | 2.37 | 0.55 |
| 2:C:406:LEU:CA | 2:C:409:ASN:ND2 | 2.61 | 0.55 |
| 1:D:401:TRP:HD1 | 1:D:404:HIS:HD2 | 1.53 | 0.55 |
| 1:D:402:ALA:O | 1:D:406:VAL:CG1 | 2.55 | 0.55 |
| 1:D:613:HIS:CE1 | 1:D:717:LEU:CD1 | 2.89 | 0.55 |
| 1:D:659:HIS:CG | 1:D:719:LEU:HD22 | 2.42 | 0.55 |
| 1:D:732:TYR:CG | 1:D:755:LYS:NZ | 2.75 | 0.55 |
| 1:D:891:VAL:CG1 | 1:D:1135:ASP:CA | 2.85 | 0.55 |
| 1:D:922:GLN:OE1 | 1:D:934:LYS:NZ | 2.39 | 0.55 |
| 2:E:263:TRP:C | 2:E:265:LYS:N | 2.58 | 0.55 |
| 2:E:324:GLY:O | 2:E:331:VAL:HG13 | 2.06 | 0.55 |
| 2:E:380:PRO:CA | 2:E:438:LEU:HD12 | 2.37 | 0.55 |
| 2:F:115:TRP:O | 2:F:118:VAL:HG12 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:116:THR:O | 2:F:120:VAL:HG13 | 2.07 | 0.55 |
| 2:F:240:VAL:CA | 2:F:336:LEU:HB3 | 2.36 | 0.55 |
| 2:F:342:LEU:CD2 | 2:F:342:LEU:C | 2.74 | 0.55 |
| 2:F:344:ARG:HA | 2:F:347:LEU:CD2 | 2.34 | 0.55 |
| 1:A:1108:TYR:HE2 | 1:A:1112:MET:CE | 2.20 | 0.54 |
| 1:A:885:THR:HB | 1:A:1146:ARG:HH21 | 1.72 | 0.54 |
| 1:A:196:VAL:C | 1:A:401:TRP:CH2 | 2.81 | 0.54 |
| 1:A:363:ARG:O | 1:A:365:TYR:CE2 | 2.59 | 0.54 |
| 1:A:616:GLU:O | 1:A:616:GLU:HG3 | 2.06 | 0.54 |
| 1:A:788:GLY:O | 1:A:792:LEU:HG | 2.07 | 0.54 |
| 1:A:815:TRP:HA | 1:A:838:GLY:HA2 | 1.87 | 0.54 |
| 1:A:79:LEU:CB | 1:A:89:GLY:CA | 2.84 | 0.54 |
| 1:A:974:THR:HG23 | 1:A:975:GLN:H | 1.72 | 0.54 |
| 2:B:283:GLY:O | 2:B:305:ASN:O | 2.25 | 0.54 |
| 2:B:456:ARG:HG2 | 2:B:463:LYS:HG3 | 1.89 | 0.54 |
| 2:B:75:ARG:HD2 | 2:B:434:GLU:CD | 2.28 | 0.54 |
| 2:C:239:LEU:C | 2:C:338:VAL:HG12 | 2.26 | 0.54 |
| 1:D:1111:LEU:HD22 | 1:D:1164:PHE:HE1 | 1.68 | 0.54 |
| 1:D:203:LEU:C | 1:D:203:LEU:CD2 | 2.74 | 0.54 |
| 1:D:273:PHE:CA | 1:D:276:ALA:H | 2.19 | 0.54 |
| 1:D:439:GLN:NE2 | 1:D:837:TYR:CE2 | 2.75 | 0.54 |
| 1:D:460:LYS:HG2 | 1:D:461:LYS:N | 2.22 | 0.54 |
| 1:D:768:LYS:C | 1:D:772:PRO:CD | 2.74 | 0.54 |
| 1:D:771:LEU:CD1 | 1:D:771:LEU:N | 2.70 | 0.54 |
| 1:D:904:ASP:OD1 | 1:D:915:ALA:CB | 2.55 | 0.54 |
| 2:E:109:ASN:HB2 | 2:E:378:LEU:CB | 2.37 | 0.54 |
| 2:E:427:GLN:HA | 2:E:430:SER:OG | 2.07 | 0.54 |
| 2:F:118:VAL:CG1 | 2:F:119:VAL:N | 2.70 | 0.54 |
| 2:F:123:GLU:OE1 | 2:F:206:TYR:HA | 2.07 | 0.54 |
| 1:D:1209:ARG:CZ | 2:F:252:LEU:HB3 | 2.37 | 0.54 |
| 2:F:375:HIS:CD2 | 2:F:377:CYS:H | 2.24 | 0.54 |
| 2:F:460:THR:CG2 | 2:F:462:MET:HB2 | 2.35 | 0.54 |
| 1:A:1006:ARG:N | 1:A:1006:ARG:HH11 | 2.06 | 0.54 |
| 1:A:189:ILE:HD12 | 1:A:258:GLN:HA | 1.89 | 0.54 |
| 1:A:456:GLN:O | 1:A:460:LYS:HD3 | 2.07 | 0.54 |
| 1:A:490:TRP:CH2 | 1:A:598:VAL:CB | 2.85 | 0.54 |
| 1:A:496:LYS:NZ | 1:A:570:PRO:O | 2.37 | 0.54 |
| 1:A:730:PRO:HD3 | 1:A:761:ASN:OD1 | 2.08 | 0.54 |
| 2:B:376:PRO:O | 2:B:378:LEU:N | 2.39 | 0.54 |
| 2:B:75:ARG:C | 2:B:76:ARG:HG2 | 2.28 | 0.54 |
| 2:C:200:VAL:O | 2:C:201:ASN:HB2 | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:266:PHE:HB3 | 2:C:378:LEU:HD11 | 1.88 | 0.54 |
| 2:C:342:LEU:CB | 2:C:344:ARG:HB2 | 2.37 | 0.54 |
| 1:D:1151:LEU:HD12 | 1:D:1230:SER:HA | 1.89 | 0.54 |
| 1:D:1190:ARG:NH1 | 1:D:1195:MET:HE3 | 2.21 | 0.54 |
| 1:D:284:ILE:H | 1:D:284:ILE:CD1 | 2.02 | 0.54 |
| 1:D:612:LEU:HB3 | 1:D:621:GLY:N | 2.22 | 0.54 |
| 1:D:739:TYR:O | 1:D:741:ASP:O | 2.25 | 0.54 |
| 1:D:808:ILE:O | 1:D:811:GLN:OE1 | 2.25 | 0.54 |
| 1:D:879:GLN:O | 1:D:1189:LEU:CD2 | 2.54 | 0.54 |
| 2:E:239:LEU:O | 2:E:240:VAL:HB | 2.06 | 0.54 |
| 2:E:382:LYS:CG | 2:E:383:VAL:H | 2.20 | 0.54 |
| 2:F:385:LEU:HD13 | 2:F:399:CYS:SG | 2.47 | 0.54 |
| 2:F:402:LEU:O | 2:F:403:PHE:C | 2.45 | 0.54 |
| 1:A:371:LYS:HA | 1:A:374:ARG:HD2 | 1.88 | 0.54 |
| 1:A:420:HIS:CE1 | 1:A:422:VAL:HG23 | 2.42 | 0.54 |
| 1:A:520:ALA:N | 1:A:521:PRO:CD | 2.71 | 0.54 |
| 1:A:652:ILE:HG23 | 1:A:655:LEU:HD11 | 1.89 | 0.54 |
| 2:B:78:PHE:CD2 | 2:B:102:LEU:HB2 | 2.42 | 0.54 |
| 2:B:67:GLU:N | 2:B:70:LEU:HB2 | 2.22 | 0.54 |
| 2:C:357:THR:C | 2:C:359:ASN:N | 2.61 | 0.54 |
| 1:D:1157:ASN:OD1 | 1:D:1161:ARG:NH2 | 2.40 | 0.54 |
| 1:D:260:ASP:C | 1:D:260:ASP:OD2 | 2.45 | 0.54 |
| 1:D:396:CYS:O | 1:D:400:VAL:HG23 | 2.06 | 0.54 |
| 1:D:437:VAL:HG12 | 1:D:438:ASN:N | 2.21 | 0.54 |
| 1:D:484:TRP:CD1 | 1:D:488:LEU:HG | 2.42 | 0.54 |
| 1:D:618:HIS:CE1 | 1:D:761:ASN:HB3 | 2.42 | 0.54 |
| 1:D:933:SER:OG | 1:D:943:ARG:CZ | 2.55 | 0.54 |
| 2:E:318:ASN:O | 2:E:319:VAL:C | 2.46 | 0.54 |
| 2:E:385:LEU:HD13 | 2:E:441:VAL:HB | 1.88 | 0.54 |
| 2:F:307:GLY:C | 2:F:308:ASP:OD2 | 2.46 | 0.54 |
| 2:F:309:HIS:HB3 | 2:F:310:GLU:OE1 | 2.06 | 0.54 |
| 2:F:425:LEU:HD12 | 2:F:425:LEU:O | 2.08 | 0.54 |
| 1:A:1008:LEU:C | 1:A:1011:PRO:HD3 | 2.28 | 0.54 |
| 1:A:1043:VAL:C | 1:A:1046:GLU:H | 2.10 | 0.54 |
| 1:A:885:THR:HB | 1:A:1146:ARG:CZ | 2.37 | 0.54 |
| 1:A:188:ALA:C | 1:A:189:ILE:HG12 | 2.27 | 0.54 |
| 1:A:196:VAL:CG1 | 1:A:401:TRP:CZ3 | 2.91 | 0.54 |
| 1:A:273:PHE:CA | 1:A:276:ALA:HB3 | 2.37 | 0.54 |
| 1:A:503:VAL:O | 1:A:504:LYS:HB3 | 2.07 | 0.54 |
| 1:A:639:THR:HB | 1:A:640:LEU:CD2 | 2.27 | 0.54 |
| 1:A:915:ALA:O | 1:A:919:MET:N | 2.26 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:307:GLY:HA2 | 2:B:334:CYS:HB3 | 1.90 | 0.54 |
| 2:C:395:LEU:CD2 | 2:C:443:VAL:HB | 2.37 | 0.54 |
| 1:D:999:ASP:C | 1:D:1001:GLY:N | 2.59 | 0.54 |
| 1:D:1063:SER:OG | 1:D:1066:THR:HB | 2.08 | 0.54 |
| 1:D:1153:LEU:N | 1:D:1153:LEU:HD23 | 2.22 | 0.54 |
| 1:D:143:ALA:HB1 | 1:D:421:PRO:O | 2.08 | 0.54 |
| 1:D:257:THR:CG2 | 1:D:257:THR:O | 2.49 | 0.54 |
| 1:D:421:PRO:O | 1:D:425:ALA:CB | 2.55 | 0.54 |
| 1:D:542:ASP:O | 1:D:546:ARG:HB2 | 2.06 | 0.54 |
| 1:D:601:LYS:HZ2 | 1:D:721:ALA:HA | 1.72 | 0.54 |
| 1:D:744:ILE:CB | 1:D:745:PRO:HD3 | 2.36 | 0.54 |
| 1:D:734:HIS:ND1 | 1:D:752:LEU:HD11 | 2.22 | 0.54 |
| 1:D:776:ASP:N | 1:D:796:LYS:NZ | 2.55 | 0.54 |
| 1:D:774:MET:O | 1:D:776:ASP:O | 2.25 | 0.54 |
| 1:D:807:ARG:HB2 | 1:D:858:THR:CG2 | 2.37 | 0.54 |
| 1:D:873:GLU:CD | 1:D:1203:PRO:HG3 | 2.28 | 0.54 |
| 2:E:240:VAL:HG12 | 2:E:242:PHE:CZ | 2.43 | 0.54 |
| 2:E:271:SER:C | 2:E:273:PHE:H | 2.10 | 0.54 |
| 2:E:280:ASP:O | 2:E:304:TRP:CH2 | 2.60 | 0.54 |
| 2:E:460:THR:O | 2:E:462:MET:HE2 | 2.07 | 0.54 |
| 2:E:127:PRO:O | 2:F:101:PRO:HA | 2.07 | 0.54 |
| 2:F:381:ILE:CG2 | 2:F:437:ILE:HG22 | 2.38 | 0.54 |
| 2:F:413:VAL:C | 2:F:415:PRO:HD2 | 2.27 | 0.54 |
| 1:A:112:LEU:HD12 | 1:A:112:LEU:N | 2.21 | 0.54 |
| 1:A:1140:LEU:CD2 | 1:A:1141:VAL:N | 2.71 | 0.54 |
| 1:A:175:TRP:HD1 | 1:A:183:GLU:HB2 | 1.71 | 0.54 |
| 1:A:371:LYS:NZ | 1:A:400:VAL:CG2 | 2.70 | 0.54 |
| 1:A:611:PRO:HG3 | 1:A:671:GLN:CG | 2.37 | 0.54 |
| 2:B:122:ARG:HB3 | 2:B:122:ARG:HH11 | 1.72 | 0.54 |
| 2:B:285:LYS:C | 2:B:305:ASN:HD22 | 2.11 | 0.54 |
| 2:B:469:SER:O | 2:B:471:LEU:N | 2.40 | 0.54 |
| 2:B:69:LEU:HA | 2:B:72:ILE:HG12 | 1.90 | 0.54 |
| 2:B:82:SER:HB3 | 2:B:85:GLN:CG | 2.38 | 0.54 |
| 2:C:208:LEU:HD12 | 2:C:208:LEU:C | 2.26 | 0.54 |
| 2:C:381:ILE:CG2 | 2:C:437:ILE:HG22 | 2.38 | 0.54 |
| 2:C:456:ARG:NH2 | 2:C:465:MET:SD | 2.80 | 0.54 |
| 1:D:1027:LYS:HB2 | 1:D:1096:ARG:CG | 2.37 | 0.54 |
| 1:D:1122:GLU:O | 1:D:1123:PHE:HB2 | 2.08 | 0.54 |
| 1:D:193:ARG:CA | 1:D:193:ARG:HH11 | 2.19 | 0.54 |
| 1:D:279:ARG:HH11 | 1:D:841:LEU:HD13 | 1.71 | 0.54 |
| 1:D:308:GLN:NE2 | 1:D:1091:GLU:N | 2.55 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:429:GLU:HG3 | 1:D:1128:ARG:HH22 | 1.68 | 0.54 |
| 1:D:434:TYR:HA | 1:D:841:LEU:HD13 | 1.89 | 0.54 |
| 1:D:483:PRO:HG3 | 1:D:712:VAL:CG1 | 2.38 | 0.54 |
| 1:D:503:VAL:C | 1:D:505:LYS:N | 2.46 | 0.54 |
| 1:D:581:ASP:OD1 | 1:D:592:LEU:HD13 | 2.08 | 0.54 |
| 1:D:730:PRO:HB3 | 1:D:761:ASN:CA | 2.38 | 0.54 |
| 1:D:945:HIS:HA | 1:D:948:ILE:HD11 | 1.88 | 0.54 |
| 2:E:187:HIS:HA | 2:E:190:LEU:CD2 | 2.31 | 0.54 |
| 2:E:427:GLN:O | 2:E:430:SER:HB2 | 2.08 | 0.54 |
| 2:F:129:ASP:HB3 | 2:F:131:LEU:HD22 | 1.88 | 0.54 |
| 2:F:383:VAL:CG2 | 2:F:384:ALA:N | 2.70 | 0.54 |
| 2:F:385:LEU:HD11 | 2:F:402:LEU:HB3 | 1.90 | 0.54 |
| 2:F:407:LEU:C | 2:F:407:LEU:CD2 | 2.76 | 0.54 |
| 2:F:473:ASP:C | 2:F:476:ILE:HG23 | 2.27 | 0.54 |
| 1:A:1006:ARG:CZ | 1:A:1010:LEU:HD11 | 2.35 | 0.54 |
| 1:A:1198:LYS:C | 1:A:1199:THR:HG23 | 2.27 | 0.54 |
| 1:A:385:ILE:CG2 | 1:A:386:ARG:N | 2.70 | 0.54 |
| 1:A:196:VAL:HG12 | 1:A:401:TRP:CZ3 | 2.43 | 0.54 |
| 1:A:613:HIS:O | 1:A:614:TYR:CB | 2.55 | 0.54 |
| 1:A:659:HIS:CD2 | 1:A:720:THR:HB | 2.43 | 0.54 |
| 1:A:845:VAL:CG1 | 1:A:848:GLY:HA3 | 2.37 | 0.54 |
| 2:B:217:PRO:HB2 | 2:B:231:ILE:CG2 | 2.38 | 0.54 |
| 2:B:315:TYR:HB2 | 2:B:322:LEU:HD11 | 1.90 | 0.54 |
| 2:B:417:TYR:OH | 2:C:122:ARG:CD | 2.40 | 0.54 |
| 2:B:373:LYS:CE | 2:B:459:ASP:HA | 2.33 | 0.54 |
| 2:C:201:ASN:O | 2:C:202:LYS:HB3 | 2.08 | 0.54 |
| 2:C:308:ASP:OD1 | 2:C:333:PRO:C | 2.46 | 0.54 |
| 2:C:197:LEU:CD1 | 2:C:322:LEU:HD21 | 2.37 | 0.54 |
| 2:C:241:TRP:CE3 | 2:C:336:LEU:HD12 | 2.43 | 0.54 |
| 1:A:560:PRO:HD2 | 2:C:452:LEU:CD2 | 2.37 | 0.54 |
| 2:C:466:MET:O | 2:C:467:HIS:C | 2.45 | 0.54 |
| 1:D:1014:ARG:HD3 | 1:D:1026:ARG:CD | 2.37 | 0.54 |
| 1:D:1052:GLY:O | 1:D:1056:GLU:N | 2.40 | 0.54 |
| 1:D:888:GLY:CA | 1:D:1138:ARG:HD3 | 2.18 | 0.54 |
| 1:D:298:HIS:CD2 | 1:D:411:LEU:CD2 | 2.90 | 0.54 |
| 1:D:348:LEU:HD13 | 1:D:350:ILE:HD11 | 1.88 | 0.54 |
| 1:D:437:VAL:CA | 1:D:441:TRP:HD1 | 2.16 | 0.54 |
| 1:D:459:MET:H | 1:D:460:LYS:NZ | 2.00 | 0.54 |
| 1:D:641:GLU:C | 1:D:645:VAL:CG2 | 2.68 | 0.54 |
| 1:D:667:GLN:C | 1:D:671:GLN:HG2 | 2.27 | 0.54 |
| 1:D:735:GLY:HA2 | 1:D:750:PHE:N | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:779:LEU:HD13 | 1:D:779:LEU:O | 2.07 | 0.54 |
| 1:D:854:ALA:O | 1:D:855:VAL:CG2 | 2.55 | 0.54 |
| 1:D:901:VAL:O | 1:D:902:LEU:C | 2.46 | 0.54 |
| 1:D:949:PHE:CD1 | 1:D:949:PHE:C | 2.80 | 0.54 |
| 2:E:101:PRO:N | 2:F:128:VAL:CG2 | 2.71 | 0.54 |
| 2:E:199:LEU:CD1 | 2:E:200:VAL:H | 2.21 | 0.54 |
| 2:E:352:ASP:CG | 2:E:352:ASP:O | 2.45 | 0.54 |
| 2:E:402:LEU:O | 2:E:403:PHE:C | 2.46 | 0.54 |
| 2:F:131:LEU:HB3 | 2:F:133:HIS:ND1 | 2.22 | 0.54 |
| 2:F:256:LEU:O | 2:F:257:ARG:C | 2.46 | 0.54 |
| 1:A:1015:THR:CA | 1:A:1016:GLU:OE2 | 2.55 | 0.54 |
| 1:A:850:ILE:CG1 | 1:A:1099:TRP:NE1 | 2.71 | 0.54 |
| 1:A:175:TRP:CG | 1:A:184:ALA:HA | 2.43 | 0.54 |
| 1:A:297:MET:HE1 | 1:A:415:LEU:CD2 | 2.38 | 0.54 |
| 1:A:730:PRO:HG3 | 1:A:760:CYS:O | 2.08 | 0.54 |
| 1:A:866:ARG:HD3 | 1:A:866:ARG:C | 2.27 | 0.54 |
| 1:A:982:ALA:O | 1:A:986:TYR:CD1 | 2.61 | 0.54 |
| 2:B:112:ALA:O | 2:B:115:TRP:CB | 2.56 | 0.54 |
| 2:B:400:GLN:HG2 | 2:B:417:TYR:CE2 | 2.43 | 0.54 |
| 2:B:447:THR:HG23 | 2:B:452:LEU:H | 1.70 | 0.54 |
| 2:C:326:ASP:OD2 | 2:C:327:GLY:N | 2.39 | 0.54 |
| 1:A:784:GLY:CA | 2:C:363:ARG:CD | 2.85 | 0.54 |
| 2:C:483:LYS:HE2 | 2:C:483:LYS:C | 2.27 | 0.54 |
| 2:C:78:PHE:CD2 | 2:C:79:LEU:HD22 | 2.42 | 0.54 |
| 1:D:301:ILE:O | 1:D:1024:ASP:CB | 2.55 | 0.54 |
| 1:D:1145:ASP:HA | 1:D:1148:ARG:HD3 | 1.90 | 0.54 |
| 1:D:148:LEU:CB | 1:D:149:PRO:HD3 | 2.38 | 0.54 |
| 1:D:286:GLY:O | 1:D:287:SER:CB | 2.56 | 0.54 |
| 1:D:371:LYS:NZ | 1:D:393:MET:HA | 2.21 | 0.54 |
| 1:D:627:ARG:O | 1:D:628:ARG:CB | 2.56 | 0.54 |
| 1:D:735:GLY:CA | 1:D:749:PHE:CA | 2.85 | 0.54 |
| 1:D:901:VAL:CG2 | 1:D:902:LEU:N | 2.70 | 0.54 |
| 2:E:214:CYS:HB2 | 2:E:236:GLU:CB | 2.37 | 0.54 |
| 2:E:428:LEU:CD1 | 2:E:428:LEU:N | 2.60 | 0.54 |
| 2:E:91:LEU:C | 2:E:93:SER:N | 2.61 | 0.54 |
| 2:F:221:THR:CG2 | 2:F:222:LYS:N | 2.71 | 0.54 |
| 1:D:1209:ARG:CZ | 2:F:252:LEU:HD22 | 2.38 | 0.54 |
| 2:F:328:ARG:HG3 | 2:F:329:LYS:HD2 | 1.90 | 0.54 |
| 1:A:1043:VAL:O | 1:A:1043:VAL:HG12 | 2.08 | 0.54 |
| 1:A:1111:LEU:O | 1:A:1112:MET:C | 2.46 | 0.54 |
| 1:A:82:GLY:O | 1:A:85:GLU:HG3 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:879:GLN:O | 1:A:1187:ARG:O | 2.26 | 0.54 |
| 1:A:977:GLU:HA | 1:A:980:GLU:OE2 | 2.08 | 0.54 |
| 2:B:252:LEU:O | 2:B:255:TRP:HB2 | 2.07 | 0.54 |
| 2:B:277:ASP:HA | 2:B:287:ASN:CG | 2.28 | 0.54 |
| 2:B:204:LEU:HD11 | 2:B:333:PRO:HB3 | 1.88 | 0.54 |
| 2:B:476:ILE:O | 2:B:480:SER:N | 2.36 | 0.54 |
| 2:B:100:GLY:HA2 | 2:C:128:VAL:HG11 | 1.90 | 0.54 |
| 2:C:234:LYS:NZ | 2:C:344:ARG:CD | 2.61 | 0.54 |
| 2:C:358:GLU:HA | 2:C:361:PHE:CB | 2.38 | 0.54 |
| 2:C:395:LEU:HD11 | 2:C:444:THR:CA | 2.36 | 0.54 |
| 2:C:81:GLY:O | 2:C:86:LEU:HD21 | 2.07 | 0.54 |
| 1:D:422:VAL:CG1 | 1:D:1111:LEU:HD12 | 2.36 | 0.54 |
| 1:D:1147:TYR:CD2 | 1:D:1147:TYR:N | 2.74 | 0.54 |
| 1:D:278:ILE:HA | 1:D:291:PHE:CD1 | 2.42 | 0.54 |
| 1:D:354:ASN:O | 1:D:355:SER:OG | 2.19 | 0.54 |
| 1:D:548:CYS:N | 1:D:551:LYS:HD3 | 2.22 | 0.54 |
| 1:D:585:TRP:CB | 1:D:587:PRO:HD2 | 2.23 | 0.54 |
| 1:D:972:ARG:C | 1:D:974:THR:HG23 | 2.28 | 0.54 |
| 2:E:193:TYR:O | 2:E:197:LEU:HB3 | 2.08 | 0.54 |
| 2:E:218:VAL:O | 2:E:230:SER:OG | 2.22 | 0.54 |
| 2:E:299:LEU:HD11 | 2:E:302:THR:HG22 | 1.89 | 0.54 |
| 2:F:146:ARG:CB | 2:F:228:VAL:HG11 | 2.38 | 0.54 |
| 2:F:328:ARG:C | 2:F:329:LYS:HD2 | 2.27 | 0.54 |
| 2:F:400:GLN:C | 2:F:400:GLN:CD | 2.66 | 0.54 |
| 1:A:307:PHE:CD2 | 1:A:1051:GLY:HA3 | 2.43 | 0.54 |
| 1:A:1128:ARG:O | 1:A:1140:LEU:N | 2.40 | 0.54 |
| 1:A:113:TRP:HA | 1:A:116:PRO:CD | 2.37 | 0.54 |
| 1:A:298:HIS:C | 1:A:298:HIS:ND1 | 2.61 | 0.54 |
| 1:A:645:VAL:HA | 1:A:650:ARG:CD | 2.38 | 0.54 |
| 1:A:792:LEU:O | 1:A:796:LYS:HG3 | 2.08 | 0.54 |
| 1:A:442:GLU:OE1 | 1:A:815:TRP:HZ2 | 1.91 | 0.54 |
| 1:A:964:ARG:O | 1:A:968:GLN:CG | 2.56 | 0.54 |
| 2:B:249:ASN:HA | 2:B:252:LEU:HD22 | 1.89 | 0.54 |
| 2:B:265:LYS:HD3 | 2:B:349:TYR:OH | 2.08 | 0.54 |
| 2:B:265:LYS:O | 2:B:266:PHE:HB2 | 2.08 | 0.54 |
| 2:B:267:ALA:HB1 | 2:B:270:PRO:HB2 | 1.90 | 0.54 |
| 2:B:418:LEU:C | 2:B:418:LEU:HD23 | 2.28 | 0.54 |
| 2:C:314:MET:HB3 | 2:C:315:TYR:CD2 | 2.43 | 0.54 |
| 2:C:336:LEU:HD23 | 2:C:337:SER:O | 2.08 | 0.54 |
| 1:D:1224:ILE:HG12 | 1:D:1227:THR:O | 2.07 | 0.54 |
| 1:D:381:THR:HG23 | 1:D:385:ILE:HB | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:395:TYR:HD1 | 1:D:395:TYR:H | 1.56 | 0.54 |
| 1:D:744:ILE:CB | 1:D:745:PRO:CD | 2.85 | 0.54 |
| 1:D:605:LEU:CD2 | 1:D:781:ALA:CB | 2.73 | 0.54 |
| 1:D:823:ARG:CZ | 1:D:824:ALA:HB3 | 2.38 | 0.54 |
| 1:D:859:TRP:N | 1:D:859:TRP:CD1 | 2.76 | 0.54 |
| 1:D:865:ALA:HB1 | 1:D:872:SER:HG | 1.71 | 0.54 |
| 2:E:99:PHE:CD1 | 2:E:107:ARG:NH2 | 2.76 | 0.54 |
| 2:E:189:ALA:HB3 | 2:E:240:VAL:HG21 | 1.89 | 0.54 |
| 2:E:115:TRP:CZ3 | 2:E:210:GLN:HA | 2.40 | 0.54 |
| 2:E:96:HIS:C | 2:E:98:GLY:H | 2.11 | 0.54 |
| 2:E:419:GLU:CA | 2:F:203:ARG:HH22 | 2.20 | 0.54 |
| 2:F:447:THR:CG2 | 2:F:448:LEU:HG | 2.35 | 0.54 |
| 1:A:1046:GLU:OE1 | 1:A:1049:TRP:CG | 2.60 | 0.54 |
| 1:A:136:ASP:HA | 1:A:139:PHE:HB2 | 1.88 | 0.54 |
| 1:A:196:VAL:HG13 | 1:A:269:HIS:HD2 | 1.67 | 0.54 |
| 1:A:563:PRO:C | 1:A:564:GLN:NE2 | 2.60 | 0.54 |
| 1:A:733:HIS:C | 1:A:735:GLY:N | 2.60 | 0.54 |
| 2:B:116:THR:HA | 2:B:120:VAL:CB | 2.38 | 0.54 |
| 2:B:200:VAL:O | 2:B:202:LYS:N | 2.41 | 0.54 |
| 2:B:267:ALA:HB1 | 2:B:270:PRO:HD2 | 1.89 | 0.54 |
| 2:C:305:ASN:HA | 2:C:335:VAL:CG1 | 2.38 | 0.54 |
| 2:C:371:VAL:HG23 | 2:C:433:ASP:CB | 2.37 | 0.54 |
| 2:C:444:THR:O | 2:C:445:GLU:C | 2.47 | 0.54 |
| 1:A:556:THR:HG22 | 2:C:467:HIS:CD2 | 2.43 | 0.54 |
| 2:C:466:MET:CE | 2:C:471:LEU:HB3 | 2.38 | 0.54 |
| 1:D:1113:LEU:CD2 | 1:D:1113:LEU:N | 2.71 | 0.54 |
| 1:D:1129:PHE:CE2 | 1:D:1139:TYR:CE2 | 2.96 | 0.54 |
| 1:D:1134:HIS:O | 1:D:1134:HIS:CD2 | 2.60 | 0.54 |
| 1:D:385:ILE:O | 1:D:388:ASN:HB2 | 2.08 | 0.54 |
| 1:D:543:VAL:O | 1:D:547:ALA:CB | 2.56 | 0.54 |
| 1:D:603:MET:O | 1:D:605:LEU:HG | 2.07 | 0.54 |
| 1:D:845:VAL:H | 1:D:855:VAL:HB | 1.73 | 0.54 |
| 1:D:853:ARG:NH1 | 1:D:1102:GLN:HA | 2.23 | 0.54 |
| 2:E:353:SER:HG | 2:E:372:LEU:HD11 | 1.73 | 0.54 |
| 2:E:75:ARG:O | 2:E:76:ARG:HB2 | 2.08 | 0.54 |
| 2:F:311:LEU:CA | 2:F:314:MET:HB2 | 2.38 | 0.54 |
| 2:F:241:TRP:CG | 2:F:336:LEU:HD12 | 2.41 | 0.54 |
| 2:F:344:ARG:HA | 2:F:347:LEU:CB | 2.36 | 0.54 |
| 2:F:74:GLN:HE21 | 2:F:75:ARG:HH21 | 1.56 | 0.54 |
| 1:A:1169:GLY:O | 1:A:1170:LEU:CB | 2.53 | 0.53 |
| 1:A:244:LEU:O | 1:A:247:LEU:CD2 | 2.56 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:316:LYS:HD3 | 1:A:350:ILE:HG12 | 1.89 | 0.53 |
| 1:A:301:ILE:CD1 | 1:A:414:PHE:CB | 2.86 | 0.53 |
| 1:A:450:GLY:O | 1:A:454:GLU:HG3 | 2.09 | 0.53 |
| 1:A:513:LEU:O | 1:A:568:GLY:CA | 2.56 | 0.53 |
| 1:A:498:LYS:CE | 1:A:518:ALA:H | 2.09 | 0.53 |
| 1:A:549:LEU:O | 1:A:553:LYS:HG3 | 2.08 | 0.53 |
| 1:A:582:ASP:OD1 | 1:A:592:LEU:HD22 | 2.08 | 0.53 |
| 1:A:783:PRO:CG | 2:C:363:ARG:CZ | 2.84 | 0.53 |
| 1:A:827:ARG:NH1 | 1:A:827:ARG:HG2 | 2.19 | 0.53 |
| 2:B:182:ARG:HG2 | 2:B:214:CYS:HA | 1.90 | 0.53 |
| 2:B:206:TYR:HA | 2:B:241:TRP:CZ3 | 2.43 | 0.53 |
| 2:B:284:ARG:NE | 2:B:284:ARG:HA | 2.22 | 0.53 |
| 2:B:78:PHE:CE1 | 2:B:103:GLY:HA2 | 2.38 | 0.53 |
| 2:C:253:ASP:HA | 2:C:256:LEU:HD23 | 1.90 | 0.53 |
| 2:C:375:HIS:HB3 | 2:C:378:LEU:CD1 | 2.35 | 0.53 |
| 2:C:416:GLY:HA2 | 2:C:419:GLU:CB | 2.37 | 0.53 |
| 2:C:446:THR:CB | 2:C:450:ASN:OD1 | 2.51 | 0.53 |
| 1:D:885:THR:HG22 | 1:D:1186:ASP:C | 2.28 | 0.53 |
| 1:D:1189:LEU:CD2 | 1:D:1189:LEU:N | 2.68 | 0.53 |
| 1:D:1204:THR:C | 1:D:1207:GLU:HB3 | 2.29 | 0.53 |
| 1:D:441:TRP:CZ3 | 1:D:1210:TYR:CE1 | 2.96 | 0.53 |
| 1:D:211:LEU:O | 1:D:212:ALA:HB2 | 2.08 | 0.53 |
| 1:D:189:ILE:HD13 | 1:D:258:GLN:HB3 | 1.91 | 0.53 |
| 1:D:269:HIS:HB2 | 1:D:274:ASP:OD1 | 2.08 | 0.53 |
| 1:D:279:ARG:HH21 | 1:D:844:VAL:HG22 | 1.72 | 0.53 |
| 1:D:472:GLN:O | 1:D:473:LEU:C | 2.47 | 0.53 |
| 1:D:495:PHE:O | 1:D:496:LYS:CD | 2.48 | 0.53 |
| 1:D:642:SER:C | 1:D:645:VAL:HB | 2.29 | 0.53 |
| 2:E:123:GLU:C | 2:E:125:VAL:N | 2.59 | 0.53 |
| 2:E:260:LEU:CD1 | 2:E:264:ARG:HD2 | 2.38 | 0.53 |
| 2:E:441:VAL:CG1 | 2:E:442:LEU:N | 2.71 | 0.53 |
| 2:F:208:LEU:C | 2:F:208:LEU:HD12 | 2.28 | 0.53 |
| 2:F:371:VAL:HG23 | 2:F:433:ASP:CB | 2.38 | 0.53 |
| 2:F:454:HIS:NE2 | 2:F:472:LYS:CD | 2.70 | 0.53 |
| 2:F:80:SER:OG | 2:F:99:PHE:O | 2.25 | 0.53 |
| 1:A:1115:ALA:O | 1:A:1118:TRP:HB3 | 2.08 | 0.53 |
| 1:A:172:ALA:O | 1:A:173:GLU:HB2 | 2.07 | 0.53 |
| 1:A:313:ILE:HD12 | 1:A:314:ALA:N | 2.23 | 0.53 |
| 1:A:371:LYS:HZ1 | 1:A:400:VAL:CG2 | 2.21 | 0.53 |
| 1:A:899:ALA:O | 1:A:1002:GLU:OE1 | 2.27 | 0.53 |
| 2:B:202:LYS:O | 2:B:325:ARG:NE | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:291:TYR:HH | 2:C:355:GLN:HG3 | 1.69 | 0.53 |
| 2:C:364:LYS:H | 2:C:364:LYS:CD | 2.08 | 0.53 |
| 2:C:426:GLU:O | 2:C:429:TYR:HB2 | 2.08 | 0.53 |
| 2:C:451:GLY:O | 2:C:452:LEU:HG | 2.09 | 0.53 |
| 1:D:1116:MET:HE2 | 1:D:1156:THR:OG1 | 2.08 | 0.53 |
| 1:D:1131:ILE:HD11 | 1:D:1138:ARG:C | 2.28 | 0.53 |
| 1:D:456:GLN:O | 1:D:460:LYS:NZ | 2.41 | 0.53 |
| 1:D:571:GLY:O | 1:D:572:TRP:HB2 | 2.08 | 0.53 |
| 1:D:731:SER:O | 1:D:732:TYR:HB2 | 2.09 | 0.53 |
| 2:E:127:PRO:HG2 | 2:F:101:PRO:HA | 1.91 | 0.53 |
| 2:E:418:LEU:HD11 | 2:F:122:ARG:CG | 2.38 | 0.53 |
| 2:E:483:LYS:NZ | 2:E:483:LYS:HB2 | 2.23 | 0.53 |
| 2:F:350:LEU:N | 2:F:350:LEU:CD1 | 2.56 | 0.53 |
| 2:F:371:VAL:HG23 | 2:F:433:ASP:O | 2.08 | 0.53 |
| 2:F:454:HIS:CG | 2:F:466:MET:HB2 | 2.40 | 0.53 |
| 1:A:1019:TRP:O | 1:A:1020:ILE:CB | 2.56 | 0.53 |
| 1:A:347:TRP:HD1 | 1:A:1030:ARG:HG2 | 1.73 | 0.53 |
| 1:A:885:THR:HB | 1:A:1146:ARG:NH2 | 2.22 | 0.53 |
| 1:A:312:TRP:HZ2 | 1:A:346:ASP:C | 2.12 | 0.53 |
| 1:A:400:VAL:HG13 | 1:A:404:HIS:NE2 | 2.22 | 0.53 |
| 1:A:420:HIS:O | 1:A:424:LEU:CG | 2.56 | 0.53 |
| 1:A:627:ARG:O | 1:A:628:ARG:CB | 2.56 | 0.53 |
| 1:A:644:GLY:O | 1:A:645:VAL:HB | 2.07 | 0.53 |
| 1:A:814:VAL:O | 1:A:838:GLY:HA3 | 2.08 | 0.53 |
| 1:A:435:LEU:HD12 | 1:A:842:PRO:CD | 2.39 | 0.53 |
| 2:C:250:GLN:OE1 | 2:C:257:ARG:NH2 | 2.29 | 0.53 |
| 2:C:343:ASP:O | 2:C:346:MET:HB3 | 2.09 | 0.53 |
| 1:D:210:THR:O | 1:D:211:LEU:CB | 2.54 | 0.53 |
| 1:D:312:TRP:CE3 | 1:D:316:LYS:CD | 2.92 | 0.53 |
| 1:D:405:GLU:O | 1:D:406:VAL:C | 2.47 | 0.53 |
| 1:D:421:PRO:HG2 | 1:D:422:VAL:N | 2.23 | 0.53 |
| 1:D:457:ARG:NH1 | 1:D:457:ARG:CB | 2.71 | 0.53 |
| 1:D:491:ASP:O | 1:D:492:LEU:C | 2.45 | 0.53 |
| 1:D:603:MET:O | 1:D:604:ALA:C | 2.46 | 0.53 |
| 1:D:732:TYR:CB | 1:D:755:LYS:NZ | 2.71 | 0.53 |
| 1:D:776:ASP:CG | 1:D:777:GLY:N | 2.61 | 0.53 |
| 1:D:279:ARG:HA | 1:D:841:LEU:HD12 | 1.91 | 0.53 |
| 1:D:932:HIS:ND1 | 1:D:933:SER:N | 2.56 | 0.53 |
| 2:E:379:ALA:N | 2:E:380:PRO:CD | 2.72 | 0.53 |
| 2:F:199:LEU:HD12 | 2:F:200:VAL:H | 1.73 | 0.53 |
| 2:F:127:PRO:HD3 | 2:F:210:GLN:HB2 | 1.82 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:286:GLY:HA3 | 2:F:303:LEU:O | 2.08 | 0.53 |
| 2:F:306:LEU:CG | 2:F:306:LEU:O | 2.50 | 0.53 |
| 2:F:372:LEU:CD1 | 2:F:374:LEU:HG | 2.38 | 0.53 |
| 2:F:416:GLY:HA2 | 2:F:419:GLU:HB3 | 1.91 | 0.53 |
| 1:A:87:ILE:HG12 | 1:A:1166:TYR:CE2 | 2.43 | 0.53 |
| 1:A:316:LYS:HB2 | 1:A:348:LEU:CD1 | 2.39 | 0.53 |
| 1:A:408:GLN:HG3 | 1:A:411:LEU:HD21 | 1.90 | 0.53 |
| 1:A:441:TRP:HE1 | 1:A:877:MET:HB3 | 1.72 | 0.53 |
| 1:A:528:GLU:O | 1:A:529:ASP:OD2 | 2.27 | 0.53 |
| 1:A:606:THR:CB | 1:A:613:HIS:N | 2.72 | 0.53 |
| 1:A:828:HIS:N | 1:A:829:PRO:CD | 2.72 | 0.53 |
| 1:A:857:PRO:O | 1:A:861:THR:OG1 | 2.20 | 0.53 |
| 1:A:920:THR:OG1 | 1:A:921:LEU:HD12 | 2.08 | 0.53 |
| 2:B:348:ALA:O | 2:B:351:TYR:N | 2.36 | 0.53 |
| 2:B:412:SER:C | 2:B:413:VAL:CG2 | 2.77 | 0.53 |
| 2:B:133:HIS:NE2 | 2:C:231:ILE:HG21 | 2.20 | 0.53 |
| 2:C:246:ARG:O | 2:C:247:THR:C | 2.45 | 0.53 |
| 2:C:274:SER:OG | 2:C:275:SER:N | 2.41 | 0.53 |
| 2:C:266:PHE:HD1 | 2:C:378:LEU:CD1 | 2.21 | 0.53 |
| 2:C:84:GLN:C | 2:C:86:LEU:H | 2.11 | 0.53 |
| 1:D:1016:GLU:HG3 | 1:D:1022:LEU:CD2 | 2.39 | 0.53 |
| 1:D:116:PRO:O | 1:D:118:VAL:HG12 | 2.08 | 0.53 |
| 1:D:136:ASP:OD1 | 1:D:140:ARG:NE | 2.41 | 0.53 |
| 1:D:278:ILE:HD13 | 1:D:282:TYR:CZ | 2.43 | 0.53 |
| 1:D:298:HIS:NE2 | 1:D:407:PHE:HB2 | 2.24 | 0.53 |
| 1:D:434:TYR:C | 1:D:1130:CYS:HB3 | 2.29 | 0.53 |
| 1:D:744:ILE:CG1 | 1:D:745:PRO:HD3 | 2.37 | 0.53 |
| 1:D:786:ALA:O | 1:D:787:SER:CB | 2.55 | 0.53 |
| 1:D:849:THR:HG21 | 1:D:851:THR:HB | 1.89 | 0.53 |
| 1:D:932:HIS:O | 1:D:935:THR:CG2 | 2.46 | 0.53 |
| 2:E:109:ASN:HD22 | 2:E:378:LEU:HB3 | 1.73 | 0.53 |
| 2:F:347:LEU:H | 2:F:347:LEU:CD1 | 2.21 | 0.53 |
| 2:F:78:PHE:CD1 | 2:F:102:LEU:CD2 | 2.90 | 0.53 |
| 1:A:1019:TRP:O | 1:A:1020:ILE:CG2 | 2.56 | 0.53 |
| 1:A:1124:ALA:CA | 1:A:1148:ARG:HH12 | 2.21 | 0.53 |
| 1:A:247:LEU:HG | 1:A:248:GLU:N | 2.12 | 0.53 |
| 1:A:411:LEU:HD12 | 1:A:411:LEU:C | 2.28 | 0.53 |
| 1:A:297:MET:CE | 1:A:415:LEU:HD21 | 2.39 | 0.53 |
| 1:A:743:ASP:HB2 | 1:A:744:ILE:HD13 | 1.91 | 0.53 |
| 1:A:207:THR:HG21 | 1:A:812:MET:CB | 2.38 | 0.53 |
| 1:A:831:TYR:HB2 | 1:A:837:TYR:OH | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:849:THR:HB | 1:A:852:ARG:H | 1.73 | 0.53 |
| 2:C:134:LYS:CB | 2:C:180:LYS:HE2 | 2.38 | 0.53 |
| 2:C:272:ASN:CA | 2:C:292:ASN:ND2 | 2.72 | 0.53 |
| 2:C:376:PRO:HG3 | 2:C:482:ALA:CB | 2.31 | 0.53 |
| 2:C:403:PHE:CD1 | 2:C:415:PRO:HG3 | 2.43 | 0.53 |
| 1:D:308:GLN:HE22 | 1:D:1027:LYS:NZ | 2.06 | 0.53 |
| 1:D:104:VAL:HG12 | 1:D:105:GLU:N | 2.24 | 0.53 |
| 1:D:576:LEU:HD22 | 2:F:481:SER:HB2 | 1.89 | 0.53 |
| 1:D:850:ILE:HG12 | 1:D:851:THR:H | 1.73 | 0.53 |
| 1:D:441:TRP:CD1 | 1:D:878:VAL:O | 2.61 | 0.53 |
| 1:D:938:THR:C | 1:D:939:VAL:HG23 | 2.29 | 0.53 |
| 2:E:299:LEU:HD23 | 2:E:300:ILE:N | 2.24 | 0.53 |
| 2:E:389:ARG:HE | 2:E:390:GLY:H | 1.48 | 0.53 |
| 2:E:400:GLN:CA | 2:E:403:PHE:HB3 | 2.38 | 0.53 |
| 1:D:472:GLN:CD | 2:F:460:THR:O | 2.47 | 0.53 |
| 2:F:86:LEU:O | 2:F:87:SER:O | 2.26 | 0.53 |
| 1:A:1019:TRP:CH2 | 1:A:1163:MET:HG2 | 2.43 | 0.53 |
| 1:A:1208:ARG:O | 2:C:253:ASP:OD2 | 2.26 | 0.53 |
| 1:A:286:GLY:O | 1:A:287:SER:CB | 2.56 | 0.53 |
| 1:A:355:SER:O | 1:A:407:PHE:HZ | 1.92 | 0.53 |
| 1:A:513:LEU:O | 1:A:568:GLY:HA3 | 2.09 | 0.53 |
| 1:A:659:HIS:ND1 | 1:A:716:PRO:CA | 2.71 | 0.53 |
| 1:A:843:GLN:O | 1:A:856:GLU:HG2 | 2.08 | 0.53 |
| 2:B:235:THR:OG1 | 2:B:343:ASP:N | 2.41 | 0.53 |
| 2:B:451:GLY:O | 2:B:468:ILE:HG22 | 2.09 | 0.53 |
| 2:B:67:GLU:CG | 2:B:69:LEU:HG | 2.39 | 0.53 |
| 1:D:1029:GLN:CD | 1:D:1030:ARG:HH21 | 2.09 | 0.53 |
| 1:D:1143:GLU:O | 1:D:1146:ARG:CG | 2.54 | 0.53 |
| 1:D:145:LYS:HB3 | 1:D:1118:TRP:HH2 | 1.73 | 0.53 |
| 1:D:430:MET:HE1 | 1:D:1132:SER:HB3 | 1.91 | 0.53 |
| 1:D:438:ASN:N | 1:D:441:TRP:HD1 | 2.00 | 0.53 |
| 1:D:449:GLN:CA | 1:D:452:TYR:HE2 | 2.13 | 0.53 |
| 1:D:588:GLY:HA3 | 1:D:806:LYS:HE3 | 1.90 | 0.53 |
| 2:E:132:HIS:HB2 | 2:F:233:GLU:OE1 | 2.08 | 0.53 |
| 2:E:332:VAL:N | 2:E:333:PRO:HD3 | 2.23 | 0.53 |
| 2:E:101:PRO:HG3 | 2:F:128:VAL:HG21 | 1.90 | 0.53 |
| 2:F:399:CYS:SG | 2:F:417:TYR:CD2 | 3.00 | 0.53 |
| 2:F:440:THR:O | 2:F:457:SER:CB | 2.54 | 0.53 |
| 1:A:1100:VAL:HG12 | 1:A:1101:VAL:N | 2.24 | 0.53 |
| 1:A:1115:ALA:O | 1:A:1119:LEU:HG | 2.08 | 0.53 |
| 1:A:1198:LYS:CG | 1:A:1204:THR:CG2 | 2.80 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:202:CYS:SG | 1:A:210:THR:CG2 | 2.94 | 0.53 |
| 1:A:371:LYS:CG | 1:A:372:GLU:HG2 | 2.39 | 0.53 |
| 1:A:594:LEU:CD2 | 1:A:594:LEU:N | 2.72 | 0.53 |
| 1:A:606:THR:HG21 | 1:A:613:HIS:H | 1.69 | 0.53 |
| 1:A:646:VAL:O | 1:A:646:VAL:HG13 | 2.09 | 0.53 |
| 1:A:950:ASN:O | 1:A:953:ARG:N | 2.41 | 0.53 |
| 2:B:189:ALA:HB1 | 2:B:208:LEU:HD21 | 1.91 | 0.53 |
| 2:B:217:PRO:HB3 | 2:B:232:GLY:H | 1.74 | 0.53 |
| 2:C:208:LEU:N | 2:C:208:LEU:HD12 | 2.24 | 0.53 |
| 2:C:114:TRP:NE1 | 2:C:259:ARG:CZ | 2.70 | 0.53 |
| 2:C:72:ILE:HG23 | 2:C:76:ARG:HD2 | 1.91 | 0.53 |
| 2:C:82:SER:O | 2:C:83:LYS:HG3 | 2.09 | 0.53 |
| 1:D:1014:ARG:HG2 | 1:D:1026:ARG:NE | 2.18 | 0.53 |
| 1:D:1019:TRP:CD1 | 1:D:1020:ILE:N | 2.76 | 0.53 |
| 1:D:249:VAL:HG22 | 1:D:250:PRO:N | 2.24 | 0.53 |
| 1:D:267:VAL:C | 1:D:269:HIS:NE2 | 2.62 | 0.53 |
| 1:D:287:SER:C | 1:D:288:ARG:NE | 2.62 | 0.53 |
| 1:D:357:ALA:C | 1:D:359:VAL:H | 2.12 | 0.53 |
| 1:D:549:LEU:O | 1:D:553:LYS:HG3 | 2.08 | 0.53 |
| 1:D:656:TYR:C | 1:D:659:HIS:CE1 | 2.81 | 0.53 |
| 1:D:808:ILE:O | 1:D:811:GLN:HB3 | 2.08 | 0.53 |
| 1:D:973:LEU:O | 1:D:977:GLU:HG3 | 2.09 | 0.53 |
| 2:E:351:TYR:C | 2:E:353:SER:N | 2.59 | 0.53 |
| 2:E:400:GLN:O | 2:E:402:LEU:N | 2.42 | 0.53 |
| 2:F:131:LEU:CG | 2:F:133:HIS:CE1 | 2.82 | 0.53 |
| 1:A:211:LEU:HD11 | 1:A:221:TYR:HB3 | 1.89 | 0.53 |
| 1:A:254:SER:O | 1:A:255:SER:HB2 | 2.08 | 0.53 |
| 1:A:451:THR:OG1 | 1:A:1202:ASN:OD1 | 2.27 | 0.53 |
| 1:A:853:ARG:O | 1:A:854:ALA:HB2 | 2.09 | 0.53 |
| 1:A:914:THR:O | 1:A:915:ALA:HB2 | 2.09 | 0.53 |
| 2:B:190:LEU:HB3 | 2:B:315:TYR:OH | 2.08 | 0.53 |
| 2:C:285:LYS:CB | 2:C:285:LYS:NZ | 2.71 | 0.53 |
| 1:D:1196:ASP:HB2 | 1:D:1204:THR:HG22 | 1.91 | 0.53 |
| 1:D:152:GLU:HA | 1:D:155:ASN:HD22 | 1.74 | 0.53 |
| 1:D:255:SER:OG | 1:D:257:THR:N | 2.41 | 0.53 |
| 1:D:369:LEU:CB | 1:D:372:GLU:HB2 | 2.39 | 0.53 |
| 1:D:472:GLN:O | 1:D:474:LEU:O | 2.27 | 0.53 |
| 1:D:493:GLN:O | 1:D:494:GLU:CG | 2.53 | 0.53 |
| 1:D:666:GLN:HG2 | 1:D:669:MET:HE2 | 1.91 | 0.53 |
| 1:D:776:ASP:CA | 1:D:796:LYS:HZ3 | 2.22 | 0.53 |
| 1:D:910:MET:HE1 | 1:D:911:HIS:CE1 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:967:MET:SD | 1:D:975:GLN:N | 2.82 | 0.53 |
| 1:D:993:ARG:NE | 1:D:994:TRP:HB2 | 2.24 | 0.53 |
| 2:E:116:THR:O | 2:E:118:VAL:N | 2.41 | 0.53 |
| 2:E:311:LEU:O | 2:E:315:TYR:N | 2.42 | 0.53 |
| 2:E:424:SER:OG | 2:E:425:LEU:N | 2.42 | 0.53 |
| 2:E:96:HIS:O | 2:E:96:HIS:HD2 | 1.92 | 0.53 |
| 2:F:206:TYR:CE1 | 2:F:208:LEU:HD23 | 2.43 | 0.53 |
| 2:F:243:THR:HB | 2:F:247:THR:OG1 | 2.08 | 0.53 |
| 2:F:241:TRP:CE3 | 2:F:336:LEU:HD12 | 2.44 | 0.53 |
| 2:F:348:ALA:O | 2:F:351:TYR:CB | 2.56 | 0.53 |
| 2:F:348:ALA:O | 2:F:351:TYR:HB2 | 2.07 | 0.53 |
| 2:F:403:PHE:CD1 | 2:F:415:PRO:HG3 | 2.44 | 0.53 |
| 2:F:442:LEU:HB2 | 2:F:455:LEU:HD22 | 1.91 | 0.53 |
| 2:F:484:ASN:C | 2:F:485:VAL:CG1 | 2.77 | 0.53 |
| 2:F:61:GLY:C | 2:F:64:GLU:HG2 | 2.29 | 0.53 |
| 1:A:1011:PRO:CD | 1:A:1012:VAL:N | 2.65 | 0.53 |
| 1:A:1143:GLU:O | 1:A:1146:ARG:CB | 2.57 | 0.53 |
| 1:A:213:VAL:CG1 | 1:A:397:ALA:CB | 2.84 | 0.53 |
| 1:A:653:GLU:CA | 1:A:656:TYR:CZ | 2.88 | 0.53 |
| 1:A:658:LYS:CB | 1:A:713:PRO:O | 2.57 | 0.53 |
| 1:A:659:HIS:CE1 | 1:A:663:GLN:CD | 2.82 | 0.53 |
| 1:A:812:MET:CG | 1:A:813:VAL:H | 2.21 | 0.53 |
| 2:B:301:GLU:HG2 | 2:B:303:LEU:CD1 | 2.39 | 0.53 |
| 2:B:76:ARG:HH21 | 2:B:431:LYS:HG3 | 1.73 | 0.53 |
| 2:B:69:LEU:CD1 | 2:B:73:CYS:SG | 2.97 | 0.53 |
| 2:B:74:GLN:HB2 | 2:B:77:HIS:CD2 | 2.43 | 0.53 |
| 2:C:131:LEU:HB3 | 2:C:133:HIS:CG | 2.44 | 0.53 |
| 2:C:387:VAL:HG13 | 2:C:399:CYS:HB2 | 1.90 | 0.53 |
| 2:C:414:TRP:O | 2:C:414:TRP:CD1 | 2.62 | 0.53 |
| 1:D:1174:PRO:HB2 | 1:D:1177:VAL:CG2 | 2.39 | 0.53 |
| 1:D:1195:MET:O | 1:D:1196:ASP:CG | 2.48 | 0.53 |
| 1:D:1232:GLU:CB | 1:D:1234:ARG:HB2 | 2.39 | 0.53 |
| 1:D:195:LEU:O | 1:D:267:VAL:HG12 | 2.09 | 0.53 |
| 1:D:293:ASP:C | 1:D:293:ASP:OD2 | 2.46 | 0.53 |
| 1:D:305:SER:OG | 1:D:1099:TRP:NE1 | 2.42 | 0.53 |
| 1:D:312:TRP:HE3 | 1:D:316:LYS:CD | 2.22 | 0.53 |
| 1:D:567:PRO:O | 1:D:568:GLY:C | 2.45 | 0.53 |
| 1:D:604:ALA:HA | 1:D:613:HIS:NE2 | 2.20 | 0.53 |
| 1:D:618:HIS:HA | 1:D:762:VAL:HG22 | 1.91 | 0.53 |
| 1:D:620:TRP:CZ2 | 1:D:751:LYS:HD3 | 2.44 | 0.53 |
| 2:E:106:LEU:C | 2:E:109:ASN:OD1 | 2.47 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:247:THR:HB | 2:E:251:TRP:CD1 | 2.42 | 0.53 |
| 2:E:91:LEU:C | 2:E:93:SER:H | 2.12 | 0.53 |
| 2:F:243:THR:CG2 | 2:F:247:THR:OG1 | 2.57 | 0.53 |
| 2:F:456:ARG:NE | 2:F:456:ARG:N | 2.56 | 0.53 |
| 1:A:107:LEU:O | 1:A:111:GLY:N | 2.41 | 0.53 |
| 1:A:1131:ILE:HG12 | 1:A:1132:SER:N | 2.24 | 0.53 |
| 1:A:1164:PHE:HB3 | 1:A:1168:LEU:HD12 | 1.91 | 0.53 |
| 1:A:1183:VAL:C | 1:A:1217:ALA:HB1 | 2.29 | 0.53 |
| 1:A:129:PRO:O | 1:A:130:LEU:HD12 | 2.09 | 0.53 |
| 1:A:213:VAL:C | 1:A:401:TRP:CZ2 | 2.74 | 0.53 |
| 1:A:235:TRP:CD1 | 1:A:236:THR:OG1 | 2.62 | 0.53 |
| 1:A:354:ASN:O | 1:A:355:SER:HB2 | 2.08 | 0.53 |
| 1:A:389:PHE:O | 1:A:390:GLN:C | 2.47 | 0.53 |
| 1:A:545:ALA:HB1 | 2:C:400:GLN:OE1 | 2.09 | 0.53 |
| 1:A:821:LEU:HD13 | 1:A:825:VAL:CG1 | 2.39 | 0.53 |
| 1:A:815:TRP:HE3 | 1:A:838:GLY:N | 2.07 | 0.53 |
| 1:A:887:VAL:HA | 1:A:1146:ARG:HH12 | 1.74 | 0.53 |
| 1:A:949:PHE:O | 1:A:953:ARG:N | 2.42 | 0.53 |
| 1:A:992:LEU:CD1 | 1:A:993:ARG:N | 2.66 | 0.53 |
| 2:B:105:GLU:HB3 | 2:B:380:PRO:CB | 2.33 | 0.53 |
| 2:B:72:ILE:HD12 | 2:B:372:LEU:HD21 | 1.90 | 0.53 |
| 2:B:69:LEU:HA | 2:B:72:ILE:CD1 | 2.39 | 0.53 |
| 2:C:273:PHE:CE1 | 2:C:291:TYR:CD1 | 2.92 | 0.53 |
| 2:C:359:ASN:O | 2:C:360:SER:HB2 | 2.07 | 0.53 |
| 1:D:1138:ARG:HH22 | 1:D:1191:LYS:HE3 | 1.73 | 0.53 |
| 1:D:172:ALA:O | 1:D:173:GLU:HB2 | 2.09 | 0.53 |
| 1:D:243:ASP:O | 1:D:246:PRO:HD2 | 2.08 | 0.53 |
| 1:D:271:VAL:N | 1:D:274:ASP:OD2 | 2.42 | 0.53 |
| 1:D:349:ASP:O | 1:D:350:ILE:C | 2.47 | 0.53 |
| 1:D:472:GLN:HB3 | 2:F:461:THR:HG23 | 1.90 | 0.53 |
| 1:D:491:ASP:OD2 | 1:D:578:PRO:CB | 2.56 | 0.53 |
| 1:D:608:ASP:N | 1:D:620:TRP:CZ3 | 2.77 | 0.53 |
| 1:D:649:TYR:C | 1:D:652:ILE:HB | 2.28 | 0.53 |
| 1:D:711:ALA:C | 1:D:713:PRO:CD | 2.77 | 0.53 |
| 1:D:827:ARG:HD3 | 1:D:828:HIS:CA | 2.38 | 0.53 |
| 1:D:890:ASP:C | 1:D:891:VAL:HG12 | 2.23 | 0.53 |
| 1:D:920:THR:HG21 | 1:D:922:GLN:OE1 | 2.10 | 0.53 |
| 2:E:389:ARG:CA | 2:E:395:LEU:HG | 2.39 | 0.53 |
| 2:F:127:PRO:CD | 2:F:209:ALA:C | 2.71 | 0.53 |
| 2:F:207:GLY:HA2 | 2:F:240:VAL:O | 2.08 | 0.53 |
| 2:F:360:SER:HA | 2:F:363:ARG:HG3 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:88:ARG:NH1 | 2:F:88:ARG:CB | 2.72 | 0.53 |
| 1:A:1026:ARG:O | 1:A:1030:ARG:CA | 2.57 | 0.52 |
| 1:A:1133:ILE:O | 1:A:1136:GLU:N | 2.37 | 0.52 |
| 1:A:1157:ASN:HA | 1:A:1160:THR:OG1 | 2.08 | 0.52 |
| 1:A:1206:MET:O | 1:A:1207:GLU:HB2 | 2.09 | 0.52 |
| 1:A:1206:MET:H | 1:A:1209:ARG:HB2 | 1.72 | 0.52 |
| 1:A:175:TRP:HB3 | 1:A:184:ALA:HA | 1.90 | 0.52 |
| 1:A:308:GLN:HB3 | 1:A:1090:GLU:CG | 2.38 | 0.52 |
| 1:A:353:VAL:HG22 | 1:A:354:ASN:N | 2.23 | 0.52 |
| 1:A:424:LEU:H | 1:A:424:LEU:HD23 | 1.69 | 0.52 |
| 1:A:515:ILE:CG2 | 1:A:516:GLU:H | 2.08 | 0.52 |
| 1:A:633:LYS:O | 1:A:634:LEU:HD13 | 2.10 | 0.52 |
| 1:A:645:VAL:HG12 | 1:A:646:VAL:N | 2.22 | 0.52 |
| 1:A:659:HIS:CE1 | 1:A:716:PRO:C | 2.82 | 0.52 |
| 1:A:657:ARG:C | 1:A:660:CYS:HB3 | 2.27 | 0.52 |
| 1:A:662:GLU:O | 1:A:666:GLN:HB2 | 2.08 | 0.52 |
| 1:A:770:PHE:O | 1:A:773:LYS:HB2 | 2.09 | 0.52 |
| 1:A:80:SER:OG | 1:A:125:LEU:CD1 | 2.56 | 0.52 |
| 1:A:829:PRO:O | 1:A:830:ASP:CB | 2.56 | 0.52 |
| 1:A:938:THR:C | 1:A:939:VAL:HG23 | 2.28 | 0.52 |
| 2:B:123:GLU:OE2 | 2:B:126:PHE:CE2 | 2.62 | 0.52 |
| 2:C:415:PRO:CB | 2:C:417:TYR:CE2 | 2.90 | 0.52 |
| 1:D:944:GLU:CG | 1:D:1071:ARG:NH1 | 2.71 | 0.52 |
| 1:D:224:CYS:SG | 1:D:228:LEU:HD22 | 2.48 | 0.52 |
| 1:D:275:ARG:HH11 | 1:D:843:GLN:HE21 | 1.48 | 0.52 |
| 1:D:279:ARG:NH2 | 1:D:433:SER:HB3 | 2.25 | 0.52 |
| 1:D:404:HIS:O | 1:D:408:GLN:HB2 | 2.09 | 0.52 |
| 1:D:795:ASN:HA | 1:D:798:ILE:HG12 | 1.91 | 0.52 |
| 1:D:836:LEU:O | 1:D:837:TYR:HD2 | 1.93 | 0.52 |
| 2:E:115:TRP:CH2 | 2:E:127:PRO:HB3 | 2.44 | 0.52 |
| 2:E:123:GLU:C | 2:E:125:VAL:H | 2.11 | 0.52 |
| 2:E:431:LYS:CG | 2:E:432:TYR:N | 2.72 | 0.52 |
| 2:E:445:GLU:CD | 2:E:446:THR:N | 2.62 | 0.52 |
| 2:F:127:PRO:O | 2:F:192:HIS:CD2 | 2.62 | 0.52 |
| 2:F:196:CYS:HB3 | 2:F:206:TYR:OH | 2.09 | 0.52 |
| 2:F:454:HIS:CD2 | 2:F:468:ILE:CA | 2.83 | 0.52 |
| 1:A:1072:THR:N | 1:A:1073:PRO:CD | 2.72 | 0.52 |
| 1:A:308:GLN:HB3 | 1:A:1090:GLU:CA | 2.37 | 0.52 |
| 1:A:1109:LEU:HD11 | 1:A:1137:VAL:HG21 | 1.91 | 0.52 |
| 1:A:1193:VAL:CG2 | 1:A:1194:THR:H | 2.21 | 0.52 |
| 1:A:203:LEU:HD12 | 1:A:380:GLY:CA | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:813:VAL:HG11 | 1:A:815:TRP:CH2 | 2.44 | 0.52 |
| 1:A:893:SER:OG | 1:A:896:LEU:HB2 | 2.09 | 0.52 |
| 2:B:180:LYS:HG3 | 2:B:181:LEU:H | 1.73 | 0.52 |
| 2:B:288:LYS:C | 2:B:289:LEU:HD22 | 2.29 | 0.52 |
| 2:B:379:ALA:O | 2:B:380:PRO:C | 2.46 | 0.52 |
| 2:C:190:LEU:O | 2:C:193:TYR:CB | 2.51 | 0.52 |
| 1:D:100:VAL:O | 1:D:103:SER:OG | 2.23 | 0.52 |
| 1:D:206:GLY:CA | 1:D:245:ILE:CG2 | 2.84 | 0.52 |
| 1:D:598:VAL:O | 1:D:601:LYS:HD3 | 2.09 | 0.52 |
| 1:D:601:LYS:NZ | 1:D:616:GLU:OE2 | 2.39 | 0.52 |
| 1:D:630:ASN:C | 1:D:630:ASN:HD22 | 2.13 | 0.52 |
| 1:D:632:ALA:CB | 1:D:657:ARG:CD | 2.87 | 0.52 |
| 1:D:732:TYR:CE1 | 1:D:755:LYS:HG3 | 2.44 | 0.52 |
| 1:D:823:ARG:O | 1:D:827:ARG:HB3 | 2.10 | 0.52 |
| 1:D:851:THR:HG21 | 1:D:853:ARG:HD3 | 1.89 | 0.52 |
| 2:E:78:PHE:CE1 | 2:E:350:LEU:HD12 | 2.44 | 0.52 |
| 2:E:94:GLY:O | 2:E:96:HIS:NE2 | 2.41 | 0.52 |
| 2:F:129:ASP:OD1 | 2:F:131:LEU:CD1 | 2.57 | 0.52 |
| 2:F:196:CYS:CB | 2:F:206:TYR:OH | 2.56 | 0.52 |
| 2:F:336:LEU:HD23 | 2:F:337:SER:CA | 2.38 | 0.52 |
| 2:F:352:ASP:OD1 | 2:F:352:ASP:C | 2.48 | 0.52 |
| 2:F:372:LEU:HD12 | 2:F:373:LYS:N | 2.25 | 0.52 |
| 2:F:81:GLY:O | 2:F:86:LEU:HD21 | 2.09 | 0.52 |
| 1:A:1004:LEU:O | 1:A:1008:LEU:HB3 | 2.09 | 0.52 |
| 1:A:1037:GLN:O | 1:A:1039:LYS:N | 2.42 | 0.52 |
| 1:A:133:ASP:O | 1:A:137:GLN:HB3 | 2.10 | 0.52 |
| 1:A:179:GLY:C | 1:A:181:GLU:N | 2.60 | 0.52 |
| 1:A:202:CYS:C | 1:A:204:ALA:H | 2.09 | 0.52 |
| 1:A:192:GLU:HB2 | 1:A:217:PRO:HD2 | 1.91 | 0.52 |
| 1:A:463:LEU:O | 1:A:464:MET:C | 2.47 | 0.52 |
| 1:A:652:ILE:HA | 1:A:655:LEU:HG | 1.88 | 0.52 |
| 1:A:787:SER:O | 1:A:790:ARG:HB2 | 2.09 | 0.52 |
| 1:A:850:ILE:HG12 | 1:A:1099:TRP:HE1 | 1.72 | 0.52 |
| 2:B:303:LEU:HA | 2:B:337:SER:O | 2.10 | 0.52 |
| 2:C:258:HIS:CA | 2:C:261:GLN:OE1 | 2.56 | 0.52 |
| 2:C:82:SER:O | 2:C:83:LYS:CG | 2.57 | 0.52 |
| 1:D:1014:ARG:HG2 | 1:D:1026:ARG:CG | 2.39 | 0.52 |
| 1:D:1135:ASP:O | 1:D:1136:GLU:CD | 2.48 | 0.52 |
| 1:D:1133:ILE:CB | 1:D:1136:GLU:HB2 | 2.12 | 0.52 |
| 1:D:128:PRO:HA | 1:D:130:LEU:CG | 2.37 | 0.52 |
| 1:D:134:ASN:O | 1:D:137:GLN:N | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:247:LEU:HA | 1:D:815:TRP:HD1 | 1.71 | 0.52 |
| 1:D:195:LEU:H | 1:D:265:LEU:CD1 | 2.22 | 0.52 |
| 1:D:271:VAL:HG22 | 1:D:295:MET:HG3 | 1.92 | 0.52 |
| 1:D:312:TRP:CB | 1:D:316:LYS:HD3 | 2.40 | 0.52 |
| 1:D:370:GLU:HB2 | 1:D:399:ASP:OD2 | 2.09 | 0.52 |
| 1:D:735:GLY:HA3 | 1:D:749:PHE:CG | 2.44 | 0.52 |
| 1:D:757:GLY:O | 1:D:758:ASN:CB | 2.57 | 0.52 |
| 1:D:801:TRP:CE3 | 1:D:870:VAL:HG12 | 2.42 | 0.52 |
| 1:D:79:LEU:HB3 | 1:D:83:LEU:CD1 | 2.40 | 0.52 |
| 2:E:188:GLY:O | 2:E:191:GLU:CG | 2.54 | 0.52 |
| 2:E:248:SER:O | 2:E:251:TRP:N | 2.42 | 0.52 |
| 2:E:331:VAL:HG22 | 2:E:333:PRO:CD | 2.28 | 0.52 |
| 2:E:349:TYR:O | 2:E:374:LEU:HD21 | 2.09 | 0.52 |
| 2:E:373:LYS:HG2 | 2:E:374:LEU:N | 2.24 | 0.52 |
| 2:F:114:TRP:HB2 | 2:F:262:TRP:CH2 | 2.43 | 0.52 |
| 2:E:104:VAL:HG21 | 2:F:128:VAL:O | 2.09 | 0.52 |
| 2:F:433:ASP:C | 2:F:435:MET:N | 2.61 | 0.52 |
| 2:F:442:LEU:O | 2:F:455:LEU:HD11 | 2.10 | 0.52 |
| 2:F:80:SER:H | 2:F:99:PHE:CA | 2.22 | 0.52 |
| 1:A:1200:PRO:CB | 1:A:1203:PRO:HD2 | 2.40 | 0.52 |
| 1:A:302:SER:O | 1:A:351:SER:HB2 | 2.09 | 0.52 |
| 1:A:440:ASN:O | 1:A:441:TRP:C | 2.47 | 0.52 |
| 1:A:455:LEU:HD12 | 1:A:798:ILE:CG2 | 2.39 | 0.52 |
| 1:A:491:ASP:OD1 | 1:A:491:ASP:N | 2.41 | 0.52 |
| 1:A:553:LYS:CD | 2:C:468:ILE:CG2 | 2.87 | 0.52 |
| 1:A:624:VAL:O | 1:A:624:VAL:HG23 | 2.09 | 0.52 |
| 1:A:616:GLU:CG | 1:A:724:GLY:HA3 | 2.39 | 0.52 |
| 1:A:767:ALA:C | 1:A:768:LYS:O | 2.43 | 0.52 |
| 1:A:949:PHE:HD2 | 1:A:949:PHE:N | 2.07 | 0.52 |
| 2:C:199:LEU:HD12 | 2:C:200:VAL:H | 1.75 | 0.52 |
| 2:C:304:TRP:CD1 | 2:C:304:TRP:N | 2.77 | 0.52 |
| 2:C:342:LEU:C | 2:C:342:LEU:CD2 | 2.78 | 0.52 |
| 2:C:88:ARG:HB2 | 2:C:88:ARG:HH11 | 1.74 | 0.52 |
| 2:C:80:SER:H | 2:C:99:PHE:CA | 2.23 | 0.52 |
| 1:D:1014:ARG:HG2 | 1:D:1026:ARG:HG2 | 1.90 | 0.52 |
| 1:D:897:TRP:HH2 | 1:D:1173:LEU:HB3 | 1.74 | 0.52 |
| 1:D:1221:TYR:O | 1:D:1225:GLU:N | 2.34 | 0.52 |
| 1:D:192:GLU:HA | 1:D:195:LEU:HD11 | 1.92 | 0.52 |
| 1:D:239:LEU:CA | 1:D:242:ALA:HB3 | 2.39 | 0.52 |
| 1:D:424:LEU:HA | 1:D:427:MET:SD | 2.49 | 0.52 |
| 1:D:457:ARG:O | 1:D:461:LYS:CD | 2.57 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:605:LEU:C | 1:D:781:ALA:HA | 2.28 | 0.52 |
| 1:D:794:ILE:HA | 1:D:797:MET:SD | 2.49 | 0.52 |
| 1:D:933:SER:C | 1:D:935:THR:N | 2.62 | 0.52 |
| 1:D:959:GLN:NE2 | 1:D:983:GLN:HE22 | 2.08 | 0.52 |
| 1:D:996:ARG:O | 1:D:996:ARG:NE | 2.34 | 0.52 |
| 2:E:119:VAL:HG23 | 2:E:120:VAL:N | 2.24 | 0.52 |
| 2:E:254:PHE:CA | 2:E:257:ARG:HB3 | 2.24 | 0.52 |
| 2:E:109:ASN:HB2 | 2:E:378:LEU:HB3 | 1.91 | 0.52 |
| 2:E:420:THR:HG23 | 2:E:421:MET:N | 2.17 | 0.52 |
| 2:E:90:SER:O | 2:E:94:GLY:N | 2.42 | 0.52 |
| 1:A:1131:ILE:CG2 | 1:A:1138:ARG:H | 2.20 | 0.52 |
| 1:A:1164:PHE:CD2 | 1:A:1168:LEU:HD11 | 2.43 | 0.52 |
| 1:A:86:GLN:C | 1:A:87:ILE:HG13 | 2.30 | 0.52 |
| 2:B:104:VAL:CG2 | 2:C:128:VAL:HG22 | 2.39 | 0.52 |
| 2:B:217:PRO:HB2 | 2:B:231:ILE:CB | 2.39 | 0.52 |
| 2:B:312:LEU:O | 2:B:315:TYR:C | 2.48 | 0.52 |
| 1:D:116:PRO:HA | 1:D:921:LEU:CD1 | 2.35 | 0.52 |
| 1:D:1174:PRO:HB2 | 1:D:1177:VAL:HG21 | 1.91 | 0.52 |
| 1:D:120:LEU:H | 1:D:120:LEU:CD2 | 2.21 | 0.52 |
| 1:D:151:LEU:O | 1:D:154:ALA:N | 2.41 | 0.52 |
| 1:D:217:PRO:O | 1:D:218:SER:CB | 2.57 | 0.52 |
| 1:D:223:TRP:HZ3 | 1:D:250:PRO:HB3 | 1.74 | 0.52 |
| 1:D:248:GLU:HB3 | 1:D:249:VAL:CB | 2.38 | 0.52 |
| 1:D:427:MET:HB2 | 1:D:846:THR:HG21 | 1.91 | 0.52 |
| 1:D:490:TRP:CZ2 | 1:D:598:VAL:CB | 2.84 | 0.52 |
| 1:D:614:TYR:CE2 | 1:D:751:LYS:NZ | 2.70 | 0.52 |
| 1:D:630:ASN:HD22 | 1:D:631:LEU:N | 2.08 | 0.52 |
| 1:D:638:THR:HG23 | 1:D:641:GLU:OE1 | 2.09 | 0.52 |
| 1:D:664:GLY:O | 1:D:667:GLN:HG3 | 2.10 | 0.52 |
| 1:D:808:ILE:HG21 | 1:D:874:LEU:CD2 | 2.40 | 0.52 |
| 2:E:201:ASN:OD1 | 2:F:422:GLN:OE1 | 2.26 | 0.52 |
| 2:E:290:TYR:HA | 2:E:298:GLU:O | 2.10 | 0.52 |
| 2:E:371:VAL:HG13 | 2:E:372:LEU:H | 1.74 | 0.52 |
| 1:D:1206:MET:CE | 2:F:257:ARG:NH1 | 2.73 | 0.52 |
| 2:F:266:PHE:HD1 | 2:F:378:LEU:CD1 | 2.22 | 0.52 |
| 1:A:1225:GLU:O | 1:A:1228:LYS:HG2 | 2.10 | 0.52 |
| 1:A:80:SER:OG | 1:A:125:LEU:CD2 | 2.57 | 0.52 |
| 1:A:214:ALA:HB2 | 1:A:219:ALA:HB3 | 1.90 | 0.52 |
| 1:A:276:ALA:C | 1:A:279:ARG:N | 2.62 | 0.52 |
| 1:A:392:LEU:HG | 1:A:395:TYR:HB2 | 1.90 | 0.52 |
| 1:A:414:PHE:O | 1:A:417:ARG:HB3 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:437:VAL:N | 1:A:878:VAL:O | 2.42 | 0.52 |
| 1:A:783:PRO:HG2 | 2:C:363:ARG:NE | 2.25 | 0.52 |
| 1:A:83:LEU:HD13 | 1:A:89:GLY:HA3 | 1.92 | 0.52 |
| 1:A:995:TYR:O | 1:A:996:ARG:HG3 | 2.10 | 0.52 |
| 2:B:114:TRP:N | 2:B:262:TRP:CZ2 | 2.77 | 0.52 |
| 2:B:311:LEU:HB2 | 2:B:315:TYR:HD2 | 1.75 | 0.52 |
| 2:B:342:LEU:O | 2:B:344:ARG:N | 2.43 | 0.52 |
| 2:B:76:ARG:NH2 | 2:B:431:LYS:HB2 | 2.24 | 0.52 |
| 2:C:193:TYR:CD1 | 2:C:242:PHE:CD2 | 2.97 | 0.52 |
| 2:C:125:VAL:HG13 | 2:C:206:TYR:HD1 | 1.74 | 0.52 |
| 2:C:307:GLY:N | 2:C:335:VAL:CG1 | 2.73 | 0.52 |
| 2:C:398:VAL:O | 2:C:402:LEU:N | 2.42 | 0.52 |
| 1:D:87:ILE:HD11 | 1:D:135:LEU:HD13 | 1.91 | 0.52 |
| 1:D:462:SER:O | 1:D:466:LEU:CD2 | 2.56 | 0.52 |
| 1:D:584:ALA:O | 1:D:585:TRP:HE3 | 1.92 | 0.52 |
| 1:D:597:ARG:CG | 1:D:617:ARG:HD2 | 2.40 | 0.52 |
| 1:D:618:HIS:CB | 1:D:725:PRO:HB2 | 2.39 | 0.52 |
| 1:D:655:LEU:O | 1:D:656:TYR:C | 2.48 | 0.52 |
| 1:D:722:ARG:CG | 1:D:722:ARG:HH11 | 2.23 | 0.52 |
| 1:D:452:TYR:CD2 | 1:D:801:TRP:NE1 | 2.76 | 0.52 |
| 1:D:823:ARG:CZ | 1:D:824:ALA:CB | 2.88 | 0.52 |
| 1:D:840:ILE:O | 1:D:841:LEU:HD23 | 2.09 | 0.52 |
| 1:D:851:THR:O | 1:D:851:THR:CG2 | 2.57 | 0.52 |
| 1:D:988:ALA:O | 1:D:998:SER:OG | 2.21 | 0.52 |
| 2:E:120:VAL:HG22 | 2:F:407:LEU:HG | 1.91 | 0.52 |
| 2:F:376:PRO:CG | 2:F:482:ALA:HB1 | 2.39 | 0.52 |
| 2:F:484:ASN:C | 2:F:485:VAL:HG13 | 2.30 | 0.52 |
| 1:A:1131:ILE:CG1 | 1:A:1137:VAL:HA | 2.40 | 0.52 |
| 1:A:157:LEU:HD21 | 1:A:216:SER:CB | 2.40 | 0.52 |
| 1:A:188:ALA:O | 1:A:189:ILE:CB | 2.56 | 0.52 |
| 1:A:404:HIS:O | 1:A:408:GLN:HB2 | 2.10 | 0.52 |
| 1:A:437:VAL:CG1 | 1:A:438:ASN:N | 2.72 | 0.52 |
| 1:A:734:HIS:HA | 1:A:752:LEU:CD1 | 2.39 | 0.52 |
| 1:A:749:PHE:N | 1:A:749:PHE:CD1 | 2.77 | 0.52 |
| 1:A:77:GLN:OE1 | 1:A:1174:PRO:HB2 | 2.10 | 0.52 |
| 1:A:795:ASN:C | 1:A:795:ASN:HD22 | 2.13 | 0.52 |
| 2:B:436:SER:OG | 2:B:458:ARG:NH1 | 2.43 | 0.52 |
| 2:C:107:ARG:HH11 | 2:C:107:ARG:HG2 | 1.75 | 0.52 |
| 2:C:246:ARG:HD3 | 2:C:246:ARG:N | 2.24 | 0.52 |
| 2:C:351:TYR:CD1 | 2:C:355:GLN:HA | 2.43 | 0.52 |
| 2:C:294:PRO:HG3 | 2:C:355:GLN:HE21 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:425:LEU:HD11 | 2:C:429:TYR:CZ | 2.45 | 0.52 |
| 1:D:1171:ASN:OD1 | 1:D:1171:ASN:N | 2.41 | 0.52 |
| 1:D:1207:GLU:CA | 1:D:1210:TYR:HB3 | 2.23 | 0.52 |
| 1:D:194:ALA:HA | 1:D:265:LEU:HB3 | 1.90 | 0.52 |
| 1:D:281:GLN:HE21 | 1:D:287:SER:HB2 | 1.75 | 0.52 |
| 1:D:598:VAL:HG12 | 1:D:602:LEU:CD1 | 2.40 | 0.52 |
| 1:D:601:LYS:HG2 | 1:D:721:ALA:CA | 2.40 | 0.52 |
| 1:D:605:LEU:O | 1:D:781:ALA:CA | 2.50 | 0.52 |
| 1:D:633:LYS:HB3 | 1:D:638:THR:CG2 | 2.40 | 0.52 |
| 1:D:775:GLU:CG | 1:D:780:GLN:CG | 2.86 | 0.52 |
| 1:D:279:ARG:HH11 | 1:D:841:LEU:HB3 | 1.75 | 0.52 |
| 1:D:85:GLU:OE2 | 1:D:130:LEU:HD22 | 2.08 | 0.52 |
| 2:E:354:PHE:CG | 2:E:355:GLN:N | 2.78 | 0.52 |
| 2:E:425:LEU:CA | 2:E:428:LEU:HD11 | 2.39 | 0.52 |
| 2:E:456:ARG:CG | 2:E:457:SER:H | 2.23 | 0.52 |
| 2:F:256:LEU:O | 2:F:257:ARG:O | 2.27 | 0.52 |
| 1:D:1208:ARG:NH1 | 2:F:285:LYS:HE2 | 2.24 | 0.52 |
| 2:F:369:ARG:HD2 | 2:F:369:ARG:H | 1.75 | 0.52 |
| 2:F:418:LEU:HD11 | 2:F:421:MET:SD | 2.49 | 0.52 |
| 2:F:446:THR:HA | 2:F:450:ASN:H | 1.73 | 0.52 |
| 1:A:1020:ILE:O | 1:A:1021:SER:HB2 | 2.08 | 0.52 |
| 1:A:1066:THR:CB | 1:A:1071:ARG:HA | 2.40 | 0.52 |
| 1:A:308:GLN:CB | 1:A:1090:GLU:HG3 | 2.39 | 0.52 |
| 1:A:253:ALA:O | 1:A:256:PRO:O | 2.27 | 0.52 |
| 1:A:732:TYR:CE1 | 1:A:755:LYS:CB | 2.87 | 0.52 |
| 1:A:973:LEU:N | 1:A:973:LEU:HD23 | 2.25 | 0.52 |
| 2:B:196:CYS:O | 2:B:199:LEU:CB | 2.57 | 0.52 |
| 2:B:261:GLN:HA | 2:B:264:ARG:HG3 | 1.90 | 0.52 |
| 2:B:311:LEU:HG | 2:B:312:LEU:HD13 | 1.91 | 0.52 |
| 2:B:313:HIS:C | 2:B:313:HIS:CD2 | 2.82 | 0.52 |
| 2:B:318:ASN:O | 2:B:321:LYS:HG2 | 2.10 | 0.52 |
| 2:B:383:VAL:O | 2:B:413:VAL:HA | 2.10 | 0.52 |
| 2:C:130:ALA:CB | 2:C:182:ARG:HH12 | 2.21 | 0.52 |
| 2:C:196:CYS:HB2 | 2:C:206:TYR:OH | 2.09 | 0.52 |
| 2:C:252:LEU:HD23 | 2:C:252:LEU:C | 2.30 | 0.52 |
| 1:A:784:GLY:HA3 | 2:C:362:THR:O | 2.10 | 0.52 |
| 2:C:466:MET:SD | 2:C:471:LEU:CD2 | 2.89 | 0.52 |
| 2:C:82:SER:O | 2:C:83:LYS:HB2 | 2.10 | 0.52 |
| 1:D:1163:MET:HE3 | 1:D:1167:LYS:HG2 | 1.92 | 0.52 |
| 1:D:1206:MET:HE3 | 1:D:1210:TYR:HA | 1.89 | 0.52 |
| 1:D:286:GLY:O | 1:D:287:SER:OG | 2.27 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:299:MET:O | 1:D:303:GLY:N | 2.36 | 0.52 |
| 1:D:454:GLU:O | 1:D:458:GLU:HG3 | 2.09 | 0.52 |
| 1:D:491:ASP:N | 1:D:491:ASP:OD1 | 2.43 | 0.52 |
| 1:D:502:LYS:HD2 | 1:D:506:GLU:CB | 2.39 | 0.52 |
| 1:D:597:ARG:CB | 1:D:616:GLU:OE1 | 2.57 | 0.52 |
| 1:D:275:ARG:CG | 1:D:843:GLN:H | 2.23 | 0.52 |
| 2:F:416:GLY:C | 2:F:419:GLU:HB3 | 2.29 | 0.52 |
| 1:A:1005:VAL:C | 1:A:1006:ARG:HH11 | 2.13 | 0.52 |
| 1:A:1095:SER:HA | 1:A:1099:TRP:CZ3 | 2.45 | 0.52 |
| 1:A:293:ASP:HB2 | 1:A:296:SER:CB | 2.40 | 0.52 |
| 1:A:365:TYR:C | 1:A:367:GLY:H | 2.13 | 0.52 |
| 1:A:509:THR:HG21 | 1:A:513:LEU:CD2 | 2.39 | 0.52 |
| 1:A:553:LYS:CD | 2:C:468:ILE:HG21 | 2.39 | 0.52 |
| 1:A:80:SER:HG | 1:A:81:ARG:H | 1.57 | 0.52 |
| 2:B:125:VAL:HG13 | 2:B:207:GLY:O | 2.09 | 0.52 |
| 2:B:249:ASN:O | 2:B:252:LEU:CB | 2.58 | 0.52 |
| 2:C:146:ARG:HB2 | 2:C:228:VAL:HG11 | 1.91 | 0.52 |
| 2:C:322:LEU:HD22 | 2:C:323:HIS:C | 2.30 | 0.52 |
| 2:C:323:HIS:C | 2:C:331:VAL:O | 2.48 | 0.52 |
| 2:C:327:GLY:O | 2:C:328:ARG:CB | 2.58 | 0.52 |
| 2:C:395:LEU:O | 2:C:397:GLN:O | 2.27 | 0.52 |
| 1:D:1054:GLU:O | 1:D:1058:PHE:N | 2.42 | 0.52 |
| 1:D:1207:GLU:C | 1:D:1210:TYR:HD2 | 2.13 | 0.52 |
| 1:D:220:TRP:NE1 | 1:D:221:TYR:CD2 | 2.78 | 0.52 |
| 1:D:312:TRP:HB3 | 1:D:316:LYS:HD3 | 1.92 | 0.52 |
| 1:D:374:ARG:O | 1:D:378:VAL:N | 2.43 | 0.52 |
| 1:D:500:ALA:CB | 1:D:521:PRO:HD3 | 2.39 | 0.52 |
| 1:D:656:TYR:HA | 1:D:659:HIS:CE1 | 2.44 | 0.52 |
| 1:D:939:VAL:O | 1:D:940:GLY:C | 2.47 | 0.52 |
| 2:E:263:TRP:C | 2:E:265:LYS:H | 2.13 | 0.52 |
| 2:E:328:ARG:H | 2:E:328:ARG:HD2 | 1.70 | 0.52 |
| 2:E:372:LEU:CG | 2:E:373:LYS:N | 2.52 | 0.52 |
| 2:E:393:LEU:HA | 2:E:396:ARG:CG | 2.40 | 0.52 |
| 2:E:450:ASN:HB3 | 2:E:452:LEU:HD21 | 1.90 | 0.52 |
| 2:E:465:MET:SD | 2:E:465:MET:N | 2.83 | 0.52 |
| 2:F:118:VAL:HG12 | 2:F:119:VAL:N | 2.25 | 0.52 |
| 2:F:201:ASN:C | 2:F:203:ARG:N | 2.58 | 0.52 |
| 2:F:342:LEU:HB2 | 2:F:344:ARG:HG3 | 1.87 | 0.52 |
| 2:F:404:ASN:O | 2:F:405:GLU:C | 2.49 | 0.52 |
| 2:F:406:LEU:HA | 2:F:409:ASN:HD22 | 1.68 | 0.52 |
| 1:D:546:ARG:CZ | 2:F:408:GLU:OE1 | 2.58 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:414:TRP:O | 2:F:414:TRP:CD1 | 2.63 | 0.52 |
| 1:A:1175:GLN:CG | 1:A:1176:SER:N | 2.71 | 0.52 |
| 1:A:213:VAL:HG11 | 1:A:397:ALA:CB | 2.40 | 0.52 |
| 1:A:192:GLU:HA | 1:A:217:PRO:HG2 | 1.92 | 0.52 |
| 1:A:545:ALA:O | 1:A:548:CYS:SG | 2.65 | 0.52 |
| 1:A:576:LEU:HD12 | 1:A:577:CYS:CB | 2.37 | 0.52 |
| 1:A:670:PRO:HA | 1:A:673:ALA:HB3 | 1.91 | 0.52 |
| 1:A:618:HIS:CD2 | 1:A:726:LYS:O | 2.63 | 0.52 |
| 1:A:727:ASP:O | 1:A:728:THR:CB | 2.56 | 0.52 |
| 1:A:964:ARG:O | 1:A:968:GLN:HG2 | 2.10 | 0.52 |
| 2:B:257:ARG:O | 2:B:258:HIS:C | 2.48 | 0.52 |
| 2:C:129:ASP:O | 2:C:130:ALA:CB | 2.58 | 0.52 |
| 2:C:217:PRO:CB | 2:C:219:PHE:CE1 | 2.90 | 0.52 |
| 2:C:455:LEU:CB | 2:C:456:ARG:NE | 2.72 | 0.52 |
| 1:D:1129:PHE:CD2 | 1:D:1139:TYR:CD2 | 2.98 | 0.52 |
| 1:D:1138:ARG:NH2 | 1:D:1191:LYS:HE2 | 2.20 | 0.52 |
| 1:D:157:LEU:HG | 1:D:194:ALA:CB | 2.40 | 0.52 |
| 1:D:655:LEU:O | 1:D:659:HIS:NE2 | 2.44 | 0.52 |
| 1:D:83:LEU:O | 1:D:87:ILE:N | 2.34 | 0.52 |
| 1:D:854:ALA:CB | 1:D:860:LEU:HD13 | 2.36 | 0.52 |
| 1:D:874:LEU:O | 1:D:875:LYS:C | 2.46 | 0.52 |
| 2:E:280:ASP:N | 2:E:280:ASP:OD1 | 2.42 | 0.52 |
| 2:F:342:LEU:O | 2:F:342:LEU:HD23 | 2.09 | 0.52 |
| 2:F:294:PRO:HG3 | 2:F:355:GLN:HE21 | 1.74 | 0.52 |
| 2:F:454:HIS:CD2 | 2:F:468:ILE:HD12 | 2.45 | 0.52 |
| 1:A:1068:ASP:N | 1:A:1071:ARG:CD | 2.73 | 0.51 |
| 1:A:192:GLU:C | 1:A:193:ARG:HG2 | 2.30 | 0.51 |
| 1:A:292:LEU:HD11 | 1:A:428:LEU:HG | 1.92 | 0.51 |
| 1:A:448:ALA:C | 1:A:870:VAL:HG11 | 2.31 | 0.51 |
| 1:A:490:TRP:CZ2 | 1:A:596:MET:CB | 2.91 | 0.51 |
| 1:A:726:LYS:O | 1:A:727:ASP:O | 2.27 | 0.51 |
| 2:B:114:TRP:N | 2:B:262:TRP:CH2 | 2.78 | 0.51 |
| 2:B:309:HIS:HB2 | 2:B:312:LEU:HB2 | 1.93 | 0.51 |
| 2:B:373:LYS:HE2 | 2:B:459:ASP:CA | 2.37 | 0.51 |
| 2:B:392:THR:HG22 | 2:B:393:LEU:HG | 1.91 | 0.51 |
| 1:D:866:ARG:CG | 1:D:1069:ILE:CG2 | 2.78 | 0.51 |
| 1:D:1092:PHE:O | 1:D:1096:ARG:NH1 | 2.43 | 0.51 |
| 1:D:1138:ARG:CG | 1:D:1138:ARG:NH1 | 2.63 | 0.51 |
| 1:D:130:LEU:HD23 | 1:D:130:LEU:H | 1.75 | 0.51 |
| 1:D:280:GLU:O | 1:D:284:ILE:HD11 | 2.10 | 0.51 |
| 1:D:410:GLN:C | 1:D:412:PRO:HD2 | 2.30 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:414:PHE:O | 1:D:417:ARG:CB | 2.56 | 0.51 |
| 1:D:601:LYS:HZ2 | 1:D:721:ALA:CA | 2.24 | 0.51 |
| 1:D:787:SER:O | 1:D:789:PRO:HD2 | 2.09 | 0.51 |
| 1:D:865:ALA:HB2 | 1:D:1197:CYS:SG | 2.50 | 0.51 |
| 1:D:867:PRO:O | 1:D:868:ASP:CG | 2.49 | 0.51 |
| 1:D:994:TRP:O | 1:D:994:TRP:HE3 | 1.93 | 0.51 |
| 2:E:118:VAL:HG13 | 2:E:119:VAL:N | 2.25 | 0.51 |
| 2:E:205:PRO:HB3 | 2:E:243:THR:CA | 2.36 | 0.51 |
| 2:E:130:ALA:HB3 | 2:E:210:GLN:OE1 | 2.10 | 0.51 |
| 2:E:388:GLY:O | 2:E:395:LEU:HD12 | 2.10 | 0.51 |
| 2:E:443:VAL:HA | 2:E:453:ILE:CG2 | 2.40 | 0.51 |
| 2:F:200:VAL:HG13 | 2:F:204:LEU:HD22 | 1.92 | 0.51 |
| 2:F:243:THR:OG1 | 2:F:334:CYS:HB3 | 2.08 | 0.51 |
| 2:F:310:GLU:OE1 | 2:F:310:GLU:N | 2.43 | 0.51 |
| 2:F:306:LEU:H | 2:F:335:VAL:HG21 | 1.75 | 0.51 |
| 2:F:415:PRO:CA | 2:F:417:TYR:HE2 | 2.23 | 0.51 |
| 2:F:67:GLU:O | 2:F:71:GLU:CB | 2.57 | 0.51 |
| 2:F:76:ARG:CG | 2:F:76:ARG:HH11 | 2.23 | 0.51 |
| 1:A:1029:GLN:HA | 1:A:1032:THR:HB | 1.92 | 0.51 |
| 1:A:564:GLN:HA | 1:A:564:GLN:HE21 | 1.73 | 0.51 |
| 1:A:601:LYS:HZ1 | 1:A:721:ALA:CB | 2.22 | 0.51 |
| 1:A:640:LEU:H | 1:A:640:LEU:CD2 | 1.92 | 0.51 |
| 1:A:786:ALA:CB | 1:A:790:ARG:CZ | 2.87 | 0.51 |
| 1:A:865:ALA:HB2 | 1:A:872:SER:O | 2.10 | 0.51 |
| 1:A:610:PHE:CZ | 1:A:972:ARG:NH2 | 2.78 | 0.51 |
| 2:B:235:THR:N | 2:B:343:ASP:HB2 | 2.25 | 0.51 |
| 2:B:323:HIS:HB3 | 2:B:332:VAL:HB | 1.92 | 0.51 |
| 2:C:344:ARG:HA | 2:C:347:LEU:CD1 | 2.40 | 0.51 |
| 2:C:389:ARG:CD | 2:C:390:GLY:N | 2.71 | 0.51 |
| 2:C:459:ASP:O | 2:C:460:THR:HG23 | 2.11 | 0.51 |
| 2:C:454:HIS:HD2 | 2:C:468:ILE:HG13 | 1.73 | 0.51 |
| 2:C:471:LEU:C | 2:C:474:PHE:H | 2.13 | 0.51 |
| 2:C:472:LYS:O | 2:C:475:LEU:HG | 2.10 | 0.51 |
| 1:D:1029:GLN:HG3 | 1:D:1030:ARG:NE | 2.14 | 0.51 |
| 1:D:214:ALA:O | 1:D:401:TRP:CH2 | 2.63 | 0.51 |
| 1:D:229:VAL:HG23 | 1:D:230:GLU:N | 2.25 | 0.51 |
| 1:D:246:PRO:O | 1:D:247:LEU:HD12 | 2.10 | 0.51 |
| 1:D:251:THR:HG23 | 1:D:280:GLU:OE1 | 2.10 | 0.51 |
| 1:D:549:LEU:CD2 | 1:D:552:LEU:HD12 | 2.40 | 0.51 |
| 1:D:612:LEU:HD11 | 1:D:622:TYR:CG | 2.45 | 0.51 |
| 2:E:270:PRO:O | 2:E:273:PHE:CD2 | 2.60 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:282:GLU:HB3 | 2:E:309:HIS:ND1 | 2.25 | 0.51 |
| 2:E:419:GLU:OE2 | 2:F:201:ASN:ND2 | 2.43 | 0.51 |
| 1:A:1175:GLN:CG | 1:A:1176:SER:H | 2.21 | 0.51 |
| 1:A:244:LEU:O | 1:A:247:LEU:HD23 | 2.10 | 0.51 |
| 1:A:606:THR:CG2 | 1:A:614:TYR:N | 2.66 | 0.51 |
| 1:A:870:VAL:C | 1:A:872:SER:N | 2.62 | 0.51 |
| 1:A:887:VAL:CA | 1:A:1146:ARG:NH1 | 2.74 | 0.51 |
| 1:A:896:LEU:HD13 | 1:A:954:ILE:HD12 | 1.91 | 0.51 |
| 1:A:930:ASP:C | 1:A:930:ASP:OD2 | 2.48 | 0.51 |
| 1:A:960:PRO:O | 1:A:963:GLU:HG3 | 2.11 | 0.51 |
| 2:B:236:GLU:HG2 | 2:B:341:ASP:CB | 2.37 | 0.51 |
| 2:B:259:ARG:CD | 2:B:262:TRP:CG | 2.93 | 0.51 |
| 2:C:266:PHE:HB2 | 2:C:349:TYR:OH | 2.11 | 0.51 |
| 2:C:406:LEU:N | 2:C:406:LEU:CD1 | 2.73 | 0.51 |
| 1:D:1020:ILE:C | 1:D:1020:ILE:HD13 | 2.27 | 0.51 |
| 1:D:1193:VAL:HG21 | 1:D:1215:GLY:H | 1.74 | 0.51 |
| 1:D:148:LEU:HB2 | 1:D:149:PRO:HD3 | 1.92 | 0.51 |
| 1:D:275:ARG:CB | 1:D:843:GLN:OE1 | 2.59 | 0.51 |
| 1:D:279:ARG:N | 1:D:279:ARG:HD3 | 2.25 | 0.51 |
| 1:D:576:LEU:CD1 | 1:D:577:CYS:N | 2.69 | 0.51 |
| 1:D:868:ASP:O | 1:D:869:ARG:CB | 2.58 | 0.51 |
| 1:D:888:GLY:HA3 | 1:D:1138:ARG:CD | 2.18 | 0.51 |
| 1:D:931:LEU:HA | 1:D:934:LYS:HE3 | 1.92 | 0.51 |
| 1:D:992:LEU:HD13 | 1:D:993:ARG:H | 1.74 | 0.51 |
| 2:E:116:THR:C | 2:E:118:VAL:H | 2.12 | 0.51 |
| 2:E:418:LEU:HD11 | 2:F:122:ARG:HG3 | 1.91 | 0.51 |
| 2:E:429:TYR:O | 2:E:433:ASP:HB2 | 2.10 | 0.51 |
| 2:F:115:TRP:CZ3 | 2:F:210:GLN:HA | 2.46 | 0.51 |
| 2:F:445:GLU:O | 2:F:447:THR:N | 2.43 | 0.51 |
| 1:A:1033:ALA:O | 1:A:1034:ARG:CB | 2.58 | 0.51 |
| 1:A:1041:TRP:NE1 | 1:A:1043:VAL:CB | 2.68 | 0.51 |
| 1:A:1069:ILE:CG2 | 1:A:1070:PRO:CD | 2.87 | 0.51 |
| 1:A:169:TRP:HD1 | 1:A:170:ALA:H | 1.57 | 0.51 |
| 1:A:441:TRP:CE3 | 1:A:445:LEU:HD12 | 2.44 | 0.51 |
| 1:A:503:VAL:CG2 | 1:A:504:LYS:N | 2.72 | 0.51 |
| 1:A:73:PRO:O | 1:A:74:LEU:HD22 | 2.10 | 0.51 |
| 1:A:868:ASP:OD2 | 1:A:1199:THR:OG1 | 2.26 | 0.51 |
| 2:B:249:ASN:O | 2:B:252:LEU:HB2 | 2.09 | 0.51 |
| 2:B:270:PRO:C | 2:B:272:ASN:H | 2.10 | 0.51 |
| 2:C:300:ILE:CG2 | 2:C:301:GLU:H | 2.15 | 0.51 |
| 2:C:383:VAL:CG2 | 2:C:384:ALA:N | 2.74 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:471:LEU:O | 2:C:474:PHE:N | 2.34 | 0.51 |
| 1:D:1121:GLU:O | 1:D:1123:PHE:N | 2.40 | 0.51 |
| 1:D:1175:GLN:O | 1:D:1177:VAL:HG23 | 2.10 | 0.51 |
| 1:D:163:PRO:O | 1:D:165:LYS:HD2 | 2.11 | 0.51 |
| 1:D:175:TRP:HB2 | 1:D:185:VAL:CG2 | 2.40 | 0.51 |
| 1:D:179:GLY:O | 1:D:181:GLU:N | 2.44 | 0.51 |
| 1:D:542:ASP:OD2 | 2:F:404:ASN:ND2 | 2.44 | 0.51 |
| 1:D:666:GLN:HG2 | 1:D:669:MET:HE3 | 1.93 | 0.51 |
| 1:D:826:ILE:HB | 1:D:831:TYR:CE2 | 2.42 | 0.51 |
| 1:D:937:THR:O | 1:D:940:GLY:N | 2.44 | 0.51 |
| 2:E:113:GLU:O | 2:E:116:THR:OG1 | 2.28 | 0.51 |
| 2:E:113:GLU:HG3 | 2:E:378:LEU:HD11 | 1.92 | 0.51 |
| 2:E:407:LEU:O | 2:E:409:ASN:N | 2.43 | 0.51 |
| 2:E:72:ILE:HD12 | 2:E:72:ILE:N | 2.25 | 0.51 |
| 2:F:115:TRP:O | 2:F:119:VAL:HG23 | 2.10 | 0.51 |
| 2:F:180:LYS:CE | 2:F:180:LYS:C | 2.64 | 0.51 |
| 2:F:134:LYS:HB2 | 2:F:180:LYS:HE2 | 1.92 | 0.51 |
| 2:F:372:LEU:HD21 | 2:F:436:SER:HB2 | 1.92 | 0.51 |
| 2:F:381:ILE:O | 2:F:437:ILE:HA | 2.10 | 0.51 |
| 2:F:381:ILE:HB | 2:F:437:ILE:HG22 | 1.93 | 0.51 |
| 1:A:1031:GLU:O | 1:A:1032:THR:CB | 2.56 | 0.51 |
| 1:A:1041:TRP:O | 1:A:1042:GLU:CB | 2.55 | 0.51 |
| 1:A:1113:LEU:N | 1:A:1113:LEU:CD2 | 2.72 | 0.51 |
| 1:A:1207:GLU:HA | 1:A:1210:TYR:CD1 | 2.39 | 0.51 |
| 1:A:1208:ARG:H | 1:A:1210:TYR:H | 1.58 | 0.51 |
| 1:A:305:SER:HB2 | 1:A:308:GLN:HG2 | 1.89 | 0.51 |
| 1:A:376:LEU:O | 1:A:378:VAL:N | 2.30 | 0.51 |
| 1:A:556:THR:HG21 | 2:C:452:LEU:HB2 | 1.93 | 0.51 |
| 1:A:592:LEU:HA | 1:A:595:GLN:CG | 2.40 | 0.51 |
| 1:A:752:LEU:CB | 1:A:753:PRO:HA | 2.39 | 0.51 |
| 1:A:81:ARG:HG3 | 1:A:81:ARG:NH1 | 2.25 | 0.51 |
| 1:A:920:THR:HG23 | 1:A:922:GLN:HB3 | 1.93 | 0.51 |
| 1:A:938:THR:O | 1:A:939:VAL:HB | 2.10 | 0.51 |
| 1:A:93:GLU:O | 1:A:95:PRO:HD3 | 2.11 | 0.51 |
| 2:B:105:GLU:O | 2:B:109:ASN:HB3 | 2.10 | 0.51 |
| 2:B:114:TRP:HZ2 | 2:B:259:ARG:HH21 | 1.59 | 0.51 |
| 2:B:123:GLU:HB2 | 2:C:403:PHE:CZ | 2.40 | 0.51 |
| 2:B:125:VAL:HG12 | 2:B:126:PHE:H | 1.75 | 0.51 |
| 2:B:320:SER:HA | 2:B:323:HIS:HD2 | 1.76 | 0.51 |
| 2:B:69:LEU:O | 2:B:72:ILE:CG1 | 2.56 | 0.51 |
| 2:C:235:THR:C | 2:C:341:ASP:CG | 2.69 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1010:LEU:C | 1:D:1012:VAL:H | 2.10 | 0.51 |
| 1:D:1065:ALA:CA | 1:D:1073:PRO:HG3 | 2.39 | 0.51 |
| 1:D:249:VAL:HG21 | 1:D:251:THR:HG22 | 1.91 | 0.51 |
| 1:D:275:ARG:HG3 | 1:D:843:GLN:N | 2.26 | 0.51 |
| 1:D:275:ARG:NH1 | 1:D:843:GLN:HE21 | 2.06 | 0.51 |
| 1:D:316:LYS:HZ2 | 1:D:348:LEU:HD23 | 1.75 | 0.51 |
| 1:D:409:GLN:O | 1:D:412:PRO:CD | 2.59 | 0.51 |
| 1:D:80:SER:O | 1:D:83:LEU:HD22 | 2.11 | 0.51 |
| 1:D:887:VAL:CG1 | 1:D:1183:VAL:CG1 | 2.89 | 0.51 |
| 1:D:888:GLY:CA | 1:D:1138:ARG:HA | 2.39 | 0.51 |
| 1:D:898:ILE:HG13 | 1:D:899:ALA:N | 2.25 | 0.51 |
| 1:D:941:ILE:HG12 | 1:D:942:SER:H | 1.75 | 0.51 |
| 2:E:185:LEU:CD1 | 2:E:237:ALA:O | 2.58 | 0.51 |
| 2:E:373:LYS:HG2 | 2:E:374:LEU:H | 1.75 | 0.51 |
| 2:E:86:LEU:CA | 2:E:90:SER:HB3 | 2.36 | 0.51 |
| 2:F:301:GLU:HG2 | 2:F:339:ASN:CB | 2.40 | 0.51 |
| 1:A:1068:ASP:C | 1:A:1070:PRO:CD | 2.78 | 0.51 |
| 1:A:1224:ILE:O | 1:A:1224:ILE:CD1 | 2.53 | 0.51 |
| 1:A:374:ARG:NH1 | 1:A:374:ARG:CG | 2.69 | 0.51 |
| 1:A:821:LEU:O | 1:A:821:LEU:CG | 2.58 | 0.51 |
| 1:A:275:ARG:NH2 | 1:A:844:VAL:O | 2.36 | 0.51 |
| 2:B:255:TRP:O | 2:B:256:LEU:C | 2.49 | 0.51 |
| 2:B:263:TRP:O | 2:B:264:ARG:C | 2.46 | 0.51 |
| 2:B:410:GLY:C | 2:B:411:ILE:HD12 | 2.31 | 0.51 |
| 2:B:456:ARG:NH2 | 2:B:457:SER:O | 2.44 | 0.51 |
| 2:C:193:TYR:CD1 | 2:C:193:TYR:C | 2.83 | 0.51 |
| 2:B:77:HIS:ND1 | 2:C:195:ASN:OD1 | 2.43 | 0.51 |
| 2:C:239:LEU:HD21 | 2:C:255:TRP:CZ2 | 2.45 | 0.51 |
| 2:C:241:TRP:H | 2:C:336:LEU:CB | 2.22 | 0.51 |
| 2:C:351:TYR:HD1 | 2:C:355:GLN:HG2 | 1.75 | 0.51 |
| 2:C:399:CYS:O | 2:C:400:GLN:C | 2.47 | 0.51 |
| 2:C:451:GLY:O | 2:C:452:LEU:CB | 2.58 | 0.51 |
| 2:C:82:SER:CA | 2:C:86:LEU:CD2 | 2.77 | 0.51 |
| 1:D:1027:LYS:NZ | 1:D:1091:GLU:CG | 2.53 | 0.51 |
| 1:D:1112:MET:HB3 | 1:D:1113:LEU:HD23 | 1.91 | 0.51 |
| 1:D:235:TRP:CD1 | 1:D:235:TRP:C | 2.84 | 0.51 |
| 1:D:242:ALA:HA | 1:D:245:ILE:H | 1.75 | 0.51 |
| 1:D:278:ILE:HG22 | 1:D:279:ARG:N | 2.26 | 0.51 |
| 1:D:287:SER:O | 1:D:288:ARG:NH2 | 2.43 | 0.51 |
| 1:D:423:THR:O | 1:D:427:MET:HG2 | 2.11 | 0.51 |
| 1:D:656:TYR:HE1 | 1:D:743:ASP:CB | 2.23 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:761:ASN:O | 1:D:762:VAL:C | 2.48 | 0.51 |
| 1:D:792:LEU:O | 1:D:795:ASN:ND2 | 2.43 | 0.51 |
| 1:D:83:LEU:N | 1:D:83:LEU:CD1 | 2.72 | 0.51 |
| 1:D:279:ARG:HG3 | 1:D:841:LEU:C | 2.30 | 0.51 |
| 1:D:993:ARG:O | 1:D:996:ARG:HD2 | 2.11 | 0.51 |
| 2:E:205:PRO:CB | 2:E:242:PHE:O | 2.59 | 0.51 |
| 2:E:270:PRO:CA | 2:E:273:PHE:HD2 | 2.21 | 0.51 |
| 2:E:293:PHE:HD1 | 2:E:295:TRP:NE1 | 2.08 | 0.51 |
| 2:E:72:ILE:HD11 | 2:E:370:LYS:NZ | 2.25 | 0.51 |
| 2:E:89:ASP:O | 2:E:93:SER:N | 2.43 | 0.51 |
| 2:F:201:ASN:O | 2:F:202:LYS:HB3 | 2.11 | 0.51 |
| 2:F:364:LYS:HD3 | 2:F:364:LYS:H | 1.76 | 0.51 |
| 1:A:389:PHE:HB2 | 1:A:393:MET:HG2 | 1.92 | 0.51 |
| 1:A:424:LEU:H | 1:A:424:LEU:CD2 | 2.23 | 0.51 |
| 1:A:564:GLN:C | 1:A:567:PRO:HD2 | 2.30 | 0.51 |
| 1:A:616:GLU:HG2 | 1:A:724:GLY:CA | 2.39 | 0.51 |
| 1:A:878:VAL:O | 1:A:879:GLN:NE2 | 2.43 | 0.51 |
| 1:A:829:PRO:HG3 | 1:A:883:GLY:HA2 | 1.92 | 0.51 |
| 1:A:973:LEU:O | 1:A:977:GLU:HG3 | 2.11 | 0.51 |
| 2:B:126:PHE:HB3 | 2:B:127:PRO:HD2 | 1.92 | 0.51 |
| 2:B:324:GLY:H | 2:B:333:PRO:HD3 | 1.76 | 0.51 |
| 2:B:86:LEU:HD23 | 2:B:97:PRO:HD2 | 1.92 | 0.51 |
| 2:C:118:VAL:CG1 | 2:C:119:VAL:N | 2.74 | 0.51 |
| 2:C:180:LYS:C | 2:C:180:LYS:CE | 2.65 | 0.51 |
| 2:C:331:VAL:HG13 | 2:C:332:VAL:N | 2.24 | 0.51 |
| 2:C:404:ASN:O | 2:C:405:GLU:C | 2.49 | 0.51 |
| 2:C:371:VAL:HG23 | 2:C:433:ASP:O | 2.11 | 0.51 |
| 2:C:76:ARG:HH11 | 2:C:76:ARG:CG | 2.24 | 0.51 |
| 1:D:1131:ILE:O | 1:D:1136:GLU:O | 2.29 | 0.51 |
| 1:D:886:LEU:CA | 1:D:1146:ARG:HH12 | 2.23 | 0.51 |
| 1:D:1162:CYS:O | 1:D:1165:ALA:HB3 | 2.10 | 0.51 |
| 1:D:902:LEU:HD13 | 1:D:1168:LEU:HD13 | 1.93 | 0.51 |
| 1:D:1147:TYR:HB3 | 1:D:1227:THR:CG2 | 2.41 | 0.51 |
| 1:D:610:PHE:CD1 | 1:D:972:ARG:NH2 | 2.77 | 0.51 |
| 1:D:735:GLY:HA3 | 1:D:749:PHE:CA | 2.40 | 0.51 |
| 2:E:447:THR:HG23 | 2:E:452:LEU:C | 2.31 | 0.51 |
| 2:F:193:TYR:CD1 | 2:F:242:PHE:CD2 | 2.98 | 0.51 |
| 2:F:290:TYR:HD1 | 2:F:299:LEU:HA | 1.76 | 0.51 |
| 2:F:354:PHE:HE1 | 2:F:370:LYS:CB | 2.23 | 0.51 |
| 2:F:464:GLU:OE2 | 2:F:466:MET:CG | 2.58 | 0.51 |
| 2:F:78:PHE:CE2 | 2:F:350:LEU:HD23 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1010:LEU:O | 1:A:1096:ARG:CZ | 2.58 | 0.51 |
| 1:A:1040:LYS:HG2 | 1:A:1044:VAL:HG11 | 1.92 | 0.51 |
| 1:A:1109:LEU:HD11 | 1:A:1137:VAL:CG2 | 2.40 | 0.51 |
| 1:A:868:ASP:OD1 | 1:A:1199:THR:HG21 | 2.11 | 0.51 |
| 1:A:1187:ARG:HB2 | 1:A:1212:ILE:CG1 | 2.40 | 0.51 |
| 1:A:259:ARG:HB3 | 1:A:261:TRP:HB2 | 1.93 | 0.51 |
| 1:A:283:LEU:HD13 | 1:A:283:LEU:O | 2.10 | 0.51 |
| 1:A:386:ARG:CG | 1:A:387:GLU:N | 2.74 | 0.51 |
| 1:A:460:LYS:C | 1:A:464:MET:HG3 | 2.31 | 0.51 |
| 1:A:472:GLN:HG3 | 2:C:460:THR:C | 2.29 | 0.51 |
| 1:A:891:VAL:CA | 1:A:1180:PHE:CE1 | 2.91 | 0.51 |
| 1:A:941:ILE:CG2 | 1:A:942:SER:N | 2.74 | 0.51 |
| 2:B:132:HIS:ND1 | 2:B:182:ARG:NH2 | 2.59 | 0.51 |
| 2:B:283:GLY:O | 2:B:284:ARG:HB2 | 2.08 | 0.51 |
| 2:C:443:VAL:HG13 | 2:C:447:THR:CG2 | 2.41 | 0.51 |
| 2:C:458:ARG:NH1 | 2:C:458:ARG:HG2 | 2.13 | 0.51 |
| 2:C:466:MET:CB | 2:C:471:LEU:CD2 | 2.77 | 0.51 |
| 1:D:1008:LEU:HA | 1:D:1011:PRO:CG | 2.39 | 0.51 |
| 1:D:1020:ILE:HD13 | 1:D:1021:SER:H | 1.61 | 0.51 |
| 1:D:1122:GLU:C | 1:D:1123:PHE:CD1 | 2.84 | 0.51 |
| 1:D:251:THR:O | 1:D:254:SER:CA | 2.58 | 0.51 |
| 1:D:272:SER:HA | 1:D:843:GLN:CG | 2.41 | 0.51 |
| 1:D:374:ARG:HE | 1:D:392:LEU:HG | 1.76 | 0.51 |
| 1:D:392:LEU:O | 1:D:395:TYR:CB | 2.51 | 0.51 |
| 1:D:484:TRP:NE1 | 1:D:488:LEU:HG | 2.26 | 0.51 |
| 1:D:715:GLN:HG2 | 1:D:717:LEU:CD1 | 2.40 | 0.51 |
| 1:D:620:TRP:C | 1:D:748:TRP:HB2 | 2.29 | 0.51 |
| 1:D:775:GLU:O | 1:D:776:ASP:CB | 2.44 | 0.51 |
| 1:D:875:LYS:HG3 | 1:D:876:ALA:N | 2.25 | 0.51 |
| 1:D:916:PHE:CE1 | 1:D:920:THR:O | 2.63 | 0.51 |
| 1:D:964:ARG:O | 1:D:968:GLN:CG | 2.59 | 0.51 |
| 1:D:990:LYS:O | 1:D:996:ARG:NH2 | 2.43 | 0.51 |
| 2:E:121:PHE:HB2 | 2:E:122:ARG:HD2 | 1.93 | 0.51 |
| 2:E:128:VAL:HG22 | 2:E:129:ASP:N | 2.24 | 0.51 |
| 2:E:218:VAL:H | 2:E:231:ILE:CA | 2.20 | 0.51 |
| 2:E:378:LEU:CD1 | 2:E:378:LEU:H | 2.24 | 0.51 |
| 1:D:1209:ARG:NH2 | 2:F:256:LEU:CD2 | 2.74 | 0.51 |
| 2:F:239:LEU:N | 2:F:338:VAL:HG21 | 2.25 | 0.51 |
| 2:F:235:THR:O | 2:F:341:ASP:OD1 | 2.28 | 0.51 |
| 2:F:372:LEU:HD21 | 2:F:436:SER:N | 2.25 | 0.51 |
| 1:D:546:ARG:HH21 | 2:F:404:ASN:HD22 | 1.58 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:454:HIS:NE2 | 2:F:472:LYS:HE3 | 2.25 | 0.51 |
| 2:F:78:PHE:CD1 | 2:F:103:GLY:CA | 2.91 | 0.51 |
| 1:A:1099:TRP:O | 1:A:1103:SER:N | 2.37 | 0.51 |
| 1:A:1111:LEU:CB | 1:A:1160:THR:HG23 | 2.40 | 0.51 |
| 1:A:1111:LEU:HB2 | 1:A:1160:THR:HG23 | 1.93 | 0.51 |
| 1:A:157:LEU:HG | 1:A:194:ALA:HB1 | 1.92 | 0.51 |
| 1:A:192:GLU:CD | 1:A:193:ARG:H | 2.13 | 0.51 |
| 1:A:313:ILE:O | 1:A:316:LYS:HG2 | 2.11 | 0.51 |
| 1:A:505:LYS:O | 1:A:506:GLU:HB2 | 2.11 | 0.51 |
| 2:B:132:HIS:HA | 2:B:182:ARG:HE | 1.75 | 0.51 |
| 2:B:259:ARG:C | 2:B:262:TRP:H | 2.14 | 0.51 |
| 2:B:84:GLN:NE2 | 2:B:84:GLN:O | 2.44 | 0.51 |
| 2:C:112:ALA:O | 2:C:116:THR:HG22 | 2.10 | 0.51 |
| 2:C:306:LEU:HD12 | 2:C:335:VAL:HB | 1.92 | 0.51 |
| 2:C:450:ASN:O | 2:C:451:GLY:C | 2.48 | 0.51 |
| 2:C:456:ARG:HG2 | 2:C:457:SER:H | 1.75 | 0.51 |
| 1:D:224:CYS:O | 1:D:228:LEU:HD23 | 2.11 | 0.51 |
| 1:D:313:ILE:CG1 | 1:D:314:ALA:N | 2.73 | 0.51 |
| 1:D:424:LEU:O | 1:D:427:MET:HG2 | 2.11 | 0.51 |
| 1:D:432:VAL:O | 1:D:433:SER:C | 2.49 | 0.51 |
| 1:D:501:LYS:HG2 | 1:D:502:LYS:H | 1.76 | 0.51 |
| 1:D:545:ALA:HA | 1:D:548:CYS:SG | 2.51 | 0.51 |
| 1:D:917:GLY:O | 1:D:920:THR:HA | 2.11 | 0.51 |
| 1:D:989:THR:HA | 1:D:998:SER:HG | 1.68 | 0.51 |
| 2:E:193:TYR:HA | 2:E:206:TYR:OH | 2.11 | 0.51 |
| 2:F:197:LEU:C | 2:F:197:LEU:HD23 | 2.30 | 0.51 |
| 2:F:203:ARG:N | 2:F:325:ARG:HD3 | 2.24 | 0.51 |
| 2:F:367:LEU:O | 2:F:369:ARG:CD | 2.59 | 0.51 |
| 2:F:439:PHE:CD1 | 2:F:458:ARG:CG | 2.93 | 0.51 |
| 2:F:454:HIS:CD2 | 2:F:468:ILE:O | 2.64 | 0.51 |
| 1:A:1160:THR:O | 1:A:1164:PHE:CD1 | 2.54 | 0.51 |
| 1:A:205:GLU:OE1 | 1:A:205:GLU:CA | 2.57 | 0.51 |
| 1:A:213:VAL:HG11 | 1:A:397:ALA:CA | 2.40 | 0.51 |
| 1:A:439:GLN:HG2 | 1:A:835:GLY:HA2 | 1.83 | 0.51 |
| 1:A:605:LEU:HB2 | 1:A:614:TYR:HD1 | 1.74 | 0.51 |
| 1:A:607:TRP:CZ2 | 1:A:671:GLN:CA | 2.93 | 0.51 |
| 1:A:612:LEU:HD23 | 1:A:614:TYR:CA | 2.40 | 0.51 |
| 1:A:646:VAL:CG1 | 1:A:646:VAL:O | 2.59 | 0.51 |
| 1:A:669:MET:O | 1:A:673:ALA:N | 2.44 | 0.51 |
| 1:A:788:GLY:O | 1:A:791:ALA:N | 2.44 | 0.51 |
| 2:B:205:PRO:HG2 | 2:B:241:TRP:HE1 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:86:LEU:HB3 | 2:B:91:LEU:HD21 | 1.92 | 0.51 |
| 2:C:415:PRO:CA | 2:C:417:TYR:HE2 | 2.24 | 0.51 |
| 2:C:455:LEU:O | 2:C:456:ARG:HD2 | 2.11 | 0.51 |
| 1:D:198:ASP:H | 1:D:213:VAL:HG12 | 1.76 | 0.51 |
| 1:D:294:THR:HA | 1:D:407:PHE:CZ | 2.46 | 0.51 |
| 1:D:429:GLU:CA | 1:D:429:GLU:OE1 | 2.59 | 0.51 |
| 1:D:500:ALA:HB1 | 1:D:520:ALA:C | 2.31 | 0.51 |
| 1:D:500:ALA:CB | 1:D:520:ALA:HB3 | 2.41 | 0.51 |
| 2:E:389:ARG:HE | 2:E:389:ARG:C | 2.10 | 0.51 |
| 2:F:255:TRP:HA | 2:F:255:TRP:CE3 | 2.46 | 0.51 |
| 2:F:357:THR:C | 2:F:359:ASN:H | 2.13 | 0.51 |
| 2:F:84:GLN:C | 2:F:86:LEU:H | 2.15 | 0.51 |
| 1:A:1027:LYS:HG3 | 1:A:1028:VAL:N | 2.26 | 0.50 |
| 1:A:891:VAL:HB | 1:A:1180:PHE:CE1 | 2.46 | 0.50 |
| 1:A:890:ASP:CG | 1:A:1191:LYS:HZ3 | 2.10 | 0.50 |
| 1:A:1193:VAL:O | 1:A:1214:GLN:HB3 | 2.10 | 0.50 |
| 1:A:199:VAL:HG21 | 1:A:277:HIS:HB2 | 1.92 | 0.50 |
| 1:A:358:LEU:HD12 | 1:A:407:PHE:HE1 | 1.76 | 0.50 |
| 1:A:490:TRP:CE2 | 1:A:596:MET:HE1 | 2.46 | 0.50 |
| 1:A:495:PHE:O | 1:A:496:LYS:HD2 | 2.11 | 0.50 |
| 1:A:604:ALA:HA | 1:A:717:LEU:HD21 | 1.93 | 0.50 |
| 1:A:844:VAL:HB | 1:A:856:GLU:OE2 | 2.10 | 0.50 |
| 1:A:83:LEU:HD13 | 1:A:89:GLY:N | 2.25 | 0.50 |
| 2:B:99:PHE:CE2 | 2:C:131:LEU:HD21 | 2.46 | 0.50 |
| 2:C:197:LEU:HD11 | 2:C:322:LEU:HD21 | 1.92 | 0.50 |
| 2:C:309:HIS:CA | 2:C:312:LEU:HD12 | 2.40 | 0.50 |
| 2:C:431:LYS:O | 2:C:435:MET:N | 2.44 | 0.50 |
| 1:D:1029:GLN:O | 1:D:1032:THR:HB | 2.11 | 0.50 |
| 1:D:1056:GLU:CB | 1:D:1057:MET:HE3 | 2.40 | 0.50 |
| 1:D:115:GLN:NE2 | 1:D:115:GLN:O | 2.44 | 0.50 |
| 1:D:121:PRO:HB2 | 1:D:1175:GLN:HE22 | 1.74 | 0.50 |
| 1:D:1198:LYS:C | 1:D:1204:THR:OG1 | 2.49 | 0.50 |
| 1:D:147:SER:O | 1:D:150:TYR:HB3 | 2.11 | 0.50 |
| 1:D:237:SER:OG | 1:D:238:GLN:N | 2.44 | 0.50 |
| 1:D:298:HIS:NE2 | 1:D:407:PHE:HA | 2.25 | 0.50 |
| 1:D:373:PRO:HD2 | 1:D:374:ARG:HG2 | 1.93 | 0.50 |
| 1:D:410:GLN:O | 1:D:414:PHE:CD2 | 2.62 | 0.50 |
| 1:D:417:ARG:HG2 | 1:D:417:ARG:HH11 | 1.75 | 0.50 |
| 1:D:550:GLN:CA | 1:D:551:LYS:HE3 | 2.41 | 0.50 |
| 1:D:624:VAL:C | 1:D:626:GLY:N | 2.49 | 0.50 |
| 1:D:82:GLY:HA3 | 1:D:125:LEU:HD12 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:886:LEU:C | 1:D:1146:ARG:NH1 | 2.50 | 0.50 |
| 1:D:939:VAL:HG12 | 1:D:939:VAL:O | 2.10 | 0.50 |
| 1:D:994:TRP:N | 1:D:996:ARG:HH11 | 2.09 | 0.50 |
| 2:E:369:ARG:CZ | 2:E:369:ARG:HB3 | 2.40 | 0.50 |
| 2:E:384:ALA:HB1 | 2:E:385:LEU:HB3 | 1.89 | 0.50 |
| 2:E:380:PRO:CD | 2:E:438:LEU:HD11 | 2.40 | 0.50 |
| 2:E:93:SER:HB3 | 2:E:95:CYS:SG | 2.51 | 0.50 |
| 2:F:123:GLU:OE1 | 2:F:205:PRO:O | 2.28 | 0.50 |
| 2:F:253:ASP:HB3 | 2:F:257:ARG:NH2 | 2.26 | 0.50 |
| 2:F:262:TRP:HZ3 | 2:F:263:TRP:CZ2 | 2.28 | 0.50 |
| 2:F:483:LYS:HG3 | 2:F:484:ASN:N | 2.26 | 0.50 |
| 1:A:1187:ARG:HB2 | 1:A:1212:ILE:HG13 | 1.93 | 0.50 |
| 1:A:270:ASN:OD1 | 1:A:270:ASN:N | 2.43 | 0.50 |
| 1:A:348:LEU:CA | 1:A:350:ILE:HD13 | 2.28 | 0.50 |
| 1:A:434:TYR:H | 1:A:1129:PHE:HD1 | 1.57 | 0.50 |
| 1:A:490:TRP:HH2 | 1:A:598:VAL:CB | 2.13 | 0.50 |
| 1:A:539:PHE:CG | 1:A:539:PHE:O | 2.64 | 0.50 |
| 1:A:576:LEU:CD1 | 1:A:577:CYS:N | 2.68 | 0.50 |
| 1:A:914:THR:HB | 1:A:999:ASP:HB3 | 1.93 | 0.50 |
| 2:B:375:HIS:CE1 | 2:B:377:CYS:SG | 3.04 | 0.50 |
| 2:C:314:MET:HE3 | 2:C:315:TYR:HE2 | 1.77 | 0.50 |
| 2:C:314:MET:HB3 | 2:C:315:TYR:CE2 | 2.45 | 0.50 |
| 2:C:78:PHE:HZ | 2:C:346:MET:HE2 | 1.75 | 0.50 |
| 2:C:266:PHE:O | 2:C:349:TYR:CE1 | 2.64 | 0.50 |
| 2:C:455:LEU:N | 2:C:455:LEU:CD1 | 2.73 | 0.50 |
| 2:C:474:PHE:CE2 | 2:C:475:LEU:HD23 | 2.46 | 0.50 |
| 1:D:1161:ARG:NH1 | 1:D:1178:ALA:O | 2.44 | 0.50 |
| 1:D:127:LEU:HD22 | 1:D:129:PRO:CG | 2.42 | 0.50 |
| 1:D:280:GLU:HB3 | 1:D:814:VAL:HG11 | 1.93 | 0.50 |
| 1:D:256:PRO:CG | 1:D:284:ILE:HD11 | 2.39 | 0.50 |
| 1:D:550:GLN:OE1 | 1:D:551:LYS:HE2 | 2.10 | 0.50 |
| 1:D:798:ILE:CA | 1:D:869:ARG:NH1 | 2.74 | 0.50 |
| 1:D:920:THR:CG2 | 1:D:922:GLN:OE1 | 2.59 | 0.50 |
| 2:E:324:GLY:O | 2:E:331:VAL:CG1 | 2.59 | 0.50 |
| 2:E:445:GLU:OE2 | 2:E:446:THR:HG22 | 2.12 | 0.50 |
| 2:F:270:PRO:HA | 2:F:273:PHE:HD2 | 1.76 | 0.50 |
| 2:F:466:MET:SD | 2:F:471:LEU:CD2 | 2.93 | 0.50 |
| 2:F:83:LYS:N | 2:F:86:LEU:HD22 | 2.27 | 0.50 |
| 1:A:1027:LYS:HD3 | 1:A:1092:PHE:CE2 | 2.46 | 0.50 |
| 1:A:1153:LEU:O | 1:A:1154:GLN:C | 2.50 | 0.50 |
| 1:A:276:ALA:C | 1:A:278:ILE:N | 2.55 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:304:LEU:HD11 | 1:A:350:ILE:O | 2.11 | 0.50 |
| 1:A:606:THR:H | 1:A:613:HIS:CA | 2.25 | 0.50 |
| 1:A:620:TRP:HD1 | 1:A:620:TRP:H | 1.58 | 0.50 |
| 1:A:652:ILE:O | 1:A:655:LEU:CG | 2.58 | 0.50 |
| 1:A:737:GLY:O | 1:A:738:PRO:C | 2.49 | 0.50 |
| 1:A:732:TYR:CE1 | 1:A:755:LYS:HA | 2.47 | 0.50 |
| 2:B:115:TRP:O | 2:B:120:VAL:HG23 | 2.11 | 0.50 |
| 2:B:284:ARG:O | 2:B:285:LYS:CB | 2.57 | 0.50 |
| 2:B:372:LEU:HB2 | 2:B:433:ASP:O | 2.10 | 0.50 |
| 2:C:349:TYR:C | 2:C:351:TYR:N | 2.62 | 0.50 |
| 2:C:375:HIS:N | 2:C:378:LEU:HB2 | 2.26 | 0.50 |
| 1:D:1108:TYR:HA | 1:D:1164:PHE:HE1 | 1.76 | 0.50 |
| 1:D:1209:ARG:HE | 2:F:253:ASP:CB | 2.24 | 0.50 |
| 1:D:437:VAL:CG1 | 1:D:438:ASN:N | 2.73 | 0.50 |
| 1:D:887:VAL:HG22 | 1:D:1185:ILE:CG2 | 2.37 | 0.50 |
| 1:D:981:LYS:HA | 1:D:984:GLN:OE1 | 2.11 | 0.50 |
| 2:E:122:ARG:HB2 | 2:E:124:GLN:HG2 | 1.93 | 0.50 |
| 2:E:375:HIS:CG | 2:E:376:PRO:HA | 2.46 | 0.50 |
| 2:E:403:PHE:O | 2:E:406:LEU:HB2 | 2.11 | 0.50 |
| 2:E:426:GLU:CD | 2:E:426:GLU:N | 2.65 | 0.50 |
| 2:E:371:VAL:CA | 2:E:433:ASP:OD2 | 2.43 | 0.50 |
| 2:F:123:GLU:HB3 | 2:F:206:TYR:HB2 | 1.93 | 0.50 |
| 2:F:245:PRO:HG2 | 2:F:246:ARG:N | 2.26 | 0.50 |
| 2:F:431:LYS:HD3 | 2:F:431:LYS:C | 2.31 | 0.50 |
| 1:A:1029:GLN:CA | 1:A:1031:GLU:O | 2.59 | 0.50 |
| 1:A:1066:THR:HB | 1:A:1071:ARG:HA | 1.92 | 0.50 |
| 1:A:167:PRO:HG2 | 1:A:177:ARG:CG | 2.25 | 0.50 |
| 1:A:276:ALA:HA | 1:A:279:ARG:HB2 | 1.88 | 0.50 |
| 1:A:296:SER:O | 1:A:299:MET:HB2 | 2.12 | 0.50 |
| 1:A:353:VAL:CG2 | 1:A:354:ASN:N | 2.75 | 0.50 |
| 1:A:648:PRO:O | 1:A:652:ILE:HG13 | 2.10 | 0.50 |
| 1:A:848:GLY:HA3 | 1:A:855:VAL:HG21 | 1.92 | 0.50 |
| 1:A:870:VAL:HG22 | 1:A:1202:ASN:ND2 | 2.24 | 0.50 |
| 1:A:916:PHE:CA | 1:A:919:MET:HB2 | 2.24 | 0.50 |
| 1:A:972:ARG:O | 1:A:974:THR:N | 2.45 | 0.50 |
| 1:A:999:ASP:O | 1:A:1000:GLU:CG | 2.57 | 0.50 |
| 2:B:206:TYR:HA | 2:B:241:TRP:CH2 | 2.45 | 0.50 |
| 2:B:105:GLU:CB | 2:B:380:PRO:HB3 | 2.32 | 0.50 |
| 2:B:447:THR:CA | 2:B:450:ASN:OD1 | 2.59 | 0.50 |
| 2:B:374:LEU:N | 2:B:458:ARG:CZ | 2.75 | 0.50 |
| 1:D:1134:HIS:O | 1:D:1134:HIS:HD2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:220:TRP:HD1 | 1:D:221:TYR:CD2 | 2.30 | 0.50 |
| 1:D:269:HIS:CE1 | 1:D:291:PHE:C | 2.84 | 0.50 |
| 1:D:271:VAL:O | 1:D:274:ASP:CB | 2.58 | 0.50 |
| 1:D:287:SER:C | 1:D:288:ARG:HE | 2.15 | 0.50 |
| 1:D:403:THR:O | 1:D:407:PHE:HB3 | 2.11 | 0.50 |
| 1:D:453:GLU:HB3 | 1:D:457:ARG:HD3 | 1.94 | 0.50 |
| 1:D:504:LYS:NZ | 1:D:525:MET:HG2 | 2.26 | 0.50 |
| 1:D:512:LYS:CE | 1:D:514:PRO:HD3 | 2.41 | 0.50 |
| 1:D:768:LYS:N | 1:D:772:PRO:HD3 | 2.27 | 0.50 |
| 1:D:78:MET:CE | 1:D:121:PRO:HB2 | 2.40 | 0.50 |
| 1:D:790:ARG:C | 1:D:792:LEU:H | 2.13 | 0.50 |
| 1:D:827:ARG:CD | 1:D:828:HIS:N | 2.73 | 0.50 |
| 1:D:891:VAL:HG22 | 1:D:891:VAL:O | 2.12 | 0.50 |
| 2:E:115:TRP:CZ2 | 2:E:127:PRO:HB3 | 2.47 | 0.50 |
| 2:E:194:VAL:CG1 | 2:E:195:ASN:N | 2.70 | 0.50 |
| 2:E:199:LEU:CG | 2:E:200:VAL:H | 2.25 | 0.50 |
| 2:E:378:LEU:HD12 | 2:E:378:LEU:N | 2.26 | 0.50 |
| 2:F:123:GLU:CD | 2:F:205:PRO:O | 2.49 | 0.50 |
| 2:F:206:TYR:CZ | 2:F:208:LEU:HD23 | 2.47 | 0.50 |
| 2:F:325:ARG:CG | 2:F:325:ARG:NH1 | 2.72 | 0.50 |
| 1:A:1131:ILE:CB | 1:A:1138:ARG:H | 2.24 | 0.50 |
| 1:A:266:VAL:HG22 | 1:A:267:VAL:N | 2.26 | 0.50 |
| 1:A:543:VAL:HG13 | 1:A:544:MET:N | 2.27 | 0.50 |
| 1:A:607:TRP:CE2 | 1:A:671:GLN:NE2 | 2.79 | 0.50 |
| 1:A:771:LEU:O | 1:A:775:GLU:HG3 | 2.11 | 0.50 |
| 1:A:786:ALA:O | 1:A:790:ARG:HG2 | 2.12 | 0.50 |
| 1:A:86:GLN:OE1 | 1:A:130:LEU:HB3 | 2.11 | 0.50 |
| 1:A:886:LEU:CA | 1:A:1146:ARG:NH2 | 2.74 | 0.50 |
| 1:A:905:ALA:HA | 1:A:910:MET:CA | 2.42 | 0.50 |
| 1:A:945:HIS:CE1 | 1:A:969:PHE:CB | 2.94 | 0.50 |
| 1:A:966:LEU:O | 1:A:970:ASN:HB2 | 2.12 | 0.50 |
| 1:A:996:ARG:NH1 | 1:A:1000:GLU:CB | 2.52 | 0.50 |
| 1:A:998:SER:OG | 1:A:999:ASP:N | 2.42 | 0.50 |
| 2:B:217:PRO:CA | 2:B:232:GLY:H | 2.24 | 0.50 |
| 2:B:259:ARG:HG2 | 2:B:262:TRP:CD1 | 2.47 | 0.50 |
| 2:B:348:ALA:O | 2:B:350:LEU:N | 2.45 | 0.50 |
| 2:B:447:THR:O | 2:B:451:GLY:N | 2.44 | 0.50 |
| 2:B:67:GLU:CA | 2:B:70:LEU:HB2 | 2.41 | 0.50 |
| 2:B:93:SER:O | 2:B:95:CYS:N | 2.44 | 0.50 |
| 2:C:126:PHE:HB2 | 2:C:128:VAL:HA | 1.92 | 0.50 |
| 2:C:241:TRP:HE3 | 2:C:336:LEU:CD1 | 2.24 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:241:TRP:CG | 2:C:336:LEU:HD12 | 2.45 | 0.50 |
| 1:D:266:VAL:HG23 | 1:D:290:ARG:O | 2.12 | 0.50 |
| 1:D:270:ASN:CA | 1:D:294:THR:OG1 | 2.59 | 0.50 |
| 1:D:436:PRO:HA | 1:D:839:ALA:CB | 2.42 | 0.50 |
| 1:D:660:CYS:CA | 1:D:745:PRO:HG3 | 2.41 | 0.50 |
| 1:D:783:PRO:CG | 1:D:784:GLY:H | 2.23 | 0.50 |
| 1:D:795:ASN:HA | 1:D:798:ILE:CG1 | 2.41 | 0.50 |
| 1:D:831:TYR:O | 1:D:831:TYR:CD1 | 2.62 | 0.50 |
| 1:D:873:GLU:OE1 | 1:D:1203:PRO:HG2 | 2.12 | 0.50 |
| 1:D:915:ALA:O | 1:D:919:MET:SD | 2.69 | 0.50 |
| 1:D:927:ARG:CG | 1:D:928:GLY:N | 2.62 | 0.50 |
| 1:D:980:GLU:O | 1:D:984:GLN:HG3 | 2.11 | 0.50 |
| 2:E:203:ARG:HH21 | 2:E:203:ARG:CG | 2.22 | 0.50 |
| 2:E:302:THR:O | 2:E:303:LEU:HD12 | 2.11 | 0.50 |
| 2:E:388:GLY:O | 2:E:395:LEU:CD1 | 2.59 | 0.50 |
| 2:F:193:TYR:O | 2:F:196:CYS:HB2 | 2.12 | 0.50 |
| 2:F:203:ARG:NE | 2:F:204:LEU:HD11 | 2.27 | 0.50 |
| 2:F:123:GLU:HB3 | 2:F:206:TYR:CB | 2.41 | 0.50 |
| 2:F:259:ARG:NE | 2:F:339:ASN:ND2 | 2.59 | 0.50 |
| 2:F:239:LEU:C | 2:F:338:VAL:HG22 | 2.27 | 0.50 |
| 2:F:357:THR:O | 2:F:358:GLU:CG | 2.60 | 0.50 |
| 2:E:120:VAL:HG13 | 2:F:407:LEU:HD21 | 1.93 | 0.50 |
| 2:F:418:LEU:O | 2:F:421:MET:CG | 2.54 | 0.50 |
| 2:F:466:MET:HE2 | 2:F:471:LEU:HB3 | 1.92 | 0.50 |
| 1:A:1121:GLU:O | 1:A:1123:PHE:N | 2.39 | 0.50 |
| 1:A:1175:GLN:O | 1:A:1178:ALA:HB3 | 2.11 | 0.50 |
| 1:A:486:TRP:HE1 | 1:A:722:ARG:HG2 | 1.77 | 0.50 |
| 1:A:657:ARG:CA | 1:A:660:CYS:HB3 | 2.41 | 0.50 |
| 1:A:662:GLU:O | 1:A:666:GLN:CB | 2.60 | 0.50 |
| 1:A:824:ALA:HB1 | 1:A:827:ARG:HG2 | 1.93 | 0.50 |
| 1:A:931:LEU:HD23 | 1:A:932:HIS:CA | 2.42 | 0.50 |
| 1:A:936:ALA:O | 1:A:939:VAL:C | 2.50 | 0.50 |
| 2:B:320:SER:HA | 2:B:323:HIS:CD2 | 2.47 | 0.50 |
| 2:B:383:VAL:CG2 | 2:B:384:ALA:H | 2.23 | 0.50 |
| 2:C:193:TYR:CG | 2:C:194:VAL:N | 2.80 | 0.50 |
| 2:C:326:ASP:CG | 2:C:329:LYS:HB2 | 2.32 | 0.50 |
| 2:C:353:SER:HG | 2:C:354:PHE:H | 1.55 | 0.50 |
| 2:C:389:ARG:CZ | 2:C:390:GLY:CA | 2.90 | 0.50 |
| 2:C:78:PHE:HZ | 2:C:346:MET:SD | 2.35 | 0.50 |
| 1:D:1131:ILE:HD13 | 1:D:1131:ILE:O | 2.11 | 0.50 |
| 1:D:1147:TYR:N | 1:D:1147:TYR:HD2 | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1187:ARG:HG3 | 1:D:1212:ILE:CG1 | 2.42 | 0.50 |
| 1:D:177:ARG:CG | 1:D:218:SER:OG | 2.60 | 0.50 |
| 1:D:194:ALA:CB | 1:D:265:LEU:HD13 | 2.39 | 0.50 |
| 1:D:272:SER:O | 1:D:273:PHE:HB2 | 2.10 | 0.50 |
| 1:D:307:PHE:O | 1:D:308:GLN:C | 2.50 | 0.50 |
| 1:D:375:GLU:OE1 | 1:D:379:LYS:HB3 | 2.11 | 0.50 |
| 1:D:472:GLN:C | 2:F:461:THR:CG2 | 2.80 | 0.50 |
| 1:D:547:ALA:O | 1:D:551:LYS:CG | 2.58 | 0.50 |
| 1:D:800:PHE:CE2 | 1:D:867:PRO:HB3 | 2.47 | 0.50 |
| 1:D:85:GLU:OE2 | 1:D:127:LEU:O | 2.30 | 0.50 |
| 2:E:425:LEU:HD23 | 2:E:426:GLU:OE1 | 2.12 | 0.50 |
| 2:E:449:GLU:CA | 2:E:449:GLU:OE1 | 2.45 | 0.50 |
| 2:E:373:LYS:HA | 2:E:458:ARG:NE | 2.25 | 0.50 |
| 2:E:88:ARG:CD | 2:E:88:ARG:H | 2.24 | 0.50 |
| 2:F:198:ASP:C | 2:F:198:ASP:OD1 | 2.48 | 0.50 |
| 1:A:1016:GLU:OE2 | 1:A:1022:LEU:HD22 | 2.12 | 0.50 |
| 1:A:1055:SER:O | 1:A:1059:ASN:CG | 2.50 | 0.50 |
| 1:A:1158:LEU:HD13 | 1:A:1179:PHE:CZ | 2.47 | 0.50 |
| 1:A:81:ARG:NH1 | 1:A:125:LEU:O | 2.45 | 0.50 |
| 1:A:660:CYS:CB | 1:A:745:PRO:CG | 2.90 | 0.50 |
| 2:B:338:VAL:C | 2:B:339:ASN:ND2 | 2.65 | 0.50 |
| 2:C:224:ILE:N | 2:C:224:ILE:HD13 | 2.27 | 0.50 |
| 2:C:213:VAL:HA | 2:C:235:THR:HA | 1.94 | 0.50 |
| 2:C:389:ARG:NH2 | 2:C:390:GLY:HA3 | 2.26 | 0.50 |
| 2:C:471:LEU:CD1 | 2:C:471:LEU:N | 2.38 | 0.50 |
| 1:D:1124:ALA:HB1 | 1:D:1148:ARG:HH12 | 1.70 | 0.50 |
| 1:D:204:ALA:O | 1:D:205:GLU:CG | 2.60 | 0.50 |
| 1:D:245:ILE:CG1 | 1:D:246:PRO:N | 2.51 | 0.50 |
| 1:D:439:GLN:CG | 1:D:836:LEU:H | 2.25 | 0.50 |
| 1:D:453:GLU:O | 1:D:454:GLU:C | 2.49 | 0.50 |
| 1:D:549:LEU:O | 1:D:552:LEU:HB2 | 2.12 | 0.50 |
| 1:D:657:ARG:O | 1:D:660:CYS:CB | 2.58 | 0.50 |
| 1:D:657:ARG:C | 1:D:660:CYS:HB3 | 2.31 | 0.50 |
| 1:D:732:TYR:HB3 | 1:D:755:LYS:HZ1 | 1.76 | 0.50 |
| 1:D:802:ARG:HG3 | 1:D:803:ASN:N | 2.27 | 0.50 |
| 1:D:827:ARG:CD | 1:D:827:ARG:C | 2.80 | 0.50 |
| 1:D:938:THR:O | 1:D:939:VAL:CG2 | 2.59 | 0.50 |
| 2:E:372:LEU:O | 2:E:458:ARG:HG2 | 2.12 | 0.50 |
| 2:F:432:TYR:C | 2:F:435:MET:H | 2.15 | 0.50 |
| 2:F:447:THR:CG2 | 2:F:448:LEU:N | 2.73 | 0.50 |
| 2:F:460:THR:O | 2:F:461:THR:C | 2.50 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1207:GLU:O | 1:A:1208:ARG:HB2 | 2.12 | 0.50 |
| 1:A:291:PHE:O | 1:A:292:LEU:CB | 2.59 | 0.50 |
| 1:A:371:LYS:C | 1:A:373:PRO:CD | 2.79 | 0.50 |
| 1:A:355:SER:C | 1:A:407:PHE:HZ | 2.15 | 0.50 |
| 1:A:564:GLN:HA | 1:A:567:PRO:CD | 2.35 | 0.50 |
| 1:A:658:LYS:O | 1:A:659:HIS:C | 2.50 | 0.50 |
| 1:A:789:PRO:O | 1:A:792:LEU:HD12 | 2.12 | 0.50 |
| 1:A:863:SER:O | 1:A:873:GLU:CG | 2.57 | 0.50 |
| 1:A:953:ARG:HD3 | 1:A:986:TYR:CD2 | 2.47 | 0.50 |
| 2:B:194:VAL:HG13 | 2:B:195:ASN:N | 2.27 | 0.50 |
| 2:B:105:GLU:HG3 | 2:B:380:PRO:C | 2.31 | 0.50 |
| 2:B:389:ARG:HG2 | 2:B:444:THR:CG2 | 2.42 | 0.50 |
| 2:B:437:ILE:N | 2:B:458:ARG:HD3 | 2.26 | 0.50 |
| 2:C:118:VAL:HG12 | 2:C:119:VAL:N | 2.27 | 0.50 |
| 2:C:307:GLY:N | 2:C:335:VAL:HG12 | 2.27 | 0.50 |
| 2:C:469:SER:C | 2:C:471:LEU:HD12 | 2.31 | 0.50 |
| 2:C:377:CYS:SG | 2:C:483:LYS:HA | 2.51 | 0.50 |
| 2:C:82:SER:C | 2:C:83:LYS:HG3 | 2.32 | 0.50 |
| 1:D:1068:ASP:OD1 | 1:D:1068:ASP:N | 2.44 | 0.50 |
| 1:D:106:HIS:HA | 1:D:109:LYS:CG | 2.41 | 0.50 |
| 1:D:429:GLU:CG | 1:D:1128:ARG:NH2 | 2.66 | 0.50 |
| 1:D:1126:ASP:CB | 1:D:1141:VAL:HG13 | 2.42 | 0.50 |
| 1:D:239:LEU:C | 1:D:242:ALA:H | 2.14 | 0.50 |
| 1:D:295:MET:O | 1:D:299:MET:N | 2.41 | 0.50 |
| 1:D:308:GLN:O | 1:D:312:TRP:HB2 | 2.12 | 0.50 |
| 1:D:428:LEU:O | 1:D:432:VAL:HG23 | 2.11 | 0.50 |
| 1:D:457:ARG:C | 1:D:460:LYS:HZ2 | 2.15 | 0.50 |
| 1:D:727:ASP:O | 1:D:728:THR:OG1 | 2.25 | 0.50 |
| 1:D:907:PHE:HE2 | 1:D:913:CYS:SG | 2.35 | 0.50 |
| 2:E:389:ARG:HE | 2:E:390:GLY:CA | 2.23 | 0.50 |
| 2:E:90:SER:OG | 2:E:96:HIS:HA | 2.12 | 0.50 |
| 2:F:196:CYS:O | 2:F:199:LEU:HB3 | 2.12 | 0.50 |
| 2:F:204:LEU:CD1 | 2:F:204:LEU:N | 2.75 | 0.50 |
| 2:F:307:GLY:HA2 | 2:F:335:VAL:HG12 | 1.94 | 0.50 |
| 2:F:354:PHE:C | 2:F:356:LEU:N | 2.60 | 0.50 |
| 2:F:447:THR:HG22 | 2:F:448:LEU:HD12 | 1.94 | 0.50 |
| 1:A:1068:ASP:CA | 1:A:1071:ARG:HD3 | 2.41 | 0.50 |
| 1:A:1140:LEU:CD2 | 1:A:1141:VAL:H | 2.20 | 0.50 |
| 1:A:183:GLU:C | 1:A:183:GLU:CD | 2.70 | 0.50 |
| 1:A:204:ALA:O | 1:A:206:GLY:N | 2.40 | 0.50 |
| 1:A:494:GLU:HB2 | 1:A:572:TRP:CD2 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:605:LEU:C | 1:A:781:ALA:CB | 2.81 | 0.50 |
| 1:A:645:VAL:HA | 1:A:650:ARG:HD2 | 1.94 | 0.50 |
| 1:A:742:VAL:HG12 | 1:A:742:VAL:O | 2.11 | 0.50 |
| 1:A:754:HIS:HD2 | 1:A:757:GLY:HA3 | 1.77 | 0.50 |
| 1:A:892:ASP:HB3 | 1:A:927:ARG:HH22 | 1.77 | 0.50 |
| 2:B:440:THR:CG2 | 2:B:441:VAL:H | 2.19 | 0.50 |
| 2:C:414:TRP:N | 2:C:415:PRO:HD2 | 2.25 | 0.50 |
| 2:C:428:LEU:HD23 | 2:C:428:LEU:N | 2.22 | 0.50 |
| 2:C:443:VAL:CG1 | 2:C:447:THR:CG2 | 2.89 | 0.50 |
| 1:D:1090:GLU:HG3 | 1:D:1092:PHE:CZ | 2.46 | 0.50 |
| 1:D:1106:VAL:O | 1:D:1107:ASP:C | 2.50 | 0.50 |
| 1:D:121:PRO:CB | 1:D:1175:GLN:NE2 | 2.73 | 0.50 |
| 1:D:131:TYR:C | 1:D:138:HIS:CE1 | 2.86 | 0.50 |
| 1:D:162:LEU:O | 1:D:162:LEU:HG | 2.12 | 0.50 |
| 1:D:262:GLN:OE1 | 1:D:262:GLN:HA | 2.11 | 0.50 |
| 1:D:278:ILE:CG1 | 1:D:291:PHE:HD1 | 2.24 | 0.50 |
| 1:D:369:LEU:HD13 | 1:D:372:GLU:CB | 2.41 | 0.50 |
| 1:D:452:TYR:CB | 1:D:801:TRP:CD1 | 2.94 | 0.50 |
| 1:D:592:LEU:O | 1:D:595:GLN:N | 2.40 | 0.50 |
| 1:D:885:THR:HG22 | 1:D:886:LEU:H | 1.75 | 0.50 |
| 2:E:192:HIS:O | 2:E:193:TYR:C | 2.49 | 0.50 |
| 2:F:241:TRP:CZ3 | 2:F:255:TRP:CZ2 | 2.99 | 0.50 |
| 2:F:272:ASN:HA | 2:F:292:ASN:ND2 | 2.26 | 0.50 |
| 2:F:348:ALA:O | 2:F:352:ASP:N | 2.41 | 0.50 |
| 2:F:375:HIS:CB | 2:F:378:LEU:HD22 | 2.40 | 0.50 |
| 2:F:388:GLY:N | 2:F:443:VAL:O | 2.42 | 0.50 |
| 1:A:1092:PHE:O | 1:A:1096:ARG:HG3 | 2.12 | 0.49 |
| 1:A:286:GLY:CA | 1:A:1128:ARG:HH22 | 2.24 | 0.49 |
| 1:A:1163:MET:HE2 | 1:A:1167:LYS:HE3 | 1.94 | 0.49 |
| 1:A:174:GLY:HA2 | 1:A:220:TRP:HB2 | 1.94 | 0.49 |
| 1:A:192:GLU:CG | 1:A:195:LEU:HD21 | 2.42 | 0.49 |
| 1:A:227:ARG:HD3 | 1:A:227:ARG:C | 2.31 | 0.49 |
| 1:A:272:SER:C | 1:A:274:ASP:H | 2.16 | 0.49 |
| 1:A:392:LEU:O | 1:A:394:GLN:N | 2.45 | 0.49 |
| 1:A:441:TRP:O | 1:A:445:LEU:HB2 | 2.12 | 0.49 |
| 1:A:452:TYR:CE2 | 1:A:453:GLU:HG2 | 2.47 | 0.49 |
| 1:A:503:VAL:HG11 | 1:A:520:ALA:CB | 2.42 | 0.49 |
| 1:A:730:PRO:HB3 | 1:A:760:CYS:O | 2.12 | 0.49 |
| 1:A:764:SER:OG | 1:A:767:ALA:HB2 | 2.11 | 0.49 |
| 2:B:114:TRP:CA | 2:B:262:TRP:CH2 | 2.95 | 0.49 |
| 2:B:472:LYS:HZ2 | 2:B:473:ASP:HA | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:306:LEU:H | 2:C:335:VAL:CG1 | 2.24 | 0.49 |
| 2:C:311:LEU:HD22 | 2:C:311:LEU:N | 2.26 | 0.49 |
| 2:C:347:LEU:CD1 | 2:C:347:LEU:H | 2.24 | 0.49 |
| 2:C:474:PHE:HA | 2:C:477:LYS:HD3 | 1.92 | 0.49 |
| 1:D:1025:LEU:O | 1:D:1027:LYS:N | 2.43 | 0.49 |
| 1:D:1055:SER:O | 1:D:1058:PHE:CD2 | 2.65 | 0.49 |
| 1:D:886:LEU:CA | 1:D:1146:ARG:NH1 | 2.75 | 0.49 |
| 1:D:116:PRO:O | 1:D:118:VAL:CG1 | 2.61 | 0.49 |
| 1:D:1207:GLU:HA | 1:D:1210:TYR:CG | 2.47 | 0.49 |
| 1:D:1213:PRO:O | 1:D:1214:GLN:CB | 2.57 | 0.49 |
| 1:D:298:HIS:CD2 | 1:D:407:PHE:CB | 2.90 | 0.49 |
| 1:D:389:PHE:CD1 | 1:D:389:PHE:C | 2.85 | 0.49 |
| 1:D:712:VAL:N | 1:D:713:PRO:CD | 2.75 | 0.49 |
| 1:D:427:MET:HB2 | 1:D:846:THR:CG2 | 2.42 | 0.49 |
| 1:D:847:ALA:C | 1:D:852:ARG:HA | 2.32 | 0.49 |
| 1:D:860:LEU:HD22 | 1:D:1133:ILE:HD12 | 1.94 | 0.49 |
| 1:D:891:VAL:HA | 1:D:894:GLN:CG | 2.41 | 0.49 |
| 2:E:109:ASN:HD22 | 2:E:378:LEU:CB | 2.26 | 0.49 |
| 2:E:374:LEU:O | 2:E:375:HIS:CB | 2.52 | 0.49 |
| 2:E:392:THR:O | 2:E:392:THR:HG22 | 2.11 | 0.49 |
| 2:E:96:HIS:CD2 | 2:E:96:HIS:O | 2.65 | 0.49 |
| 2:E:418:LEU:HD11 | 2:F:122:ARG:HE | 1.74 | 0.49 |
| 2:F:244:PRO:N | 2:F:247:THR:HG21 | 2.27 | 0.49 |
| 2:F:349:TYR:C | 2:F:351:TYR:N | 2.62 | 0.49 |
| 2:F:346:MET:O | 2:F:350:LEU:HD11 | 2.12 | 0.49 |
| 2:F:357:THR:O | 2:F:359:ASN:N | 2.42 | 0.49 |
| 2:F:447:THR:CA | 2:F:452:LEU:CA | 2.81 | 0.49 |
| 2:F:457:SER:O | 2:F:458:ARG:C | 2.50 | 0.49 |
| 2:F:483:LYS:O | 2:F:485:VAL:HG12 | 2.12 | 0.49 |
| 1:A:246:PRO:O | 1:A:250:PRO:HD2 | 2.12 | 0.49 |
| 1:A:304:LEU:HB2 | 1:A:309:ARG:HB3 | 1.94 | 0.49 |
| 1:A:421:PRO:CG | 1:A:422:VAL:N | 2.75 | 0.49 |
| 1:A:789:PRO:O | 1:A:793:GLU:HB2 | 2.12 | 0.49 |
| 1:A:960:PRO:HA | 1:A:963:GLU:CG | 2.43 | 0.49 |
| 1:A:755:LYS:CD | 1:A:964:ARG:HH11 | 2.23 | 0.49 |
| 2:B:208:LEU:N | 2:B:208:LEU:HD23 | 2.26 | 0.49 |
| 2:B:425:LEU:HB3 | 2:B:426:GLU:OE1 | 2.11 | 0.49 |
| 2:C:127:PRO:O | 2:C:192:HIS:CD2 | 2.65 | 0.49 |
| 1:D:1027:LYS:O | 1:D:1031:GLU:HG2 | 2.12 | 0.49 |
| 1:D:1031:GLU:OE2 | 1:D:1092:PHE:HD2 | 1.95 | 0.49 |
| 1:D:1116:MET:HE3 | 1:D:1156:THR:HB | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:252:GLY:O | 1:D:256:PRO:CG | 2.58 | 0.49 |
| 1:D:270:ASN:C | 1:D:274:ASP:OD1 | 2.50 | 0.49 |
| 1:D:298:HIS:CE1 | 1:D:362:LEU:CD1 | 2.95 | 0.49 |
| 1:D:359:VAL:HG22 | 1:D:406:VAL:CG2 | 2.42 | 0.49 |
| 1:D:371:LYS:CA | 1:D:374:ARG:CD | 2.77 | 0.49 |
| 1:D:407:PHE:CE1 | 1:D:411:LEU:HD21 | 2.46 | 0.49 |
| 1:D:607:TRP:CE3 | 1:D:607:TRP:HA | 2.47 | 0.49 |
| 1:D:607:TRP:O | 1:D:608:ASP:OD1 | 2.30 | 0.49 |
| 1:D:275:ARG:CG | 1:D:843:GLN:N | 2.75 | 0.49 |
| 1:D:441:TRP:CD1 | 1:D:879:GLN:HA | 2.45 | 0.49 |
| 2:E:200:VAL:HG12 | 2:F:418:LEU:HD21 | 1.92 | 0.49 |
| 2:E:249:ASN:O | 2:E:252:LEU:HB3 | 2.12 | 0.49 |
| 2:E:307:GLY:HA2 | 2:E:334:CYS:HB2 | 1.94 | 0.49 |
| 2:E:239:LEU:CB | 2:E:338:VAL:HB | 2.42 | 0.49 |
| 2:F:308:ASP:OD1 | 2:F:333:PRO:C | 2.50 | 0.49 |
| 2:F:358:GLU:CG | 2:F:359:ASN:N | 2.75 | 0.49 |
| 2:F:413:VAL:CG1 | 2:F:414:TRP:N | 2.76 | 0.49 |
| 2:F:384:ALA:CB | 2:F:437:ILE:HD12 | 2.42 | 0.49 |
| 2:F:471:LEU:O | 2:F:474:PHE:N | 2.39 | 0.49 |
| 1:A:1065:ALA:O | 1:A:1066:THR:OG1 | 2.22 | 0.49 |
| 1:A:1144:GLU:O | 1:A:1146:ARG:N | 2.45 | 0.49 |
| 1:A:1209:ARG:HE | 1:A:1209:ARG:HA | 1.78 | 0.49 |
| 1:A:228:LEU:N | 1:A:228:LEU:CD2 | 2.73 | 0.49 |
| 1:A:421:PRO:HG2 | 1:A:422:VAL:HG23 | 1.93 | 0.49 |
| 1:A:541:GLN:O | 1:A:544:MET:HB3 | 2.12 | 0.49 |
| 1:A:583:PRO:O | 1:A:584:ALA:HB3 | 2.12 | 0.49 |
| 1:A:599:THR:O | 1:A:602:LEU:HB2 | 2.12 | 0.49 |
| 1:A:630:ASN:HD21 | 1:A:632:ALA:N | 2.11 | 0.49 |
| 1:A:732:TYR:HE1 | 1:A:755:LYS:CG | 2.24 | 0.49 |
| 1:A:762:VAL:O | 1:A:764:SER:N | 2.38 | 0.49 |
| 1:A:821:LEU:HD11 | 1:A:826:ILE:N | 2.27 | 0.49 |
| 1:A:275:ARG:NH2 | 1:A:845:VAL:N | 2.60 | 0.49 |
| 1:A:866:ARG:HB2 | 1:A:1069:ILE:HG21 | 1.94 | 0.49 |
| 1:A:878:VAL:HG12 | 1:A:879:GLN:HE22 | 1.77 | 0.49 |
| 1:A:919:MET:C | 1:A:920:THR:O | 2.51 | 0.49 |
| 1:A:95:PRO:O | 1:A:96:GLY:O | 2.30 | 0.49 |
| 2:B:205:PRO:HG2 | 2:B:241:TRP:NE1 | 2.27 | 0.49 |
| 2:B:259:ARG:HB3 | 2:B:259:ARG:NH1 | 2.27 | 0.49 |
| 2:B:336:LEU:HD23 | 2:B:336:LEU:C | 2.32 | 0.49 |
| 2:B:463:LYS:HD2 | 2:B:463:LYS:N | 2.27 | 0.49 |
| 2:C:270:PRO:HA | 2:C:273:PHE:HD2 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:425:LEU:O | 2:C:428:LEU:HB2 | 2.12 | 0.49 |
| 1:D:1092:PHE:HA | 1:D:1096:ARG:NH2 | 2.27 | 0.49 |
| 1:D:260:ASP:OD2 | 1:D:261:TRP:CD2 | 2.65 | 0.49 |
| 1:D:298:HIS:HD2 | 1:D:407:PHE:CD1 | 2.30 | 0.49 |
| 1:D:561:LYS:O | 1:D:562:ARG:CB | 2.60 | 0.49 |
| 1:D:643:ALA:N | 1:D:645:VAL:HB | 2.26 | 0.49 |
| 1:D:756:ASP:N | 1:D:756:ASP:OD1 | 2.44 | 0.49 |
| 1:D:275:ARG:HB3 | 1:D:843:GLN:OE1 | 2.12 | 0.49 |
| 1:D:853:ARG:HH12 | 1:D:1105:ALA:HB3 | 1.76 | 0.49 |
| 1:D:931:LEU:HA | 1:D:934:LYS:HB3 | 1.93 | 0.49 |
| 2:E:216:HIS:CD2 | 2:E:216:HIS:N | 2.79 | 0.49 |
| 2:E:385:LEU:HB2 | 2:E:440:THR:HA | 1.93 | 0.49 |
| 2:E:380:PRO:HG3 | 2:E:438:LEU:CD1 | 2.40 | 0.49 |
| 2:E:74:GLN:O | 2:E:77:HIS:N | 2.44 | 0.49 |
| 2:F:258:HIS:HA | 2:F:261:GLN:OE1 | 2.12 | 0.49 |
| 2:F:306:LEU:O | 2:F:335:VAL:HB | 2.11 | 0.49 |
| 2:F:350:LEU:O | 2:F:353:SER:OG | 2.30 | 0.49 |
| 2:F:389:ARG:O | 2:F:395:LEU:HD11 | 2.12 | 0.49 |
| 2:F:393:LEU:O | 2:F:396:ARG:N | 2.46 | 0.49 |
| 2:F:405:GLU:C | 2:F:405:GLU:OE1 | 2.51 | 0.49 |
| 2:F:76:ARG:NH1 | 2:F:434:GLU:OE1 | 2.45 | 0.49 |
| 1:A:1026:ARG:CG | 1:A:1029:GLN:CD | 2.81 | 0.49 |
| 1:A:1093:MET:C | 1:A:1097:VAL:HG23 | 2.32 | 0.49 |
| 1:A:1113:LEU:CB | 1:A:1117:LYS:NZ | 2.74 | 0.49 |
| 1:A:1232:GLU:CD | 1:A:1234:ARG:NH2 | 2.65 | 0.49 |
| 1:A:240:SER:HB3 | 1:A:241:PRO:CD | 2.42 | 0.49 |
| 1:A:298:HIS:NE2 | 1:A:351:SER:O | 2.45 | 0.49 |
| 1:A:353:VAL:O | 1:A:354:ASN:CB | 2.60 | 0.49 |
| 1:A:434:TYR:HA | 1:A:841:LEU:CD2 | 2.41 | 0.49 |
| 1:A:580:LEU:HD23 | 1:A:596:MET:CE | 2.42 | 0.49 |
| 1:A:76:ILE:HG21 | 1:A:911:HIS:CE1 | 2.47 | 0.49 |
| 1:A:772:PRO:HG2 | 1:A:773:LYS:H | 1.77 | 0.49 |
| 1:A:79:LEU:HB2 | 1:A:89:GLY:C | 2.32 | 0.49 |
| 2:B:342:LEU:O | 2:B:343:ASP:C | 2.50 | 0.49 |
| 2:B:414:TRP:C | 2:B:414:TRP:CD1 | 2.86 | 0.49 |
| 1:A:572:TRP:CD1 | 2:C:477:LYS:HE2 | 2.47 | 0.49 |
| 2:C:477:LYS:O | 2:C:478:TYR:C | 2.49 | 0.49 |
| 1:D:1051:GLY:O | 1:D:1055:SER:N | 2.45 | 0.49 |
| 1:D:1116:MET:HG3 | 1:D:1139:TYR:OH | 2.13 | 0.49 |
| 1:D:1218:LEU:HB2 | 1:D:1223:ILE:HG22 | 1.90 | 0.49 |
| 1:D:371:LYS:O | 1:D:372:GLU:CB | 2.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:735:GLY:HA2 | 1:D:749:PHE:CA | 2.43 | 0.49 |
| 1:D:779:LEU:CD2 | 1:D:779:LEU:C | 2.79 | 0.49 |
| 1:D:840:ILE:O | 1:D:841:LEU:CD2 | 2.60 | 0.49 |
| 2:E:270:PRO:C | 2:E:273:PHE:HD2 | 2.15 | 0.49 |
| 2:E:432:TYR:HA | 2:E:435:MET:CA | 2.41 | 0.49 |
| 2:E:456:ARG:HD2 | 2:E:461:THR:CA | 2.42 | 0.49 |
| 2:F:239:LEU:H | 2:F:338:VAL:HG11 | 1.53 | 0.49 |
| 2:F:239:LEU:HG | 2:F:336:LEU:HD13 | 1.94 | 0.49 |
| 2:F:424:SER:N | 2:F:427:GLN:OE1 | 2.45 | 0.49 |
| 2:F:442:LEU:O | 2:F:443:VAL:C | 2.50 | 0.49 |
| 2:F:389:ARG:CG | 2:F:445:GLU:OE2 | 2.58 | 0.49 |
| 2:F:74:GLN:CG | 2:F:75:ARG:N | 2.75 | 0.49 |
| 2:F:78:PHE:CD2 | 2:F:79:LEU:CD2 | 2.95 | 0.49 |
| 2:F:80:SER:H | 2:F:99:PHE:HA | 1.78 | 0.49 |
| 2:F:82:SER:C | 2:F:83:LYS:HG3 | 2.33 | 0.49 |
| 1:A:185:VAL:O | 1:A:185:VAL:HG22 | 2.12 | 0.49 |
| 1:A:219:ALA:O | 1:A:220:TRP:HE3 | 1.93 | 0.49 |
| 1:A:420:HIS:CG | 1:A:421:PRO:HD2 | 2.47 | 0.49 |
| 1:A:467:ALA:CB | 1:A:602:LEU:HD13 | 2.42 | 0.49 |
| 1:A:504:LYS:HD3 | 1:A:523:ASP:HB3 | 1.92 | 0.49 |
| 1:A:591:LEU:HD21 | 1:A:802:ARG:CZ | 2.42 | 0.49 |
| 1:A:713:PRO:CA | 1:A:719:LEU:HD13 | 2.42 | 0.49 |
| 1:A:773:LYS:NZ | 1:A:1057:MET:CE | 2.75 | 0.49 |
| 1:A:856:GLU:OE1 | 1:A:859:TRP:HB2 | 2.11 | 0.49 |
| 2:B:78:PHE:CD1 | 2:B:102:LEU:HB2 | 2.48 | 0.49 |
| 2:B:403:PHE:CE1 | 2:B:413:VAL:HB | 2.47 | 0.49 |
| 2:B:79:LEU:HA | 2:B:100:GLY:N | 2.27 | 0.49 |
| 2:C:123:GLU:HG2 | 2:C:204:LEU:CD1 | 2.42 | 0.49 |
| 2:C:289:LEU:HD12 | 2:C:301:GLU:CB | 2.35 | 0.49 |
| 2:C:347:LEU:O | 2:C:350:LEU:HD13 | 2.12 | 0.49 |
| 2:C:431:LYS:HZ3 | 2:C:435:MET:CG | 2.24 | 0.49 |
| 2:C:456:ARG:CB | 2:C:463:LYS:C | 2.79 | 0.49 |
| 1:D:1010:LEU:C | 1:D:1012:VAL:N | 2.63 | 0.49 |
| 1:D:273:PHE:N | 1:D:275:ARG:HB3 | 2.23 | 0.49 |
| 1:D:412:PRO:CG | 1:D:413:LEU:H | 2.23 | 0.49 |
| 1:D:748:TRP:CZ3 | 1:D:750:PHE:CE2 | 2.99 | 0.49 |
| 1:D:829:PRO:HG3 | 1:D:831:TYR:CE1 | 2.47 | 0.49 |
| 1:D:904:ASP:OD1 | 1:D:915:ALA:HB2 | 2.13 | 0.49 |
| 2:E:391:PRO:CD | 2:E:395:LEU:HB2 | 2.39 | 0.49 |
| 2:E:404:ASN:C | 2:E:406:LEU:N | 2.66 | 0.49 |
| 2:E:466:MET:HG2 | 2:E:467:HIS:N | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:E:481:SER:HA | 2:E:484:ASN:CG | 2.33 | 0.49 |
| 2:E:79:LEU:HD12 | 2:E:79:LEU:C | 2.33 | 0.49 |
| 2:F:289:LEU:HD12 | 2:F:301:GLU:CB | 2.32 | 0.49 |
| 2:F:291:TYR:HB2 | 2:F:300:ILE:HD11 | 1.95 | 0.49 |
| 2:F:368:HIS:NE2 | 2:F:370:LYS:CE | 2.75 | 0.49 |
| 2:F:372:LEU:HD12 | 2:F:372:LEU:C | 2.33 | 0.49 |
| 2:F:453:ILE:CG2 | 2:F:454:HIS:N | 2.75 | 0.49 |
| 2:F:458:ARG:HD3 | 2:F:459:ASP:N | 2.28 | 0.49 |
| 2:F:90:SER:HA | 2:F:93:SER:OG | 2.12 | 0.49 |
| 1:A:1043:VAL:CB | 1:A:1046:GLU:HB3 | 2.41 | 0.49 |
| 1:A:1148:ARG:CG | 1:A:1148:ARG:NH1 | 2.62 | 0.49 |
| 1:A:1223:ILE:HD13 | 1:A:1224:ILE:N | 2.27 | 0.49 |
| 1:A:260:ASP:H | 1:A:264:GLN:HE22 | 1.57 | 0.49 |
| 1:A:420:HIS:CE1 | 1:A:421:PRO:HD2 | 2.47 | 0.49 |
| 1:A:485:LEU:O | 1:A:489:GLU:OE2 | 2.31 | 0.49 |
| 1:A:719:LEU:CD2 | 1:A:719:LEU:H | 2.23 | 0.49 |
| 1:A:657:ARG:HG2 | 1:A:744:ILE:HG21 | 1.94 | 0.49 |
| 1:A:795:ASN:ND2 | 1:A:795:ASN:C | 2.65 | 0.49 |
| 1:A:853:ARG:HH22 | 1:A:1105:ALA:HB3 | 1.72 | 0.49 |
| 1:A:869:ARG:O | 1:A:1200:PRO:CA | 2.58 | 0.49 |
| 2:B:206:TYR:HD1 | 2:B:207:GLY:O | 1.94 | 0.49 |
| 2:C:387:VAL:HG23 | 2:C:417:TYR:HA | 1.95 | 0.49 |
| 2:C:414:TRP:O | 2:C:415:PRO:C | 2.50 | 0.49 |
| 2:C:78:PHE:CD1 | 2:C:103:GLY:CA | 2.93 | 0.49 |
| 1:D:1047:ARG:O | 1:D:1051:GLY:N | 2.43 | 0.49 |
| 1:D:1114:VAL:HA | 1:D:1117:LYS:HD2 | 1.95 | 0.49 |
| 1:D:1118:TRP:CE2 | 1:D:1122:GLU:OE1 | 2.65 | 0.49 |
| 1:D:444:TYR:HE2 | 1:D:1210:TYR:HB2 | 1.78 | 0.49 |
| 1:D:1210:TYR:CD1 | 1:D:1211:GLY:N | 2.80 | 0.49 |
| 1:D:1224:ILE:CD1 | 1:D:1228:LYS:HE3 | 2.42 | 0.49 |
| 1:D:194:ALA:C | 1:D:195:LEU:HG | 2.33 | 0.49 |
| 1:D:361:ARG:NH2 | 1:D:362:LEU:HG | 2.28 | 0.49 |
| 1:D:430:MET:O | 1:D:430:MET:SD | 2.70 | 0.49 |
| 1:D:435:LEU:O | 1:D:839:ALA:CB | 2.58 | 0.49 |
| 1:D:443:ARG:O | 1:D:447:GLU:N | 2.43 | 0.49 |
| 1:D:494:GLU:H | 1:D:573:TYR:HB2 | 1.77 | 0.49 |
| 1:D:635:PRO:O | 1:D:636:THR:HB | 2.11 | 0.49 |
| 1:D:655:LEU:O | 1:D:657:ARG:N | 2.46 | 0.49 |
| 1:D:615:SER:O | 1:D:725:PRO:HG3 | 2.12 | 0.49 |
| 1:D:768:LYS:HE2 | 1:D:769:ASP:H | 1.76 | 0.49 |
| 1:D:868:ASP:OD1 | 1:D:1199:THR:CG2 | 2.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:891:VAL:HA | 1:D:894:GLN:OE1 | 2.10 | 0.49 |
| 1:D:95:PRO:HG2 | 1:D:99:ALA:HB2 | 1.89 | 0.49 |
| 2:E:323:HIS:O | 2:E:325:ARG:N | 2.45 | 0.49 |
| 2:E:328:ARG:N | 2:E:328:ARG:CD | 2.68 | 0.49 |
| 2:E:443:VAL:HG12 | 2:E:444:THR:N | 2.28 | 0.49 |
| 2:E:462:MET:CE | 2:E:462:MET:HA | 2.42 | 0.49 |
| 2:E:86:LEU:HD23 | 2:E:97:PRO:HD2 | 1.95 | 0.49 |
| 2:E:88:ARG:CD | 2:E:88:ARG:N | 2.75 | 0.49 |
| 2:F:145:PHE:O | 2:F:146:ARG:HG3 | 2.12 | 0.49 |
| 2:F:251:TRP:CZ3 | 2:F:254:PHE:CG | 3.00 | 0.49 |
| 2:F:336:LEU:CD2 | 2:F:337:SER:O | 2.61 | 0.49 |
| 2:F:371:VAL:CG2 | 2:F:433:ASP:O | 2.60 | 0.49 |
| 2:F:449:GLU:OE1 | 2:F:450:ASN:N | 2.46 | 0.49 |
| 1:A:1029:GLN:CD | 1:A:1096:ARG:NH2 | 2.65 | 0.49 |
| 1:A:307:PHE:HB3 | 1:A:1055:SER:OG | 2.13 | 0.49 |
| 1:A:235:TRP:C | 1:A:235:TRP:CD1 | 2.85 | 0.49 |
| 1:A:296:SER:HB2 | 1:A:847:ALA:CB | 2.36 | 0.49 |
| 1:A:500:ALA:O | 1:A:501:LYS:HB2 | 2.12 | 0.49 |
| 1:A:515:ILE:O | 1:A:516:GLU:C | 2.50 | 0.49 |
| 1:A:659:HIS:CG | 1:A:716:PRO:HA | 2.47 | 0.49 |
| 1:A:613:HIS:NE2 | 1:A:716:PRO:HG3 | 2.28 | 0.49 |
| 1:A:455:LEU:CD1 | 1:A:798:ILE:HG22 | 2.40 | 0.49 |
| 1:A:869:ARG:N | 1:A:872:SER:CB | 2.75 | 0.49 |
| 1:A:877:MET:O | 1:A:878:VAL:C | 2.51 | 0.49 |
| 1:A:947:LYS:O | 1:A:951:TYR:HD1 | 1.95 | 0.49 |
| 2:C:186:LEU:O | 2:C:189:ALA:HB3 | 2.12 | 0.49 |
| 2:C:192:HIS:C | 2:C:196:CYS:SG | 2.91 | 0.49 |
| 2:C:123:GLU:HG2 | 2:C:204:LEU:HD12 | 1.95 | 0.49 |
| 2:C:397:GLN:O | 2:C:398:VAL:CG2 | 2.55 | 0.49 |
| 2:C:447:THR:HG22 | 2:C:455:LEU:CD1 | 2.43 | 0.49 |
| 2:C:452:LEU:O | 2:C:453:ILE:HB | 2.13 | 0.49 |
| 1:D:1067:SER:CB | 1:D:1073:PRO:HG2 | 2.42 | 0.49 |
| 1:D:1162:CYS:O | 1:D:1165:ALA:N | 2.46 | 0.49 |
| 1:D:175:TRP:C | 1:D:185:VAL:HG11 | 2.32 | 0.49 |
| 1:D:213:VAL:CB | 1:D:401:TRP:CZ2 | 2.96 | 0.49 |
| 1:D:288:ARG:NH1 | 1:D:290:ARG:NH2 | 2.61 | 0.49 |
| 1:D:203:LEU:HB2 | 1:D:379:LYS:O | 2.13 | 0.49 |
| 1:D:383:LYS:HD3 | 1:D:383:LYS:N | 2.27 | 0.49 |
| 1:D:453:GLU:O | 1:D:457:ARG:CG | 2.59 | 0.49 |
| 1:D:459:MET:HB3 | 1:D:460:LYS:NZ | 2.27 | 0.49 |
| 1:D:578:PRO:O | 1:D:579:ARG:C | 2.50 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:719:LEU:HD12 | 1:D:720:THR:CB | 2.43 | 0.49 |
| 1:D:735:GLY:HA2 | 1:D:750:PHE:H | 1.77 | 0.49 |
| 1:D:765:PRO:HG2 | 1:D:766:PHE:CE1 | 2.48 | 0.49 |
| 1:D:854:ALA:C | 1:D:855:VAL:HG23 | 2.33 | 0.49 |
| 2:E:129:ASP:HB2 | 2:F:99:PHE:O | 2.12 | 0.49 |
| 2:E:183:GLU:CG | 2:E:216:HIS:CD2 | 2.96 | 0.49 |
| 2:F:128:VAL:HG12 | 2:F:129:ASP:N | 2.27 | 0.49 |
| 2:F:246:ARG:N | 2:F:246:ARG:HD3 | 2.27 | 0.49 |
| 2:F:344:ARG:HA | 2:F:347:LEU:CD1 | 2.39 | 0.49 |
| 2:F:466:MET:O | 2:F:467:HIS:C | 2.50 | 0.49 |
| 1:A:196:VAL:CB | 1:A:401:TRP:CZ3 | 2.86 | 0.49 |
| 1:A:212:ALA:H | 1:A:221:TYR:HA | 1.78 | 0.49 |
| 1:A:215:ILE:O | 1:A:216:SER:C | 2.51 | 0.49 |
| 1:A:355:SER:O | 1:A:407:PHE:CZ | 2.66 | 0.49 |
| 1:A:616:GLU:C | 1:A:725:PRO:HG3 | 2.33 | 0.49 |
| 1:A:732:TYR:CE1 | 1:A:755:LYS:CG | 2.95 | 0.49 |
| 1:A:776:ASP:OD1 | 1:A:777:GLY:N | 2.46 | 0.49 |
| 1:A:900:ALA:C | 1:A:915:ALA:HB1 | 2.32 | 0.49 |
| 1:A:992:LEU:HD13 | 1:A:993:ARG:N | 2.26 | 0.49 |
| 2:B:128:VAL:HG21 | 2:B:208:LEU:HD12 | 1.94 | 0.49 |
| 2:B:280:ASP:HB3 | 2:B:281:GLU:HB2 | 1.93 | 0.49 |
| 2:B:432:TYR:HA | 2:B:437:ILE:HD12 | 1.95 | 0.49 |
| 2:B:450:ASN:HD22 | 2:B:452:LEU:CD2 | 2.22 | 0.49 |
| 2:B:67:GLU:HB3 | 2:B:70:LEU:CD1 | 2.43 | 0.49 |
| 1:D:1065:ALA:O | 1:D:1073:PRO:CG | 2.59 | 0.49 |
| 1:D:873:GLU:OE1 | 1:D:1200:PRO:HG3 | 2.13 | 0.49 |
| 1:D:177:ARG:CB | 1:D:218:SER:HB3 | 2.26 | 0.49 |
| 1:D:374:ARG:CG | 1:D:374:ARG:HH11 | 2.25 | 0.49 |
| 1:D:374:ARG:NE | 1:D:392:LEU:HG | 2.27 | 0.49 |
| 1:D:439:GLN:CG | 1:D:835:GLY:HA3 | 2.40 | 0.49 |
| 1:D:453:GLU:O | 1:D:457:ARG:N | 2.46 | 0.49 |
| 1:D:483:PRO:HG3 | 1:D:712:VAL:HG13 | 1.95 | 0.49 |
| 1:D:493:GLN:HG2 | 1:D:494:GLU:N | 2.28 | 0.49 |
| 1:D:513:LEU:HB2 | 1:D:568:GLY:CA | 2.32 | 0.49 |
| 1:D:515:ILE:HG12 | 1:D:568:GLY:O | 2.13 | 0.49 |
| 1:D:564:GLN:O | 1:D:565:HIS:C | 2.51 | 0.49 |
| 1:D:656:TYR:CA | 1:D:659:HIS:CE1 | 2.95 | 0.49 |
| 1:D:791:ALA:C | 1:D:792:LEU:HD12 | 2.32 | 0.49 |
| 1:D:801:TRP:CH2 | 1:D:805:HIS:ND1 | 2.75 | 0.49 |
| 1:D:950:ASN:OD1 | 1:D:953:ARG:HD2 | 2.13 | 0.49 |
| 1:D:959:GLN:HG2 | 1:D:983:GLN:NE2 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:E:325:ARG:HG2 | 2:E:330:ASN:N | 2.27 | 0.49 |
| 2:E:113:GLU:HG3 | 2:E:378:LEU:CD1 | 2.42 | 0.49 |
| 2:F:354:PHE:CD2 | 2:F:354:PHE:O | 2.66 | 0.49 |
| 2:F:385:LEU:CD2 | 2:F:402:LEU:HD23 | 2.42 | 0.49 |
| 2:F:432:TYR:HB3 | 2:F:437:ILE:CD1 | 2.41 | 0.49 |
| 1:A:233:TYR:O | 1:A:234:SER:HB2 | 2.13 | 0.49 |
| 1:A:274:ASP:O | 1:A:277:HIS:N | 2.45 | 0.49 |
| 1:A:369:PRO:O | 1:A:371:LYS:O | 2.31 | 0.49 |
| 1:A:214:ALA:CA | 1:A:401:TRP:HZ2 | 2.20 | 0.49 |
| 1:A:421:PRO:CG | 1:A:422:VAL:H | 2.26 | 0.49 |
| 1:A:438:ASN:C | 1:A:440:ASN:N | 2.64 | 0.49 |
| 1:A:548:CYS:O | 1:A:552:LEU:HG | 2.12 | 0.49 |
| 1:A:616:GLU:O | 1:A:725:PRO:HD3 | 2.13 | 0.49 |
| 1:A:618:HIS:HB3 | 1:A:725:PRO:HB2 | 1.90 | 0.49 |
| 1:A:730:PRO:HG3 | 1:A:760:CYS:C | 2.33 | 0.49 |
| 2:B:403:PHE:CD1 | 2:B:415:PRO:HD3 | 2.48 | 0.49 |
| 2:C:203:ARG:O | 2:C:204:LEU:HB3 | 2.09 | 0.49 |
| 2:C:243:THR:CG2 | 2:C:247:THR:OG1 | 2.61 | 0.49 |
| 2:C:306:LEU:HG | 2:C:335:VAL:CG2 | 2.43 | 0.49 |
| 2:C:351:TYR:CA | 2:C:355:GLN:HB2 | 2.42 | 0.49 |
| 2:C:357:THR:HA | 2:C:370:LYS:HZ3 | 1.73 | 0.49 |
| 2:C:389:ARG:NE | 2:C:390:GLY:N | 2.60 | 0.49 |
| 2:C:416:GLY:HA2 | 2:C:419:GLU:HB2 | 1.93 | 0.49 |
| 1:D:259:ARG:CA | 1:D:259:ARG:NE | 2.72 | 0.49 |
| 1:D:267:VAL:CG2 | 1:D:291:PHE:HE2 | 2.23 | 0.49 |
| 1:D:412:PRO:CG | 1:D:413:LEU:N | 2.76 | 0.49 |
| 1:D:455:LEU:O | 1:D:459:MET:HB2 | 2.12 | 0.49 |
| 1:D:630:ASN:HD21 | 1:D:632:ALA:HB2 | 1.76 | 0.49 |
| 2:E:268:MET:SD | 2:E:373:LYS:HD3 | 2.52 | 0.49 |
| 2:E:67:GLU:N | 2:E:67:GLU:CD | 2.67 | 0.49 |
| 2:E:67:GLU:CG | 2:E:70:LEU:HD11 | 2.37 | 0.49 |
| 2:F:130:ALA:O | 2:F:131:LEU:HD13 | 2.13 | 0.49 |
| 2:F:208:LEU:CD2 | 2:F:242:PHE:CE2 | 2.93 | 0.49 |
| 2:F:293:PHE:C | 2:F:295:TRP:H | 2.17 | 0.49 |
| 2:F:363:ARG:CZ | 2:F:363:ARG:CB | 2.90 | 0.49 |
| 1:D:546:ARG:NH2 | 2:F:408:GLU:OE2 | 2.45 | 0.49 |
| 2:F:435:MET:O | 2:F:435:MET:SD | 2.71 | 0.49 |
| 1:A:1024:ASP:HA | 1:A:1026:ARG:CZ | 2.43 | 0.49 |
| 1:A:1064:ILE:HD12 | 1:A:1064:ILE:N | 2.27 | 0.49 |
| 1:A:301:ILE:CG2 | 1:A:302:SER:H | 2.26 | 0.49 |
| 1:A:371:LYS:O | 1:A:372:GLU:HG2 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:384:ASP:O | 1:A:387:GLU:HG3 | 2.12 | 0.49 |
| 1:A:410:GLN:O | 1:A:414:PHE:CE2 | 2.66 | 0.49 |
| 1:A:614:TYR:CE2 | 1:A:620:TRP:CE3 | 3.01 | 0.49 |
| 1:A:789:PRO:O | 1:A:793:GLU:CG | 2.61 | 0.49 |
| 1:A:848:GLY:C | 1:A:849:THR:O | 2.49 | 0.49 |
| 1:A:879:GLN:CB | 1:A:1189:LEU:HD21 | 2.43 | 0.49 |
| 1:A:436:PRO:HB2 | 1:A:879:GLN:HE21 | 1.78 | 0.49 |
| 1:A:914:THR:OG1 | 1:A:999:ASP:CB | 2.60 | 0.49 |
| 2:B:217:PRO:CB | 2:B:232:GLY:H | 2.26 | 0.49 |
| 2:C:336:LEU:HD23 | 2:C:337:SER:CA | 2.43 | 0.49 |
| 2:C:375:HIS:CD2 | 2:C:377:CYS:HB2 | 2.47 | 0.49 |
| 2:C:407:LEU:C | 2:C:407:LEU:CD2 | 2.81 | 0.49 |
| 2:C:70:LEU:HD13 | 2:C:70:LEU:C | 2.33 | 0.49 |
| 1:D:1026:ARG:O | 1:D:1029:GLN:HB2 | 2.13 | 0.49 |
| 1:D:1141:VAL:N | 1:D:1146:ARG:NH2 | 2.57 | 0.49 |
| 1:D:1208:ARG:HH22 | 2:F:285:LYS:HD2 | 1.72 | 0.49 |
| 1:D:169:TRP:O | 1:D:169:TRP:CG | 2.66 | 0.49 |
| 1:D:406:VAL:O | 1:D:410:GLN:HB2 | 2.12 | 0.49 |
| 1:D:297:MET:HG2 | 1:D:411:LEU:CD1 | 2.43 | 0.49 |
| 1:D:505:LYS:O | 1:D:506:GLU:HB3 | 2.13 | 0.49 |
| 1:D:649:TYR:CE2 | 1:D:652:ILE:HG21 | 2.47 | 0.49 |
| 1:D:749:PHE:N | 1:D:749:PHE:CD1 | 2.80 | 0.49 |
| 1:D:807:ARG:HH22 | 1:D:1061:LEU:HD12 | 1.78 | 0.49 |
| 1:D:279:ARG:CG | 1:D:841:LEU:HB3 | 2.43 | 0.49 |
| 1:D:907:PHE:CD1 | 1:D:907:PHE:N | 2.80 | 0.49 |
| 2:F:115:TRP:CD1 | 2:F:119:VAL:HG21 | 2.48 | 0.49 |
| 2:F:341:ASP:OD1 | 2:F:342:LEU:N | 2.41 | 0.49 |
| 2:F:342:LEU:HB3 | 2:F:344:ARG:HD3 | 1.92 | 0.49 |
| 1:A:1024:ASP:O | 1:A:1026:ARG:CD | 2.61 | 0.48 |
| 1:A:1164:PHE:O | 1:A:1168:LEU:HG | 2.12 | 0.48 |
| 1:A:127:LEU:HD23 | 1:A:128:PRO:CD | 2.37 | 0.48 |
| 1:A:175:TRP:HB2 | 1:A:184:ALA:N | 2.27 | 0.48 |
| 1:A:201:VAL:HG22 | 1:A:208:CYS:C | 2.33 | 0.48 |
| 1:A:214:ALA:HA | 1:A:401:TRP:CH2 | 2.47 | 0.48 |
| 1:A:461:LYS:O | 1:A:462:SER:C | 2.52 | 0.48 |
| 1:A:564:GLN:CA | 1:A:564:GLN:NE2 | 2.75 | 0.48 |
| 1:A:605:LEU:N | 1:A:717:LEU:HD21 | 2.27 | 0.48 |
| 1:A:656:TYR:CD1 | 1:A:744:ILE:CD1 | 2.92 | 0.48 |
| 1:A:744:ILE:HG12 | 1:A:745:PRO:HD2 | 1.94 | 0.48 |
| 1:A:754:HIS:CE1 | 1:A:762:VAL:HA | 2.48 | 0.48 |
| 2:B:182:ARG:O | 2:B:215:PHE:N | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:217:PRO:CB | 2:B:231:ILE:HB | 2.43 | 0.48 |
| 2:B:205:PRO:CG | 2:B:241:TRP:HE1 | 2.26 | 0.48 |
| 2:B:387:VAL:CG1 | 2:B:396:ARG:HB2 | 2.43 | 0.48 |
| 2:B:81:GLY:CA | 2:B:86:LEU:HD11 | 2.44 | 0.48 |
| 2:C:145:PHE:O | 2:C:146:ARG:CG | 2.61 | 0.48 |
| 2:C:127:PRO:CD | 2:C:209:ALA:C | 2.76 | 0.48 |
| 2:C:325:ARG:NH1 | 2:C:325:ARG:CG | 2.70 | 0.48 |
| 2:C:243:THR:N | 2:C:334:CYS:H | 2.11 | 0.48 |
| 1:A:549:LEU:CD1 | 2:C:401:GLY:HA3 | 2.43 | 0.48 |
| 1:D:306:SER:HB2 | 1:D:1058:PHE:CZ | 2.48 | 0.48 |
| 1:D:1069:ILE:CG2 | 1:D:1070:PRO:N | 2.74 | 0.48 |
| 1:D:113:TRP:HZ3 | 1:D:116:PRO:HD2 | 1.76 | 0.48 |
| 1:D:192:GLU:OE2 | 1:D:258:GLN:NE2 | 2.46 | 0.48 |
| 1:D:281:GLN:HA | 1:D:284:ILE:HD11 | 1.95 | 0.48 |
| 1:D:301:ILE:HG22 | 1:D:302:SER:N | 2.28 | 0.48 |
| 1:D:768:LYS:H | 1:D:772:PRO:HD3 | 1.77 | 0.48 |
| 1:D:920:THR:OG1 | 1:D:921:LEU:HD12 | 2.13 | 0.48 |
| 2:E:407:LEU:CA | 2:E:411:ILE:O | 2.61 | 0.48 |
| 2:F:127:PRO:CD | 2:F:210:GLN:CB | 2.72 | 0.48 |
| 2:F:88:ARG:CZ | 2:F:88:ARG:HB3 | 2.42 | 0.48 |
| 1:A:1016:GLU:OE2 | 1:A:1022:LEU:HD21 | 2.14 | 0.48 |
| 1:A:1156:THR:O | 1:A:1160:THR:OG1 | 2.31 | 0.48 |
| 1:A:659:HIS:CD2 | 1:A:720:THR:HG22 | 2.48 | 0.48 |
| 1:A:789:PRO:HA | 1:A:792:LEU:CD1 | 2.38 | 0.48 |
| 1:A:853:ARG:NH2 | 1:A:1105:ALA:HB1 | 2.28 | 0.48 |
| 1:A:916:PHE:CD1 | 1:A:919:MET:CB | 2.96 | 0.48 |
| 1:A:967:MET:CG | 1:A:978:ALA:HB2 | 2.43 | 0.48 |
| 2:B:234:LYS:CG | 2:B:341:ASP:OD2 | 2.61 | 0.48 |
| 2:C:203:ARG:HG2 | 2:C:325:ARG:NE | 2.28 | 0.48 |
| 2:C:251:TRP:HE3 | 2:C:254:PHE:HB3 | 1.78 | 0.48 |
| 2:C:357:THR:O | 2:C:359:ASN:N | 2.43 | 0.48 |
| 2:C:385:LEU:O | 2:C:416:GLY:CA | 2.54 | 0.48 |
| 1:D:1212:ILE:HD12 | 1:D:1213:PRO:HD3 | 1.94 | 0.48 |
| 1:D:192:GLU:CD | 1:D:258:GLN:NE2 | 2.66 | 0.48 |
| 1:D:274:ASP:O | 1:D:278:ILE:HG12 | 2.13 | 0.48 |
| 1:D:549:LEU:N | 1:D:551:LYS:CD | 2.75 | 0.48 |
| 1:D:592:LEU:H | 1:D:592:LEU:HD12 | 1.77 | 0.48 |
| 1:D:712:VAL:O | 1:D:712:VAL:HG12 | 2.13 | 0.48 |
| 1:D:849:THR:CG2 | 1:D:851:THR:HB | 2.43 | 0.48 |
| 1:D:887:VAL:CG2 | 1:D:1146:ARG:NH1 | 2.76 | 0.48 |
| 1:D:987:ALA:O | 1:D:991:GLY:CA | 2.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:306:LEU:HB2 | 2:E:335:VAL:CG1 | 2.43 | 0.48 |
| 2:F:125:VAL:CG2 | 2:F:208:LEU:CA | 2.75 | 0.48 |
| 2:F:264:ARG:HA | 2:F:270:PRO:CB | 2.43 | 0.48 |
| 2:F:308:ASP:OD2 | 2:F:334:CYS:HA | 2.12 | 0.48 |
| 2:F:395:LEU:CB | 2:F:443:VAL:CG2 | 2.86 | 0.48 |
| 1:A:1027:LYS:O | 1:A:1031:GLU:HB2 | 2.13 | 0.48 |
| 1:A:1198:LYS:HG3 | 1:A:1204:THR:HG23 | 1.89 | 0.48 |
| 1:A:1200:PRO:O | 1:A:1201:SER:C | 2.51 | 0.48 |
| 1:A:347:TRP:O | 1:A:348:LEU:O | 2.31 | 0.48 |
| 1:A:422:VAL:O | 1:A:423:THR:C | 2.49 | 0.48 |
| 1:A:449:GLN:CA | 1:A:452:TYR:CE1 | 2.95 | 0.48 |
| 1:A:556:THR:HG23 | 2:C:452:LEU:CD2 | 2.43 | 0.48 |
| 1:A:610:PHE:HB3 | 1:A:671:GLN:OE1 | 2.13 | 0.48 |
| 1:A:788:GLY:HA2 | 1:A:791:ALA:CB | 2.43 | 0.48 |
| 1:A:866:ARG:HB3 | 1:A:867:PRO:CD | 2.35 | 0.48 |
| 1:A:907:PHE:O | 1:A:908:ALA:HB3 | 2.14 | 0.48 |
| 2:B:259:ARG:HD2 | 2:B:262:TRP:CG | 2.49 | 0.48 |
| 2:B:236:GLU:CG | 2:B:341:ASP:CB | 2.91 | 0.48 |
| 2:B:234:LYS:HB3 | 2:B:341:ASP:OD2 | 2.14 | 0.48 |
| 2:B:391:PRO:HD2 | 2:B:392:THR:H | 1.78 | 0.48 |
| 2:B:400:GLN:NE2 | 2:B:417:TYR:CB | 2.77 | 0.48 |
| 2:B:87:SER:O | 2:B:89:ASP:N | 2.46 | 0.48 |
| 2:C:342:LEU:O | 2:C:342:LEU:HD23 | 2.13 | 0.48 |
| 2:C:371:VAL:CG2 | 2:C:433:ASP:O | 2.62 | 0.48 |
| 2:C:395:LEU:HD21 | 2:C:443:VAL:C | 2.34 | 0.48 |
| 1:A:560:PRO:CG | 2:C:452:LEU:HD21 | 2.43 | 0.48 |
| 2:C:454:HIS:CA | 2:C:466:MET:O | 2.61 | 0.48 |
| 1:D:1003:TRP:CH2 | 1:D:1101:VAL:HG22 | 2.48 | 0.48 |
| 1:D:1141:VAL:O | 1:D:1142:ARG:C | 2.52 | 0.48 |
| 1:D:1155:ILE:O | 1:D:1156:THR:C | 2.52 | 0.48 |
| 1:D:423:THR:HG22 | 1:D:424:LEU:HD23 | 1.95 | 0.48 |
| 1:D:432:VAL:O | 1:D:433:SER:O | 2.31 | 0.48 |
| 1:D:484:TRP:NE1 | 1:D:488:LEU:HD11 | 2.28 | 0.48 |
| 1:D:791:ALA:O | 1:D:795:ASN:ND2 | 2.38 | 0.48 |
| 1:D:993:ARG:HD3 | 1:D:993:ARG:C | 2.34 | 0.48 |
| 2:F:257:ARG:O | 2:F:261:GLN:OE1 | 2.31 | 0.48 |
| 2:F:289:LEU:O | 2:F:299:LEU:O | 2.32 | 0.48 |
| 2:F:335:VAL:HG13 | 2:F:335:VAL:O | 2.13 | 0.48 |
| 1:A:1029:GLN:H | 1:A:1029:GLN:HG3 | 1.16 | 0.48 |
| 1:A:1196:ASP:OD2 | 1:A:1197:CYS:N | 2.46 | 0.48 |
| 1:A:1219:ASP:C | 1:A:1220:ILE:HD12 | 2.34 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:235:TRP:HD1 | 1:A:236:THR:HG1 | 1.61 | 0.48 |
| 1:A:275:ARG:O | 1:A:278:ILE:HB | 2.14 | 0.48 |
| 1:A:301:ILE:O | 1:A:1024:ASP:OD2 | 2.32 | 0.48 |
| 1:A:309:ARG:C | 1:A:313:ILE:HG23 | 2.31 | 0.48 |
| 1:A:393:MET:CE | 1:A:396:CYS:SG | 3.02 | 0.48 |
| 1:A:490:TRP:CA | 1:A:580:LEU:HB2 | 2.41 | 0.48 |
| 1:A:596:MET:O | 1:A:597:ARG:C | 2.51 | 0.48 |
| 1:A:638:THR:HG23 | 1:A:642:SER:HG | 1.75 | 0.48 |
| 1:A:793:GLU:O | 1:A:797:MET:HG3 | 2.13 | 0.48 |
| 1:A:863:SER:O | 1:A:875:LYS:HD2 | 2.14 | 0.48 |
| 1:A:930:ASP:OD2 | 1:A:930:ASP:O | 2.32 | 0.48 |
| 1:A:960:PRO:HD2 | 1:A:961:PHE:CD1 | 2.48 | 0.48 |
| 1:A:992:LEU:HB2 | 1:A:997:LEU:CB | 2.43 | 0.48 |
| 2:B:200:VAL:HB | 2:B:203:ARG:HG2 | 1.95 | 0.48 |
| 2:B:309:HIS:CB | 2:B:312:LEU:HB2 | 2.43 | 0.48 |
| 2:B:418:LEU:O | 2:B:419:GLU:C | 2.50 | 0.48 |
| 2:B:419:GLU:HA | 2:C:203:ARG:HD2 | 1.95 | 0.48 |
| 2:C:99:PHE:HB2 | 2:C:103:GLY:HA3 | 1.95 | 0.48 |
| 1:D:1008:LEU:C | 1:D:1011:PRO:CD | 2.79 | 0.48 |
| 1:D:110:HIS:O | 1:D:112:LEU:HD12 | 2.13 | 0.48 |
| 1:D:1191:LYS:HA | 1:D:1191:LYS:HE2 | 1.95 | 0.48 |
| 1:D:376:LEU:HD12 | 1:D:379:LYS:NZ | 2.28 | 0.48 |
| 1:D:407:PHE:CE1 | 1:D:411:LEU:HD11 | 2.49 | 0.48 |
| 1:D:512:LYS:HE2 | 1:D:514:PRO:HD3 | 1.95 | 0.48 |
| 1:D:623:LEU:H | 1:D:623:LEU:HD23 | 1.78 | 0.48 |
| 2:E:456:ARG:CA | 2:E:462:MET:O | 2.57 | 0.48 |
| 2:E:471:LEU:HA | 2:E:474:PHE:HB3 | 1.95 | 0.48 |
| 2:E:69:LEU:O | 2:E:70:LEU:C | 2.50 | 0.48 |
| 2:F:196:CYS:O | 2:F:199:LEU:CB | 2.61 | 0.48 |
| 2:F:254:PHE:HA | 2:F:257:ARG:CD | 2.43 | 0.48 |
| 2:F:371:VAL:CG2 | 2:F:433:ASP:HB3 | 2.43 | 0.48 |
| 2:F:459:ASP:C | 2:F:460:THR:HG22 | 2.34 | 0.48 |
| 1:D:473:LEU:HA | 2:F:461:THR:CG2 | 2.44 | 0.48 |
| 2:F:471:LEU:CA | 2:F:474:PHE:HB3 | 2.42 | 0.48 |
| 1:A:1026:ARG:HG2 | 1:A:1029:GLN:CD | 2.33 | 0.48 |
| 1:A:278:ILE:O | 1:A:278:ILE:HG22 | 2.14 | 0.48 |
| 1:A:389:PHE:CG | 1:A:390:GLN:N | 2.82 | 0.48 |
| 1:A:421:PRO:HG2 | 1:A:422:VAL:CG2 | 2.43 | 0.48 |
| 1:A:570:PRO:HG2 | 1:A:571:GLY:H | 1.78 | 0.48 |
| 2:B:134:LYS:NZ | 2:B:137:PRO:HD2 | 2.29 | 0.48 |
| 2:B:277:ASP:HA | 2:B:287:ASN:OD1 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:248:SER:OG | 2:C:249:ASN:N | 2.46 | 0.48 |
| 2:C:306:LEU:HG | 2:C:335:VAL:HG21 | 1.94 | 0.48 |
| 2:C:346:MET:O | 2:C:350:LEU:CD1 | 2.62 | 0.48 |
| 2:C:399:CYS:SG | 2:C:417:TYR:CG | 3.07 | 0.48 |
| 1:A:549:LEU:HD11 | 2:C:401:GLY:HA3 | 1.94 | 0.48 |
| 2:C:440:THR:O | 2:C:457:SER:CB | 2.61 | 0.48 |
| 1:D:1015:THR:HG21 | 1:D:1026:ARG:HB3 | 1.95 | 0.48 |
| 1:D:347:TRP:CZ2 | 1:D:1030:ARG:NH1 | 2.82 | 0.48 |
| 1:D:1060:LYS:O | 1:D:1063:SER:O | 2.31 | 0.48 |
| 1:D:1131:ILE:HD11 | 1:D:1138:ARG:O | 2.13 | 0.48 |
| 1:D:1133:ILE:HB | 1:D:1136:GLU:CB | 2.12 | 0.48 |
| 1:D:248:GLU:OE1 | 1:D:250:PRO:HD2 | 2.12 | 0.48 |
| 1:D:277:HIS:HB3 | 1:D:291:PHE:CZ | 2.48 | 0.48 |
| 1:D:547:ALA:CA | 1:D:551:LYS:CE | 2.88 | 0.48 |
| 1:D:634:LEU:HD22 | 1:D:635:PRO:CD | 2.34 | 0.48 |
| 1:D:776:ASP:CA | 1:D:796:LYS:NZ | 2.76 | 0.48 |
| 1:D:920:THR:CG2 | 1:D:922:GLN:CD | 2.82 | 0.48 |
| 1:D:946:ALA:CA | 1:D:949:PHE:CE2 | 2.83 | 0.48 |
| 2:E:267:ALA:O | 2:E:270:PRO:HD3 | 2.13 | 0.48 |
| 2:E:382:LYS:O | 2:E:383:VAL:HG23 | 2.13 | 0.48 |
| 2:E:386:ASP:O | 2:E:387:VAL:HG13 | 2.14 | 0.48 |
| 2:E:380:PRO:CA | 2:E:438:LEU:CD1 | 2.92 | 0.48 |
| 2:E:448:LEU:O | 2:E:449:GLU:C | 2.52 | 0.48 |
| 2:F:127:PRO:HG2 | 2:F:128:VAL:N | 2.28 | 0.48 |
| 2:E:101:PRO:HG3 | 2:F:128:VAL:CG2 | 2.43 | 0.48 |
| 2:F:241:TRP:CB | 2:F:336:LEU:CD1 | 2.59 | 0.48 |
| 2:F:360:SER:HA | 2:F:363:ARG:CG | 2.44 | 0.48 |
| 2:F:415:PRO:CB | 2:F:417:TYR:CE2 | 2.91 | 0.48 |
| 2:F:265:LYS:HG3 | 2:F:485:VAL:HG11 | 1.95 | 0.48 |
| 2:F:86:LEU:O | 2:F:91:LEU:HB2 | 2.13 | 0.48 |
| 1:A:996:ARG:CZ | 1:A:1003:TRP:CB | 2.87 | 0.48 |
| 1:A:1006:ARG:HH11 | 1:A:1006:ARG:HA | 1.62 | 0.48 |
| 1:A:214:ALA:N | 1:A:401:TRP:CZ2 | 2.82 | 0.48 |
| 1:A:176:THR:O | 1:A:220:TRP:CZ3 | 2.66 | 0.48 |
| 1:A:267:VAL:HG12 | 1:A:269:HIS:CE1 | 2.49 | 0.48 |
| 1:A:269:HIS:O | 1:A:294:THR:N | 2.45 | 0.48 |
| 1:A:274:ASP:C | 1:A:276:ALA:H | 2.12 | 0.48 |
| 1:A:400:VAL:C | 1:A:403:THR:HG23 | 2.33 | 0.48 |
| 1:A:556:THR:O | 1:A:559:LEU:HB3 | 2.13 | 0.48 |
| 1:A:640:LEU:N | 1:A:640:LEU:CD2 | 2.64 | 0.48 |
| 1:A:914:THR:N | 1:A:918:TRP:HB2 | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:116:THR:O | 2:B:121:PHE:CD2 | 2.63 | 0.48 |
| 2:B:80:SER:N | 2:B:100:GLY:HA3 | 2.29 | 0.48 |
| 2:B:90:SER:CA | 2:B:93:SER:OG | 2.59 | 0.48 |
| 2:C:127:PRO:CD | 2:C:210:GLN:CB | 2.78 | 0.48 |
| 2:C:131:LEU:O | 2:C:182:ARG:HD3 | 2.13 | 0.48 |
| 1:A:783:PRO:HG2 | 2:C:363:ARG:HD2 | 1.96 | 0.48 |
| 2:C:375:HIS:HB3 | 2:C:378:LEU:HD22 | 1.94 | 0.48 |
| 2:C:90:SER:HA | 2:C:93:SER:OG | 2.13 | 0.48 |
| 1:D:1193:VAL:CG2 | 1:D:1215:GLY:H | 2.26 | 0.48 |
| 1:D:253:ALA:O | 1:D:254:SER:CB | 2.60 | 0.48 |
| 1:D:375:GLU:O | 1:D:379:LYS:CG | 2.55 | 0.48 |
| 1:D:410:GLN:O | 1:D:414:PHE:HD2 | 1.97 | 0.48 |
| 1:D:439:GLN:C | 1:D:441:TRP:N | 2.66 | 0.48 |
| 1:D:604:ALA:CA | 1:D:613:HIS:HE1 | 2.11 | 0.48 |
| 1:D:829:PRO:O | 1:D:829:PRO:HD2 | 2.14 | 0.48 |
| 1:D:869:ARG:CA | 1:D:1200:PRO:CB | 2.91 | 0.48 |
| 2:E:191:GLU:HG3 | 2:E:192:HIS:CD2 | 2.49 | 0.48 |
| 2:E:346:MET:SD | 2:E:346:MET:C | 2.91 | 0.48 |
| 2:E:347:LEU:C | 2:E:350:LEU:HB3 | 2.34 | 0.48 |
| 2:E:407:LEU:C | 2:E:409:ASN:N | 2.67 | 0.48 |
| 2:E:429:TYR:C | 2:E:431:LYS:N | 2.64 | 0.48 |
| 2:F:126:PHE:C | 2:F:128:VAL:N | 2.59 | 0.48 |
| 2:F:146:ARG:HB2 | 2:F:228:VAL:HG11 | 1.95 | 0.48 |
| 2:F:266:PHE:HB2 | 2:F:349:TYR:OH | 2.14 | 0.48 |
| 1:D:1208:ARG:NH1 | 2:F:285:LYS:CD | 2.57 | 0.48 |
| 2:F:414:TRP:N | 2:F:415:PRO:HD2 | 2.28 | 0.48 |
| 1:A:106:HIS:O | 1:A:113:TRP:NE1 | 2.32 | 0.48 |
| 1:A:1157:ASN:HB3 | 1:A:1161:ARG:NH1 | 2.28 | 0.48 |
| 1:A:128:PRO:N | 1:A:129:PRO:CD | 2.76 | 0.48 |
| 1:A:165:LYS:CG | 1:A:178:TYR:HB2 | 2.44 | 0.48 |
| 1:A:358:LEU:N | 1:A:358:LEU:HD23 | 2.28 | 0.48 |
| 1:A:414:PHE:CA | 1:A:417:ARG:HB2 | 2.44 | 0.48 |
| 1:A:954:ILE:HG22 | 1:A:955:TYR:N | 2.28 | 0.48 |
| 2:B:110:LEU:O | 2:B:111:ALA:C | 2.52 | 0.48 |
| 2:B:245:PRO:O | 2:B:248:SER:HB3 | 2.14 | 0.48 |
| 2:B:336:LEU:HG | 2:B:337:SER:H | 1.79 | 0.48 |
| 2:C:193:TYR:OH | 2:C:333:PRO:HG3 | 2.13 | 0.48 |
| 2:C:239:LEU:CA | 2:C:338:VAL:HG12 | 2.41 | 0.48 |
| 1:D:102:ARG:O | 1:D:106:HIS:HD2 | 1.96 | 0.48 |
| 1:D:860:LEU:CD2 | 1:D:1133:ILE:HD12 | 2.44 | 0.48 |
| 1:D:1133:ILE:HG22 | 1:D:1134:HIS:HD2 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:1159:LEU:O | 1:D:1162:CYS:HB2 | 2.14 | 0.48 |
| 1:D:1222:GLN:O | 1:D:1226:LEU:CD2 | 2.55 | 0.48 |
| 1:D:168:ALA:O | 1:D:169:TRP:C | 2.52 | 0.48 |
| 1:D:316:LYS:HZ1 | 1:D:348:LEU:HD23 | 1.76 | 0.48 |
| 1:D:779:LEU:HD22 | 1:D:780:GLN:HA | 1.94 | 0.48 |
| 1:D:829:PRO:O | 1:D:830:ASP:OD2 | 2.32 | 0.48 |
| 1:D:868:ASP:OD1 | 1:D:1199:THR:HB | 2.14 | 0.48 |
| 1:D:923:GLY:O | 1:D:931:LEU:HD11 | 2.12 | 0.48 |
| 2:E:120:VAL:HG22 | 2:F:407:LEU:CD2 | 2.43 | 0.48 |
| 2:E:243:THR:CG2 | 2:E:248:SER:HA | 2.44 | 0.48 |
| 2:E:247:THR:HG23 | 2:E:250:GLN:HG3 | 1.96 | 0.48 |
| 2:E:294:PRO:HD2 | 2:E:351:TYR:CD2 | 2.49 | 0.48 |
| 2:E:389:ARG:NH2 | 2:E:391:PRO:C | 2.67 | 0.48 |
| 2:F:190:LEU:O | 2:F:193:TYR:CB | 2.49 | 0.48 |
| 2:F:347:LEU:N | 2:F:347:LEU:CD1 | 2.77 | 0.48 |
| 2:E:203:ARG:CZ | 2:F:418:LEU:HD13 | 2.43 | 0.48 |
| 1:A:1144:GLU:HG3 | 1:A:1145:ASP:OD1 | 2.14 | 0.48 |
| 1:A:1224:ILE:HD12 | 1:A:1224:ILE:C | 2.33 | 0.48 |
| 1:A:287:SER:O | 1:A:288:ARG:NE | 2.47 | 0.48 |
| 1:A:377:PHE:O | 1:A:378:VAL:CB | 2.61 | 0.48 |
| 1:A:423:THR:O | 1:A:427:MET:HG2 | 2.13 | 0.48 |
| 1:A:547:ALA:HA | 1:A:550:GLN:OE1 | 2.14 | 0.48 |
| 1:A:626:GLY:O | 1:A:627:ARG:HB3 | 2.13 | 0.48 |
| 1:A:727:ASP:O | 1:A:728:THR:OG1 | 2.31 | 0.48 |
| 1:A:795:ASN:ND2 | 1:A:796:LYS:HG3 | 2.28 | 0.48 |
| 1:A:822:PRO:O | 1:A:823:ARG:HB3 | 2.14 | 0.48 |
| 1:A:79:LEU:HB3 | 1:A:83:LEU:HD21 | 1.96 | 0.48 |
| 1:A:867:PRO:HG2 | 1:A:1067:SER:OG | 2.12 | 0.48 |
| 2:B:285:LYS:O | 2:B:305:ASN:HB2 | 2.13 | 0.48 |
| 2:C:246:ARG:C | 2:C:248:SER:N | 2.59 | 0.48 |
| 2:C:190:LEU:CB | 2:C:314:MET:HE1 | 2.44 | 0.48 |
| 2:C:327:GLY:O | 2:C:328:ARG:HB3 | 2.14 | 0.48 |
| 2:C:397:GLN:O | 2:C:399:CYS:N | 2.46 | 0.48 |
| 2:C:419:GLU:CG | 2:C:432:TYR:OH | 2.61 | 0.48 |
| 2:C:435:MET:CE | 2:C:435:MET:CA | 2.84 | 0.48 |
| 2:C:70:LEU:O | 2:C:73:CYS:HB2 | 2.14 | 0.48 |
| 1:D:1005:VAL:HG23 | 1:D:1006:ARG:N | 2.28 | 0.48 |
| 1:D:1058:PHE:CD2 | 1:D:1059:ASN:N | 2.82 | 0.48 |
| 1:D:886:LEU:HA | 1:D:1146:ARG:NH2 | 2.28 | 0.48 |
| 1:D:293:ASP:C | 1:D:296:SER:HB3 | 2.34 | 0.48 |
| 1:D:297:MET:HG2 | 1:D:411:LEU:HD13 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:520:ALA:N | 1:D:521:PRO:HD3 | 2.28 | 0.48 |
| 1:D:575:LYS:HG2 | 1:D:581:ASP:O | 2.14 | 0.48 |
| 1:D:624:VAL:C | 1:D:745:PRO:O | 2.52 | 0.48 |
| 1:D:630:ASN:C | 1:D:630:ASN:ND2 | 2.67 | 0.48 |
| 1:D:633:LYS:HD3 | 1:D:638:THR:HG21 | 1.92 | 0.48 |
| 2:E:105:GLU:O | 2:E:109:ASN:OD1 | 2.31 | 0.48 |
| 2:E:120:VAL:HG12 | 2:E:121:PHE:HD1 | 1.79 | 0.48 |
| 2:E:194:VAL:CG1 | 2:E:195:ASN:H | 2.26 | 0.48 |
| 2:E:332:VAL:N | 2:E:333:PRO:CD | 2.76 | 0.48 |
| 2:F:239:LEU:HB3 | 2:F:338:VAL:HG13 | 1.96 | 0.48 |
| 2:F:245:PRO:C | 2:F:248:SER:HB2 | 2.32 | 0.48 |
| 2:F:353:SER:OG | 2:F:354:PHE:N | 2.47 | 0.48 |
| 2:F:351:TYR:O | 2:F:355:GLN:HB2 | 2.10 | 0.48 |
| 2:F:375:HIS:CD2 | 2:F:377:CYS:HB2 | 2.49 | 0.48 |
| 2:E:203:ARG:NH2 | 2:F:418:LEU:HD11 | 2.29 | 0.48 |
| 2:F:416:GLY:HA2 | 2:F:419:GLU:HB2 | 1.95 | 0.48 |
| 2:F:88:ARG:CZ | 2:F:88:ARG:CB | 2.91 | 0.48 |
| 1:A:996:ARG:NH1 | 1:A:1000:GLU:O | 2.25 | 0.48 |
| 1:A:1169:GLY:C | 1:A:1170:LEU:HD12 | 2.34 | 0.48 |
| 1:A:304:LEU:HD23 | 1:A:1025:LEU:HD13 | 1.96 | 0.48 |
| 1:A:595:GLN:O | 1:A:597:ARG:N | 2.47 | 0.48 |
| 1:A:755:LYS:O | 1:A:758:ASN:HA | 2.14 | 0.48 |
| 1:A:807:ARG:C | 1:A:810:SER:OG | 2.53 | 0.48 |
| 1:A:879:GLN:HB2 | 1:A:1189:LEU:HD21 | 1.96 | 0.48 |
| 2:B:453:ILE:H | 2:B:453:ILE:CD1 | 2.24 | 0.48 |
| 2:C:303:LEU:HD12 | 2:C:339:ASN:OD1 | 2.14 | 0.48 |
| 2:C:399:CYS:SG | 2:C:417:TYR:CD2 | 3.07 | 0.48 |
| 2:C:456:ARG:CB | 2:C:463:LYS:HB3 | 2.44 | 0.48 |
| 2:C:84:GLN:C | 2:C:86:LEU:N | 2.67 | 0.48 |
| 1:D:1207:GLU:C | 1:D:1210:TYR:CD2 | 2.86 | 0.48 |
| 1:D:256:PRO:CG | 1:D:281:GLN:HA | 2.44 | 0.48 |
| 1:D:454:GLU:CA | 1:D:457:ARG:HG3 | 2.43 | 0.48 |
| 1:D:671:GLN:CA | 1:D:671:GLN:NE2 | 2.75 | 0.48 |
| 1:D:895:GLU:CD | 1:D:895:GLU:C | 2.73 | 0.48 |
| 1:D:900:ALA:O | 1:D:915:ALA:CB | 2.62 | 0.48 |
| 2:E:441:VAL:HG22 | 2:E:455:LEU:HB3 | 1.96 | 0.48 |
| 2:F:217:PRO:CB | 2:F:219:PHE:CE1 | 2.90 | 0.48 |
| 2:F:243:THR:CA | 2:F:334:CYS:HB2 | 2.44 | 0.48 |
| 2:F:290:TYR:CD1 | 2:F:299:LEU:HD22 | 2.49 | 0.48 |
| 2:F:372:LEU:HD11 | 2:F:436:SER:OG | 2.11 | 0.48 |
| 2:F:387:VAL:HG11 | 2:F:396:ARG:HA | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:402:LEU:C | 2:F:406:LEU:HD22 | 2.35 | 0.48 |
| 1:A:1054:GLU:O | 1:A:1058:PHE:CD2 | 2.65 | 0.48 |
| 1:A:121:PRO:O | 1:A:1175:GLN:NE2 | 2.35 | 0.48 |
| 1:A:210:THR:HB | 1:A:224:CYS:SG | 2.53 | 0.48 |
| 1:A:301:ILE:HD11 | 1:A:414:PHE:HB3 | 1.96 | 0.48 |
| 1:A:346:ASP:HB3 | 1:A:1040:LYS:HZ2 | 1.67 | 0.48 |
| 1:A:445:LEU:C | 1:A:448:ALA:HB3 | 2.33 | 0.48 |
| 1:A:483:PRO:HB3 | 1:A:712:VAL:CG1 | 2.42 | 0.48 |
| 1:A:605:LEU:O | 1:A:781:ALA:HB3 | 2.14 | 0.48 |
| 1:A:658:LYS:O | 1:A:660:CYS:N | 2.47 | 0.48 |
| 1:A:624:VAL:HG21 | 1:A:747:CYS:SG | 2.54 | 0.48 |
| 1:A:764:SER:O | 1:A:767:ALA:HB2 | 2.13 | 0.48 |
| 1:A:916:PHE:O | 1:A:920:THR:CA | 2.62 | 0.48 |
| 2:B:213:VAL:HA | 2:B:235:THR:CA | 2.43 | 0.48 |
| 2:B:313:HIS:O | 2:B:316:PRO:CD | 2.55 | 0.48 |
| 2:B:315:TYR:CB | 2:B:322:LEU:HD11 | 2.44 | 0.48 |
| 2:B:450:ASN:ND2 | 2:B:452:LEU:HD23 | 2.24 | 0.48 |
| 2:B:437:ILE:O | 2:B:458:ARG:CZ | 2.62 | 0.48 |
| 2:B:74:GLN:HE21 | 2:B:77:HIS:CD2 | 2.32 | 0.48 |
| 2:C:306:LEU:H | 2:C:335:VAL:HG21 | 1.77 | 0.48 |
| 2:C:74:GLN:CG | 2:C:75:ARG:N | 2.76 | 0.48 |
| 2:C:78:PHE:CD2 | 2:C:79:LEU:CD2 | 2.97 | 0.48 |
| 1:D:1002:GLU:HG2 | 1:D:1003:TRP:H | 1.79 | 0.48 |
| 1:D:101:ARG:O | 1:D:102:ARG:C | 2.52 | 0.48 |
| 1:D:1198:LYS:CA | 1:D:1204:THR:CB | 2.85 | 0.48 |
| 1:D:195:LEU:H | 1:D:265:LEU:CG | 2.27 | 0.48 |
| 1:D:195:LEU:HD21 | 1:D:217:PRO:HD2 | 1.96 | 0.48 |
| 1:D:242:ALA:CB | 1:D:245:ILE:CG2 | 2.92 | 0.48 |
| 1:D:282:TYR:CE2 | 1:D:432:VAL:CA | 2.93 | 0.48 |
| 1:D:282:TYR:O | 1:D:285:GLN:HG2 | 2.12 | 0.48 |
| 1:D:282:TYR:CD2 | 1:D:432:VAL:O | 2.66 | 0.48 |
| 1:D:450:GLY:O | 1:D:454:GLU:HG3 | 2.14 | 0.48 |
| 1:D:456:GLN:O | 1:D:460:LYS:CD | 2.62 | 0.48 |
| 1:D:484:TRP:NE1 | 1:D:488:LEU:CD1 | 2.77 | 0.48 |
| 1:D:607:TRP:O | 1:D:608:ASP:CG | 2.51 | 0.48 |
| 1:D:741:ASP:OD1 | 1:D:741:ASP:N | 2.47 | 0.48 |
| 1:D:743:ASP:HB2 | 1:D:744:ILE:CD1 | 2.43 | 0.48 |
| 1:D:73:PRO:HG2 | 1:D:90:GLN:HG2 | 1.90 | 0.48 |
| 2:E:131:LEU:HD23 | 2:E:132:HIS:H | 1.79 | 0.48 |
| 2:E:297:LYS:O | 2:E:298:GLU:CB | 2.62 | 0.48 |
| 2:F:183:GLU:HA | 2:F:183:GLU:OE2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:243:THR:CB | 2:F:334:CYS:HB2 | 2.44 | 0.48 |
| 2:F:368:HIS:CG | 2:F:368:HIS:O | 2.65 | 0.48 |
| 2:F:86:LEU:O | 2:F:87:SER:C | 2.51 | 0.48 |
| 1:A:1006:ARG:O | 1:A:1010:LEU:HB2 | 2.14 | 0.47 |
| 1:A:313:ILE:HG13 | 1:A:314:ALA:H | 1.79 | 0.47 |
| 1:A:463:LEU:HD22 | 1:A:464:MET:N | 2.29 | 0.47 |
| 1:A:526:ASP:OD2 | 1:A:526:ASP:C | 2.52 | 0.47 |
| 1:A:620:TRP:C | 1:A:748:TRP:HB2 | 2.35 | 0.47 |
| 1:A:756:ASP:OD1 | 1:A:756:ASP:N | 2.47 | 0.47 |
| 1:A:795:ASN:HD21 | 1:A:796:LYS:HG3 | 1.78 | 0.47 |
| 1:A:900:ALA:CA | 1:A:915:ALA:CB | 2.80 | 0.47 |
| 1:A:972:ARG:C | 1:A:974:THR:N | 2.66 | 0.47 |
| 2:B:196:CYS:O | 2:B:197:LEU:C | 2.53 | 0.47 |
| 2:B:261:GLN:O | 2:B:261:GLN:CG | 2.61 | 0.47 |
| 2:B:383:VAL:CG2 | 2:B:384:ALA:N | 2.76 | 0.47 |
| 2:B:435:MET:O | 2:B:436:SER:C | 2.51 | 0.47 |
| 2:B:82:SER:H | 2:B:85:GLN:HG3 | 1.78 | 0.47 |
| 2:C:384:ALA:HB2 | 2:C:437:ILE:CD1 | 2.38 | 0.47 |
| 1:D:308:GLN:NE2 | 1:D:1027:LYS:HZ1 | 2.10 | 0.47 |
| 1:D:1028:VAL:CG2 | 1:D:1096:ARG:CZ | 2.89 | 0.47 |
| 1:D:1111:LEU:CD1 | 1:D:1111:LEU:H | 2.27 | 0.47 |
| 1:D:301:ILE:CG2 | 1:D:302:SER:N | 2.77 | 0.47 |
| 1:D:497:GLN:OE1 | 1:D:516:GLU:O | 2.32 | 0.47 |
| 1:D:904:ASP:OD1 | 1:D:904:ASP:N | 2.34 | 0.47 |
| 2:E:94:GLY:CA | 2:E:234:LYS:HE2 | 2.43 | 0.47 |
| 2:E:270:PRO:CA | 2:E:273:PHE:CD2 | 2.88 | 0.47 |
| 2:E:440:THR:HG22 | 2:E:441:VAL:N | 2.29 | 0.47 |
| 2:E:448:LEU:CD2 | 2:E:448:LEU:C | 2.82 | 0.47 |
| 2:E:86:LEU:CG | 2:E:97:PRO:HD2 | 2.43 | 0.47 |
| 2:F:236:GLU:HB3 | 2:F:341:ASP:HB3 | 1.95 | 0.47 |
| 2:F:331:VAL:HG13 | 2:F:332:VAL:N | 2.28 | 0.47 |
| 2:F:454:HIS:CA | 2:F:466:MET:O | 2.62 | 0.47 |
| 2:F:90:SER:O | 2:F:93:SER:OG | 2.27 | 0.47 |
| 1:A:1014:ARG:HB2 | 1:A:1026:ARG:NE | 2.27 | 0.47 |
| 1:A:1136:GLU:N | 1:A:1136:GLU:OE2 | 2.47 | 0.47 |
| 1:A:81:ARG:NH2 | 1:A:126:ARG:HA | 2.29 | 0.47 |
| 1:A:226:GLN:CD | 1:A:226:GLN:C | 2.73 | 0.47 |
| 1:A:302:SER:HB2 | 1:A:351:SER:HB3 | 1.96 | 0.47 |
| 1:A:389:PHE:CB | 1:A:393:MET:HG2 | 2.44 | 0.47 |
| 1:A:406:VAL:HG22 | 1:A:407:PHE:CD2 | 2.48 | 0.47 |
| 1:A:503:VAL:HG21 | 1:A:521:PRO:C | 2.35 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:601:LYS:CE | 1:A:616:GLU:OE2 | 2.61 | 0.47 |
| 1:A:774:MET:CA | 1:A:777:GLY:HA3 | 2.32 | 0.47 |
| 1:A:869:ARG:N | 1:A:872:SER:HB2 | 2.28 | 0.47 |
| 2:B:72:ILE:C | 2:B:75:ARG:HG3 | 2.33 | 0.47 |
| 2:C:375:HIS:HD2 | 2:C:377:CYS:HB2 | 1.78 | 0.47 |
| 1:A:484:TRP:HH2 | 2:C:461:THR:O | 1.97 | 0.47 |
| 1:D:1008:LEU:CD2 | 1:D:1008:LEU:C | 2.82 | 0.47 |
| 1:D:1044:VAL:O | 1:D:1047:ARG:CB | 2.62 | 0.47 |
| 1:D:1122:GLU:O | 1:D:1123:PHE:CB | 2.63 | 0.47 |
| 1:D:78:MET:HB2 | 1:D:1175:GLN:HB3 | 1.96 | 0.47 |
| 1:D:877:MET:HE1 | 1:D:1203:PRO:HA | 1.96 | 0.47 |
| 1:D:1221:TYR:CA | 1:D:1224:ILE:CG2 | 2.73 | 0.47 |
| 1:D:257:THR:O | 1:D:258:GLN:C | 2.53 | 0.47 |
| 1:D:293:ASP:HB3 | 1:D:296:SER:CB | 2.42 | 0.47 |
| 1:D:357:ALA:O | 1:D:359:VAL:N | 2.47 | 0.47 |
| 1:D:389:PHE:HD1 | 1:D:389:PHE:C | 2.16 | 0.47 |
| 1:D:420:HIS:ND1 | 1:D:421:PRO:CD | 2.47 | 0.47 |
| 1:D:451:THR:O | 1:D:454:GLU:HB2 | 2.13 | 0.47 |
| 1:D:459:MET:CB | 1:D:460:LYS:NZ | 2.77 | 0.47 |
| 1:D:485:LEU:HD12 | 1:D:489:GLU:CD | 2.34 | 0.47 |
| 1:D:486:TRP:CZ3 | 1:D:598:VAL:CG2 | 2.97 | 0.47 |
| 1:D:607:TRP:HA | 1:D:607:TRP:HE3 | 1.80 | 0.47 |
| 1:D:771:LEU:O | 1:D:775:GLU:N | 2.47 | 0.47 |
| 1:D:774:MET:HB3 | 1:D:779:LEU:CD1 | 2.44 | 0.47 |
| 1:D:992:LEU:O | 1:D:996:ARG:CZ | 2.62 | 0.47 |
| 2:E:389:ARG:HH21 | 2:E:390:GLY:C | 2.17 | 0.47 |
| 2:E:431:LYS:CG | 2:E:432:TYR:H | 2.27 | 0.47 |
| 2:F:193:TYR:CZ | 2:F:333:PRO:HG3 | 2.49 | 0.47 |
| 2:F:219:PHE:O | 2:F:220:ASP:O | 2.31 | 0.47 |
| 2:F:311:LEU:CD2 | 2:F:311:LEU:H | 2.26 | 0.47 |
| 2:F:99:PHE:N | 2:F:99:PHE:CD2 | 2.82 | 0.47 |
| 1:A:1016:GLU:N | 1:A:1016:GLU:OE2 | 2.46 | 0.47 |
| 1:A:141:LEU:O | 1:A:144:GLN:CB | 2.63 | 0.47 |
| 1:A:373:PRO:HD2 | 1:A:374:ARG:HG2 | 1.94 | 0.47 |
| 1:A:372:GLU:C | 1:A:374:ARG:O | 2.52 | 0.47 |
| 1:A:374:ARG:C | 1:A:376:LEU:H | 2.17 | 0.47 |
| 1:A:383:LYS:O | 1:A:386:ARG:NH1 | 2.48 | 0.47 |
| 1:A:462:SER:O | 1:A:463:LEU:C | 2.52 | 0.47 |
| 1:A:503:VAL:CG2 | 1:A:521:PRO:CA | 2.82 | 0.47 |
| 1:A:587:PRO:O | 1:A:588:GLY:O | 2.31 | 0.47 |
| 1:A:596:MET:HB3 | 1:A:596:MET:HE2 | 1.59 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:670:PRO:HA | 1:A:673:ALA:CB | 2.44 | 0.47 |
| 1:A:753:PRO:HD2 | 1:A:770:PHE:CD2 | 2.49 | 0.47 |
| 1:A:275:ARG:HG2 | 1:A:843:GLN:HB2 | 1.95 | 0.47 |
| 1:A:958:GLY:HA2 | 1:A:986:TYR:CZ | 2.49 | 0.47 |
| 2:B:305:ASN:C | 2:B:307:GLY:H | 2.17 | 0.47 |
| 2:B:386:ASP:OD1 | 2:B:387:VAL:HG22 | 2.14 | 0.47 |
| 2:B:469:SER:OG | 2:B:470:LYS:N | 2.46 | 0.47 |
| 2:C:239:LEU:C | 2:C:338:VAL:CG1 | 2.82 | 0.47 |
| 2:C:364:LYS:N | 2:C:364:LYS:CD | 2.76 | 0.47 |
| 2:C:388:GLY:O | 2:C:444:THR:CA | 2.54 | 0.47 |
| 1:D:97:GLU:C | 1:D:101:ARG:HG3 | 2.35 | 0.47 |
| 1:D:1026:ARG:O | 1:D:1026:ARG:HG2 | 2.14 | 0.47 |
| 1:D:1040:LYS:HA | 1:D:1040:LYS:HE3 | 1.97 | 0.47 |
| 1:D:162:LEU:HD12 | 1:D:162:LEU:C | 2.34 | 0.47 |
| 1:D:172:ALA:O | 1:D:173:GLU:CB | 2.62 | 0.47 |
| 1:D:275:ARG:HH11 | 1:D:843:GLN:CG | 2.20 | 0.47 |
| 1:D:384:ASP:N | 1:D:384:ASP:OD1 | 2.42 | 0.47 |
| 1:D:459:MET:CA | 1:D:460:LYS:HZ1 | 2.23 | 0.47 |
| 1:D:550:GLN:H | 1:D:551:LYS:CE | 2.21 | 0.47 |
| 1:D:633:LYS:HB3 | 1:D:638:THR:CB | 2.44 | 0.47 |
| 1:D:656:TYR:HD1 | 1:D:744:ILE:CD1 | 2.24 | 0.47 |
| 1:D:247:LEU:HA | 1:D:815:TRP:HB2 | 1.97 | 0.47 |
| 1:D:900:ALA:O | 1:D:915:ALA:HB2 | 2.14 | 0.47 |
| 1:D:923:GLY:HA2 | 1:D:931:LEU:CD1 | 2.44 | 0.47 |
| 2:E:108:LYS:HG3 | 2:E:109:ASN:N | 2.29 | 0.47 |
| 2:E:186:LEU:O | 2:E:187:HIS:C | 2.51 | 0.47 |
| 2:E:289:LEU:O | 2:E:290:TYR:CG | 2.68 | 0.47 |
| 2:E:425:LEU:C | 2:E:428:LEU:HD11 | 2.34 | 0.47 |
| 2:F:200:VAL:CG1 | 2:F:204:LEU:HD22 | 2.43 | 0.47 |
| 2:F:300:ILE:CG2 | 2:F:301:GLU:HG3 | 2.31 | 0.47 |
| 2:F:82:SER:O | 2:F:83:LYS:HB2 | 2.12 | 0.47 |
| 1:A:1137:VAL:HG12 | 1:A:1139:TYR:CZ | 2.48 | 0.47 |
| 1:A:885:THR:CA | 1:A:1146:ARG:HE | 2.23 | 0.47 |
| 1:A:420:HIS:O | 1:A:424:LEU:HD11 | 2.14 | 0.47 |
| 1:A:441:TRP:CE3 | 1:A:445:LEU:CD1 | 2.96 | 0.47 |
| 1:A:468:ASN:O | 1:A:469:ASP:C | 2.52 | 0.47 |
| 1:A:664:GLY:HA2 | 1:A:667:GLN:NE2 | 2.28 | 0.47 |
| 1:A:792:LEU:C | 1:A:796:LYS:HD3 | 2.35 | 0.47 |
| 1:A:914:THR:HA | 1:A:918:TRP:CB | 2.29 | 0.47 |
| 1:A:951:TYR:O | 1:A:955:TYR:CD1 | 2.67 | 0.47 |
| 2:B:336:LEU:HD23 | 2:B:337:SER:N | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:193:TYR:CD1 | 2:C:242:PHE:CE2 | 3.02 | 0.47 |
| 2:C:291:TYR:CG | 2:C:348:ALA:HB1 | 2.50 | 0.47 |
| 2:C:314:MET:O | 2:C:316:PRO:HD3 | 2.14 | 0.47 |
| 2:C:342:LEU:HD23 | 2:C:342:LEU:C | 2.35 | 0.47 |
| 2:C:371:VAL:HG13 | 2:C:372:LEU:O | 2.14 | 0.47 |
| 2:C:405:GLU:OE1 | 2:C:405:GLU:C | 2.53 | 0.47 |
| 2:C:428:LEU:HB3 | 2:C:432:TYR:CE1 | 2.50 | 0.47 |
| 2:C:455:LEU:CB | 2:C:456:ARG:HE | 2.26 | 0.47 |
| 2:C:456:ARG:HG3 | 2:C:463:LYS:HB3 | 1.96 | 0.47 |
| 2:C:59:ALA:O | 2:C:62:SER:OG | 2.28 | 0.47 |
| 1:D:306:SER:HB2 | 1:D:1058:PHE:CE2 | 2.49 | 0.47 |
| 1:D:164:PRO:CD | 1:D:165:LYS:N | 2.73 | 0.47 |
| 1:D:197:PHE:CD1 | 1:D:213:VAL:O | 2.67 | 0.47 |
| 1:D:273:PHE:O | 1:D:276:ALA:HB3 | 2.14 | 0.47 |
| 1:D:312:TRP:HB3 | 1:D:316:LYS:CD | 2.44 | 0.47 |
| 1:D:348:LEU:CD2 | 1:D:350:ILE:CG1 | 2.85 | 0.47 |
| 1:D:891:VAL:CG2 | 1:D:891:VAL:O | 2.62 | 0.47 |
| 2:E:193:TYR:O | 2:E:197:LEU:HB2 | 2.14 | 0.47 |
| 2:E:322:LEU:HB3 | 2:E:332:VAL:HG13 | 1.96 | 0.47 |
| 2:E:382:LYS:HE2 | 2:E:412:SER:C | 2.23 | 0.47 |
| 2:E:468:ILE:O | 2:E:469:SER:OG | 2.25 | 0.47 |
| 2:F:219:PHE:HE2 | 2:F:228:VAL:C | 2.17 | 0.47 |
| 2:F:219:PHE:O | 2:F:220:ASP:C | 2.50 | 0.47 |
| 1:D:1209:ARG:HD2 | 2:F:249:ASN:CA | 2.45 | 0.47 |
| 2:F:344:ARG:HG2 | 2:F:347:LEU:HD22 | 1.96 | 0.47 |
| 2:F:351:TYR:HD1 | 2:F:355:GLN:HA | 1.78 | 0.47 |
| 2:F:365:LYS:HB3 | 2:F:367:LEU:HD21 | 1.96 | 0.47 |
| 1:D:472:GLN:CB | 2:F:460:THR:O | 2.56 | 0.47 |
| 1:A:1056:GLU:HG3 | 1:A:1059:ASN:HD21 | 1.79 | 0.47 |
| 1:A:1154:GLN:HE21 | 1:A:1220:ILE:HG13 | 1.77 | 0.47 |
| 1:A:420:HIS:O | 1:A:424:LEU:CD1 | 2.62 | 0.47 |
| 1:A:454:GLU:C | 1:A:458:GLU:HG3 | 2.34 | 0.47 |
| 1:A:741:ASP:OD2 | 1:A:742:VAL:HG23 | 2.14 | 0.47 |
| 1:A:784:GLY:CA | 2:C:363:ARG:HD3 | 2.44 | 0.47 |
| 1:A:801:TRP:O | 1:A:802:ARG:C | 2.50 | 0.47 |
| 1:A:907:PHE:CZ | 1:A:1001:GLY:HA3 | 2.50 | 0.47 |
| 2:B:289:LEU:HB2 | 2:B:301:GLU:H | 1.80 | 0.47 |
| 2:B:338:VAL:O | 2:B:338:VAL:HG12 | 2.14 | 0.47 |
| 2:B:379:ALA:HB3 | 2:B:438:LEU:HD11 | 1.96 | 0.47 |
| 2:B:475:LEU:O | 2:B:476:ILE:C | 2.51 | 0.47 |
| 2:C:120:VAL:CG2 | 2:C:121:PHE:H | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:290:TYR:HD1 | 2:C:299:LEU:HA | 1.80 | 0.47 |
| 2:C:403:PHE:CD2 | 2:C:407:LEU:HB2 | 2.50 | 0.47 |
| 2:C:403:PHE:O | 2:C:406:LEU:HB2 | 2.14 | 0.47 |
| 1:D:1041:TRP:CD1 | 1:D:1044:VAL:HG11 | 2.50 | 0.47 |
| 1:D:1132:SER:O | 1:D:1132:SER:OG | 2.33 | 0.47 |
| 1:D:1208:ARG:CG | 1:D:1209:ARG:N | 2.77 | 0.47 |
| 1:D:127:LEU:HD23 | 1:D:128:PRO:N | 2.29 | 0.47 |
| 1:D:224:CYS:SG | 1:D:228:LEU:HD23 | 2.54 | 0.47 |
| 1:D:525:MET:HG3 | 1:D:526:ASP:OD1 | 2.15 | 0.47 |
| 1:D:556:THR:HG23 | 1:D:559:LEU:HD23 | 1.95 | 0.47 |
| 1:D:724:GLY:HA2 | 1:D:725:PRO:HA | 1.64 | 0.47 |
| 1:D:801:TRP:CH2 | 1:D:805:HIS:CD2 | 3.02 | 0.47 |
| 1:D:846:THR:O | 1:D:847:ALA:C | 2.52 | 0.47 |
| 1:D:115:GLN:NE2 | 1:D:924:ARG:NH1 | 2.61 | 0.47 |
| 2:E:131:LEU:CD2 | 2:E:132:HIS:H | 2.26 | 0.47 |
| 2:E:272:ASN:HB3 | 2:E:292:ASN:HB2 | 1.97 | 0.47 |
| 2:F:199:LEU:HD12 | 2:F:200:VAL:N | 2.30 | 0.47 |
| 2:F:204:LEU:O | 2:F:205:PRO:C | 2.53 | 0.47 |
| 2:F:350:LEU:H | 2:F:350:LEU:CD1 | 2.16 | 0.47 |
| 2:F:458:ARG:HH11 | 2:F:458:ARG:CG | 2.27 | 0.47 |
| 1:A:996:ARG:HH12 | 1:A:1004:LEU:N | 2.12 | 0.47 |
| 1:A:1131:ILE:CG1 | 1:A:1132:SER:N | 2.77 | 0.47 |
| 1:A:81:ARG:CD | 1:A:125:LEU:O | 2.57 | 0.47 |
| 1:A:247:LEU:HD12 | 1:A:251:THR:HG23 | 1.93 | 0.47 |
| 1:A:258:GLN:CD | 1:A:258:GLN:N | 2.67 | 0.47 |
| 1:A:506:GLU:HG3 | 1:A:507:PRO:N | 2.29 | 0.47 |
| 1:A:583:PRO:C | 1:A:585:TRP:H | 2.14 | 0.47 |
| 1:A:821:LEU:CD1 | 1:A:825:VAL:CG1 | 2.92 | 0.47 |
| 2:C:99:PHE:CB | 2:C:103:GLY:HA3 | 2.44 | 0.47 |
| 2:C:206:TYR:N | 2:C:206:TYR:CD2 | 2.52 | 0.47 |
| 2:C:236:GLU:CA | 2:C:341:ASP:CG | 2.82 | 0.47 |
| 2:C:389:ARG:HG3 | 2:C:390:GLY:N | 2.27 | 0.47 |
| 2:C:385:LEU:CD2 | 2:C:402:LEU:HD23 | 2.38 | 0.47 |
| 2:C:431:LYS:HZ3 | 2:C:435:MET:HG2 | 1.72 | 0.47 |
| 1:D:1024:ASP:C | 1:D:1026:ARG:H | 2.18 | 0.47 |
| 1:D:253:ALA:O | 1:D:254:SER:HB3 | 2.14 | 0.47 |
| 1:D:361:ARG:HH22 | 1:D:362:LEU:HD21 | 1.80 | 0.47 |
| 1:D:458:GLU:N | 1:D:460:LYS:HE3 | 2.29 | 0.47 |
| 1:D:888:GLY:O | 1:D:889:ALA:HB2 | 2.13 | 0.47 |
| 2:F:110:LEU:O | 2:F:111:ALA:C | 2.51 | 0.47 |
| 2:F:207:GLY:CA | 2:F:239:LEU:HD11 | 2.43 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:305:ASN:C | 2:F:307:GLY:N | 2.68 | 0.47 |
| 1:A:1011:PRO:CD | 1:A:1012:VAL:H | 2.24 | 0.47 |
| 1:A:1141:VAL:HB | 1:A:1146:ARG:HD3 | 1.94 | 0.47 |
| 1:A:1196:ASP:C | 1:A:1196:ASP:OD2 | 2.52 | 0.47 |
| 1:A:1223:ILE:HA | 1:A:1226:LEU:CD2 | 2.43 | 0.47 |
| 1:A:157:LEU:HG | 1:A:194:ALA:CB | 2.44 | 0.47 |
| 1:A:386:ARG:HD3 | 1:A:387:GLU:N | 2.27 | 0.47 |
| 1:A:213:VAL:HG11 | 1:A:401:TRP:NE1 | 2.26 | 0.47 |
| 1:A:515:ILE:CG1 | 1:A:565:HIS:O | 2.56 | 0.47 |
| 1:A:655:LEU:CD1 | 1:A:719:LEU:O | 2.62 | 0.47 |
| 1:A:727:ASP:N | 1:A:727:ASP:OD2 | 2.33 | 0.47 |
| 1:A:451:THR:CB | 1:A:869:ARG:HH22 | 2.28 | 0.47 |
| 1:A:884:TYR:OH | 1:A:1142:ARG:NH1 | 2.48 | 0.47 |
| 1:A:916:PHE:O | 1:A:920:THR:N | 2.48 | 0.47 |
| 2:B:186:LEU:O | 2:B:190:LEU:HD23 | 2.15 | 0.47 |
| 2:B:320:SER:O | 2:B:323:HIS:NE2 | 2.47 | 0.47 |
| 2:B:389:ARG:HG2 | 2:B:444:THR:HG22 | 1.96 | 0.47 |
| 2:B:461:THR:OG1 | 2:B:463:LYS:CE | 2.62 | 0.47 |
| 2:B:81:GLY:HA3 | 2:B:86:LEU:HD11 | 1.96 | 0.47 |
| 2:C:186:LEU:O | 2:C:190:LEU:HG | 2.15 | 0.47 |
| 2:B:419:GLU:OE2 | 2:C:201:ASN:ND2 | 2.48 | 0.47 |
| 2:C:479:ILE:H | 2:C:479:ILE:HG13 | 1.47 | 0.47 |
| 1:D:1002:GLU:CG | 1:D:1003:TRP:H | 2.28 | 0.47 |
| 1:D:1107:ASP:C | 1:D:1111:LEU:HD13 | 2.35 | 0.47 |
| 1:D:121:PRO:O | 1:D:122:ASP:OD2 | 2.32 | 0.47 |
| 1:D:255:SER:HB3 | 1:D:256:PRO:CA | 2.43 | 0.47 |
| 1:D:195:LEU:O | 1:D:267:VAL:CG1 | 2.63 | 0.47 |
| 1:D:484:TRP:HE1 | 1:D:488:LEU:CD1 | 2.28 | 0.47 |
| 1:D:499:LYS:NZ | 1:D:499:LYS:CB | 2.76 | 0.47 |
| 1:D:550:GLN:CG | 1:D:551:LYS:HE3 | 2.45 | 0.47 |
| 1:D:808:ILE:HG22 | 1:D:811:GLN:OE1 | 2.14 | 0.47 |
| 1:D:821:LEU:HB3 | 1:D:822:PRO:HA | 1.95 | 0.47 |
| 1:D:851:THR:OG1 | 1:D:1102:GLN:HG2 | 2.15 | 0.47 |
| 1:D:848:GLY:HA3 | 1:D:855:VAL:HG21 | 1.97 | 0.47 |
| 1:D:921:LEU:CD1 | 1:D:921:LEU:H | 2.27 | 0.47 |
| 1:D:945:HIS:HE1 | 1:D:969:PHE:HB2 | 1.79 | 0.47 |
| 2:E:129:ASP:OD2 | 2:F:97:PRO:O | 2.33 | 0.47 |
| 2:E:481:SER:HA | 2:E:484:ASN:OD1 | 2.14 | 0.47 |
| 2:E:78:PHE:CZ | 2:E:350:LEU:HD12 | 2.49 | 0.47 |
| 2:F:356:LEU:HB3 | 2:F:359:ASN:HB2 | 1.96 | 0.47 |
| 2:F:432:TYR:O | 2:F:435:MET:N | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:F:459:ASP:OD1 | 2:F:461:THR:N | 2.40 | 0.47 |
| 1:A:1068:ASP:O | 1:A:1069:ILE:CB | 2.63 | 0.47 |
| 1:A:119:PRO:C | 1:A:121:PRO:HD3 | 2.35 | 0.47 |
| 1:A:293:ASP:CB | 1:A:296:SER:OG | 2.63 | 0.47 |
| 1:A:305:SER:O | 1:A:309:ARG:HG2 | 2.13 | 0.47 |
| 1:A:557:GLU:C | 1:A:559:LEU:N | 2.67 | 0.47 |
| 1:A:572:TRP:CA | 1:A:572:TRP:CE3 | 2.98 | 0.47 |
| 1:A:581:ASP:OD1 | 1:A:581:ASP:O | 2.32 | 0.47 |
| 1:A:793:GLU:N | 1:A:796:LYS:HD3 | 2.30 | 0.47 |
| 1:A:824:ALA:HA | 1:A:827:ARG:HB3 | 1.96 | 0.47 |
| 1:A:848:GLY:O | 1:A:849:THR:CB | 2.59 | 0.47 |
| 1:A:76:ILE:HG12 | 1:A:911:HIS:NE2 | 2.30 | 0.47 |
| 1:A:950:ASN:O | 1:A:954:ILE:N | 2.31 | 0.47 |
| 1:A:948:ILE:O | 1:A:951:TYR:HB2 | 2.14 | 0.47 |
| 1:A:992:LEU:HB2 | 1:A:997:LEU:HB2 | 1.97 | 0.47 |
| 2:B:246:ARG:C | 2:B:246:ARG:NE | 2.68 | 0.47 |
| 2:B:254:PHE:O | 2:B:257:ARG:N | 2.46 | 0.47 |
| 2:B:445:GLU:C | 2:B:447:THR:N | 2.68 | 0.47 |
| 2:C:216:HIS:O | 2:C:232:GLY:N | 2.40 | 0.47 |
| 2:C:441:VAL:CG1 | 2:C:454:HIS:CE1 | 2.88 | 0.47 |
| 2:C:466:MET:HE2 | 2:C:471:LEU:HB3 | 1.96 | 0.47 |
| 2:C:79:LEU:HD12 | 2:C:98:GLY:O | 2.15 | 0.47 |
| 1:D:1109:LEU:HD21 | 1:D:1137:VAL:CG2 | 2.44 | 0.47 |
| 1:D:1136:GLU:HG3 | 1:D:1138:ARG:NH1 | 2.29 | 0.47 |
| 1:D:1203:PRO:O | 1:D:1204:THR:C | 2.52 | 0.47 |
| 1:D:1204:THR:O | 1:D:1205:GLY:O | 2.32 | 0.47 |
| 1:D:188:ALA:O | 1:D:189:ILE:C | 2.52 | 0.47 |
| 1:D:515:ILE:HG22 | 1:D:565:HIS:ND1 | 2.30 | 0.47 |
| 1:D:733:HIS:CE1 | 1:D:750:PHE:CE1 | 3.02 | 0.47 |
| 1:D:787:SER:O | 1:D:789:PRO:CD | 2.63 | 0.47 |
| 1:D:807:ARG:NH1 | 1:D:1062:GLU:HG2 | 2.30 | 0.47 |
| 1:D:865:ALA:CA | 1:D:872:SER:O | 2.63 | 0.47 |
| 1:D:967:MET:SD | 1:D:975:GLN:HA | 2.55 | 0.47 |
| 1:D:987:ALA:HA | 1:D:991:GLY:HA2 | 1.96 | 0.47 |
| 2:E:246:ARG:HD2 | 2:E:326:ASP:OD1 | 2.13 | 0.47 |
| 2:E:272:ASN:CA | 2:E:292:ASN:HD22 | 2.26 | 0.47 |
| 2:E:193:TYR:HE2 | 2:E:322:LEU:CB | 2.28 | 0.47 |
| 2:F:208:LEU:HD22 | 2:F:242:PHE:CD2 | 2.48 | 0.47 |
| 2:F:311:LEU:O | 2:F:312:LEU:C | 2.52 | 0.47 |
| 2:F:456:ARG:N | 2:F:456:ARG:CD | 2.78 | 0.47 |
| 2:F:458:ARG:CD | 2:F:459:ASP:N | 2.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:468:ILE:O | 2:F:471:LEU:HD13 | 2.15 | 0.47 |
| 1:A:114:GLY:N | 1:A:116:PRO:CD | 2.73 | 0.47 |
| 1:A:81:ARG:HH12 | 1:A:127:LEU:H | 1.61 | 0.47 |
| 1:A:230:GLU:CG | 1:A:231:GLU:N | 2.78 | 0.47 |
| 1:A:371:LYS:O | 1:A:372:GLU:CG | 2.63 | 0.47 |
| 1:A:392:LEU:HD22 | 1:A:393:MET:CE | 2.44 | 0.47 |
| 1:A:500:ALA:HA | 1:A:521:PRO:HD3 | 1.97 | 0.47 |
| 1:A:633:LYS:HZ2 | 1:A:634:LEU:HB2 | 1.80 | 0.47 |
| 1:A:824:ALA:CA | 1:A:827:ARG:HB3 | 2.44 | 0.47 |
| 1:A:830:ASP:C | 1:A:831:TYR:CD1 | 2.83 | 0.47 |
| 1:A:860:LEU:CD2 | 1:A:1133:ILE:HA | 2.44 | 0.47 |
| 1:A:925:LYS:HG2 | 1:A:926:SER:H | 1.78 | 0.47 |
| 1:A:959:GLN:N | 1:A:986:TYR:CE1 | 2.83 | 0.47 |
| 2:B:251:TRP:HA | 2:B:251:TRP:CE3 | 2.49 | 0.47 |
| 2:B:236:GLU:CG | 2:B:341:ASP:HB2 | 2.43 | 0.47 |
| 2:B:81:GLY:O | 2:B:86:LEU:HD11 | 2.14 | 0.47 |
| 2:C:452:LEU:HD12 | 2:C:453:ILE:CA | 2.44 | 0.47 |
| 1:D:1027:LYS:HZ3 | 1:D:1091:GLU:CG | 2.20 | 0.47 |
| 1:D:1055:SER:O | 1:D:1058:PHE:HD2 | 1.97 | 0.47 |
| 1:D:271:VAL:HG22 | 1:D:295:MET:CG | 2.44 | 0.47 |
| 1:D:275:ARG:HG3 | 1:D:279:ARG:HG3 | 1.96 | 0.47 |
| 1:D:307:PHE:O | 1:D:310:SER:OG | 2.23 | 0.47 |
| 1:D:308:GLN:HE22 | 1:D:1027:LYS:HZ2 | 1.63 | 0.47 |
| 1:D:515:ILE:O | 1:D:565:HIS:ND1 | 2.48 | 0.47 |
| 1:D:455:LEU:HD22 | 1:D:794:ILE:HB | 1.96 | 0.47 |
| 1:D:80:SER:O | 1:D:81:ARG:C | 2.52 | 0.47 |
| 1:D:966:LEU:CA | 1:D:970:ASN:HD22 | 2.28 | 0.47 |
| 2:E:254:PHE:HD1 | 2:E:257:ARG:HE | 1.63 | 0.47 |
| 2:F:347:LEU:HD12 | 2:F:347:LEU:N | 2.30 | 0.47 |
| 2:F:360:SER:HB3 | 2:F:364:LYS:CE | 2.44 | 0.47 |
| 2:F:406:LEU:O | 2:F:407:LEU:C | 2.54 | 0.47 |
| 1:A:1019:TRP:O | 1:A:1020:ILE:HB | 2.15 | 0.47 |
| 1:A:867:PRO:HG3 | 1:A:1067:SER:OG | 2.14 | 0.47 |
| 1:A:1144:GLU:H | 1:A:1144:GLU:HG2 | 1.32 | 0.47 |
| 1:A:1150:ALA:CB | 1:A:1223:ILE:HG13 | 2.44 | 0.47 |
| 1:A:132:GLY:CA | 1:A:138:HIS:CE1 | 2.98 | 0.47 |
| 1:A:175:TRP:HB3 | 1:A:186:PRO:CG | 2.45 | 0.47 |
| 1:A:256:PRO:HD2 | 1:A:257:THR:N | 2.19 | 0.47 |
| 1:A:197:PHE:CB | 1:A:277:HIS:CD2 | 2.98 | 0.47 |
| 1:A:295:MET:O | 1:A:299:MET:HG2 | 2.15 | 0.47 |
| 1:A:369:PRO:O | 1:A:370:PRO:C | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:441:TRP:CD1 | 1:A:877:MET:HB3 | 2.49 | 0.47 |
| 1:A:481:GLU:C | 1:A:482:ASP:CG | 2.73 | 0.47 |
| 1:A:79:LEU:HB3 | 1:A:83:LEU:CD2 | 2.45 | 0.47 |
| 1:A:866:ARG:CB | 1:A:867:PRO:HD3 | 2.35 | 0.47 |
| 2:B:400:GLN:CA | 2:B:400:GLN:OE1 | 2.63 | 0.47 |
| 2:C:188:GLY:O | 2:C:190:LEU:N | 2.48 | 0.47 |
| 2:C:241:TRP:CZ3 | 2:C:255:TRP:CE2 | 2.99 | 0.47 |
| 2:C:394:GLU:OE1 | 2:C:394:GLU:N | 2.48 | 0.47 |
| 2:C:398:VAL:HA | 2:C:401:GLY:CA | 2.43 | 0.47 |
| 2:C:469:SER:O | 2:C:472:LYS:HB2 | 2.15 | 0.47 |
| 1:D:1002:GLU:HG3 | 1:D:1003:TRP:N | 2.28 | 0.47 |
| 1:D:948:ILE:CG2 | 1:D:1071:ARG:O | 2.63 | 0.47 |
| 1:D:114:GLY:O | 1:D:116:PRO:HD3 | 2.13 | 0.47 |
| 1:D:249:VAL:CG1 | 1:D:251:THR:HG22 | 2.45 | 0.47 |
| 1:D:497:GLN:O | 1:D:517:GLY:HA2 | 2.15 | 0.47 |
| 1:D:627:ARG:O | 1:D:627:ARG:HG3 | 2.15 | 0.47 |
| 1:D:597:ARG:NH1 | 1:D:725:PRO:CD | 2.78 | 0.47 |
| 2:E:109:ASN:CB | 2:E:378:LEU:HB3 | 2.44 | 0.47 |
| 2:E:182:ARG:N | 2:E:215:PHE:CZ | 2.83 | 0.47 |
| 2:E:319:VAL:CG1 | 2:E:320:SER:N | 2.78 | 0.47 |
| 2:F:303:LEU:CA | 2:F:337:SER:CB | 2.92 | 0.47 |
| 2:F:413:VAL:HG12 | 2:F:414:TRP:H | 1.80 | 0.47 |
| 1:A:290:ARG:O | 1:A:291:PHE:HD2 | 1.98 | 0.47 |
| 1:A:439:GLN:HG2 | 1:A:835:GLY:C | 2.34 | 0.47 |
| 1:A:456:GLN:HE21 | 1:A:798:ILE:CD1 | 2.27 | 0.47 |
| 1:A:465:ASP:CG | 1:A:466:LEU:N | 2.67 | 0.47 |
| 1:A:503:VAL:CG1 | 1:A:520:ALA:C | 2.65 | 0.47 |
| 1:A:576:LEU:CD1 | 1:A:577:CYS:HB2 | 2.41 | 0.47 |
| 1:A:719:LEU:CD2 | 1:A:719:LEU:N | 2.73 | 0.47 |
| 1:A:736:ASN:ND2 | 1:A:736:ASN:N | 2.63 | 0.47 |
| 1:A:739:TYR:O | 1:A:741:ASP:N | 2.25 | 0.47 |
| 1:A:843:GLN:O | 1:A:843:GLN:CG | 2.55 | 0.47 |
| 2:B:257:ARG:O | 2:B:258:HIS:O | 2.33 | 0.47 |
| 2:C:247:THR:HG1 | 2:C:251:TRP:HD1 | 1.58 | 0.47 |
| 2:C:308:ASP:OD1 | 2:C:333:PRO:O | 2.33 | 0.47 |
| 2:C:397:GLN:HG2 | 2:C:398:VAL:N | 2.29 | 0.47 |
| 2:C:94:GLY:HA2 | 2:C:96:HIS:CE1 | 2.49 | 0.47 |
| 1:D:1000:GLU:C | 1:D:1004:LEU:HD13 | 2.35 | 0.47 |
| 1:D:1019:TRP:HD1 | 1:D:1020:ILE:H | 1.63 | 0.47 |
| 1:D:1107:ASP:O | 1:D:1108:TYR:C | 2.53 | 0.47 |
| 1:D:1111:LEU:HD22 | 1:D:1164:PHE:CD1 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1133:ILE:CD1 | 1:D:1133:ILE:N | 2.78 | 0.47 |
| 1:D:196:VAL:CG1 | 1:D:268:GLY:H | 2.27 | 0.47 |
| 1:D:306:SER:CB | 1:D:1058:PHE:CZ | 2.98 | 0.47 |
| 1:D:498:LYS:HD3 | 1:D:521:PRO:HG3 | 1.97 | 0.47 |
| 1:D:616:GLU:O | 1:D:617:ARG:HG3 | 2.14 | 0.47 |
| 1:D:646:VAL:HG12 | 1:D:647:CYS:H | 1.79 | 0.47 |
| 1:D:909:GLY:O | 1:D:912:GLY:N | 2.48 | 0.47 |
| 1:D:923:GLY:HA2 | 1:D:931:LEU:HD11 | 1.96 | 0.47 |
| 1:D:922:GLN:HG3 | 1:D:931:LEU:HD22 | 1.96 | 0.47 |
| 2:E:86:LEU:HB2 | 2:E:91:LEU:HD21 | 1.96 | 0.47 |
| 2:F:406:LEU:CA | 2:F:409:ASN:HD21 | 2.19 | 0.47 |
| 2:F:470:LYS:CE | 2:F:471:LEU:HD21 | 2.45 | 0.47 |
| 1:A:1057:MET:CA | 1:A:1064:ILE:HG21 | 2.45 | 0.46 |
| 1:A:386:ARG:CZ | 1:A:387:GLU:CG | 2.93 | 0.46 |
| 1:A:407:PHE:O | 1:A:411:LEU:HB3 | 2.15 | 0.46 |
| 1:A:465:ASP:C | 1:A:465:ASP:OD1 | 2.54 | 0.46 |
| 1:A:484:TRP:C | 1:A:488:LEU:HG | 2.33 | 0.46 |
| 1:A:601:LYS:HZ3 | 1:A:616:GLU:CG | 2.24 | 0.46 |
| 1:A:752:LEU:CB | 1:A:753:PRO:CA | 2.93 | 0.46 |
| 1:A:879:GLN:CA | 1:A:879:GLN:NE2 | 2.77 | 0.46 |
| 1:A:935:THR:HG21 | 1:A:950:ASN:HD21 | 1.78 | 0.46 |
| 1:A:966:LEU:O | 1:A:970:ASN:N | 2.46 | 0.46 |
| 2:B:283:GLY:HA2 | 2:B:306:LEU:HD23 | 1.97 | 0.46 |
| 2:C:440:THR:O | 2:C:457:SER:OG | 2.24 | 0.46 |
| 1:D:1019:TRP:C | 1:D:1019:TRP:CD1 | 2.87 | 0.46 |
| 1:D:1025:LEU:O | 1:D:1027:LYS:CD | 2.57 | 0.46 |
| 1:D:1040:LYS:C | 1:D:1042:GLU:H | 2.17 | 0.46 |
| 1:D:1209:ARG:HE | 2:F:253:ASP:HB2 | 1.80 | 0.46 |
| 1:D:78:MET:SD | 1:D:121:PRO:HB2 | 2.55 | 0.46 |
| 1:D:1147:TYR:HB3 | 1:D:1227:THR:HG22 | 1.97 | 0.46 |
| 1:D:175:TRP:H | 1:D:220:TRP:HB2 | 1.80 | 0.46 |
| 1:D:173:GLU:OE2 | 1:D:223:TRP:NE1 | 2.48 | 0.46 |
| 1:D:235:TRP:O | 1:D:236:THR:HG23 | 2.15 | 0.46 |
| 1:D:359:VAL:CG1 | 1:D:363:TYR:HB3 | 2.44 | 0.46 |
| 1:D:930:ASP:OD2 | 1:D:930:ASP:O | 2.34 | 0.46 |
| 1:D:963:GLU:HB3 | 1:D:978:ALA:O | 2.15 | 0.46 |
| 2:E:323:HIS:C | 2:E:331:VAL:O | 2.52 | 0.46 |
| 2:E:403:PHE:CE1 | 2:E:407:LEU:HD11 | 2.50 | 0.46 |
| 2:E:461:THR:C | 2:E:462:MET:HE2 | 2.36 | 0.46 |
| 2:F:228:VAL:O | 2:F:228:VAL:HG23 | 2.15 | 0.46 |
| 2:F:343:ASP:O | 2:F:346:MET:HB3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:86:LEU:N | 2:F:86:LEU:HD12 | 2.30 | 0.46 |
| 1:A:1158:LEU:C | 1:A:1162:CYS:SG | 2.93 | 0.46 |
| 1:A:403:THR:O | 1:A:404:HIS:C | 2.53 | 0.46 |
| 1:A:612:LEU:HD23 | 1:A:614:TYR:HA | 1.96 | 0.46 |
| 1:A:657:ARG:O | 1:A:660:CYS:CB | 2.51 | 0.46 |
| 1:A:757:GLY:O | 1:A:758:ASN:CB | 2.62 | 0.46 |
| 1:A:618:HIS:CA | 1:A:762:VAL:HG21 | 2.42 | 0.46 |
| 2:C:109:ASN:O | 2:C:113:GLU:N | 2.31 | 0.46 |
| 2:C:130:ALA:HB1 | 2:C:182:ARG:NH1 | 2.24 | 0.46 |
| 2:C:78:PHE:CE2 | 2:C:350:LEU:HD23 | 2.50 | 0.46 |
| 1:D:1042:GLU:C | 1:D:1044:VAL:H | 2.19 | 0.46 |
| 1:D:1064:ILE:O | 1:D:1064:ILE:CG2 | 2.62 | 0.46 |
| 1:D:944:GLU:OE1 | 1:D:1071:ARG:NH1 | 2.49 | 0.46 |
| 1:D:1122:GLU:O | 1:D:1123:PHE:CD1 | 2.68 | 0.46 |
| 1:D:1187:ARG:HG3 | 1:D:1212:ILE:HG12 | 1.96 | 0.46 |
| 1:D:307:PHE:CD2 | 1:D:1048:ALA:HB1 | 2.50 | 0.46 |
| 1:D:417:ARG:CG | 1:D:417:ARG:HH11 | 2.28 | 0.46 |
| 1:D:648:PRO:CG | 1:D:649:TYR:N | 2.78 | 0.46 |
| 1:D:735:GLY:CA | 1:D:749:PHE:CB | 2.79 | 0.46 |
| 2:E:303:LEU:N | 2:E:303:LEU:HD12 | 2.29 | 0.46 |
| 2:E:96:HIS:C | 2:E:98:GLY:N | 2.68 | 0.46 |
| 2:F:349:TYR:O | 2:F:352:ASP:HB3 | 2.14 | 0.46 |
| 2:F:447:THR:HA | 2:F:452:LEU:C | 2.35 | 0.46 |
| 1:A:1019:TRP:C | 1:A:1020:ILE:HG22 | 2.35 | 0.46 |
| 1:A:1048:ALA:HB3 | 1:A:1092:PHE:CE1 | 2.48 | 0.46 |
| 1:A:1094:THR:O | 1:A:1095:SER:C | 2.53 | 0.46 |
| 1:A:1113:LEU:HD23 | 1:A:1113:LEU:H | 1.78 | 0.46 |
| 1:A:1124:ALA:CA | 1:A:1148:ARG:NH1 | 2.78 | 0.46 |
| 1:A:1124:ALA:O | 1:A:1126:ASP:OD1 | 2.34 | 0.46 |
| 1:A:1131:ILE:HD13 | 1:A:1137:VAL:CA | 2.46 | 0.46 |
| 1:A:237:SER:O | 1:A:238:GLN:HB2 | 2.15 | 0.46 |
| 1:A:272:SER:CA | 1:A:275:ARG:HB2 | 2.35 | 0.46 |
| 1:A:294:THR:HG22 | 1:A:411:LEU:CD2 | 2.46 | 0.46 |
| 1:A:887:VAL:HG23 | 1:A:1146:ARG:NH1 | 2.20 | 0.46 |
| 2:B:212:GLY:O | 2:B:235:THR:O | 2.34 | 0.46 |
| 2:B:99:PHE:CE2 | 2:C:131:LEU:HD11 | 2.44 | 0.46 |
| 2:C:208:LEU:HD11 | 2:C:240:VAL:CA | 2.45 | 0.46 |
| 2:C:272:ASN:CB | 2:C:292:ASN:HB2 | 2.43 | 0.46 |
| 2:C:344:ARG:CB | 2:C:347:LEU:HD22 | 2.46 | 0.46 |
| 2:C:402:LEU:O | 2:C:403:PHE:C | 2.54 | 0.46 |
| 2:C:464:GLU:OE2 | 2:C:466:MET:SD | 2.74 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:88:ARG:NH1 | 2:C:88:ARG:CB | 2.78 | 0.46 |
| 2:C:90:SER:O | 2:C:93:SER:OG | 2.26 | 0.46 |
| 1:D:1020:ILE:HD13 | 1:D:1021:SER:HA | 1.94 | 0.46 |
| 1:D:1030:ARG:C | 1:D:1032:THR:N | 2.68 | 0.46 |
| 1:D:1060:LYS:HD2 | 1:D:1060:LYS:H | 1.80 | 0.46 |
| 1:D:118:VAL:CG2 | 1:D:121:PRO:HD3 | 2.45 | 0.46 |
| 1:D:1224:ILE:O | 1:D:1227:THR:C | 2.54 | 0.46 |
| 1:D:184:ALA:C | 1:D:185:VAL:CG1 | 2.84 | 0.46 |
| 1:D:486:TRP:CA | 1:D:489:GLU:OE2 | 2.56 | 0.46 |
| 1:D:524:PRO:O | 1:D:525:MET:CB | 2.53 | 0.46 |
| 1:D:668:LEU:HD23 | 1:D:668:LEU:N | 2.30 | 0.46 |
| 1:D:656:TYR:CG | 1:D:744:ILE:HD12 | 2.49 | 0.46 |
| 1:D:73:PRO:O | 1:D:74:LEU:HD22 | 2.15 | 0.46 |
| 1:D:768:LYS:CA | 1:D:772:PRO:CG | 2.93 | 0.46 |
| 1:D:886:LEU:HA | 1:D:1146:ARG:HH22 | 1.81 | 0.46 |
| 2:F:256:LEU:HD12 | 2:F:256:LEU:HA | 1.82 | 0.46 |
| 2:F:314:MET:CE | 2:F:315:TYR:CE2 | 2.94 | 0.46 |
| 2:F:242:PHE:CB | 2:F:333:PRO:HB2 | 2.25 | 0.46 |
| 1:D:546:ARG:HH22 | 2:F:408:GLU:CD | 2.19 | 0.46 |
| 2:F:421:MET:HE3 | 2:F:421:MET:HB2 | 1.85 | 0.46 |
| 2:F:454:HIS:NE2 | 2:F:472:LYS:CE | 2.78 | 0.46 |
| 2:F:470:LYS:HB2 | 2:F:471:LEU:HG | 1.96 | 0.46 |
| 2:F:84:GLN:C | 2:F:86:LEU:N | 2.68 | 0.46 |
| 1:A:1068:ASP:O | 1:A:1069:ILE:CG2 | 2.64 | 0.46 |
| 1:A:430:MET:HA | 1:A:1130:CYS:SG | 2.55 | 0.46 |
| 1:A:77:GLN:HB3 | 1:A:1174:PRO:HB3 | 1.96 | 0.46 |
| 1:A:134:ASN:O | 1:A:137:GLN:N | 2.47 | 0.46 |
| 1:A:196:VAL:HG11 | 1:A:404:HIS:CB | 2.45 | 0.46 |
| 1:A:259:ARG:CA | 1:A:259:ARG:HE | 2.27 | 0.46 |
| 1:A:273:PHE:C | 1:A:276:ALA:CB | 2.83 | 0.46 |
| 1:A:752:LEU:HB3 | 1:A:753:PRO:HA | 1.98 | 0.46 |
| 1:A:827:ARG:CG | 1:A:828:HIS:N | 2.78 | 0.46 |
| 1:A:873:GLU:OE1 | 1:A:875:LYS:HG2 | 2.15 | 0.46 |
| 1:A:949:PHE:HD2 | 1:A:949:PHE:H | 1.62 | 0.46 |
| 1:A:960:PRO:HD2 | 1:A:961:PHE:HE1 | 1.79 | 0.46 |
| 2:B:117:SER:CB | 2:B:262:TRP:HE1 | 2.21 | 0.46 |
| 2:C:134:LYS:HB2 | 2:C:180:LYS:HE2 | 1.96 | 0.46 |
| 2:C:184:ASN:C | 2:C:186:LEU:N | 2.67 | 0.46 |
| 2:C:201:ASN:O | 2:C:202:LYS:CB | 2.64 | 0.46 |
| 2:C:400:GLN:CD | 2:C:400:GLN:C | 2.74 | 0.46 |
| 2:C:428:LEU:O | 2:C:429:TYR:C | 2.52 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:448:LEU:O | 2:C:449:GLU:HG3 | 2.16 | 0.46 |
| 2:C:474:PHE:CE1 | 2:C:478:TYR:CD2 | 2.94 | 0.46 |
| 2:C:67:GLU:O | 2:C:71:GLU:N | 2.46 | 0.46 |
| 1:D:1019:TRP:CZ2 | 1:D:1167:LYS:HG3 | 2.51 | 0.46 |
| 1:D:1030:ARG:HA | 1:D:1030:ARG:HD3 | 1.54 | 0.46 |
| 1:D:1157:ASN:O | 1:D:1158:LEU:C | 2.54 | 0.46 |
| 1:D:1209:ARG:NH1 | 2:F:285:LYS:NZ | 2.63 | 0.46 |
| 1:D:253:ALA:HB2 | 1:D:281:GLN:N | 2.30 | 0.46 |
| 1:D:271:VAL:HG22 | 1:D:295:MET:CB | 2.46 | 0.46 |
| 1:D:307:PHE:C | 1:D:311:LEU:HD12 | 2.34 | 0.46 |
| 1:D:309:ARG:O | 1:D:310:SER:C | 2.49 | 0.46 |
| 1:D:720:THR:C | 1:D:721:ALA:O | 2.32 | 0.46 |
| 1:D:794:ILE:O | 1:D:798:ILE:HG23 | 2.15 | 0.46 |
| 1:D:945:HIS:CE1 | 1:D:969:PHE:CB | 2.99 | 0.46 |
| 2:E:184:ASN:C | 2:E:186:LEU:N | 2.68 | 0.46 |
| 2:E:293:PHE:O | 2:E:295:TRP:N | 2.49 | 0.46 |
| 2:E:345:GLY:O | 2:E:348:ALA:HB3 | 2.15 | 0.46 |
| 2:E:353:SER:OG | 2:E:372:LEU:HD21 | 2.15 | 0.46 |
| 2:E:460:THR:C | 2:E:461:THR:HG22 | 2.35 | 0.46 |
| 2:F:145:PHE:O | 2:F:146:ARG:CG | 2.64 | 0.46 |
| 2:F:197:LEU:O | 2:F:202:LYS:CA | 2.60 | 0.46 |
| 2:F:213:VAL:CG2 | 2:F:235:THR:OG1 | 2.63 | 0.46 |
| 2:F:317:GLY:C | 2:F:319:VAL:N | 2.56 | 0.46 |
| 2:F:414:TRP:O | 2:F:415:PRO:O | 2.34 | 0.46 |
| 1:D:472:GLN:C | 2:F:461:THR:HG23 | 2.36 | 0.46 |
| 1:A:1017:GLY:C | 1:A:1019:TRP:N | 2.69 | 0.46 |
| 1:A:1020:ILE:CG1 | 1:A:1021:SER:H | 2.28 | 0.46 |
| 1:A:1165:ALA:HB2 | 1:A:1173:LEU:HD11 | 1.97 | 0.46 |
| 1:A:1222:GLN:O | 1:A:1225:GLU:HB2 | 2.15 | 0.46 |
| 1:A:192:GLU:OE2 | 1:A:193:ARG:N | 2.48 | 0.46 |
| 1:A:213:VAL:N | 1:A:221:TYR:HE2 | 2.11 | 0.46 |
| 1:A:313:ILE:HD12 | 1:A:313:ILE:C | 2.36 | 0.46 |
| 1:A:452:TYR:HA | 1:A:869:ARG:NH2 | 2.19 | 0.46 |
| 1:A:634:LEU:CB | 1:A:635:PRO:CA | 2.78 | 0.46 |
| 1:A:666:GLN:HA | 1:A:669:MET:CE | 2.45 | 0.46 |
| 1:A:711:ALA:C | 1:A:713:PRO:CD | 2.65 | 0.46 |
| 1:A:720:THR:CG2 | 1:A:721:ALA:H | 2.28 | 0.46 |
| 1:A:959:GLN:CB | 1:A:960:PRO:CD | 2.60 | 0.46 |
| 1:A:967:MET:O | 1:A:970:ASN:O | 2.33 | 0.46 |
| 2:B:102:LEU:HD12 | 2:B:102:LEU:N | 2.19 | 0.46 |
| 2:B:306:LEU:O | 2:B:335:VAL:HB | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:336:LEU:HG | 2:B:337:SER:N | 2.30 | 0.46 |
| 2:C:236:GLU:CB | 2:C:341:ASP:HB3 | 2.45 | 0.46 |
| 2:C:360:SER:HB3 | 2:C:364:LYS:HE2 | 1.97 | 0.46 |
| 1:D:1042:GLU:C | 1:D:1044:VAL:N | 2.69 | 0.46 |
| 1:D:1058:PHE:CG | 1:D:1059:ASN:N | 2.82 | 0.46 |
| 1:D:1124:ALA:CB | 1:D:1148:ARG:HH12 | 2.26 | 0.46 |
| 1:D:192:GLU:HG2 | 1:D:193:ARG:N | 2.31 | 0.46 |
| 1:D:272:SER:HB3 | 1:D:843:GLN:OE1 | 2.15 | 0.46 |
| 1:D:429:GLU:HG2 | 1:D:1117:LYS:CE | 2.42 | 0.46 |
| 1:D:460:LYS:HG2 | 1:D:461:LYS:H | 1.80 | 0.46 |
| 1:D:599:THR:C | 1:D:602:LEU:HD12 | 2.36 | 0.46 |
| 1:D:751:LYS:HE2 | 1:D:751:LYS:HB3 | 1.55 | 0.46 |
| 1:D:865:ALA:HB1 | 1:D:872:SER:CB | 2.45 | 0.46 |
| 1:D:995:TYR:H | 1:D:996:ARG:HH11 | 1.58 | 0.46 |
| 2:E:116:THR:C | 2:E:118:VAL:N | 2.69 | 0.46 |
| 2:E:315:TYR:O | 2:E:316:PRO:O | 2.34 | 0.46 |
| 2:E:84:GLN:NE2 | 2:E:84:GLN:O | 2.49 | 0.46 |
| 2:F:233:GLU:O | 2:F:234:LYS:CG | 2.61 | 0.46 |
| 2:F:367:LEU:HD12 | 2:F:367:LEU:C | 2.36 | 0.46 |
| 2:F:454:HIS:HB2 | 2:F:466:MET:CA | 2.45 | 0.46 |
| 1:A:1030:ARG:CD | 1:A:1040:LYS:HZ2 | 2.29 | 0.46 |
| 1:A:1043:VAL:HG22 | 1:A:1046:GLU:HB3 | 1.98 | 0.46 |
| 1:A:285:GLN:HA | 1:A:1128:ARG:NH2 | 2.31 | 0.46 |
| 1:A:860:LEU:HD23 | 1:A:1133:ILE:HG12 | 1.96 | 0.46 |
| 1:A:1190:ARG:CZ | 1:A:1190:ARG:HB2 | 2.45 | 0.46 |
| 1:A:132:GLY:HA2 | 1:A:138:HIS:CE1 | 2.50 | 0.46 |
| 1:A:195:LEU:CD2 | 1:A:217:PRO:CD | 2.87 | 0.46 |
| 1:A:252:GLY:O | 1:A:253:ALA:CB | 2.64 | 0.46 |
| 1:A:309:ARG:HA | 1:A:312:TRP:HB2 | 1.98 | 0.46 |
| 1:A:313:ILE:HG13 | 1:A:314:ALA:N | 2.31 | 0.46 |
| 1:A:441:TRP:HE1 | 1:A:878:VAL:N | 2.13 | 0.46 |
| 1:A:503:VAL:CB | 1:A:521:PRO:CA | 2.76 | 0.46 |
| 1:A:569:HIS:CB | 1:A:570:PRO:HD2 | 2.45 | 0.46 |
| 1:A:570:PRO:HG3 | 1:A:572:TRP:CZ3 | 2.51 | 0.46 |
| 1:A:649:TYR:HA | 1:A:652:ILE:HB | 1.97 | 0.46 |
| 1:A:817:PRO:HG2 | 1:A:818:ARG:N | 2.30 | 0.46 |
| 1:A:973:LEU:CB | 1:A:977:GLU:HB2 | 2.45 | 0.46 |
| 2:B:187:HIS:O | 2:B:190:LEU:HB2 | 2.16 | 0.46 |
| 2:B:423:SER:HG | 2:B:428:LEU:HD22 | 1.79 | 0.46 |
| 2:B:74:GLN:O | 2:B:75:ARG:C | 2.53 | 0.46 |
| 2:C:185:LEU:CG | 2:C:214:CYS:SG | 3.03 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:300:ILE:CA | 2:C:342:LEU:HD12 | 2.42 | 0.46 |
| 2:C:375:HIS:NE2 | 2:C:377:CYS:SG | 2.87 | 0.46 |
| 1:D:1014:ARG:NE | 1:D:1022:LEU:HD22 | 2.30 | 0.46 |
| 1:D:1019:TRP:CE3 | 1:D:1168:LEU:CG | 2.75 | 0.46 |
| 1:D:1151:LEU:HD11 | 1:D:1227:THR:OG1 | 2.15 | 0.46 |
| 1:D:157:LEU:N | 1:D:157:LEU:HD23 | 2.30 | 0.46 |
| 1:D:163:PRO:HB2 | 1:D:165:LYS:CG | 2.36 | 0.46 |
| 1:D:179:GLY:C | 1:D:182:GLY:N | 2.69 | 0.46 |
| 1:D:345:TRP:N | 1:D:1040:LYS:HZ2 | 2.13 | 0.46 |
| 1:D:503:VAL:O | 1:D:505:LYS:O | 2.33 | 0.46 |
| 1:D:636:THR:CG2 | 1:D:637:GLY:N | 2.74 | 0.46 |
| 1:D:719:LEU:O | 1:D:722:ARG:HD3 | 2.15 | 0.46 |
| 1:D:720:THR:HA | 1:D:721:ALA:O | 2.15 | 0.46 |
| 1:D:827:ARG:CG | 1:D:828:HIS:N | 2.79 | 0.46 |
| 2:E:283:GLY:HA3 | 2:E:306:LEU:HD23 | 1.98 | 0.46 |
| 2:E:311:LEU:N | 2:E:314:MET:HG3 | 2.31 | 0.46 |
| 2:E:326:ASP:O | 2:E:327:GLY:C | 2.54 | 0.46 |
| 2:F:280:ASP:C | 2:F:282:GLU:H | 2.19 | 0.46 |
| 2:F:322:LEU:HD22 | 2:F:323:HIS:N | 2.31 | 0.46 |
| 2:F:431:LYS:O | 2:F:434:GLU:HB2 | 2.15 | 0.46 |
| 2:F:477:LYS:O | 2:F:478:TYR:C | 2.53 | 0.46 |
| 2:F:61:GLY:HA2 | 2:F:64:GLU:HG2 | 1.97 | 0.46 |
| 1:A:773:LYS:HZ1 | 1:A:1057:MET:HE3 | 1.81 | 0.46 |
| 1:A:1123:PHE:C | 1:A:1125:ILE:H | 2.19 | 0.46 |
| 1:A:1171:ASN:O | 1:A:1172:ASP:OD1 | 2.33 | 0.46 |
| 1:A:265:LEU:C | 1:A:265:LEU:HD12 | 2.36 | 0.46 |
| 1:A:297:MET:HE2 | 1:A:297:MET:HB3 | 1.62 | 0.46 |
| 1:A:311:LEU:HD22 | 1:A:1047:ARG:HD2 | 1.97 | 0.46 |
| 1:A:363:ARG:HH21 | 1:A:410:GLN:HG2 | 1.81 | 0.46 |
| 1:A:439:GLN:NE2 | 1:A:837:TYR:CE2 | 2.79 | 0.46 |
| 1:A:599:THR:HB | 1:A:600:PRO:HD3 | 1.96 | 0.46 |
| 1:A:657:ARG:HD3 | 1:A:744:ILE:CG2 | 2.45 | 0.46 |
| 1:A:731:SER:O | 1:A:732:TYR:C | 2.52 | 0.46 |
| 1:A:751:LYS:HB3 | 1:A:751:LYS:HE2 | 1.57 | 0.46 |
| 1:A:70:ARG:HD3 | 1:A:81:ARG:CB | 2.44 | 0.46 |
| 2:B:132:HIS:HA | 2:B:182:ARG:CZ | 2.46 | 0.46 |
| 2:B:475:LEU:CA | 2:B:479:ILE:HD13 | 2.46 | 0.46 |
| 2:C:115:TRP:NE1 | 2:C:119:VAL:CG2 | 2.79 | 0.46 |
| 2:C:243:THR:HG21 | 2:C:247:THR:HG1 | 1.80 | 0.46 |
| 1:D:1192:GLU:O | 1:D:1192:GLU:CG | 2.59 | 0.46 |
| 1:D:1206:MET:SD | 1:D:1206:MET:C | 2.93 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:1206:MET:SD | 2:F:257:ARG:NH1 | 2.88 | 0.46 |
| 1:D:201:VAL:HG13 | 1:D:202:CYS:N | 2.31 | 0.46 |
| 1:D:271:VAL:CG2 | 1:D:295:MET:HG3 | 2.46 | 0.46 |
| 1:D:375:GLU:HG3 | 1:D:379:LYS:HG3 | 1.93 | 0.46 |
| 1:D:623:LEU:HB3 | 1:D:667:GLN:HE22 | 1.71 | 0.46 |
| 1:D:658:LYS:HE3 | 1:D:713:PRO:HG3 | 1.98 | 0.46 |
| 1:D:748:TRP:CE3 | 1:D:748:TRP:O | 2.69 | 0.46 |
| 1:D:444:TYR:CZ | 1:D:877:MET:HE1 | 2.51 | 0.46 |
| 1:D:943:ARG:O | 1:D:946:ALA:N | 2.49 | 0.46 |
| 2:E:116:THR:C | 2:E:120:VAL:HG12 | 2.36 | 0.46 |
| 2:E:325:ARG:HG2 | 2:E:330:ASN:H | 1.80 | 0.46 |
| 2:E:373:LYS:O | 2:E:374:LEU:HG | 2.16 | 0.46 |
| 2:E:99:PHE:O | 2:F:128:VAL:CG1 | 2.63 | 0.46 |
| 2:F:115:TRP:CD1 | 2:F:119:VAL:CG2 | 2.98 | 0.46 |
| 2:F:295:TRP:O | 2:F:295:TRP:CD1 | 2.69 | 0.46 |
| 2:F:300:ILE:HA | 2:F:342:LEU:HD12 | 1.97 | 0.46 |
| 2:F:344:ARG:O | 2:F:345:GLY:C | 2.52 | 0.46 |
| 2:F:354:PHE:HD1 | 2:F:371:VAL:O | 1.98 | 0.46 |
| 2:F:455:LEU:HB3 | 2:F:456:ARG:NE | 2.29 | 0.46 |
| 2:F:459:ASP:O | 2:F:460:THR:HB | 2.16 | 0.46 |
| 2:F:70:LEU:HD13 | 2:F:70:LEU:C | 2.36 | 0.46 |
| 1:A:1141:VAL:HG12 | 1:A:1142:ARG:N | 2.31 | 0.46 |
| 1:A:282:TYR:CE2 | 1:A:291:PHE:CE1 | 3.04 | 0.46 |
| 1:A:302:SER:HB2 | 1:A:351:SER:CB | 2.45 | 0.46 |
| 1:A:369:PRO:O | 1:A:371:LYS:N | 2.49 | 0.46 |
| 1:A:539:PHE:O | 1:A:540:GLN:HB2 | 2.16 | 0.46 |
| 1:A:630:ASN:ND2 | 1:A:631:LEU:N | 2.62 | 0.46 |
| 1:A:658:LYS:O | 1:A:662:GLU:CD | 2.53 | 0.46 |
| 1:A:732:TYR:HD1 | 1:A:755:LYS:NZ | 2.08 | 0.46 |
| 1:A:657:ARG:HD3 | 1:A:744:ILE:HG22 | 1.98 | 0.46 |
| 1:A:829:PRO:O | 1:A:830:ASP:HB2 | 2.15 | 0.46 |
| 1:A:933:SER:CB | 1:A:943:ARG:CZ | 2.91 | 0.46 |
| 1:A:993:ARG:HG3 | 1:A:994:TRP:HD1 | 1.81 | 0.46 |
| 2:B:126:PHE:HB3 | 2:C:101:PRO:HB3 | 1.98 | 0.46 |
| 2:B:261:GLN:O | 2:B:262:TRP:O | 2.34 | 0.46 |
| 2:B:289:LEU:HB3 | 2:B:300:ILE:HG13 | 1.97 | 0.46 |
| 2:B:378:LEU:CD1 | 2:B:378:LEU:N | 2.78 | 0.46 |
| 2:B:454:HIS:N | 2:B:454:HIS:ND1 | 2.63 | 0.46 |
| 2:C:115:TRP:NE1 | 2:C:119:VAL:HG21 | 2.31 | 0.46 |
| 2:C:221:THR:CG2 | 2:C:222:LYS:H | 2.28 | 0.46 |
| 2:C:291:TYR:CD1 | 2:C:348:ALA:HB1 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:348:ALA:O | 2:C:351:TYR:CB | 2.63 | 0.46 |
| 2:C:361:PHE:CD2 | 2:C:362:THR:HG23 | 2.48 | 0.46 |
| 2:C:455:LEU:HD12 | 2:C:455:LEU:H | 1.81 | 0.46 |
| 1:D:1050:LYS:O | 1:D:1053:THR:HB | 2.16 | 0.46 |
| 1:D:877:MET:HE3 | 1:D:1207:GLU:HB2 | 1.97 | 0.46 |
| 1:D:1207:GLU:CB | 1:D:1210:TYR:HD2 | 2.28 | 0.46 |
| 1:D:270:ASN:N | 1:D:294:THR:HG23 | 2.30 | 0.46 |
| 1:D:374:ARG:NE | 1:D:392:LEU:HD21 | 2.31 | 0.46 |
| 1:D:559:LEU:CD1 | 1:D:560:PRO:HD3 | 2.39 | 0.46 |
| 1:D:597:ARG:HG2 | 1:D:617:ARG:HD2 | 1.98 | 0.46 |
| 1:D:622:TYR:O | 1:D:746:GLY:HA2 | 2.14 | 0.46 |
| 1:D:649:TYR:O | 1:D:653:GLU:N | 2.45 | 0.46 |
| 1:D:664:GLY:CA | 1:D:667:GLN:HG3 | 2.45 | 0.46 |
| 1:D:729:GLN:HB3 | 1:D:731:SER:OG | 2.16 | 0.46 |
| 2:E:230:SER:O | 2:E:231:ILE:HB | 2.15 | 0.46 |
| 2:E:344:ARG:O | 2:E:346:MET:N | 2.49 | 0.46 |
| 2:E:390:GLY:HA3 | 2:E:395:LEU:HD23 | 1.98 | 0.46 |
| 2:E:428:LEU:O | 2:E:431:LYS:CB | 2.57 | 0.46 |
| 2:F:389:ARG:CD | 2:F:390:GLY:H | 2.28 | 0.46 |
| 1:D:457:ARG:NH2 | 2:F:485:VAL:HG23 | 2.20 | 0.46 |
| 1:A:1067:SER:O | 1:A:1068:ASP:CB | 2.62 | 0.46 |
| 1:A:1068:ASP:H | 1:A:1071:ARG:CD | 2.28 | 0.46 |
| 1:A:1111:LEU:N | 1:A:1111:LEU:CD1 | 2.79 | 0.46 |
| 1:A:1198:LYS:O | 1:A:1199:THR:OG1 | 2.33 | 0.46 |
| 1:A:598:VAL:N | 1:A:616:GLU:OE1 | 2.49 | 0.46 |
| 1:A:801:TRP:O | 1:A:805:HIS:CB | 2.64 | 0.46 |
| 1:A:879:GLN:HG3 | 1:A:886:LEU:CD1 | 2.46 | 0.46 |
| 1:A:76:ILE:CG2 | 1:A:911:HIS:CE1 | 2.98 | 0.46 |
| 2:B:79:LEU:HA | 2:B:100:GLY:HA3 | 1.98 | 0.46 |
| 2:B:259:ARG:O | 2:B:260:LEU:O | 2.34 | 0.46 |
| 2:B:283:GLY:O | 2:B:284:ARG:CB | 2.64 | 0.46 |
| 2:B:447:THR:HG23 | 2:B:451:GLY:C | 2.35 | 0.46 |
| 1:A:604:ALA:HB3 | 2:C:363:ARG:NH2 | 2.30 | 0.46 |
| 1:D:1024:ASP:O | 1:D:1026:ARG:N | 2.48 | 0.46 |
| 1:D:1162:CYS:O | 1:D:1166:TYR:CE1 | 2.69 | 0.46 |
| 1:D:1172:ASP:O | 1:D:1173:LEU:CG | 2.44 | 0.46 |
| 1:D:1198:LYS:O | 1:D:1201:SER:O | 2.34 | 0.46 |
| 1:D:868:ASP:OD1 | 1:D:1199:THR:CB | 2.63 | 0.46 |
| 1:D:140:ARG:NH1 | 1:D:140:ARG:CG | 2.74 | 0.46 |
| 1:D:277:HIS:C | 1:D:291:PHE:CE1 | 2.89 | 0.46 |
| 1:D:293:ASP:CB | 1:D:296:SER:CB | 2.94 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:400:VAL:O | 1:D:400:VAL:HG12 | 2.16 | 0.46 |
| 1:D:550:GLN:OE1 | 1:D:551:LYS:HE3 | 2.16 | 0.46 |
| 1:D:794:ILE:HA | 1:D:797:MET:HG3 | 1.96 | 0.46 |
| 1:D:822:PRO:N | 1:D:825:VAL:HB | 2.31 | 0.46 |
| 1:D:865:ALA:CB | 1:D:872:SER:O | 2.63 | 0.46 |
| 1:D:88:PHE:O | 1:D:1172:ASP:OD1 | 2.33 | 0.46 |
| 1:D:116:PRO:CA | 1:D:921:LEU:HD13 | 2.40 | 0.46 |
| 2:E:114:TRP:CZ2 | 2:E:238:SER:O | 2.69 | 0.46 |
| 2:E:386:ASP:N | 2:E:414:TRP:O | 2.49 | 0.46 |
| 2:F:259:ARG:HE | 2:F:339:ASN:ND2 | 2.14 | 0.46 |
| 2:F:92:LEU:CD2 | 2:F:344:ARG:HE | 2.27 | 0.46 |
| 1:A:176:THR:O | 1:A:177:ARG:HG2 | 2.16 | 0.46 |
| 1:A:811:GLN:HB2 | 1:A:840:ILE:CG2 | 2.33 | 0.46 |
| 1:A:821:LEU:CG | 1:A:826:ILE:HG23 | 2.43 | 0.46 |
| 1:A:845:VAL:CG2 | 1:A:855:VAL:HB | 2.45 | 0.46 |
| 1:A:952:GLY:HA2 | 1:A:955:TYR:HD1 | 1.81 | 0.46 |
| 1:A:987:ALA:HA | 1:A:991:GLY:HA3 | 1.98 | 0.46 |
| 2:B:182:ARG:O | 2:B:215:PHE:HB2 | 2.15 | 0.46 |
| 2:B:245:PRO:O | 2:B:248:SER:CB | 2.64 | 0.46 |
| 2:B:400:GLN:O | 2:B:403:PHE:HB3 | 2.15 | 0.46 |
| 2:B:374:LEU:N | 2:B:458:ARG:NH1 | 2.64 | 0.46 |
| 2:C:130:ALA:CA | 2:C:182:ARG:NH1 | 2.79 | 0.46 |
| 2:C:350:LEU:N | 2:C:350:LEU:CD1 | 2.58 | 0.46 |
| 2:C:444:THR:H | 2:C:447:THR:CG2 | 2.23 | 0.46 |
| 2:C:452:LEU:HD12 | 2:C:453:ILE:HG13 | 1.98 | 0.46 |
| 2:C:74:GLN:NE2 | 2:C:75:ARG:HH21 | 2.14 | 0.46 |
| 1:D:1034:ARG:O | 1:D:1035:LYS:HB2 | 2.16 | 0.46 |
| 1:D:1118:TRP:C | 1:D:1122:GLU:HG2 | 2.35 | 0.46 |
| 1:D:150:TYR:CE1 | 1:D:266:VAL:HG21 | 2.51 | 0.46 |
| 1:D:279:ARG:O | 1:D:841:LEU:CG | 2.54 | 0.46 |
| 1:D:368:PRO:CB | 1:D:369:LEU:CD2 | 2.94 | 0.46 |
| 1:D:627:ARG:O | 1:D:627:ARG:CG | 2.64 | 0.46 |
| 1:D:652:ILE:HA | 1:D:655:LEU:CB | 2.46 | 0.46 |
| 1:D:665:LYS:O | 1:D:669:MET:N | 2.38 | 0.46 |
| 1:D:770:PHE:O | 1:D:773:LYS:CG | 2.64 | 0.46 |
| 1:D:801:TRP:CD2 | 1:D:870:VAL:CG1 | 2.99 | 0.46 |
| 1:D:904:ASP:OD1 | 1:D:915:ALA:HB3 | 2.16 | 0.46 |
| 1:D:935:THR:O | 1:D:938:THR:OG1 | 2.33 | 0.46 |
| 1:D:932:HIS:CE1 | 1:D:947:LYS:HG2 | 2.51 | 0.46 |
| 1:D:986:TYR:CD1 | 1:D:990:LYS:HD2 | 2.51 | 0.46 |
| 2:E:254:PHE:CZ | 2:E:258:HIS:HB2 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:263:TRP:CH2 | 2:E:300:ILE:HD12 | 2.51 | 0.46 |
| 2:E:419:GLU:OE1 | 2:E:420:THR:HG22 | 2.16 | 0.46 |
| 2:F:246:ARG:C | 2:F:248:SER:N | 2.56 | 0.46 |
| 2:F:306:LEU:HB3 | 2:F:335:VAL:HG21 | 1.98 | 0.46 |
| 2:F:423:SER:OG | 2:F:424:SER:N | 2.47 | 0.46 |
| 2:F:63:GLY:O | 2:F:67:GLU:HG3 | 2.16 | 0.46 |
| 2:F:76:ARG:CG | 2:F:76:ARG:NH1 | 2.79 | 0.46 |
| 1:A:1069:ILE:O | 1:A:1069:ILE:HD13 | 2.16 | 0.45 |
| 1:A:1109:LEU:HD13 | 1:A:1109:LEU:HA | 1.60 | 0.45 |
| 1:A:1198:LYS:HA | 1:A:1204:THR:HG23 | 1.98 | 0.45 |
| 1:A:1227:THR:O | 1:A:1228:LYS:O | 2.35 | 0.45 |
| 1:A:185:VAL:N | 1:A:186:PRO:CD | 2.80 | 0.45 |
| 1:A:238:GLN:CB | 1:A:239:LEU:HG | 2.42 | 0.45 |
| 1:A:407:PHE:N | 1:A:407:PHE:CD2 | 2.83 | 0.45 |
| 1:A:438:ASN:O | 1:A:439:GLN:C | 2.55 | 0.45 |
| 1:A:600:PRO:HG3 | 1:A:765:PRO:HG3 | 1.98 | 0.45 |
| 1:A:608:ASP:CA | 1:A:620:TRP:HH2 | 2.29 | 0.45 |
| 1:A:77:GLN:O | 1:A:79:LEU:HG | 2.16 | 0.45 |
| 1:A:788:GLY:O | 1:A:791:ALA:HB3 | 2.16 | 0.45 |
| 1:A:808:ILE:O | 1:A:811:GLN:NE2 | 2.49 | 0.45 |
| 1:A:857:PRO:O | 1:A:861:THR:CB | 2.64 | 0.45 |
| 1:A:94:MET:SD | 1:A:909:GLY:HA3 | 2.56 | 0.45 |
| 1:A:943:ARG:O | 1:A:946:ALA:N | 2.49 | 0.45 |
| 2:B:246:ARG:O | 2:B:248:SER:N | 2.49 | 0.45 |
| 2:B:439:PHE:HD1 | 2:B:456:ARG:O | 1.98 | 0.45 |
| 2:C:310:GLU:CD | 2:C:310:GLU:N | 2.70 | 0.45 |
| 2:C:394:GLU:CA | 2:C:397:GLN:HB3 | 2.45 | 0.45 |
| 2:C:432:TYR:O | 2:C:436:SER:N | 2.48 | 0.45 |
| 2:C:395:LEU:CD2 | 2:C:443:VAL:CG1 | 2.89 | 0.45 |
| 2:C:471:LEU:O | 2:C:472:LYS:C | 2.55 | 0.45 |
| 2:C:470:LYS:O | 2:C:474:PHE:N | 2.49 | 0.45 |
| 1:D:1028:VAL:HA | 1:D:1031:GLU:HG2 | 1.98 | 0.45 |
| 1:D:1206:MET:O | 1:D:1210:TYR:CA | 2.64 | 0.45 |
| 1:D:375:GLU:O | 1:D:376:LEU:C | 2.54 | 0.45 |
| 1:D:407:PHE:HD1 | 1:D:411:LEU:CG | 2.29 | 0.45 |
| 1:D:461:LYS:HA | 1:D:464:MET:HE2 | 1.96 | 0.45 |
| 1:D:608:ASP:OD1 | 1:D:611:PRO:C | 2.55 | 0.45 |
| 1:D:614:TYR:HB3 | 1:D:615:SER:O | 2.16 | 0.45 |
| 1:D:645:VAL:HG13 | 1:D:650:ARG:CD | 2.45 | 0.45 |
| 1:D:768:LYS:O | 1:D:769:ASP:CB | 2.63 | 0.45 |
| 2:E:211:ILE:N | 2:E:211:ILE:CD1 | 2.79 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:128:VAL:CG1 | 2:F:129:ASP:N | 2.79 | 0.45 |
| 2:F:131:LEU:O | 2:F:132:HIS:C | 2.54 | 0.45 |
| 2:F:138:LEU:N | 2:F:138:LEU:HD22 | 2.31 | 0.45 |
| 2:F:72:ILE:HD12 | 2:F:76:ARG:HE | 1.81 | 0.45 |
| 1:A:1102:GLN:O | 1:A:1103:SER:C | 2.53 | 0.45 |
| 1:A:1173:LEU:HA | 1:A:1174:PRO:HD3 | 1.65 | 0.45 |
| 1:A:1190:ARG:HD2 | 1:A:1195:MET:CE | 2.45 | 0.45 |
| 1:A:1231:LEU:CG | 1:A:1232:GLU:H | 2.16 | 0.45 |
| 1:A:278:ILE:HG23 | 1:A:291:PHE:HE1 | 1.80 | 0.45 |
| 1:A:350:ILE:O | 1:A:351:SER:C | 2.54 | 0.45 |
| 1:A:386:ARG:NH1 | 1:A:387:GLU:CG | 2.79 | 0.45 |
| 1:A:623:LEU:CG | 1:A:623:LEU:O | 2.45 | 0.45 |
| 1:A:630:ASN:HB2 | 1:A:744:ILE:C | 2.37 | 0.45 |
| 1:A:651:ALA:O | 1:A:655:LEU:HD23 | 2.16 | 0.45 |
| 1:A:604:ALA:HB2 | 1:A:717:LEU:HD13 | 1.99 | 0.45 |
| 1:A:788:GLY:O | 1:A:789:PRO:C | 2.51 | 0.45 |
| 1:A:439:GLN:CG | 1:A:835:GLY:CA | 2.75 | 0.45 |
| 1:A:944:GLU:N | 1:A:947:LYS:HE3 | 2.31 | 0.45 |
| 2:B:186:LEU:CD1 | 2:B:337:SER:HB2 | 2.37 | 0.45 |
| 2:C:131:LEU:O | 2:C:132:HIS:C | 2.54 | 0.45 |
| 2:C:314:MET:HE3 | 2:C:315:TYR:CE2 | 2.52 | 0.45 |
| 2:C:432:TYR:HB3 | 2:C:437:ILE:CG1 | 2.46 | 0.45 |
| 2:C:458:ARG:CG | 2:C:458:ARG:HH11 | 2.20 | 0.45 |
| 2:C:86:LEU:O | 2:C:91:LEU:HB2 | 2.16 | 0.45 |
| 1:D:1131:ILE:CD1 | 1:D:1138:ARG:O | 2.63 | 0.45 |
| 1:D:1207:GLU:C | 1:D:1210:TYR:H | 2.19 | 0.45 |
| 1:D:271:VAL:CG1 | 1:D:272:SER:N | 2.49 | 0.45 |
| 1:D:370:GLU:HB2 | 1:D:399:ASP:CG | 2.37 | 0.45 |
| 1:D:608:ASP:O | 1:D:609:GLY:O | 2.34 | 0.45 |
| 1:D:739:TYR:O | 1:D:740:ASN:ND2 | 2.49 | 0.45 |
| 1:D:801:TRP:CH2 | 1:D:805:HIS:CB | 2.99 | 0.45 |
| 2:E:106:LEU:HD12 | 2:E:109:ASN:HD21 | 1.80 | 0.45 |
| 2:F:129:ASP:OD1 | 2:F:131:LEU:HD11 | 2.17 | 0.45 |
| 2:F:351:TYR:CA | 2:F:355:GLN:HB2 | 2.44 | 0.45 |
| 2:F:389:ARG:C | 2:F:395:LEU:HD11 | 2.36 | 0.45 |
| 1:A:1020:ILE:O | 1:A:1021:SER:CB | 2.64 | 0.45 |
| 1:A:1200:PRO:HB2 | 1:A:1203:PRO:HD2 | 1.98 | 0.45 |
| 1:A:268:GLY:O | 1:A:269:HIS:CD2 | 2.69 | 0.45 |
| 1:A:313:ILE:CG1 | 1:A:314:ALA:N | 2.79 | 0.45 |
| 1:A:297:MET:HE3 | 1:A:411:LEU:HD22 | 1.98 | 0.45 |
| 1:A:712:VAL:N | 1:A:713:PRO:CD | 2.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:879:GLN:CB | 1:A:886:LEU:CD1 | 2.92 | 0.45 |
| 1:A:79:LEU:CB | 1:A:89:GLY:O | 2.64 | 0.45 |
| 1:A:918:TRP:CD1 | 1:A:918:TRP:O | 2.69 | 0.45 |
| 1:A:996:ARG:NH2 | 1:A:1003:TRP:CB | 2.68 | 0.45 |
| 2:B:122:ARG:HD3 | 2:B:124:GLN:HE22 | 1.81 | 0.45 |
| 2:B:192:HIS:O | 2:B:195:ASN:HB3 | 2.17 | 0.45 |
| 2:C:194:VAL:O | 2:C:197:LEU:CB | 2.63 | 0.45 |
| 1:A:783:PRO:CG | 2:C:363:ARG:NH1 | 2.79 | 0.45 |
| 2:C:416:GLY:HA2 | 2:C:419:GLU:HB3 | 1.98 | 0.45 |
| 2:C:443:VAL:CB | 2:C:447:THR:HG21 | 2.44 | 0.45 |
| 2:C:86:LEU:HD12 | 2:C:86:LEU:N | 2.31 | 0.45 |
| 1:D:1070:PRO:HD3 | 1:D:1071:ARG:NH1 | 2.30 | 0.45 |
| 1:D:1136:GLU:HG3 | 1:D:1138:ARG:HH12 | 1.81 | 0.45 |
| 1:D:1193:VAL:O | 1:D:1194:THR:C | 2.53 | 0.45 |
| 1:D:1195:MET:O | 1:D:1196:ASP:CB | 2.63 | 0.45 |
| 1:D:157:LEU:CG | 1:D:194:ALA:CB | 2.95 | 0.45 |
| 1:D:179:GLY:O | 1:D:180:PRO:C | 2.53 | 0.45 |
| 1:D:201:VAL:CG1 | 1:D:202:CYS:N | 2.80 | 0.45 |
| 1:D:479:TYR:HE1 | 1:D:480:LYS:HE2 | 1.82 | 0.45 |
| 1:D:502:LYS:HD2 | 1:D:506:GLU:HB3 | 1.98 | 0.45 |
| 1:D:575:LYS:HE3 | 1:D:581:ASP:HB3 | 1.97 | 0.45 |
| 1:D:649:TYR:CD2 | 1:D:652:ILE:CD1 | 2.99 | 0.45 |
| 1:D:632:ALA:HB2 | 1:D:657:ARG:HD2 | 1.98 | 0.45 |
| 1:D:665:LYS:O | 1:D:669:MET:O | 2.34 | 0.45 |
| 1:D:810:SER:O | 1:D:811:GLN:C | 2.54 | 0.45 |
| 1:D:922:GLN:CD | 1:D:931:LEU:HD13 | 2.35 | 0.45 |
| 2:E:387:VAL:O | 2:E:442:LEU:CD2 | 2.62 | 0.45 |
| 2:E:422:GLN:HG2 | 2:E:424:SER:CA | 2.47 | 0.45 |
| 2:F:234:LYS:HZ1 | 2:F:344:ARG:CG | 2.28 | 0.45 |
| 1:A:1005:VAL:O | 1:A:1006:ARG:NH1 | 2.50 | 0.45 |
| 1:A:857:PRO:HB3 | 1:A:1062:GLU:CD | 2.37 | 0.45 |
| 1:A:1069:ILE:HG23 | 1:A:1070:PRO:HG3 | 1.98 | 0.45 |
| 1:A:271:VAL:HG22 | 1:A:295:MET:CE | 2.46 | 0.45 |
| 1:A:515:ILE:HG12 | 1:A:565:HIS:C | 2.37 | 0.45 |
| 1:A:720:THR:HG22 | 1:A:721:ALA:H | 1.82 | 0.45 |
| 1:A:79:LEU:HD13 | 1:A:1172:ASP:OD2 | 2.16 | 0.45 |
| 1:A:850:ILE:HD11 | 1:A:1099:TRP:CE2 | 2.51 | 0.45 |
| 1:A:869:ARG:HG2 | 1:A:870:VAL:CG2 | 2.37 | 0.45 |
| 2:B:115:TRP:CZ2 | 2:C:108:LYS:CD | 2.98 | 0.45 |
| 2:B:196:CYS:O | 2:B:199:LEU:N | 2.43 | 0.45 |
| 2:B:243:THR:OG1 | 2:B:244:PRO:HD2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:425:LEU:HD23 | 2:B:425:LEU:C | 2.36 | 0.45 |
| 2:B:447:THR:HA | 2:B:450:ASN:CG | 2.37 | 0.45 |
| 2:B:127:PRO:HG2 | 2:C:104:VAL:HB | 1.97 | 0.45 |
| 2:C:264:ARG:HG2 | 2:C:270:PRO:HB2 | 1.98 | 0.45 |
| 2:C:317:GLY:HA2 | 2:C:320:SER:CB | 2.42 | 0.45 |
| 2:C:308:ASP:CG | 2:C:334:CYS:HA | 2.37 | 0.45 |
| 2:C:78:PHE:CE2 | 2:C:350:LEU:CD2 | 2.99 | 0.45 |
| 2:C:372:LEU:CG | 2:C:436:SER:HB2 | 2.46 | 0.45 |
| 2:C:456:ARG:HB3 | 2:C:463:LYS:O | 2.16 | 0.45 |
| 2:C:476:ILE:HD13 | 2:C:477:LYS:H | 1.79 | 0.45 |
| 1:D:1099:TRP:CE3 | 1:D:1099:TRP:HA | 2.51 | 0.45 |
| 1:D:1023:GLN:OE1 | 1:D:1100:VAL:HG22 | 2.17 | 0.45 |
| 1:D:258:GLN:O | 1:D:259:ARG:HB3 | 2.16 | 0.45 |
| 1:D:316:LYS:HZ1 | 1:D:348:LEU:CD2 | 2.29 | 0.45 |
| 1:D:461:LYS:O | 1:D:465:ASP:OD2 | 2.34 | 0.45 |
| 1:D:586:THR:O | 1:D:586:THR:CG2 | 2.65 | 0.45 |
| 1:D:606:THR:HG1 | 1:D:614:TYR:HH | 1.58 | 0.45 |
| 1:D:652:ILE:O | 1:D:655:LEU:HB2 | 2.17 | 0.45 |
| 1:D:279:ARG:NH1 | 1:D:841:LEU:HD13 | 2.31 | 0.45 |
| 1:D:893:SER:OG | 1:D:894:GLN:N | 2.48 | 0.45 |
| 2:E:272:ASN:OD1 | 2:E:292:ASN:ND2 | 2.46 | 0.45 |
| 2:E:285:LYS:O | 2:E:304:TRP:CE3 | 2.70 | 0.45 |
| 2:E:329:LYS:O | 2:E:330:ASN:O | 2.34 | 0.45 |
| 2:E:450:ASN:ND2 | 2:E:452:LEU:HD21 | 2.27 | 0.45 |
| 2:E:478:TYR:HD1 | 2:E:478:TYR:O | 1.98 | 0.45 |
| 2:F:199:LEU:O | 2:F:200:VAL:HB | 2.17 | 0.45 |
| 1:D:784:GLY:C | 2:F:363:ARG:HG2 | 2.37 | 0.45 |
| 1:A:1038:TRP:CZ3 | 1:A:1041:TRP:CG | 3.04 | 0.45 |
| 1:A:1207:GLU:C | 1:A:1210:TYR:CE1 | 2.90 | 0.45 |
| 1:A:242:ALA:O | 1:A:245:ILE:HG23 | 2.17 | 0.45 |
| 1:A:269:HIS:C | 1:A:294:THR:OG1 | 2.55 | 0.45 |
| 1:A:441:TRP:CZ2 | 1:A:874:LEU:HB3 | 2.51 | 0.45 |
| 1:A:577:CYS:HB3 | 1:A:578:PRO:HD3 | 1.87 | 0.45 |
| 1:A:591:LEU:CD1 | 1:A:594:LEU:HD11 | 2.47 | 0.45 |
| 1:A:652:ILE:O | 1:A:656:TYR:CD2 | 2.70 | 0.45 |
| 2:B:184:ASN:C | 2:B:186:LEU:N | 2.69 | 0.45 |
| 2:B:285:LYS:O | 2:B:305:ASN:N | 2.49 | 0.45 |
| 2:B:69:LEU:HD21 | 2:B:351:TYR:CE1 | 2.51 | 0.45 |
| 2:C:454:HIS:HB3 | 2:C:466:MET:C | 2.36 | 0.45 |
| 2:C:471:LEU:HA | 2:C:474:PHE:CB | 2.34 | 0.45 |
| 2:C:88:ARG:CB | 2:C:88:ARG:CZ | 2.94 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1126:ASP:HB2 | 1:D:1141:VAL:HG13 | 1.98 | 0.45 |
| 1:D:1140:LEU:HD23 | 1:D:1141:VAL:H | 1.81 | 0.45 |
| 1:D:1231:LEU:HD21 | 1:D:1236:GLN:HE22 | 1.81 | 0.45 |
| 1:D:214:ALA:HB3 | 1:D:219:ALA:N | 2.31 | 0.45 |
| 1:D:248:GLU:HB3 | 1:D:249:VAL:CA | 2.07 | 0.45 |
| 1:D:279:ARG:HD2 | 1:D:841:LEU:CD1 | 2.46 | 0.45 |
| 1:D:271:VAL:HG22 | 1:D:295:MET:HB2 | 1.98 | 0.45 |
| 1:D:365:GLY:C | 1:D:367:PRO:HD3 | 2.36 | 0.45 |
| 1:D:424:LEU:O | 1:D:428:LEU:HD12 | 2.15 | 0.45 |
| 1:D:652:ILE:CG2 | 1:D:656:TYR:CE2 | 2.99 | 0.45 |
| 1:D:76:ILE:CG1 | 1:D:77:GLN:N | 2.79 | 0.45 |
| 1:D:897:TRP:CZ3 | 1:D:1177:VAL:CG1 | 2.98 | 0.45 |
| 1:D:916:PHE:CD1 | 1:D:920:THR:O | 2.69 | 0.45 |
| 2:E:125:VAL:HG22 | 2:E:241:TRP:CZ3 | 2.50 | 0.45 |
| 2:E:254:PHE:HA | 2:E:257:ARG:NE | 2.30 | 0.45 |
| 2:E:259:ARG:NH1 | 2:E:263:TRP:NE1 | 2.64 | 0.45 |
| 2:E:280:ASP:N | 2:E:304:TRP:CZ3 | 2.84 | 0.45 |
| 2:E:110:LEU:HA | 2:E:378:LEU:HD23 | 1.97 | 0.45 |
| 2:F:76:ARG:O | 2:F:102:LEU:HD13 | 2.16 | 0.45 |
| 2:F:131:LEU:O | 2:F:182:ARG:HD3 | 2.15 | 0.45 |
| 2:F:399:CYS:SG | 2:F:417:TYR:CE2 | 3.09 | 0.45 |
| 2:F:384:ALA:HA | 2:F:414:TRP:HB3 | 1.98 | 0.45 |
| 2:F:413:VAL:HG12 | 2:F:415:PRO:CD | 2.46 | 0.45 |
| 2:F:446:THR:C | 2:F:450:ASN:H | 2.19 | 0.45 |
| 2:F:78:PHE:O | 2:F:99:PHE:HB3 | 2.17 | 0.45 |
| 1:A:107:LEU:HD13 | 1:A:107:LEU:N | 2.32 | 0.45 |
| 1:A:240:SER:O | 1:A:243:ASP:CG | 2.54 | 0.45 |
| 1:A:288:ARG:CZ | 1:A:290:ARG:HH21 | 2.29 | 0.45 |
| 1:A:386:ARG:CG | 1:A:390:GLN:HE22 | 2.29 | 0.45 |
| 1:A:597:ARG:HE | 1:A:597:ARG:HB2 | 1.28 | 0.45 |
| 1:A:788:GLY:O | 1:A:792:LEU:N | 2.49 | 0.45 |
| 2:B:78:PHE:CE1 | 2:B:103:GLY:N | 2.85 | 0.45 |
| 2:B:130:ALA:HB1 | 2:B:188:GLY:HA3 | 1.99 | 0.45 |
| 2:B:301:GLU:HG2 | 2:B:303:LEU:HD12 | 1.99 | 0.45 |
| 2:B:336:LEU:CG | 2:B:337:SER:N | 2.79 | 0.45 |
| 2:B:77:HIS:CG | 2:C:195:ASN:OD1 | 2.69 | 0.45 |
| 2:C:241:TRP:CG | 2:C:243:THR:HG23 | 2.51 | 0.45 |
| 2:C:342:LEU:HD23 | 2:C:345:GLY:N | 2.17 | 0.45 |
| 1:D:1103:SER:O | 1:D:1106:VAL:N | 2.50 | 0.45 |
| 1:D:887:VAL:N | 1:D:1139:TYR:O | 2.48 | 0.45 |
| 1:D:897:TRP:CH2 | 1:D:1173:LEU:HB3 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1198:LYS:N | 1:D:1204:THR:CG2 | 2.78 | 0.45 |
| 1:D:190:PRO:O | 1:D:192:GLU:N | 2.49 | 0.45 |
| 1:D:277:HIS:HB3 | 1:D:291:PHE:CD2 | 2.52 | 0.45 |
| 1:D:253:ALA:HB2 | 1:D:280:GLU:C | 2.37 | 0.45 |
| 1:D:375:GLU:CD | 1:D:379:LYS:HA | 2.37 | 0.45 |
| 1:D:389:PHE:CA | 1:D:393:MET:HG2 | 2.45 | 0.45 |
| 1:D:576:LEU:CD1 | 1:D:577:CYS:SG | 3.05 | 0.45 |
| 1:D:597:ARG:HH12 | 1:D:725:PRO:N | 2.14 | 0.45 |
| 1:D:793:GLU:O | 1:D:797:MET:CG | 2.64 | 0.45 |
| 1:D:992:LEU:HB2 | 1:D:997:LEU:HB2 | 1.98 | 0.45 |
| 2:E:109:ASN:HB2 | 2:E:378:LEU:C | 2.37 | 0.45 |
| 2:E:322:LEU:O | 2:E:323:HIS:C | 2.52 | 0.45 |
| 2:E:372:LEU:O | 2:E:458:ARG:CD | 2.63 | 0.45 |
| 2:F:111:ALA:O | 2:F:115:TRP:HB2 | 2.15 | 0.45 |
| 2:F:236:GLU:HA | 2:F:341:ASP:CG | 2.35 | 0.45 |
| 2:F:353:SER:HG | 2:F:354:PHE:H | 1.65 | 0.45 |
| 2:F:375:HIS:HE2 | 2:F:377:CYS:HG | 1.64 | 0.45 |
| 2:F:455:LEU:CB | 2:F:456:ARG:NE | 2.74 | 0.45 |
| 1:A:1006:ARG:N | 1:A:1006:ARG:HD2 | 2.31 | 0.45 |
| 1:A:1042:GLU:OE1 | 1:A:1042:GLU:HA | 2.17 | 0.45 |
| 1:A:1109:LEU:CD1 | 1:A:1113:LEU:HD21 | 2.38 | 0.45 |
| 1:A:1131:ILE:CG2 | 1:A:1137:VAL:CA | 2.84 | 0.45 |
| 1:A:1158:LEU:HD11 | 1:A:1179:PHE:CE1 | 2.51 | 0.45 |
| 1:A:1188:CYS:C | 1:A:1189:LEU:CD2 | 2.75 | 0.45 |
| 1:A:170:ALA:CB | 1:A:175:TRP:CZ2 | 2.67 | 0.45 |
| 1:A:460:LYS:NZ | 1:A:594:LEU:HD21 | 2.32 | 0.45 |
| 1:A:462:SER:HG | 1:A:463:LEU:H | 1.61 | 0.45 |
| 1:A:577:CYS:HB3 | 1:A:578:PRO:HD2 | 1.97 | 0.45 |
| 1:A:586:THR:O | 1:A:587:PRO:C | 2.54 | 0.45 |
| 1:A:612:LEU:HD21 | 1:A:614:TYR:C | 2.36 | 0.45 |
| 1:A:606:THR:OG1 | 1:A:613:HIS:CA | 2.65 | 0.45 |
| 1:A:607:TRP:HZ2 | 1:A:670:PRO:C | 2.20 | 0.45 |
| 1:A:784:GLY:HA3 | 2:C:362:THR:C | 2.36 | 0.45 |
| 1:A:304:LEU:O | 1:A:850:ILE:HG21 | 2.17 | 0.45 |
| 1:A:892:ASP:CB | 1:A:927:ARG:HH22 | 2.30 | 0.45 |
| 1:A:931:LEU:O | 1:A:934:LYS:N | 2.49 | 0.45 |
| 1:A:972:ARG:C | 1:A:974:THR:H | 2.20 | 0.45 |
| 1:A:984:GLN:O | 1:A:987:ALA:HB3 | 2.17 | 0.45 |
| 2:B:122:ARG:CB | 2:B:124:GLN:HE21 | 2.26 | 0.45 |
| 2:B:261:GLN:N | 2:B:264:ARG:HD3 | 2.29 | 0.45 |
| 2:B:320:SER:O | 2:B:323:HIS:CD2 | 2.70 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:385:LEU:N | 2:B:414:TRP:O | 2.49 | 0.45 |
| 2:C:187:HIS:HA | 2:C:190:LEU:CD1 | 2.46 | 0.45 |
| 2:C:197:LEU:O | 2:C:202:LYS:HA | 2.17 | 0.45 |
| 2:C:200:VAL:HG11 | 2:C:204:LEU:CD1 | 2.44 | 0.45 |
| 2:C:320:SER:HB3 | 2:C:321:LYS:CG | 2.38 | 0.45 |
| 1:D:103:SER:OG | 1:D:104:VAL:N | 2.49 | 0.45 |
| 1:D:1040:LYS:HE3 | 1:D:1040:LYS:CA | 2.46 | 0.45 |
| 1:D:944:GLU:CB | 1:D:1071:ARG:HD3 | 2.44 | 0.45 |
| 1:D:1157:ASN:C | 1:D:1161:ARG:HD2 | 2.36 | 0.45 |
| 1:D:1209:ARG:NH1 | 2:F:252:LEU:HD22 | 2.32 | 0.45 |
| 1:D:179:GLY:N | 1:D:180:PRO:CD | 2.79 | 0.45 |
| 1:D:251:THR:O | 1:D:254:SER:N | 2.49 | 0.45 |
| 1:D:466:LEU:O | 1:D:470:ALA:HB3 | 2.17 | 0.45 |
| 1:D:635:PRO:HA | 1:D:639:THR:HG1 | 1.77 | 0.45 |
| 1:D:652:ILE:HG12 | 1:D:655:LEU:HG | 1.98 | 0.45 |
| 1:D:653:GLU:HA | 1:D:656:TYR:CD2 | 2.51 | 0.45 |
| 1:D:439:GLN:HG3 | 1:D:836:LEU:H | 1.82 | 0.45 |
| 1:D:877:MET:CE | 1:D:1203:PRO:C | 2.84 | 0.45 |
| 2:E:382:LYS:HE3 | 2:E:383:VAL:C | 2.37 | 0.45 |
| 2:E:69:LEU:O | 2:E:72:ILE:HB | 2.17 | 0.45 |
| 2:F:193:TYR:CD1 | 2:F:242:PHE:CE2 | 3.04 | 0.45 |
| 2:F:322:LEU:HD22 | 2:F:324:GLY:N | 2.32 | 0.45 |
| 2:F:78:PHE:CE2 | 2:F:350:LEU:CD2 | 2.99 | 0.45 |
| 2:F:363:ARG:HB3 | 2:F:363:ARG:HH11 | 1.77 | 0.45 |
| 2:F:399:CYS:O | 2:F:400:GLN:C | 2.55 | 0.45 |
| 1:A:1005:VAL:O | 1:A:1006:ARG:C | 2.54 | 0.45 |
| 1:A:1074:VAL:CG2 | 1:A:1098:ASN:HD21 | 2.30 | 0.45 |
| 1:A:145:LYS:CG | 1:A:1118:TRP:CH2 | 2.92 | 0.45 |
| 1:A:298:HIS:O | 1:A:299:MET:C | 2.54 | 0.45 |
| 1:A:408:GLN:C | 1:A:411:LEU:HG | 2.36 | 0.45 |
| 1:A:436:PRO:HB3 | 1:A:880:ALA:H | 1.81 | 0.45 |
| 1:A:633:LYS:CD | 1:A:634:LEU:N | 2.78 | 0.45 |
| 1:A:800:PHE:CE2 | 1:A:867:PRO:CB | 3.00 | 0.45 |
| 1:A:296:SER:CB | 1:A:846:THR:OG1 | 2.64 | 0.45 |
| 1:A:851:THR:O | 1:A:852:ARG:HG3 | 2.16 | 0.45 |
| 1:A:808:ILE:HG21 | 1:A:874:LEU:HD13 | 1.99 | 0.45 |
| 1:A:995:TYR:C | 1:A:996:ARG:HG3 | 2.37 | 0.45 |
| 2:B:301:GLU:HA | 2:B:340:GLY:CA | 2.33 | 0.45 |
| 2:B:312:LEU:HA | 2:B:312:LEU:HD12 | 1.71 | 0.45 |
| 2:B:338:VAL:O | 2:B:339:ASN:ND2 | 2.40 | 0.45 |
| 2:C:200:VAL:HG11 | 2:C:204:LEU:CB | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:784:GLY:HA3 | 2:C:363:ARG:CD | 2.47 | 0.45 |
| 1:D:1158:LEU:CG | 1:D:1159:LEU:H | 2.27 | 0.45 |
| 1:D:1200:PRO:CG | 1:D:1200:PRO:O | 2.65 | 0.45 |
| 1:D:877:MET:HE1 | 1:D:1203:PRO:CA | 2.47 | 0.45 |
| 1:D:163:PRO:C | 1:D:165:LYS:N | 2.64 | 0.45 |
| 1:D:225:SER:HA | 1:D:228:LEU:CD2 | 2.44 | 0.45 |
| 1:D:228:LEU:HG | 1:D:229:VAL:H | 1.82 | 0.45 |
| 1:D:196:VAL:HA | 1:D:267:VAL:HG12 | 1.99 | 0.45 |
| 1:D:580:LEU:CD1 | 1:D:580:LEU:C | 2.75 | 0.45 |
| 1:D:630:ASN:C | 1:D:631:LEU:HD23 | 2.37 | 0.45 |
| 1:D:655:LEU:C | 1:D:659:HIS:NE2 | 2.70 | 0.45 |
| 1:D:805:HIS:O | 1:D:806:LYS:C | 2.53 | 0.45 |
| 2:E:104:VAL:CG2 | 2:F:128:VAL:O | 2.65 | 0.45 |
| 2:E:199:LEU:HG | 2:E:200:VAL:H | 1.80 | 0.45 |
| 2:E:230:SER:OG | 2:E:231:ILE:N | 2.49 | 0.45 |
| 2:E:407:LEU:HD21 | 2:E:412:SER:HA | 1.93 | 0.45 |
| 2:E:425:LEU:C | 2:E:426:GLU:OE1 | 2.55 | 0.45 |
| 2:F:124:GLN:C | 2:F:125:VAL:CG1 | 2.85 | 0.45 |
| 2:F:452:LEU:O | 2:F:453:ILE:CB | 2.64 | 0.45 |
| 1:A:1108:TYR:CE2 | 1:A:1112:MET:CE | 2.99 | 0.45 |
| 1:A:1131:ILE:HG23 | 1:A:1137:VAL:HA | 1.94 | 0.45 |
| 1:A:1108:TYR:CA | 1:A:1164:PHE:HZ | 2.29 | 0.45 |
| 1:A:197:PHE:HB3 | 1:A:277:HIS:HD2 | 1.79 | 0.45 |
| 1:A:296:SER:OG | 1:A:297:MET:N | 2.50 | 0.45 |
| 1:A:312:TRP:CH2 | 1:A:346:ASP:N | 2.85 | 0.45 |
| 1:A:316:LYS:HB2 | 1:A:348:LEU:HD12 | 1.97 | 0.45 |
| 1:A:424:LEU:N | 1:A:424:LEU:CD2 | 2.64 | 0.45 |
| 1:A:452:TYR:CD1 | 1:A:801:TRP:NE1 | 2.83 | 0.45 |
| 1:A:462:SER:C | 1:A:466:LEU:CD2 | 2.81 | 0.45 |
| 1:A:559:LEU:CG | 1:A:560:PRO:HD3 | 2.46 | 0.45 |
| 1:A:611:PRO:HG3 | 1:A:671:GLN:HG3 | 1.99 | 0.45 |
| 1:A:821:LEU:CD1 | 1:A:825:VAL:CB | 2.92 | 0.45 |
| 1:A:869:ARG:O | 1:A:870:VAL:C | 2.55 | 0.45 |
| 1:A:875:LYS:HA | 1:A:878:VAL:CG2 | 2.47 | 0.45 |
| 2:B:348:ALA:C | 2:B:350:LEU:H | 2.20 | 0.45 |
| 2:B:391:PRO:CD | 2:B:392:THR:H | 2.29 | 0.45 |
| 2:B:405:GLU:OE1 | 2:B:405:GLU:HA | 2.16 | 0.45 |
| 2:B:431:LYS:O | 2:B:431:LYS:HG2 | 2.16 | 0.45 |
| 2:C:121:PHE:C | 2:C:123:GLU:N | 2.69 | 0.45 |
| 2:B:99:PHE:O | 2:C:128:VAL:CG1 | 2.65 | 0.45 |
| 2:C:185:LEU:HD12 | 2:C:236:GLU:HB2 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:325:ARG:NH2 | 2:C:327:GLY:CA | 2.80 | 0.45 |
| 2:C:484:ASN:O | 2:C:485:VAL:C | 2.55 | 0.45 |
| 1:D:104:VAL:CG1 | 1:D:105:GLU:N | 2.79 | 0.45 |
| 1:D:1154:GLN:HG2 | 1:D:1179:PHE:CD2 | 2.52 | 0.45 |
| 1:D:294:THR:CB | 1:D:407:PHE:CE2 | 2.99 | 0.45 |
| 1:D:346:ASP:H | 1:D:1040:LYS:CD | 2.24 | 0.45 |
| 1:D:361:ARG:NH2 | 1:D:362:LEU:CG | 2.79 | 0.45 |
| 1:D:461:LYS:H | 1:D:461:LYS:HD2 | 1.82 | 0.45 |
| 1:D:482:ASP:CB | 1:D:483:PRO:CD | 2.95 | 0.45 |
| 1:D:815:TRP:CZ3 | 1:D:836:LEU:CB | 2.99 | 0.45 |
| 2:E:196:CYS:O | 2:E:197:LEU:C | 2.55 | 0.45 |
| 2:E:214:CYS:SG | 2:E:236:GLU:CB | 3.05 | 0.45 |
| 2:E:258:HIS:O | 2:E:261:GLN:HB2 | 2.17 | 0.45 |
| 2:E:322:LEU:HD12 | 2:E:332:VAL:HG11 | 1.98 | 0.45 |
| 2:E:91:LEU:HD22 | 2:E:91:LEU:N | 2.32 | 0.45 |
| 2:F:146:ARG:HD2 | 2:F:228:VAL:HG21 | 1.98 | 0.45 |
| 2:F:389:ARG:NH2 | 2:F:390:GLY:HA3 | 2.32 | 0.45 |
| 2:F:431:LYS:CE | 2:F:435:MET:HG2 | 2.47 | 0.45 |
| 2:F:69:LEU:HD12 | 2:F:69:LEU:O | 2.17 | 0.45 |
| 2:F:72:ILE:O | 2:F:75:ARG:O | 2.35 | 0.45 |
| 1:A:131:TYR:CD2 | 1:A:131:TYR:N | 2.79 | 0.45 |
| 1:A:406:VAL:CG2 | 1:A:407:PHE:HD2 | 2.30 | 0.45 |
| 1:A:614:TYR:HE2 | 1:A:620:TRP:CE3 | 2.35 | 0.45 |
| 1:A:657:ARG:O | 1:A:658:LYS:C | 2.53 | 0.45 |
| 1:A:828:HIS:O | 1:A:830:ASP:OD2 | 2.36 | 0.45 |
| 1:A:875:LYS:CA | 1:A:878:VAL:HG23 | 2.47 | 0.45 |
| 1:A:979:ALA:O | 1:A:980:GLU:C | 2.55 | 0.45 |
| 1:A:98:ALA:O | 1:A:102:ARG:CG | 2.57 | 0.45 |
| 2:B:106:LEU:O | 2:B:109:ASN:CB | 2.65 | 0.45 |
| 2:B:250:GLN:O | 2:B:252:LEU:N | 2.42 | 0.45 |
| 2:B:114:TRP:HD1 | 2:B:262:TRP:CE3 | 2.35 | 0.45 |
| 2:C:114:TRP:HB2 | 2:C:262:TRP:CZ2 | 2.51 | 0.45 |
| 2:C:275:SER:CB | 2:C:287:ASN:ND2 | 2.75 | 0.45 |
| 2:C:306:LEU:N | 2:C:335:VAL:CG1 | 2.69 | 0.45 |
| 2:C:353:SER:HB3 | 2:C:373:LYS:O | 2.17 | 0.45 |
| 2:C:476:ILE:HD13 | 2:C:477:LYS:HG3 | 1.99 | 0.45 |
| 1:D:1184:ASP:OD1 | 1:D:1184:ASP:N | 2.48 | 0.45 |
| 1:D:138:HIS:HA | 1:D:141:LEU:CD1 | 2.47 | 0.45 |
| 1:D:208:CYS:SG | 1:D:245:ILE:HG22 | 2.57 | 0.45 |
| 1:D:173:GLU:C | 1:D:220:TRP:HB3 | 2.38 | 0.45 |
| 1:D:457:ARG:O | 1:D:461:LYS:HD2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:539:PHE:O | 1:D:540:GLN:HB2 | 2.17 | 0.45 |
| 1:D:807:ARG:HH22 | 1:D:1061:LEU:CD1 | 2.30 | 0.45 |
| 1:D:822:PRO:CD | 1:D:825:VAL:CG2 | 2.78 | 0.45 |
| 1:D:80:SER:C | 1:D:83:LEU:HD22 | 2.37 | 0.45 |
| 1:D:438:ASN:HD21 | 1:D:882:PRO:HD3 | 1.82 | 0.45 |
| 1:D:972:ARG:C | 1:D:974:THR:H | 2.20 | 0.45 |
| 2:E:193:TYR:CE2 | 2:E:322:LEU:HB3 | 2.49 | 0.45 |
| 2:E:431:LYS:HD3 | 2:E:434:GLU:HG3 | 1.99 | 0.45 |
| 2:F:126:PHE:HB2 | 2:F:128:VAL:HG23 | 1.98 | 0.45 |
| 2:F:317:GLY:O | 2:F:318:ASN:C | 2.55 | 0.45 |
| 1:A:1030:ARG:CG | 1:A:1040:LYS:NZ | 2.62 | 0.44 |
| 1:A:252:GLY:O | 1:A:256:PRO:HB3 | 2.17 | 0.44 |
| 1:A:348:LEU:HD13 | 1:A:350:ILE:CD1 | 2.45 | 0.44 |
| 1:A:371:LYS:C | 1:A:372:GLU:CG | 2.79 | 0.44 |
| 1:A:412:PRO:O | 1:A:416:GLU:HG3 | 2.17 | 0.44 |
| 1:A:444:TYR:O | 1:A:448:ALA:HB2 | 2.17 | 0.44 |
| 1:A:498:LYS:CG | 1:A:518:ALA:HB3 | 2.47 | 0.44 |
| 1:A:83:LEU:O | 1:A:86:GLN:N | 2.50 | 0.44 |
| 1:A:897:TRP:O | 1:A:900:ALA:CB | 2.53 | 0.44 |
| 1:A:938:THR:O | 1:A:939:VAL:CG2 | 2.65 | 0.44 |
| 2:B:214:CYS:HB3 | 2:B:236:GLU:CD | 2.38 | 0.44 |
| 2:B:243:THR:O | 2:B:334:CYS:HB2 | 2.18 | 0.44 |
| 2:B:453:ILE:HD13 | 2:B:466:MET:O | 2.17 | 0.44 |
| 2:B:76:ARG:O | 2:B:77:HIS:O | 2.35 | 0.44 |
| 2:C:251:TRP:CZ3 | 2:C:254:PHE:CG | 3.04 | 0.44 |
| 2:C:382:LYS:HD3 | 2:C:411:ILE:CD1 | 2.46 | 0.44 |
| 2:C:431:LYS:CE | 2:C:435:MET:HG2 | 2.44 | 0.44 |
| 2:C:70:LEU:O | 2:C:73:CYS:N | 2.46 | 0.44 |
| 2:C:83:LYS:O | 2:C:86:LEU:HB2 | 2.17 | 0.44 |
| 1:D:429:GLU:CG | 1:D:1117:LYS:HE2 | 2.43 | 0.44 |
| 1:D:1139:TYR:CD1 | 1:D:1153:LEU:HD13 | 2.53 | 0.44 |
| 1:D:189:ILE:CG2 | 1:D:258:GLN:CB | 2.89 | 0.44 |
| 1:D:282:TYR:CD1 | 1:D:282:TYR:N | 2.84 | 0.44 |
| 1:D:295:MET:CE | 1:D:354:ASN:HA | 2.46 | 0.44 |
| 1:D:374:ARG:CD | 1:D:392:LEU:CD2 | 2.87 | 0.44 |
| 1:D:375:GLU:C | 1:D:378:VAL:H | 2.19 | 0.44 |
| 1:D:416:GLU:C | 1:D:418:CYS:N | 2.69 | 0.44 |
| 1:D:612:LEU:HD23 | 1:D:620:TRP:O | 2.17 | 0.44 |
| 1:D:743:ASP:CB | 1:D:744:ILE:HD13 | 2.46 | 0.44 |
| 1:D:733:HIS:O | 1:D:750:PHE:O | 2.35 | 0.44 |
| 1:D:829:PRO:CD | 1:D:829:PRO:O | 2.66 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:770:PHE:CE1 | 1:D:968:GLN:C | 2.91 | 0.44 |
| 2:F:229:LYS:O | 2:F:230:SER:HB2 | 2.17 | 0.44 |
| 2:F:307:GLY:N | 2:F:335:VAL:CG1 | 2.80 | 0.44 |
| 2:F:326:ASP:CG | 2:F:329:LYS:CB | 2.86 | 0.44 |
| 2:F:344:ARG:CG | 2:F:347:LEU:HD22 | 2.47 | 0.44 |
| 2:F:375:HIS:NE2 | 2:F:377:CYS:SG | 2.89 | 0.44 |
| 2:F:429:TYR:O | 2:F:432:TYR:HB2 | 2.17 | 0.44 |
| 2:F:471:LEU:O | 2:F:472:LYS:C | 2.56 | 0.44 |
| 2:F:474:PHE:CD2 | 2:F:475:LEU:HD23 | 2.53 | 0.44 |
| 1:A:1035:LYS:HG3 | 1:A:1039:LYS:HE2 | 0.80 | 0.44 |
| 1:A:773:LYS:HZ2 | 1:A:1057:MET:HE1 | 1.83 | 0.44 |
| 1:A:1048:ALA:CB | 1:A:1092:PHE:CE1 | 3.00 | 0.44 |
| 1:A:273:PHE:N | 1:A:273:PHE:CD2 | 2.85 | 0.44 |
| 1:A:316:LYS:HZ2 | 1:A:350:ILE:HG21 | 1.82 | 0.44 |
| 1:A:392:LEU:CG | 1:A:395:TYR:HB2 | 2.47 | 0.44 |
| 1:A:490:TRP:HH2 | 1:A:597:ARG:O | 1.99 | 0.44 |
| 1:A:630:ASN:HD21 | 1:A:632:ALA:CB | 2.30 | 0.44 |
| 1:A:659:HIS:CD2 | 1:A:720:THR:CG2 | 3.00 | 0.44 |
| 1:A:724:GLY:HA2 | 1:A:725:PRO:HA | 1.55 | 0.44 |
| 2:B:289:LEU:N | 2:B:301:GLU:O | 2.48 | 0.44 |
| 2:B:105:GLU:HG3 | 2:B:380:PRO:O | 2.17 | 0.44 |
| 2:C:214:CYS:SG | 2:C:236:GLU:CG | 3.05 | 0.44 |
| 2:C:243:THR:HB | 2:C:247:THR:HG21 | 1.99 | 0.44 |
| 2:C:280:ASP:C | 2:C:282:GLU:H | 2.21 | 0.44 |
| 2:C:320:SER:CB | 2:C:321:LYS:HG3 | 2.35 | 0.44 |
| 2:C:348:ALA:O | 2:C:351:TYR:HB2 | 2.17 | 0.44 |
| 2:C:83:LYS:N | 2:C:86:LEU:HD22 | 2.32 | 0.44 |
| 1:D:1067:SER:HB3 | 1:D:1073:PRO:HD2 | 1.98 | 0.44 |
| 1:D:1099:TRP:HE3 | 1:D:1099:TRP:HA | 1.82 | 0.44 |
| 1:D:1108:TYR:O | 1:D:1109:LEU:C | 2.54 | 0.44 |
| 1:D:1131:ILE:HG13 | 1:D:1138:ARG:HB2 | 1.99 | 0.44 |
| 1:D:1155:ILE:O | 1:D:1157:ASN:N | 2.50 | 0.44 |
| 1:D:1180:PHE:O | 1:D:1181:SER:C | 2.56 | 0.44 |
| 1:D:887:VAL:CG1 | 1:D:1183:VAL:HG11 | 2.47 | 0.44 |
| 1:D:223:TRP:CZ3 | 1:D:250:PRO:HB3 | 2.49 | 0.44 |
| 1:D:267:VAL:CG2 | 1:D:291:PHE:CE2 | 2.99 | 0.44 |
| 1:D:486:TRP:CE3 | 1:D:598:VAL:HG21 | 2.53 | 0.44 |
| 1:D:529:ASP:O | 1:D:530:LEU:CB | 2.57 | 0.44 |
| 1:D:542:ASP:O | 1:D:546:ARG:CB | 2.65 | 0.44 |
| 1:D:576:LEU:H | 1:D:579:ARG:HD2 | 1.83 | 0.44 |
| 1:D:840:ILE:C | 1:D:841:LEU:HD23 | 2.37 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:311:LEU:H | 2:E:313:HIS:HB3 | 1.82 | 0.44 |
| 2:E:318:ASN:C | 2:E:320:SER:N | 2.70 | 0.44 |
| 2:E:380:PRO:CG | 2:E:438:LEU:CD1 | 2.96 | 0.44 |
| 2:F:389:ARG:CD | 2:F:390:GLY:N | 2.81 | 0.44 |
| 2:F:484:ASN:O | 2:F:485:VAL:C | 2.56 | 0.44 |
| 2:E:199:LEU:CB | 2:F:77:HIS:NE2 | 2.74 | 0.44 |
| 1:A:907:PHE:CZ | 1:A:1001:GLY:CA | 2.99 | 0.44 |
| 1:A:1068:ASP:N | 1:A:1071:ARG:HG2 | 2.02 | 0.44 |
| 1:A:129:PRO:O | 1:A:131:TYR:CE2 | 2.70 | 0.44 |
| 1:A:196:VAL:O | 1:A:401:TRP:CH2 | 2.61 | 0.44 |
| 1:A:210:THR:HA | 1:A:224:CYS:HB2 | 1.95 | 0.44 |
| 1:A:266:VAL:HG22 | 1:A:267:VAL:H | 1.82 | 0.44 |
| 1:A:470:ALA:O | 1:A:474:LEU:HD13 | 2.17 | 0.44 |
| 1:A:549:LEU:HD23 | 1:A:549:LEU:HA | 1.54 | 0.44 |
| 1:A:656:TYR:HA | 1:A:659:HIS:CD2 | 2.51 | 0.44 |
| 1:A:439:GLN:HG2 | 1:A:836:LEU:H | 1.78 | 0.44 |
| 2:B:385:LEU:O | 2:B:415:PRO:HA | 2.17 | 0.44 |
| 2:C:450:ASN:OD1 | 2:C:453:ILE:HD12 | 2.17 | 0.44 |
| 2:C:87:SER:O | 2:C:90:SER:N | 2.49 | 0.44 |
| 1:D:1015:THR:HB | 1:D:1016:GLU:H | 1.19 | 0.44 |
| 1:D:1046:GLU:O | 1:D:1049:TRP:CD1 | 2.70 | 0.44 |
| 1:D:886:LEU:N | 1:D:1146:ARG:NH1 | 2.66 | 0.44 |
| 1:D:127:LEU:HD23 | 1:D:128:PRO:HD2 | 1.98 | 0.44 |
| 1:D:220:TRP:NE1 | 1:D:221:TYR:HD2 | 2.14 | 0.44 |
| 1:D:221:TYR:O | 1:D:222:SER:CB | 2.65 | 0.44 |
| 1:D:257:THR:C | 1:D:258:GLN:CG | 2.85 | 0.44 |
| 1:D:515:ILE:CG2 | 1:D:565:HIS:CG | 3.00 | 0.44 |
| 1:D:711:ALA:O | 1:D:712:VAL:HB | 2.17 | 0.44 |
| 1:D:823:ARG:NH1 | 1:D:824:ALA:CB | 2.80 | 0.44 |
| 1:D:992:LEU:C | 1:D:996:ARG:CD | 2.86 | 0.44 |
| 2:E:293:PHE:O | 2:E:294:PRO:C | 2.56 | 0.44 |
| 2:F:196:CYS:HB2 | 2:F:206:TYR:OH | 2.18 | 0.44 |
| 2:F:239:LEU:N | 2:F:338:VAL:HG13 | 2.22 | 0.44 |
| 2:F:385:LEU:HA | 2:F:385:LEU:HD23 | 1.75 | 0.44 |
| 2:F:407:LEU:HD13 | 2:F:408:GLU:OE2 | 2.17 | 0.44 |
| 1:D:546:ARG:NH2 | 2:F:408:GLU:CD | 2.71 | 0.44 |
| 2:F:59:ALA:N | 2:F:60:PRO:HD2 | 2.32 | 0.44 |
| 1:A:1133:ILE:O | 1:A:1133:ILE:HG23 | 2.18 | 0.44 |
| 1:A:1146:ARG:HG3 | 1:A:1146:ARG:HH11 | 1.82 | 0.44 |
| 1:A:1209:ARG:HH22 | 2:C:256:LEU:HG | 1.82 | 0.44 |
| 1:A:215:ILE:HD12 | 1:A:401:TRP:CE3 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:248:GLU:O | 1:A:249:VAL:C | 2.54 | 0.44 |
| 1:A:316:LYS:CD | 1:A:350:ILE:CG1 | 2.85 | 0.44 |
| 1:A:477:GLU:CG | 1:A:478:ARG:N | 2.32 | 0.44 |
| 1:A:497:GLN:O | 1:A:497:GLN:OE1 | 2.35 | 0.44 |
| 1:A:504:LYS:O | 1:A:505:LYS:HG3 | 2.17 | 0.44 |
| 1:A:515:ILE:HG13 | 1:A:568:GLY:O | 2.17 | 0.44 |
| 1:A:464:MET:SD | 1:A:578:PRO:O | 2.76 | 0.44 |
| 1:A:579:ARG:NH1 | 1:A:579:ARG:HG2 | 2.33 | 0.44 |
| 1:A:580:LEU:HD23 | 1:A:596:MET:SD | 2.58 | 0.44 |
| 1:A:612:LEU:HD22 | 1:A:620:TRP:CA | 2.45 | 0.44 |
| 1:A:646:VAL:O | 1:A:647:CYS:HB2 | 2.17 | 0.44 |
| 1:A:737:GLY:N | 1:A:750:PHE:HE1 | 2.16 | 0.44 |
| 1:A:801:TRP:CE2 | 1:A:805:HIS:HB2 | 2.53 | 0.44 |
| 1:A:862:ALA:HB1 | 1:A:875:LYS:CE | 2.46 | 0.44 |
| 1:A:945:HIS:NE2 | 1:A:969:PHE:CG | 2.85 | 0.44 |
| 1:A:980:GLU:O | 1:A:984:GLN:HG3 | 2.18 | 0.44 |
| 1:A:993:ARG:HG3 | 1:A:994:TRP:CD1 | 2.52 | 0.44 |
| 2:B:251:TRP:HA | 2:B:251:TRP:HE3 | 1.83 | 0.44 |
| 2:C:185:LEU:CD2 | 2:C:214:CYS:SG | 3.05 | 0.44 |
| 2:C:241:TRP:CZ3 | 2:C:255:TRP:CZ2 | 3.06 | 0.44 |
| 2:C:92:LEU:CD2 | 2:C:344:ARG:HE | 2.28 | 0.44 |
| 2:C:375:HIS:CD2 | 2:C:377:CYS:H | 2.36 | 0.44 |
| 1:A:472:GLN:CG | 2:C:460:THR:HB | 2.41 | 0.44 |
| 1:D:1111:LEU:N | 1:D:1111:LEU:HD12 | 2.32 | 0.44 |
| 1:D:1111:LEU:CD1 | 1:D:1111:LEU:N | 2.80 | 0.44 |
| 1:D:1166:TYR:CE2 | 1:D:1171:ASN:HA | 2.53 | 0.44 |
| 1:D:249:VAL:HG11 | 1:D:251:THR:CG2 | 2.47 | 0.44 |
| 1:D:305:SER:HB2 | 1:D:308:GLN:CD | 2.38 | 0.44 |
| 1:D:803:ASN:OD1 | 1:D:803:ASN:N | 2.50 | 0.44 |
| 1:D:958:GLY:O | 1:D:959:GLN:C | 2.56 | 0.44 |
| 2:E:94:GLY:CA | 2:E:96:HIS:CE1 | 2.97 | 0.44 |
| 2:F:405:GLU:OE1 | 2:F:406:LEU:HD12 | 2.16 | 0.44 |
| 2:F:407:LEU:HD23 | 2:F:407:LEU:O | 2.17 | 0.44 |
| 1:A:1014:ARG:O | 1:A:1014:ARG:HG2 | 2.17 | 0.44 |
| 1:A:247:LEU:HD11 | 1:A:251:THR:HG21 | 1.96 | 0.44 |
| 1:A:484:TRP:O | 1:A:488:LEU:CG | 2.57 | 0.44 |
| 1:A:515:ILE:HG12 | 1:A:565:HIS:HA | 1.99 | 0.44 |
| 1:A:467:ALA:HB2 | 1:A:602:LEU:HD13 | 2.00 | 0.44 |
| 1:A:756:ASP:OD1 | 1:A:770:PHE:HZ | 2.00 | 0.44 |
| 1:A:762:VAL:HG23 | 1:A:763:GLY:N | 2.32 | 0.44 |
| 1:A:893:SER:O | 1:A:894:GLN:C | 2.55 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:79:LEU:C | 2:B:100:GLY:HA3 | 2.38 | 0.44 |
| 2:B:461:THR:CG2 | 2:B:463:LYS:NZ | 2.80 | 0.44 |
| 2:B:100:GLY:CA | 2:C:128:VAL:HG11 | 2.47 | 0.44 |
| 2:C:395:LEU:CD1 | 2:C:444:THR:CA | 2.90 | 0.44 |
| 2:C:449:GLU:H | 2:C:451:GLY:N | 2.15 | 0.44 |
| 2:C:459:ASP:O | 2:C:460:THR:OG1 | 2.32 | 0.44 |
| 1:D:1027:LYS:CB | 1:D:1091:GLU:CA | 2.85 | 0.44 |
| 1:D:1129:PHE:HB2 | 1:D:1138:ARG:O | 2.17 | 0.44 |
| 1:D:897:TRP:CH2 | 1:D:1173:LEU:HD22 | 2.53 | 0.44 |
| 1:D:876:ALA:O | 1:D:1189:LEU:HD23 | 2.18 | 0.44 |
| 1:D:1209:ARG:NH1 | 2:F:252:LEU:CD1 | 2.64 | 0.44 |
| 1:D:1224:ILE:HD11 | 1:D:1228:LYS:HE3 | 2.00 | 0.44 |
| 1:D:192:GLU:HG2 | 1:D:193:ARG:C | 2.38 | 0.44 |
| 1:D:301:ILE:HG13 | 1:D:415:LEU:HD12 | 1.99 | 0.44 |
| 1:D:384:ASP:O | 1:D:388:ASN:OD1 | 2.36 | 0.44 |
| 1:D:549:LEU:C | 1:D:551:LYS:HD2 | 2.38 | 0.44 |
| 1:D:726:LYS:O | 1:D:727:ASP:HB3 | 2.17 | 0.44 |
| 1:D:786:ALA:O | 1:D:787:SER:HB3 | 2.17 | 0.44 |
| 1:D:826:ILE:O | 1:D:829:PRO:HB3 | 2.18 | 0.44 |
| 2:E:109:ASN:CB | 2:E:378:LEU:O | 2.66 | 0.44 |
| 2:E:382:LYS:CD | 2:E:383:VAL:H | 2.31 | 0.44 |
| 2:E:382:LYS:HG3 | 2:E:383:VAL:H | 1.68 | 0.44 |
| 2:E:384:ALA:HB1 | 2:E:385:LEU:H | 1.13 | 0.44 |
| 2:E:441:VAL:HG22 | 2:E:455:LEU:HD13 | 2.00 | 0.44 |
| 2:F:129:ASP:OD1 | 2:F:131:LEU:HD13 | 2.18 | 0.44 |
| 2:F:138:LEU:HB3 | 2:F:139:LEU:H | 1.57 | 0.44 |
| 2:F:263:TRP:CZ3 | 2:F:349:TYR:CE2 | 3.06 | 0.44 |
| 2:F:394:GLU:N | 2:F:394:GLU:OE1 | 2.51 | 0.44 |
| 2:F:426:GLU:O | 2:F:429:TYR:HB2 | 2.17 | 0.44 |
| 2:F:444:THR:O | 2:F:447:THR:HG21 | 2.12 | 0.44 |
| 2:F:454:HIS:CD2 | 2:F:468:ILE:HG13 | 2.53 | 0.44 |
| 1:A:1026:ARG:CA | 1:A:1029:GLN:NE2 | 2.80 | 0.44 |
| 1:A:1041:TRP:CD1 | 1:A:1043:VAL:CB | 2.97 | 0.44 |
| 1:A:1146:ARG:HH22 | 1:A:1186:ASP:H | 1.65 | 0.44 |
| 1:A:652:ILE:O | 1:A:655:LEU:HD12 | 2.17 | 0.44 |
| 1:A:655:LEU:HA | 1:A:713:PRO:HB3 | 2.00 | 0.44 |
| 1:A:905:ALA:CA | 1:A:910:MET:HB3 | 2.47 | 0.44 |
| 1:A:933:SER:HB2 | 1:A:943:ARG:NH1 | 2.33 | 0.44 |
| 1:A:934:LYS:HE3 | 1:A:934:LYS:HB2 | 1.77 | 0.44 |
| 1:A:973:LEU:HD13 | 1:A:977:GLU:OE1 | 2.18 | 0.44 |
| 2:B:132:HIS:CD2 | 2:B:182:ARG:NH1 | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:217:PRO:HB2 | 2:B:231:ILE:HB | 1.97 | 0.44 |
| 2:B:259:ARG:HD2 | 2:B:262:TRP:CB | 2.48 | 0.44 |
| 2:C:199:LEU:HD12 | 2:C:200:VAL:N | 2.32 | 0.44 |
| 1:A:1208:ARG:CZ | 2:C:277:ASP:OD1 | 2.65 | 0.44 |
| 2:C:483:LYS:O | 2:C:485:VAL:CG1 | 2.66 | 0.44 |
| 1:D:1027:LYS:HD3 | 1:D:1027:LYS:N | 2.33 | 0.44 |
| 1:D:1118:TRP:NE1 | 1:D:1122:GLU:OE1 | 2.51 | 0.44 |
| 1:D:1163:MET:CE | 1:D:1167:LYS:CG | 2.95 | 0.44 |
| 1:D:368:PRO:HA | 1:D:369:LEU:HA | 1.41 | 0.44 |
| 1:D:518:ALA:O | 1:D:521:PRO:HD2 | 2.17 | 0.44 |
| 1:D:597:ARG:O | 1:D:600:PRO:HD2 | 2.17 | 0.44 |
| 1:D:598:VAL:N | 1:D:616:GLU:OE1 | 2.49 | 0.44 |
| 1:D:801:TRP:CD2 | 1:D:870:VAL:HG12 | 2.53 | 0.44 |
| 1:D:83:LEU:C | 1:D:87:ILE:O | 2.56 | 0.44 |
| 1:D:985:MET:O | 1:D:986:TYR:C | 2.56 | 0.44 |
| 2:E:386:ASP:HB3 | 2:E:441:VAL:O | 2.18 | 0.44 |
| 2:F:241:TRP:HE3 | 2:F:336:LEU:CD1 | 2.30 | 0.44 |
| 2:F:259:ARG:CZ | 2:F:339:ASN:HD21 | 2.31 | 0.44 |
| 2:F:79:LEU:HD13 | 2:F:79:LEU:HA | 1.72 | 0.44 |
| 1:A:1064:ILE:C | 1:A:1066:THR:H | 2.21 | 0.44 |
| 1:A:1179:PHE:O | 1:A:1220:ILE:CD1 | 2.65 | 0.44 |
| 1:A:184:ALA:O | 1:A:185:VAL:CG1 | 2.58 | 0.44 |
| 1:A:188:ALA:O | 1:A:189:ILE:CG1 | 2.65 | 0.44 |
| 1:A:192:GLU:HB3 | 1:A:195:LEU:HD21 | 1.95 | 0.44 |
| 1:A:316:LYS:NZ | 1:A:350:ILE:CG1 | 2.80 | 0.44 |
| 1:A:316:LYS:CB | 1:A:348:LEU:HD11 | 2.47 | 0.44 |
| 1:A:515:ILE:HG12 | 1:A:565:HIS:CA | 2.48 | 0.44 |
| 1:A:623:LEU:H | 1:A:623:LEU:CD2 | 2.29 | 0.44 |
| 1:A:630:ASN:O | 1:A:631:LEU:HD23 | 2.18 | 0.44 |
| 1:A:741:ASP:O | 1:A:742:VAL:CB | 2.50 | 0.44 |
| 1:A:792:LEU:O | 1:A:796:LYS:CG | 2.66 | 0.44 |
| 1:A:70:ARG:HD3 | 1:A:81:ARG:HB3 | 1.99 | 0.44 |
| 1:A:901:VAL:HA | 1:A:904:ASP:OD2 | 2.18 | 0.44 |
| 1:A:992:LEU:HD12 | 1:A:993:ARG:N | 2.28 | 0.44 |
| 2:B:132:HIS:CG | 2:B:182:ARG:CZ | 3.01 | 0.44 |
| 2:B:259:ARG:HH11 | 2:B:259:ARG:CB | 2.29 | 0.44 |
| 2:B:277:ASP:HA | 2:B:287:ASN:ND2 | 2.33 | 0.44 |
| 2:B:343:ASP:CG | 2:B:344:ARG:HH21 | 2.18 | 0.44 |
| 2:B:423:SER:O | 2:B:424:SER:HB3 | 2.17 | 0.44 |
| 2:C:200:VAL:HB | 2:C:204:LEU:HD22 | 1.99 | 0.44 |
| 2:C:254:PHE:HE2 | 2:C:255:TRP:CE2 | 2.36 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:293:PHE:HB3 | 2:C:294:PRO:CD | 2.47 | 0.44 |
| 2:C:363:ARG:NH1 | 2:C:363:ARG:CB | 2.81 | 0.44 |
| 2:C:387:VAL:CG1 | 2:C:395:LEU:O | 2.66 | 0.44 |
| 1:D:1190:ARG:NH1 | 1:D:1195:MET:SD | 2.90 | 0.44 |
| 1:D:1200:PRO:O | 1:D:1203:PRO:CD | 2.40 | 0.44 |
| 1:D:1204:THR:C | 1:D:1207:GLU:H | 2.21 | 0.44 |
| 1:D:120:LEU:N | 1:D:121:PRO:HD2 | 2.33 | 0.44 |
| 1:D:127:LEU:HA | 1:D:128:PRO:HD3 | 1.56 | 0.44 |
| 1:D:143:ALA:HA | 1:D:146:GLN:HG3 | 1.99 | 0.44 |
| 1:D:225:SER:O | 1:D:229:VAL:HG22 | 2.18 | 0.44 |
| 1:D:416:GLU:HG3 | 1:D:416:GLU:H | 1.66 | 0.44 |
| 1:D:448:ALA:HB1 | 1:D:870:VAL:CB | 2.37 | 0.44 |
| 1:D:515:ILE:O | 1:D:565:HIS:CE1 | 2.70 | 0.44 |
| 1:D:728:THR:HG22 | 1:D:729:GLN:N | 2.32 | 0.44 |
| 2:E:203:ARG:NH2 | 2:E:203:ARG:CG | 2.79 | 0.44 |
| 2:E:299:LEU:HD23 | 2:E:299:LEU:C | 2.38 | 0.44 |
| 2:E:325:ARG:HA | 2:E:331:VAL:HG12 | 1.98 | 0.44 |
| 2:E:437:ILE:CG2 | 2:E:439:PHE:O | 2.66 | 0.44 |
| 2:E:90:SER:OG | 2:E:96:HIS:N | 2.51 | 0.44 |
| 2:F:106:LEU:O | 2:F:107:ARG:C | 2.53 | 0.44 |
| 2:F:128:VAL:HG12 | 2:F:129:ASP:H | 1.83 | 0.44 |
| 2:F:78:PHE:HZ | 2:F:346:MET:CE | 2.29 | 0.44 |
| 1:D:784:GLY:O | 2:F:363:ARG:HG2 | 2.17 | 0.44 |
| 1:A:1065:ALA:O | 1:A:1071:ARG:HB3 | 2.17 | 0.44 |
| 1:A:106:HIS:C | 1:A:108:GLN:H | 2.20 | 0.44 |
| 1:A:79:LEU:CD1 | 1:A:1172:ASP:OD2 | 2.66 | 0.44 |
| 1:A:170:ALA:HB1 | 1:A:175:TRP:CH2 | 2.47 | 0.44 |
| 1:A:634:LEU:CD1 | 1:A:638:THR:HG21 | 2.47 | 0.44 |
| 1:A:617:ARG:HB2 | 1:A:725:PRO:HD3 | 2.00 | 0.44 |
| 1:A:869:ARG:HB3 | 1:A:872:SER:OG | 2.18 | 0.44 |
| 1:A:930:ASP:C | 1:A:933:SER:HB3 | 2.39 | 0.44 |
| 1:A:967:MET:HG2 | 1:A:978:ALA:HB2 | 1.99 | 0.44 |
| 1:A:967:MET:SD | 1:A:978:ALA:HB2 | 2.57 | 0.44 |
| 2:B:114:TRP:C | 2:B:116:THR:N | 2.69 | 0.44 |
| 2:B:229:LYS:N | 2:B:229:LYS:CD | 2.78 | 0.44 |
| 2:B:236:GLU:CG | 2:B:341:ASP:HB3 | 2.48 | 0.44 |
| 2:B:468:ILE:CG2 | 2:B:468:ILE:O | 2.62 | 0.44 |
| 2:C:331:VAL:CG1 | 2:C:332:VAL:N | 2.79 | 0.44 |
| 2:C:348:ALA:O | 2:C:352:ASP:N | 2.48 | 0.44 |
| 2:C:351:TYR:O | 2:C:355:GLN:HB2 | 2.09 | 0.44 |
| 2:C:361:PHE:HD2 | 2:C:362:THR:CG2 | 2.30 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:367:LEU:C | 2:C:367:LEU:HD12 | 2.38 | 0.44 |
| 1:D:1019:TRP:HE3 | 1:D:1168:LEU:CD1 | 2.30 | 0.44 |
| 1:D:175:TRP:CZ2 | 1:D:183:GLU:CG | 3.01 | 0.44 |
| 1:D:195:LEU:C | 1:D:267:VAL:HG12 | 2.38 | 0.44 |
| 1:D:242:ALA:O | 1:D:246:PRO:CD | 2.57 | 0.44 |
| 1:D:269:HIS:C | 1:D:294:THR:CG2 | 2.79 | 0.44 |
| 1:D:279:ARG:NH1 | 1:D:841:LEU:HA | 2.33 | 0.44 |
| 1:D:293:ASP:OD2 | 1:D:294:THR:N | 2.51 | 0.44 |
| 1:D:482:ASP:HB2 | 1:D:483:PRO:CD | 2.46 | 0.44 |
| 1:D:547:ALA:C | 1:D:551:LYS:CD | 2.85 | 0.44 |
| 1:D:585:TRP:N | 1:D:585:TRP:CE3 | 2.86 | 0.44 |
| 1:D:728:THR:CG2 | 1:D:741:ASP:OD2 | 2.64 | 0.44 |
| 1:D:790:ARG:C | 1:D:792:LEU:N | 2.71 | 0.44 |
| 1:D:866:ARG:CB | 1:D:867:PRO:HD3 | 2.29 | 0.44 |
| 1:D:870:VAL:HG22 | 1:D:874:LEU:HD22 | 2.00 | 0.44 |
| 1:D:927:ARG:HH11 | 1:D:927:ARG:HG3 | 1.83 | 0.44 |
| 2:E:125:VAL:HG22 | 2:E:241:TRP:HZ3 | 1.82 | 0.44 |
| 2:E:185:LEU:HD12 | 2:E:237:ALA:O | 2.17 | 0.44 |
| 2:E:128:VAL:CB | 2:E:208:LEU:HB3 | 2.35 | 0.44 |
| 2:E:215:PHE:C | 2:E:216:HIS:HD2 | 2.21 | 0.44 |
| 2:E:335:VAL:CG2 | 2:E:336:LEU:H | 2.31 | 0.44 |
| 2:E:404:ASN:C | 2:E:406:LEU:H | 2.21 | 0.44 |
| 2:F:270:PRO:O | 2:F:273:PHE:HD2 | 2.01 | 0.44 |
| 2:F:451:GLY:O | 2:F:452:LEU:CB | 2.55 | 0.44 |
| 2:F:476:ILE:HD13 | 2:F:477:LYS:H | 1.82 | 0.44 |
| 1:A:1030:ARG:NH2 | 1:A:1044:VAL:CG1 | 2.81 | 0.44 |
| 1:A:1179:PHE:HB3 | 1:A:1220:ILE:CG1 | 2.31 | 0.44 |
| 1:A:195:LEU:HA | 1:A:216:SER:OG | 2.18 | 0.44 |
| 1:A:241:PRO:C | 1:A:244:LEU:HB2 | 2.38 | 0.44 |
| 1:A:493:GLN:O | 1:A:495:PHE:CD1 | 2.71 | 0.44 |
| 1:A:494:GLU:HB2 | 1:A:572:TRP:CE2 | 2.52 | 0.44 |
| 1:A:612:LEU:C | 1:A:612:LEU:HD12 | 2.38 | 0.44 |
| 1:A:635:PRO:C | 1:A:637:GLY:N | 2.71 | 0.44 |
| 1:A:730:PRO:CB | 1:A:760:CYS:O | 2.66 | 0.44 |
| 1:A:789:PRO:O | 1:A:793:GLU:CB | 2.65 | 0.44 |
| 1:A:950:ASN:O | 1:A:951:TYR:O | 2.35 | 0.44 |
| 1:A:963:GLU:HA | 1:A:966:LEU:HG | 1.99 | 0.44 |
| 1:A:97:GLU:O | 1:A:98:ALA:C | 2.54 | 0.44 |
| 2:B:79:LEU:HA | 2:B:100:GLY:CA | 2.48 | 0.44 |
| 2:B:206:TYR:CE1 | 2:B:242:PHE:HZ | 2.36 | 0.44 |
| 2:B:418:LEU:O | 2:B:418:LEU:HD23 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:115:TRP:CD1 | 2:C:119:VAL:HG21 | 2.53 | 0.44 |
| 2:C:204:LEU:HG | 2:C:206:TYR:CG | 2.53 | 0.44 |
| 1:D:873:GLU:HB2 | 1:D:1203:PRO:HB3 | 2.00 | 0.44 |
| 1:D:404:HIS:O | 1:D:408:GLN:CB | 2.66 | 0.44 |
| 1:D:601:LYS:CE | 1:D:721:ALA:HB1 | 2.32 | 0.44 |
| 1:D:768:LYS:CA | 1:D:772:PRO:CD | 2.96 | 0.44 |
| 1:D:904:ASP:OD2 | 1:D:915:ALA:CB | 2.63 | 0.44 |
| 1:D:914:THR:HA | 1:D:918:TRP:CB | 2.48 | 0.44 |
| 2:F:279:GLN:NE2 | 2:F:279:GLN:HA | 2.33 | 0.44 |
| 2:F:342:LEU:HD23 | 2:F:342:LEU:C | 2.38 | 0.44 |
| 1:A:1195:MET:O | 1:A:1196:ASP:CG | 2.56 | 0.43 |
| 1:A:1218:LEU:O | 1:A:1219:ASP:CB | 2.46 | 0.43 |
| 1:A:480:LYS:HA | 1:A:484:TRP:HD1 | 1.82 | 0.43 |
| 1:A:486:TRP:CZ3 | 1:A:598:VAL:CG2 | 2.96 | 0.43 |
| 1:A:498:LYS:HG2 | 1:A:518:ALA:H | 1.83 | 0.43 |
| 1:A:560:PRO:CB | 2:C:452:LEU:HD21 | 2.47 | 0.43 |
| 1:A:80:SER:H | 1:A:83:LEU:CD1 | 2.08 | 0.43 |
| 1:A:877:MET:HA | 1:A:877:MET:HE3 | 2.00 | 0.43 |
| 2:B:182:ARG:CD | 2:B:214:CYS:HA | 2.48 | 0.43 |
| 2:B:461:THR:HG23 | 2:B:461:THR:O | 2.18 | 0.43 |
| 2:B:471:LEU:HD12 | 2:B:474:PHE:HD2 | 1.83 | 0.43 |
| 2:C:262:TRP:HZ3 | 2:C:263:TRP:CZ2 | 2.35 | 0.43 |
| 2:C:294:PRO:HG3 | 2:C:355:GLN:NE2 | 2.32 | 0.43 |
| 2:C:346:MET:CE | 2:C:347:LEU:HD12 | 2.48 | 0.43 |
| 2:C:444:THR:N | 2:C:447:THR:HG21 | 2.33 | 0.43 |
| 2:C:90:SER:HB2 | 2:C:95:CYS:SG | 2.59 | 0.43 |
| 1:D:119:PRO:HG2 | 1:D:120:LEU:HD22 | 1.99 | 0.43 |
| 1:D:166:PRO:HA | 1:D:167:PRO:HD3 | 1.47 | 0.43 |
| 1:D:247:LEU:N | 1:D:815:TRP:HD1 | 2.14 | 0.43 |
| 1:D:553:LYS:HD3 | 2:F:468:ILE:HG21 | 1.99 | 0.43 |
| 1:D:588:GLY:N | 1:D:806:LYS:HZ1 | 2.16 | 0.43 |
| 1:D:776:ASP:C | 1:D:776:ASP:OD1 | 2.57 | 0.43 |
| 1:D:79:LEU:HD11 | 1:D:1173:LEU:C | 2.33 | 0.43 |
| 1:D:80:SER:N | 1:D:83:LEU:HD11 | 2.33 | 0.43 |
| 1:D:770:PHE:HE1 | 1:D:968:GLN:CA | 2.30 | 0.43 |
| 1:D:990:LYS:HE2 | 1:D:1000:GLU:OE2 | 2.14 | 0.43 |
| 2:E:235:THR:H | 2:E:343:ASP:CG | 2.22 | 0.43 |
| 2:E:72:ILE:CD1 | 2:E:72:ILE:N | 2.80 | 0.43 |
| 2:F:186:LEU:O | 2:F:187:HIS:C | 2.56 | 0.43 |
| 2:F:191:GLU:CD | 2:F:315:TYR:HH | 2.21 | 0.43 |
| 2:F:251:TRP:HZ3 | 2:F:254:PHE:CG | 2.35 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:253:ASP:OD1 | 2:F:256:LEU:HD23 | 2.18 | 0.43 |
| 2:F:326:ASP:OD1 | 2:F:329:LYS:CG | 2.56 | 0.43 |
| 2:F:387:VAL:HG11 | 2:F:399:CYS:HB2 | 1.98 | 0.43 |
| 2:F:415:PRO:HA | 2:F:417:TYR:HE2 | 1.82 | 0.43 |
| 2:F:471:LEU:CA | 2:F:474:PHE:CD2 | 2.91 | 0.43 |
| 2:F:70:LEU:O | 2:F:73:CYS:N | 2.47 | 0.43 |
| 1:A:1046:GLU:CD | 1:A:1049:TRP:CD1 | 2.91 | 0.43 |
| 1:A:1181:SER:O | 1:A:1182:ALA:HB2 | 2.18 | 0.43 |
| 1:A:1227:THR:O | 1:A:1235:SER:OG | 2.34 | 0.43 |
| 1:A:267:VAL:CG2 | 1:A:291:PHE:CE2 | 3.01 | 0.43 |
| 1:A:402:ALA:O | 1:A:403:THR:C | 2.56 | 0.43 |
| 1:A:585:TRP:N | 1:A:585:TRP:CE3 | 2.83 | 0.43 |
| 1:A:601:LYS:HG2 | 1:A:721:ALA:HB3 | 1.98 | 0.43 |
| 1:A:70:ARG:N | 1:A:81:ARG:HD2 | 2.33 | 0.43 |
| 1:A:749:PHE:N | 1:A:749:PHE:HD1 | 2.15 | 0.43 |
| 1:A:790:ARG:O | 1:A:794:ILE:HG13 | 2.18 | 0.43 |
| 1:A:836:LEU:O | 1:A:837:TYR:HD2 | 2.02 | 0.43 |
| 1:A:892:ASP:O | 1:A:893:SER:OG | 2.27 | 0.43 |
| 1:A:931:LEU:O | 1:A:932:HIS:C | 2.56 | 0.43 |
| 1:A:995:TYR:O | 1:A:996:ARG:CG | 2.66 | 0.43 |
| 2:B:117:SER:OG | 2:B:259:ARG:HD3 | 2.18 | 0.43 |
| 2:B:132:HIS:CE1 | 2:B:182:ARG:HH22 | 2.36 | 0.43 |
| 2:B:194:VAL:HG13 | 2:B:195:ASN:H | 1.83 | 0.43 |
| 2:B:246:ARG:C | 2:B:248:SER:N | 2.71 | 0.43 |
| 2:B:259:ARG:NH1 | 2:B:259:ARG:CB | 2.81 | 0.43 |
| 2:B:261:GLN:O | 2:B:262:TRP:C | 2.55 | 0.43 |
| 2:C:207:GLY:CA | 2:C:239:LEU:HD11 | 2.45 | 0.43 |
| 2:C:386:ASP:OD2 | 2:C:441:VAL:N | 2.51 | 0.43 |
| 2:C:76:ARG:NE | 2:C:434:GLU:HB3 | 2.32 | 0.43 |
| 1:D:1010:LEU:H | 1:D:1011:PRO:CD | 2.28 | 0.43 |
| 1:D:768:LYS:HZ2 | 1:D:1064:ILE:HG22 | 1.83 | 0.43 |
| 1:D:76:ILE:HD11 | 1:D:1174:PRO:N | 2.33 | 0.43 |
| 1:D:1195:MET:C | 1:D:1196:ASP:O | 2.49 | 0.43 |
| 1:D:1151:LEU:CG | 1:D:1223:ILE:HD11 | 2.48 | 0.43 |
| 1:D:180:PRO:O | 1:D:181:GLU:OE2 | 2.36 | 0.43 |
| 1:D:175:TRP:CB | 1:D:185:VAL:HG22 | 2.47 | 0.43 |
| 1:D:265:LEU:HD21 | 1:D:267:VAL:CB | 2.48 | 0.43 |
| 1:D:353:VAL:HG23 | 1:D:354:ASN:OD1 | 2.19 | 0.43 |
| 1:D:363:TYR:O | 1:D:364:VAL:CB | 2.65 | 0.43 |
| 1:D:424:LEU:HD23 | 1:D:424:LEU:H | 1.82 | 0.43 |
| 1:D:437:VAL:HG13 | 1:D:441:TRP:HB2 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:592:LEU:HA | 1:D:595:GLN:HG2 | 1.93 | 0.43 |
| 1:D:779:LEU:HD22 | 1:D:780:GLN:CA | 2.46 | 0.43 |
| 1:D:826:ILE:CB | 1:D:831:TYR:HE2 | 2.26 | 0.43 |
| 1:D:444:TYR:CZ | 1:D:877:MET:CE | 3.01 | 0.43 |
| 1:D:878:VAL:O | 1:D:879:GLN:HB3 | 2.18 | 0.43 |
| 1:D:950:ASN:O | 1:D:953:ARG:HB2 | 2.18 | 0.43 |
| 1:D:954:ILE:HG22 | 1:D:955:TYR:N | 2.33 | 0.43 |
| 1:D:989:THR:C | 1:D:998:SER:HB3 | 2.38 | 0.43 |
| 2:E:100:GLY:O | 2:E:104:VAL:N | 2.48 | 0.43 |
| 2:E:131:LEU:O | 2:E:182:ARG:NH2 | 2.47 | 0.43 |
| 2:E:252:LEU:HD13 | 2:E:252:LEU:O | 2.18 | 0.43 |
| 2:E:289:LEU:C | 2:E:290:TYR:CG | 2.91 | 0.43 |
| 2:E:344:ARG:C | 2:E:346:MET:N | 2.70 | 0.43 |
| 2:E:406:LEU:HB2 | 2:E:413:VAL:HG23 | 2.00 | 0.43 |
| 2:E:406:LEU:HB2 | 2:E:413:VAL:CG2 | 2.48 | 0.43 |
| 2:E:448:LEU:HD23 | 2:E:449:GLU:CA | 2.48 | 0.43 |
| 2:F:245:PRO:CG | 2:F:246:ARG:N | 2.81 | 0.43 |
| 2:F:331:VAL:CG1 | 2:F:332:VAL:N | 2.78 | 0.43 |
| 2:F:431:LYS:HZ3 | 2:F:435:MET:CG | 2.32 | 0.43 |
| 2:F:386:ASP:OD2 | 2:F:441:VAL:N | 2.51 | 0.43 |
| 1:A:1151:LEU:O | 1:A:1152:ALA:C | 2.56 | 0.43 |
| 1:A:175:TRP:O | 1:A:176:THR:HB | 2.18 | 0.43 |
| 1:A:282:TYR:CZ | 1:A:291:PHE:CZ | 3.06 | 0.43 |
| 1:A:346:ASP:HB2 | 1:A:1040:LYS:HG3 | 2.00 | 0.43 |
| 1:A:542:ASP:O | 1:A:546:ARG:HG3 | 2.18 | 0.43 |
| 1:A:570:PRO:CG | 1:A:572:TRP:CZ3 | 3.02 | 0.43 |
| 1:A:601:LYS:C | 1:A:602:LEU:O | 2.45 | 0.43 |
| 1:A:610:PHE:HB2 | 1:A:611:PRO:HD3 | 2.00 | 0.43 |
| 1:A:588:GLY:N | 1:A:806:LYS:HZ1 | 2.15 | 0.43 |
| 1:A:813:VAL:HG13 | 1:A:815:TRP:CZ2 | 2.52 | 0.43 |
| 1:A:79:LEU:HB2 | 1:A:89:GLY:O | 2.19 | 0.43 |
| 1:A:904:ASP:OD1 | 1:A:915:ALA:HB3 | 2.19 | 0.43 |
| 1:A:916:PHE:CE2 | 1:A:920:THR:O | 2.72 | 0.43 |
| 2:B:213:VAL:HG13 | 2:B:213:VAL:O | 2.18 | 0.43 |
| 2:B:78:PHE:CE1 | 2:B:103:GLY:CA | 3.01 | 0.43 |
| 2:C:121:PHE:C | 2:C:123:GLU:H | 2.21 | 0.43 |
| 2:C:280:ASP:HB3 | 2:C:282:GLU:O | 2.18 | 0.43 |
| 2:C:322:LEU:C | 2:C:322:LEU:HD13 | 2.36 | 0.43 |
| 2:C:372:LEU:HD21 | 2:C:436:SER:CB | 2.46 | 0.43 |
| 1:A:560:PRO:HG2 | 2:C:452:LEU:HD21 | 2.00 | 0.43 |
| 1:D:113:TRP:CE3 | 1:D:114:GLY:N | 2.58 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:352:SER:HB3 | 1:D:352:SER:C | 2.36 | 0.43 |
| 1:D:440:ASN:CB | 1:D:441:TRP:CE3 | 3.02 | 0.43 |
| 1:D:441:TRP:CE3 | 1:D:441:TRP:N | 2.86 | 0.43 |
| 1:D:802:ARG:CG | 1:D:803:ASN:N | 2.81 | 0.43 |
| 1:D:874:LEU:HG | 1:D:878:VAL:HG13 | 2.01 | 0.43 |
| 1:D:926:SER:O | 1:D:929:THR:HG22 | 2.18 | 0.43 |
| 2:E:312:LEU:CD1 | 2:E:312:LEU:H | 2.32 | 0.43 |
| 2:E:371:VAL:O | 2:E:372:LEU:HB2 | 2.18 | 0.43 |
| 2:E:389:ARG:C | 2:E:389:ARG:NE | 2.70 | 0.43 |
| 2:E:476:ILE:O | 2:E:480:SER:CB | 2.66 | 0.43 |
| 2:F:247:THR:OG1 | 2:F:251:TRP:HB2 | 2.18 | 0.43 |
| 2:F:396:ARG:CZ | 2:F:397:GLN:HA | 2.48 | 0.43 |
| 2:F:433:ASP:C | 2:F:435:MET:H | 2.21 | 0.43 |
| 2:F:76:ARG:HD3 | 2:F:434:GLU:HB2 | 2.00 | 0.43 |
| 2:F:449:GLU:O | 2:F:451:GLY:N | 2.46 | 0.43 |
| 2:F:479:ILE:HG13 | 2:F:479:ILE:H | 1.47 | 0.43 |
| 2:F:69:LEU:HD23 | 2:F:351:TYR:CD1 | 2.53 | 0.43 |
| 2:F:70:LEU:O | 2:F:71:GLU:C | 2.57 | 0.43 |
| 1:A:1040:LYS:C | 1:A:1042:GLU:H | 2.20 | 0.43 |
| 1:A:1108:TYR:HE2 | 1:A:1112:MET:HE1 | 1.81 | 0.43 |
| 1:A:1118:TRP:CZ3 | 1:A:1121:GLU:OE1 | 2.72 | 0.43 |
| 1:A:401:TRP:O | 1:A:402:ALA:C | 2.56 | 0.43 |
| 1:A:359:ALA:CB | 1:A:407:PHE:HE2 | 2.22 | 0.43 |
| 1:A:407:PHE:N | 1:A:407:PHE:HD2 | 2.16 | 0.43 |
| 1:A:459:MET:O | 1:A:462:SER:OG | 2.29 | 0.43 |
| 1:A:531:GLY:HA2 | 1:A:532:PRO:HD3 | 1.77 | 0.43 |
| 1:A:564:GLN:N | 1:A:564:GLN:NE2 | 2.61 | 0.43 |
| 1:A:588:GLY:HA3 | 1:A:589:PRO:HD2 | 1.78 | 0.43 |
| 1:A:610:PHE:H | 1:A:610:PHE:HD2 | 1.59 | 0.43 |
| 1:A:769:ASP:O | 1:A:772:PRO:CD | 2.66 | 0.43 |
| 1:A:79:LEU:HA | 1:A:79:LEU:HD23 | 1.65 | 0.43 |
| 1:A:81:ARG:HA | 1:A:84:HIS:CD2 | 2.52 | 0.43 |
| 1:A:83:LEU:HD22 | 1:A:89:GLY:CA | 2.39 | 0.43 |
| 1:A:960:PRO:HA | 1:A:963:GLU:HG3 | 1.99 | 0.43 |
| 2:B:382:LYS:N | 2:B:412:SER:OG | 2.50 | 0.43 |
| 2:B:95:CYS:O | 2:B:96:HIS:C | 2.56 | 0.43 |
| 1:D:1008:LEU:O | 1:D:1012:VAL:CG2 | 2.63 | 0.43 |
| 1:D:1091:GLU:O | 1:D:1092:PHE:CD2 | 2.71 | 0.43 |
| 1:D:887:VAL:N | 1:D:1146:ARG:HH22 | 2.09 | 0.43 |
| 1:D:1232:GLU:HB2 | 1:D:1234:ARG:N | 2.33 | 0.43 |
| 1:D:136:ASP:C | 1:D:136:ASP:OD1 | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:370:GLU:O | 1:D:371:LYS:CB | 2.60 | 0.43 |
| 1:D:169:TRP:CD1 | 1:D:390:GLN:O | 2.71 | 0.43 |
| 1:D:545:ALA:O | 1:D:548:CYS:SG | 2.75 | 0.43 |
| 1:D:576:LEU:HB3 | 1:D:579:ARG:HD2 | 2.00 | 0.43 |
| 1:D:604:ALA:O | 1:D:782:GLY:N | 2.48 | 0.43 |
| 1:D:876:ALA:O | 1:D:878:VAL:N | 2.51 | 0.43 |
| 1:D:878:VAL:O | 1:D:879:GLN:CB | 2.61 | 0.43 |
| 2:E:205:PRO:CG | 2:E:241:TRP:NE1 | 2.79 | 0.43 |
| 2:E:215:PHE:CD1 | 2:E:215:PHE:O | 2.71 | 0.43 |
| 2:E:339:ASN:N | 2:E:339:ASN:HD22 | 2.17 | 0.43 |
| 2:E:374:LEU:HB3 | 2:E:375:HIS:H | 1.59 | 0.43 |
| 2:E:422:GLN:O | 2:E:424:SER:N | 2.51 | 0.43 |
| 2:E:379:ALA:CB | 2:E:438:LEU:HD21 | 2.49 | 0.43 |
| 2:E:462:MET:HA | 2:E:462:MET:HE1 | 2.01 | 0.43 |
| 2:F:262:TRP:O | 2:F:266:PHE:HD2 | 2.02 | 0.43 |
| 2:F:403:PHE:HD2 | 2:F:404:ASN:N | 2.15 | 0.43 |
| 2:F:427:GLN:C | 2:F:430:SER:HG | 2.21 | 0.43 |
| 1:A:1218:LEU:O | 1:A:1222:GLN:CD | 2.57 | 0.43 |
| 1:A:172:ALA:O | 1:A:173:GLU:CB | 2.67 | 0.43 |
| 1:A:249:VAL:HB | 1:A:250:PRO:HD3 | 2.00 | 0.43 |
| 1:A:307:PHE:CD1 | 1:A:307:PHE:N | 2.81 | 0.43 |
| 1:A:350:ILE:HA | 1:A:350:ILE:HD12 | 1.67 | 0.43 |
| 1:A:371:LYS:HG2 | 1:A:372:GLU:HG2 | 1.99 | 0.43 |
| 1:A:415:LEU:C | 1:A:417:ARG:H | 2.21 | 0.43 |
| 1:A:420:HIS:ND1 | 1:A:422:VAL:HG23 | 2.33 | 0.43 |
| 1:A:498:LYS:HG2 | 1:A:518:ALA:N | 2.33 | 0.43 |
| 1:A:539:PHE:C | 1:A:539:PHE:CD2 | 2.92 | 0.43 |
| 1:A:543:VAL:HG13 | 1:A:544:MET:H | 1.82 | 0.43 |
| 1:A:761:ASN:O | 1:A:762:VAL:C | 2.55 | 0.43 |
| 1:A:77:GLN:HB2 | 1:A:1174:PRO:CG | 2.48 | 0.43 |
| 1:A:811:GLN:HG3 | 1:A:840:ILE:HD13 | 2.00 | 0.43 |
| 1:A:878:VAL:C | 1:A:879:GLN:HE21 | 2.21 | 0.43 |
| 1:A:876:ALA:O | 1:A:878:VAL:N | 2.52 | 0.43 |
| 1:A:905:ALA:HA | 1:A:910:MET:CB | 2.48 | 0.43 |
| 1:A:968:GLN:O | 1:A:970:ASN:O | 2.37 | 0.43 |
| 2:B:101:PRO:HB2 | 2:B:102:LEU:HD12 | 2.01 | 0.43 |
| 2:B:206:TYR:CD1 | 2:B:207:GLY:O | 2.70 | 0.43 |
| 2:B:343:ASP:OD2 | 2:B:344:ARG:NH2 | 2.33 | 0.43 |
| 2:B:433:ASP:O | 2:B:436:SER:N | 2.51 | 0.43 |
| 2:B:87:SER:O | 2:B:91:LEU:HG | 2.18 | 0.43 |
| 2:C:136:GLY:HA2 | 2:C:137:PRO:HD3 | 1.74 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:204:LEU:HG | 2:C:206:TYR:CD2 | 2.54 | 0.43 |
| 2:B:133:HIS:CG | 2:C:231:ILE:HG21 | 2.52 | 0.43 |
| 2:C:241:TRP:HZ3 | 2:C:255:TRP:CZ2 | 2.35 | 0.43 |
| 2:C:338:VAL:C | 2:C:339:ASN:O | 2.52 | 0.43 |
| 2:C:341:ASP:O | 2:C:342:LEU:CB | 2.66 | 0.43 |
| 2:C:344:ARG:O | 2:C:347:LEU:N | 2.52 | 0.43 |
| 2:C:456:ARG:NE | 2:C:456:ARG:N | 2.64 | 0.43 |
| 1:D:1047:ARG:O | 1:D:1048:ALA:C | 2.56 | 0.43 |
| 1:D:1051:GLY:HA2 | 1:D:1054:GLU:CG | 2.36 | 0.43 |
| 1:D:1056:GLU:HA | 1:D:1059:ASN:ND2 | 2.22 | 0.43 |
| 1:D:1126:ASP:O | 1:D:1142:ARG:HG3 | 2.19 | 0.43 |
| 1:D:177:ARG:HE | 1:D:216:SER:N | 2.13 | 0.43 |
| 1:D:214:ALA:CB | 1:D:219:ALA:HB3 | 2.48 | 0.43 |
| 1:D:281:GLN:NE2 | 1:D:287:SER:OG | 2.51 | 0.43 |
| 1:D:359:VAL:CG1 | 1:D:406:VAL:HG21 | 2.48 | 0.43 |
| 1:D:559:LEU:CD1 | 1:D:560:PRO:CD | 2.96 | 0.43 |
| 1:D:597:ARG:O | 1:D:598:VAL:C | 2.56 | 0.43 |
| 1:D:598:VAL:HG22 | 1:D:601:LYS:HE2 | 2.00 | 0.43 |
| 1:D:774:MET:HB3 | 1:D:779:LEU:HD13 | 2.01 | 0.43 |
| 1:D:783:PRO:CG | 1:D:784:GLY:N | 2.81 | 0.43 |
| 1:D:921:LEU:H | 1:D:921:LEU:HD12 | 1.84 | 0.43 |
| 1:D:954:ILE:CG2 | 1:D:955:TYR:N | 2.82 | 0.43 |
| 1:D:770:PHE:HE1 | 1:D:968:GLN:C | 2.21 | 0.43 |
| 2:E:401:GLY:O | 2:E:405:GLU:HB2 | 2.18 | 0.43 |
| 2:F:278:CYS:SG | 2:F:279:GLN:N | 2.92 | 0.43 |
| 2:F:203:ARG:CG | 2:F:325:ARG:HD3 | 2.49 | 0.43 |
| 2:F:259:ARG:HE | 2:F:339:ASN:HD21 | 1.66 | 0.43 |
| 2:F:235:THR:O | 2:F:341:ASP:CG | 2.57 | 0.43 |
| 2:F:351:TYR:O | 2:F:355:GLN:CB | 2.65 | 0.43 |
| 2:F:446:THR:CB | 2:F:450:ASN:CB | 2.80 | 0.43 |
| 1:A:1123:PHE:N | 1:A:1123:PHE:CD1 | 2.86 | 0.43 |
| 1:A:1131:ILE:HD13 | 1:A:1137:VAL:C | 2.38 | 0.43 |
| 1:A:1161:ARG:O | 1:A:1162:CYS:C | 2.55 | 0.43 |
| 1:A:1170:LEU:N | 1:A:1170:LEU:CD1 | 2.82 | 0.43 |
| 1:A:1231:LEU:CD1 | 1:A:1235:SER:CB | 2.97 | 0.43 |
| 1:A:165:LYS:HG3 | 1:A:178:TYR:HB2 | 2.00 | 0.43 |
| 1:A:167:PRO:CB | 1:A:177:ARG:NE | 2.81 | 0.43 |
| 1:A:168:ALA:C | 1:A:169:TRP:CG | 2.91 | 0.43 |
| 1:A:448:ALA:HA | 1:A:1202:ASN:HD21 | 1.84 | 0.43 |
| 1:A:583:PRO:C | 1:A:585:TRP:N | 2.71 | 0.43 |
| 1:A:845:VAL:HG11 | 1:A:848:GLY:CA | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:847:ALA:C | 1:A:848:GLY:O | 2.55 | 0.43 |
| 1:A:891:VAL:HG22 | 1:A:894:GLN:CB | 2.48 | 0.43 |
| 1:A:893:SER:OG | 1:A:893:SER:O | 2.36 | 0.43 |
| 1:A:897:TRP:HE1 | 1:A:901:VAL:HG11 | 1.81 | 0.43 |
| 1:A:904:ASP:HB2 | 1:A:910:MET:C | 2.37 | 0.43 |
| 1:A:76:ILE:HD13 | 1:A:911:HIS:CD2 | 2.54 | 0.43 |
| 2:B:419:GLU:CD | 2:C:201:ASN:ND2 | 2.71 | 0.43 |
| 2:C:102:LEU:HG | 2:C:380:PRO:HG3 | 1.99 | 0.43 |
| 2:B:108:LYS:HE3 | 2:C:115:TRP:CZ2 | 2.54 | 0.43 |
| 2:C:256:LEU:O | 2:C:257:ARG:C | 2.57 | 0.43 |
| 2:C:364:LYS:HD3 | 2:C:364:LYS:N | 2.18 | 0.43 |
| 2:C:475:LEU:H | 2:C:475:LEU:HG | 1.50 | 0.43 |
| 1:D:907:PHE:CE1 | 1:D:1002:GLU:HB3 | 2.52 | 0.43 |
| 1:D:1024:ASP:C | 1:D:1026:ARG:N | 2.71 | 0.43 |
| 1:D:897:TRP:CZ2 | 1:D:1177:VAL:HG11 | 2.50 | 0.43 |
| 1:D:177:ARG:NH2 | 1:D:216:SER:HA | 2.34 | 0.43 |
| 1:D:231:GLU:HA | 1:D:231:GLU:OE1 | 2.19 | 0.43 |
| 1:D:256:PRO:HB3 | 1:D:281:GLN:HA | 2.00 | 0.43 |
| 1:D:405:GLU:OE2 | 1:D:405:GLU:CA | 2.66 | 0.43 |
| 1:D:458:GLU:N | 1:D:460:LYS:CE | 2.82 | 0.43 |
| 1:D:629:ASP:OD2 | 1:D:744:ILE:O | 2.37 | 0.43 |
| 1:D:916:PHE:O | 1:D:916:PHE:CD1 | 2.70 | 0.43 |
| 1:D:989:THR:C | 1:D:998:SER:CB | 2.87 | 0.43 |
| 2:E:214:CYS:SG | 2:E:236:GLU:OE1 | 2.77 | 0.43 |
| 2:E:260:LEU:O | 2:E:264:ARG:HG3 | 2.19 | 0.43 |
| 2:E:326:ASP:N | 2:E:331:VAL:HG12 | 2.29 | 0.43 |
| 2:E:79:LEU:C | 2:E:100:GLY:CA | 2.86 | 0.43 |
| 2:F:78:PHE:HD1 | 2:F:102:LEU:CD2 | 2.30 | 0.43 |
| 2:F:193:TYR:CB | 2:F:242:PHE:CE2 | 2.97 | 0.43 |
| 1:D:786:ALA:CB | 2:F:358:GLU:OE2 | 2.67 | 0.43 |
| 2:F:454:HIS:HD2 | 2:F:468:ILE:CG1 | 2.31 | 0.43 |
| 1:A:1030:ARG:NE | 1:A:1040:LYS:NZ | 2.66 | 0.43 |
| 1:A:139:PHE:CE2 | 1:A:1111:LEU:HG | 2.54 | 0.43 |
| 1:A:1190:ARG:HD2 | 1:A:1195:MET:HG2 | 2.00 | 0.43 |
| 1:A:166:PRO:CG | 1:A:398:GLN:NE2 | 2.48 | 0.43 |
| 1:A:197:PHE:CZ | 1:A:214:ALA:HB2 | 2.54 | 0.43 |
| 1:A:461:LYS:HE2 | 1:A:461:LYS:HB3 | 1.80 | 0.43 |
| 1:A:513:LEU:HB2 | 1:A:568:GLY:HA3 | 1.84 | 0.43 |
| 1:A:606:THR:CG2 | 1:A:620:TRP:CE3 | 2.78 | 0.43 |
| 1:A:739:TYR:HB3 | 1:A:740:ASN:H | 1.51 | 0.43 |
| 1:A:784:GLY:HA3 | 2:C:363:ARG:CG | 2.46 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:964:ARG:O | 1:A:968:GLN:HG3 | 2.18 | 0.43 |
| 1:A:914:THR:CB | 1:A:999:ASP:HB3 | 2.48 | 0.43 |
| 2:B:257:ARG:HG2 | 2:B:258:HIS:N | 2.34 | 0.43 |
| 2:B:269:SER:O | 2:B:272:ASN:CG | 2.57 | 0.43 |
| 2:C:78:PHE:HD1 | 2:C:102:LEU:HD22 | 1.79 | 0.43 |
| 2:C:374:LEU:HB3 | 2:C:378:LEU:CB | 2.36 | 0.43 |
| 1:D:1046:GLU:HG2 | 1:D:1049:TRP:NE1 | 2.34 | 0.43 |
| 1:D:285:GLN:HE21 | 1:D:1128:ARG:HG2 | 1.74 | 0.43 |
| 1:D:1212:ILE:HA | 1:D:1212:ILE:HD12 | 1.80 | 0.43 |
| 1:D:420:HIS:O | 1:D:424:LEU:CD1 | 2.66 | 0.43 |
| 1:D:421:PRO:HG2 | 1:D:422:VAL:HG23 | 2.00 | 0.43 |
| 1:D:509:THR:O | 1:D:510:ALA:O | 2.36 | 0.43 |
| 1:D:486:TRP:CZ2 | 1:D:722:ARG:CA | 2.81 | 0.43 |
| 1:D:740:ASN:HB2 | 1:D:741:ASP:H | 1.56 | 0.43 |
| 1:D:788:GLY:O | 1:D:791:ALA:CA | 2.67 | 0.43 |
| 1:D:922:GLN:HB2 | 1:D:924:ARG:HD3 | 2.01 | 0.43 |
| 1:D:955:TYR:O | 1:D:956:GLY:O | 2.37 | 0.43 |
| 1:D:993:ARG:NH2 | 1:D:994:TRP:CD1 | 2.87 | 0.43 |
| 1:D:994:TRP:O | 1:D:994:TRP:CE3 | 2.71 | 0.43 |
| 2:E:109:ASN:CG | 2:E:378:LEU:HB3 | 2.39 | 0.43 |
| 2:E:205:PRO:HG2 | 2:E:241:TRP:NE1 | 2.33 | 0.43 |
| 2:E:437:ILE:CG2 | 2:E:439:PHE:C | 2.86 | 0.43 |
| 2:E:447:THR:HG22 | 2:E:451:GLY:HA2 | 2.00 | 0.43 |
| 2:E:456:ARG:CZ | 2:E:463:LYS:CE | 2.83 | 0.43 |
| 2:E:475:LEU:O | 2:E:479:ILE:HG13 | 2.19 | 0.43 |
| 2:F:374:LEU:O | 2:F:375:HIS:C | 2.57 | 0.43 |
| 2:F:454:HIS:CD2 | 2:F:472:LYS:HE3 | 2.54 | 0.43 |
| 2:F:474:PHE:HA | 2:F:477:LYS:CG | 2.49 | 0.43 |
| 1:A:1060:LYS:HE2 | 1:A:1065:ALA:H | 1.76 | 0.43 |
| 1:A:177:ARG:O | 1:A:178:TYR:C | 2.56 | 0.43 |
| 1:A:276:ALA:O | 1:A:279:ARG:N | 2.44 | 0.43 |
| 1:A:275:ARG:C | 1:A:278:ILE:HB | 2.39 | 0.43 |
| 1:A:313:ILE:HA | 1:A:316:LYS:CE | 2.45 | 0.43 |
| 1:A:618:HIS:NE2 | 1:A:726:LYS:O | 2.52 | 0.43 |
| 1:A:653:GLU:OE2 | 1:A:657:ARG:CZ | 2.67 | 0.43 |
| 1:A:737:GLY:N | 1:A:750:PHE:CE1 | 2.86 | 0.43 |
| 1:A:608:ASP:C | 1:A:779:LEU:HD22 | 2.39 | 0.43 |
| 2:B:280:ASP:HB3 | 2:B:281:GLU:CB | 2.49 | 0.43 |
| 2:C:115:TRP:CH2 | 2:C:210:GLN:HA | 2.54 | 0.43 |
| 2:C:293:PHE:HB3 | 2:C:294:PRO:HD2 | 2.01 | 0.43 |
| 2:C:432:TYR:C | 2:C:435:MET:H | 2.21 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:464:GLU:OE2 | 2:C:466:MET:CG | 2.64 | 0.43 |
| 2:C:468:ILE:C | 2:C:471:LEU:HD13 | 2.39 | 0.43 |
| 2:C:76:ARG:NH1 | 2:C:76:ARG:CG | 2.81 | 0.43 |
| 1:D:1007:GLU:C | 1:D:1011:PRO:HD3 | 2.34 | 0.43 |
| 1:D:1073:PRO:O | 1:D:1074:VAL:C | 2.57 | 0.43 |
| 1:D:1131:ILE:CG1 | 1:D:1138:ARG:HB2 | 2.48 | 0.43 |
| 1:D:1136:GLU:CG | 1:D:1138:ARG:HH12 | 2.32 | 0.43 |
| 1:D:220:TRP:HD1 | 1:D:221:TYR:HD2 | 1.62 | 0.43 |
| 1:D:253:ALA:CA | 1:D:280:GLU:HB2 | 2.49 | 0.43 |
| 1:D:275:ARG:O | 1:D:279:ARG:HG2 | 2.18 | 0.43 |
| 1:D:401:TRP:CD1 | 1:D:404:HIS:CD2 | 2.96 | 0.43 |
| 1:D:477:GLU:HG2 | 1:D:478:ARG:N | 2.34 | 0.43 |
| 1:D:482:ASP:OD1 | 1:D:484:TRP:HB3 | 2.19 | 0.43 |
| 1:D:501:LYS:HG2 | 1:D:502:LYS:N | 2.33 | 0.43 |
| 1:D:525:MET:C | 1:D:526:ASP:CG | 2.77 | 0.43 |
| 1:D:549:LEU:O | 1:D:552:LEU:N | 2.51 | 0.43 |
| 1:D:559:LEU:CB | 1:D:560:PRO:CD | 2.97 | 0.43 |
| 1:D:715:GLN:O | 1:D:716:PRO:C | 2.57 | 0.43 |
| 1:D:788:GLY:O | 1:D:791:ALA:CB | 2.64 | 0.43 |
| 1:D:427:MET:C | 1:D:846:THR:HG21 | 2.38 | 0.43 |
| 1:D:851:THR:O | 1:D:852:ARG:CB | 2.66 | 0.43 |
| 1:D:932:HIS:HE1 | 1:D:943:ARG:HB3 | 1.83 | 0.43 |
| 2:E:271:SER:C | 2:E:273:PHE:N | 2.71 | 0.43 |
| 2:E:471:LEU:O | 2:E:474:PHE:HB3 | 2.18 | 0.43 |
| 2:F:248:SER:OG | 2:F:249:ASN:N | 2.47 | 0.43 |
| 2:F:302:THR:H | 2:F:339:ASN:HA | 1.82 | 0.43 |
| 2:F:338:VAL:HG12 | 2:F:339:ASN:N | 2.34 | 0.43 |
| 2:F:438:LEU:CD2 | 2:F:438:LEU:N | 2.81 | 0.43 |
| 2:F:472:LYS:O | 2:F:475:LEU:CG | 2.67 | 0.43 |
| 1:A:1133:ILE:HD13 | 1:A:1134:HIS:N | 2.34 | 0.43 |
| 1:A:225:SER:HA | 1:A:228:LEU:CD1 | 2.31 | 0.43 |
| 1:A:255:SER:N | 1:A:256:PRO:CA | 2.81 | 0.43 |
| 1:A:262:GLN:HB3 | 1:A:263:GLU:H | 1.54 | 0.43 |
| 1:A:386:ARG:CA | 1:A:389:PHE:HB3 | 2.46 | 0.43 |
| 1:A:444:TYR:CD2 | 1:A:874:LEU:CD2 | 2.85 | 0.43 |
| 1:A:616:GLU:OE2 | 1:A:724:GLY:N | 2.48 | 0.43 |
| 1:A:618:HIS:N | 1:A:725:PRO:CG | 2.57 | 0.43 |
| 1:A:600:PRO:CG | 1:A:765:PRO:HG3 | 2.49 | 0.43 |
| 1:A:754:HIS:HA | 1:A:770:PHE:HE2 | 1.83 | 0.43 |
| 1:A:798:ILE:O | 1:A:799:SER:C | 2.57 | 0.43 |
| 1:A:824:ALA:C | 1:A:827:ARG:H | 2.22 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:944:GLU:HG2 | 1:A:947:LYS:HZ2 | 1.83 | 0.43 |
| 2:B:204:LEU:HG | 2:B:325:ARG:CZ | 2.48 | 0.43 |
| 2:B:234:LYS:O | 2:B:236:GLU:CG | 2.63 | 0.43 |
| 2:B:285:LYS:CG | 2:B:286:GLY:N | 2.37 | 0.43 |
| 2:B:311:LEU:HD13 | 2:B:322:LEU:HD13 | 2.00 | 0.43 |
| 2:B:375:HIS:HA | 2:B:376:PRO:HD2 | 1.76 | 0.43 |
| 2:B:76:ARG:HH21 | 2:B:431:LYS:HB2 | 1.84 | 0.43 |
| 2:B:72:ILE:HA | 2:B:75:ARG:CD | 2.42 | 0.43 |
| 2:C:108:LYS:O | 2:C:109:ASN:C | 2.56 | 0.43 |
| 2:C:341:ASP:C | 2:C:342:LEU:HD22 | 2.39 | 0.43 |
| 2:C:234:LYS:HZ1 | 2:C:344:ARG:CD | 2.28 | 0.43 |
| 2:C:375:HIS:O | 2:C:376:PRO:C | 2.55 | 0.43 |
| 2:C:406:LEU:N | 2:C:406:LEU:HD13 | 2.34 | 0.43 |
| 2:C:466:MET:CE | 2:C:471:LEU:HD23 | 2.49 | 0.43 |
| 1:D:1119:LEU:N | 1:D:1119:LEU:HD23 | 2.34 | 0.43 |
| 1:D:162:LEU:CG | 1:D:162:LEU:O | 2.67 | 0.43 |
| 1:D:248:GLU:OE1 | 1:D:250:PRO:CD | 2.67 | 0.43 |
| 1:D:368:PRO:HB3 | 1:D:369:LEU:HD23 | 2.00 | 0.43 |
| 1:D:376:LEU:C | 1:D:378:VAL:H | 2.22 | 0.43 |
| 1:D:440:ASN:HB2 | 1:D:441:TRP:CE3 | 2.53 | 0.43 |
| 1:D:469:ASP:O | 1:D:473:LEU:HG | 2.18 | 0.43 |
| 1:D:771:LEU:CD1 | 1:D:771:LEU:H | 2.32 | 0.43 |
| 1:D:433:SER:HB3 | 1:D:844:VAL:HG21 | 2.00 | 0.43 |
| 1:D:844:VAL:HG13 | 1:D:856:GLU:HG3 | 2.00 | 0.43 |
| 1:D:909:GLY:O | 1:D:912:GLY:CA | 2.66 | 0.43 |
| 1:D:961:PHE:CD1 | 1:D:961:PHE:N | 2.83 | 0.43 |
| 2:E:183:GLU:O | 2:E:214:CYS:SG | 2.70 | 0.43 |
| 2:F:108:LYS:O | 2:F:109:ASN:C | 2.55 | 0.43 |
| 1:A:1036:SER:O | 1:A:1039:LYS:HA | 2.19 | 0.43 |
| 1:A:1208:ARG:CZ | 2:C:277:ASP:CG | 2.87 | 0.43 |
| 1:A:293:ASP:CB | 1:A:296:SER:CB | 2.97 | 0.43 |
| 1:A:348:LEU:CD1 | 1:A:350:ILE:HD13 | 2.45 | 0.43 |
| 1:A:599:THR:O | 1:A:603:MET:HB2 | 2.19 | 0.43 |
| 1:A:624:VAL:CG2 | 1:A:747:CYS:SG | 3.06 | 0.43 |
| 1:A:716:PRO:O | 1:A:717:LEU:C | 2.56 | 0.43 |
| 1:A:601:LYS:CA | 1:A:717:LEU:HB3 | 2.41 | 0.43 |
| 1:A:817:PRO:CG | 1:A:818:ARG:H | 2.32 | 0.43 |
| 1:A:444:TYR:CB | 1:A:877:MET:HG3 | 2.49 | 0.43 |
| 1:A:986:TYR:O | 1:A:990:LYS:HG3 | 2.18 | 0.43 |
| 2:B:180:LYS:HG3 | 2:B:181:LEU:N | 2.34 | 0.43 |
| 2:B:235:THR:OG1 | 2:B:343:ASP:CA | 2.66 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:373:LYS:HE2 | 2:B:459:ASP:O | 2.18 | 0.43 |
| 2:B:81:GLY:C | 2:B:86:LEU:HD11 | 2.38 | 0.43 |
| 2:C:123:GLU:O | 2:C:124:GLN:HB3 | 2.19 | 0.43 |
| 2:C:128:VAL:HG12 | 2:C:192:HIS:NE2 | 2.34 | 0.43 |
| 1:D:1157:ASN:HB3 | 1:D:1161:ARG:CZ | 2.48 | 0.43 |
| 1:D:444:TYR:HH | 1:D:1206:MET:CG | 2.31 | 0.43 |
| 1:D:441:TRP:HZ3 | 1:D:1210:TYR:CE1 | 2.36 | 0.43 |
| 1:D:80:SER:CB | 1:D:125:LEU:HG | 2.43 | 0.43 |
| 1:D:525:MET:HE2 | 1:D:525:MET:HB3 | 1.90 | 0.43 |
| 1:D:666:GLN:HA | 1:D:669:MET:CG | 2.48 | 0.43 |
| 1:D:919:MET:O | 1:D:920:THR:O | 2.36 | 0.43 |
| 1:D:955:TYR:HB2 | 1:D:956:GLY:H | 1.43 | 0.43 |
| 2:E:78:PHE:HD2 | 2:E:102:LEU:CD1 | 2.29 | 0.43 |
| 2:E:113:GLU:HG3 | 2:E:377:CYS:SG | 2.59 | 0.43 |
| 2:E:212:GLY:O | 2:E:236:GLU:N | 2.52 | 0.43 |
| 2:E:398:VAL:O | 2:E:402:LEU:N | 2.49 | 0.43 |
| 2:F:300:ILE:CG2 | 2:F:301:GLU:N | 2.63 | 0.43 |
| 2:F:342:LEU:HD21 | 2:F:345:GLY:H | 1.70 | 0.43 |
| 2:F:372:LEU:CD2 | 2:F:436:SER:HB2 | 2.48 | 0.43 |
| 2:F:446:THR:O | 2:F:449:GLU:N | 2.47 | 0.43 |
| 1:A:285:GLN:C | 1:A:1128:ARG:HH22 | 2.12 | 0.42 |
| 1:A:382:MET:HE3 | 1:A:383:LYS:HA | 2.00 | 0.42 |
| 1:A:468:ASN:HB3 | 2:C:460:THR:HG22 | 2.01 | 0.42 |
| 1:A:497:GLN:OE1 | 1:A:516:GLU:HB3 | 2.19 | 0.42 |
| 1:A:659:HIS:O | 1:A:662:GLU:HG2 | 2.18 | 0.42 |
| 1:A:656:TYR:HD2 | 1:A:720:THR:HG1 | 1.55 | 0.42 |
| 1:A:728:THR:C | 1:A:729:GLN:NE2 | 2.72 | 0.42 |
| 1:A:772:PRO:HG2 | 1:A:773:LYS:N | 2.33 | 0.42 |
| 1:A:788:GLY:N | 1:A:789:PRO:CD | 2.82 | 0.42 |
| 1:A:824:ALA:O | 1:A:827:ARG:N | 2.51 | 0.42 |
| 1:A:856:GLU:O | 1:A:857:PRO:C | 2.56 | 0.42 |
| 1:A:448:ALA:C | 1:A:870:VAL:CG1 | 2.86 | 0.42 |
| 1:A:996:ARG:NH2 | 1:A:1000:GLU:OE2 | 2.52 | 0.42 |
| 2:B:116:THR:HG23 | 2:B:120:VAL:HB | 2.00 | 0.42 |
| 2:B:386:ASP:OD1 | 2:B:387:VAL:N | 2.42 | 0.42 |
| 2:C:100:GLY:O | 2:C:103:GLY:N | 2.52 | 0.42 |
| 2:C:267:ALA:CB | 2:C:270:PRO:HB3 | 2.47 | 0.42 |
| 1:D:1025:LEU:C | 1:D:1026:ARG:HD3 | 2.37 | 0.42 |
| 1:D:1027:LYS:CD | 1:D:1027:LYS:N | 2.78 | 0.42 |
| 1:D:1065:ALA:HA | 1:D:1073:PRO:HG3 | 2.00 | 0.42 |
| 1:D:1193:VAL:C | 1:D:1195:MET:HE2 | 2.40 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:204:ALA:O | 1:D:205:GLU:CB | 2.66 | 0.42 |
| 1:D:457:ARG:N | 1:D:460:LYS:NZ | 2.46 | 0.42 |
| 1:D:576:LEU:HG | 1:D:579:ARG:NE | 2.32 | 0.42 |
| 1:D:598:VAL:C | 1:D:600:PRO:HD2 | 2.39 | 0.42 |
| 1:D:613:HIS:CE1 | 1:D:717:LEU:HD22 | 2.53 | 0.42 |
| 1:D:648:PRO:HG2 | 1:D:649:TYR:N | 2.34 | 0.42 |
| 1:D:851:THR:C | 1:D:852:ARG:HG3 | 2.39 | 0.42 |
| 1:D:85:GLU:OE1 | 1:D:130:LEU:CD2 | 2.63 | 0.42 |
| 1:D:959:GLN:O | 1:D:962:ALA:HB3 | 2.19 | 0.42 |
| 2:E:128:VAL:CG1 | 2:E:208:LEU:O | 2.66 | 0.42 |
| 2:E:315:TYR:CD1 | 2:E:316:PRO:HD2 | 2.51 | 0.42 |
| 2:E:372:LEU:O | 2:E:458:ARG:CG | 2.67 | 0.42 |
| 2:E:385:LEU:O | 2:E:386:ASP:HB3 | 2.17 | 0.42 |
| 2:E:456:ARG:HG3 | 2:E:462:MET:O | 2.18 | 0.42 |
| 2:E:86:LEU:HB3 | 2:E:97:PRO:HD2 | 2.01 | 0.42 |
| 2:F:136:GLY:HA2 | 2:F:137:PRO:HD3 | 1.71 | 0.42 |
| 2:F:389:ARG:CZ | 2:F:390:GLY:N | 2.82 | 0.42 |
| 1:A:1049:TRP:CG | 1:A:1050:LYS:N | 2.87 | 0.42 |
| 1:A:756:ASP:CG | 1:A:1057:MET:HG2 | 2.38 | 0.42 |
| 1:A:1007:GLU:CD | 1:A:1093:MET:HE2 | 2.39 | 0.42 |
| 1:A:1157:ASN:HD22 | 1:A:1157:ASN:N | 2.17 | 0.42 |
| 1:A:120:LEU:HD13 | 1:A:120:LEU:N | 2.34 | 0.42 |
| 1:A:304:LEU:O | 1:A:850:ILE:CG2 | 2.67 | 0.42 |
| 1:A:369:PRO:O | 1:A:369:PRO:HG2 | 2.20 | 0.42 |
| 1:A:477:GLU:CD | 1:A:478:ARG:HG2 | 2.39 | 0.42 |
| 1:A:499:LYS:HB2 | 1:A:499:LYS:HE3 | 1.85 | 0.42 |
| 1:A:612:LEU:HB2 | 1:A:621:GLY:N | 2.34 | 0.42 |
| 1:A:656:TYR:CA | 1:A:720:THR:HB | 2.49 | 0.42 |
| 2:B:241:TRP:CD2 | 2:B:255:TRP:HH2 | 2.36 | 0.42 |
| 2:B:301:GLU:HG2 | 2:B:303:LEU:HD11 | 2.01 | 0.42 |
| 2:B:303:LEU:CD1 | 2:B:303:LEU:N | 2.79 | 0.42 |
| 2:B:306:LEU:O | 2:B:308:ASP:O | 2.37 | 0.42 |
| 2:C:443:VAL:HG13 | 2:C:447:THR:HG21 | 2.00 | 0.42 |
| 2:C:451:GLY:O | 2:C:452:LEU:CG | 2.67 | 0.42 |
| 2:C:87:SER:O | 2:C:88:ARG:C | 2.58 | 0.42 |
| 1:D:1108:TYR:CE1 | 1:D:1160:THR:CG2 | 3.02 | 0.42 |
| 1:D:1148:ARG:CZ | 1:D:1231:LEU:CD2 | 2.97 | 0.42 |
| 1:D:916:PHE:CD2 | 1:D:1174:PRO:HG2 | 2.53 | 0.42 |
| 1:D:1208:ARG:NH1 | 2:F:285:LYS:CE | 2.81 | 0.42 |
| 1:D:249:VAL:HG22 | 1:D:250:PRO:HD2 | 1.78 | 0.42 |
| 1:D:267:VAL:CB | 1:D:269:HIS:NE2 | 2.81 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:304:LEU:H | 1:D:309:ARG:HH21 | 1.59 | 0.42 |
| 1:D:458:GLU:OE2 | 2:F:270:PRO:HG3 | 2.18 | 0.42 |
| 1:D:479:TYR:C | 1:D:481:GLU:H | 2.22 | 0.42 |
| 1:D:547:ALA:HA | 1:D:551:LYS:CE | 2.39 | 0.42 |
| 1:D:577:CYS:HB3 | 1:D:578:PRO:CD | 2.46 | 0.42 |
| 1:D:614:TYR:HE2 | 1:D:620:TRP:CD2 | 2.35 | 0.42 |
| 1:D:718:ALA:O | 1:D:722:ARG:NE | 2.52 | 0.42 |
| 1:D:618:HIS:CA | 1:D:762:VAL:HG21 | 2.46 | 0.42 |
| 1:D:776:ASP:N | 1:D:796:LYS:HZ3 | 2.16 | 0.42 |
| 1:D:83:LEU:HB3 | 1:D:88:PHE:C | 2.39 | 0.42 |
| 1:D:967:MET:SD | 1:D:974:THR:C | 2.97 | 0.42 |
| 1:D:996:ARG:CA | 1:D:996:ARG:NE | 2.82 | 0.42 |
| 2:E:120:VAL:HG12 | 2:E:121:PHE:CD1 | 2.53 | 0.42 |
| 2:E:130:ALA:CB | 2:E:210:GLN:NE2 | 2.82 | 0.42 |
| 2:E:264:ARG:NH2 | 2:E:273:PHE:O | 2.52 | 0.42 |
| 2:F:145:PHE:CD1 | 2:F:145:PHE:N | 2.87 | 0.42 |
| 2:F:221:THR:CG2 | 2:F:222:LYS:H | 2.32 | 0.42 |
| 2:F:262:TRP:O | 2:F:265:LYS:HB3 | 2.19 | 0.42 |
| 2:F:197:LEU:CD1 | 2:F:322:LEU:HD11 | 2.50 | 0.42 |
| 2:F:435:MET:CE | 2:F:435:MET:CA | 2.90 | 0.42 |
| 1:A:1129:PHE:CG | 1:A:1130:CYS:N | 2.87 | 0.42 |
| 1:A:202:CYS:C | 1:A:204:ALA:N | 2.71 | 0.42 |
| 1:A:209:PRO:C | 1:A:210:THR:HG23 | 2.39 | 0.42 |
| 1:A:304:LEU:CB | 1:A:309:ARG:HB3 | 2.50 | 0.42 |
| 1:A:513:LEU:O | 1:A:568:GLY:C | 2.58 | 0.42 |
| 1:A:627:ARG:O | 1:A:627:ARG:CG | 2.67 | 0.42 |
| 1:A:824:ALA:O | 1:A:825:VAL:C | 2.58 | 0.42 |
| 1:A:829:PRO:HG3 | 1:A:883:GLY:CA | 2.49 | 0.42 |
| 1:A:905:ALA:CA | 1:A:910:MET:HA | 2.49 | 0.42 |
| 2:B:262:TRP:O | 2:B:265:LYS:CA | 2.66 | 0.42 |
| 2:C:124:GLN:C | 2:C:125:VAL:CG1 | 2.88 | 0.42 |
| 2:C:355:GLN:OE1 | 2:C:356:LEU:HD23 | 2.19 | 0.42 |
| 2:C:358:GLU:CA | 2:C:361:PHE:HB2 | 2.47 | 0.42 |
| 2:C:372:LEU:HD21 | 2:C:436:SER:N | 2.32 | 0.42 |
| 2:C:419:GLU:OE2 | 2:C:428:LEU:CD1 | 2.50 | 0.42 |
| 2:C:80:SER:H | 2:C:99:PHE:HA | 1.82 | 0.42 |
| 1:D:1020:ILE:O | 1:D:1021:SER:HB2 | 2.20 | 0.42 |
| 1:D:1150:ALA:O | 1:D:1153:LEU:HB2 | 2.19 | 0.42 |
| 1:D:274:ASP:HA | 1:D:277:HIS:CD2 | 2.54 | 0.42 |
| 1:D:292:LEU:HD23 | 1:D:297:MET:HE3 | 1.98 | 0.42 |
| 1:D:395:TYR:N | 1:D:395:TYR:CD1 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:421:PRO:CG | 1:D:422:VAL:N | 2.81 | 0.42 |
| 1:D:439:GLN:O | 1:D:440:ASN:C | 2.57 | 0.42 |
| 1:D:549:LEU:C | 1:D:551:LYS:HZ2 | 2.22 | 0.42 |
| 1:D:581:ASP:OD2 | 1:D:593:SER:HB2 | 2.18 | 0.42 |
| 1:D:586:THR:N | 1:D:587:PRO:HD2 | 2.29 | 0.42 |
| 1:D:475:SER:C | 1:D:712:VAL:HG23 | 2.40 | 0.42 |
| 2:E:254:PHE:HA | 2:E:257:ARG:CB | 2.27 | 0.42 |
| 2:E:350:LEU:C | 2:E:350:LEU:HD23 | 2.40 | 0.42 |
| 2:E:382:LYS:O | 2:E:383:VAL:CG2 | 2.67 | 0.42 |
| 2:E:404:ASN:O | 2:E:407:LEU:N | 2.53 | 0.42 |
| 2:E:419:GLU:HA | 2:F:203:ARG:HH21 | 1.75 | 0.42 |
| 2:E:474:PHE:CG | 2:E:475:LEU:N | 2.88 | 0.42 |
| 2:F:118:VAL:HG12 | 2:F:119:VAL:HG23 | 2.01 | 0.42 |
| 2:F:251:TRP:HE3 | 2:F:254:PHE:HB3 | 1.85 | 0.42 |
| 2:F:357:THR:C | 2:F:359:ASN:N | 2.72 | 0.42 |
| 1:A:1026:ARG:CG | 1:A:1029:GLN:NE2 | 2.82 | 0.42 |
| 1:A:1065:ALA:C | 1:A:1066:THR:HG1 | 2.18 | 0.42 |
| 1:A:1134:HIS:HB2 | 1:A:1136:GLU:OE2 | 2.18 | 0.42 |
| 1:A:1180:PHE:HB3 | 1:A:1181:SER:H | 1.26 | 0.42 |
| 1:A:377:PHE:HD2 | 1:A:377:PHE:HA | 1.41 | 0.42 |
| 1:A:512:LYS:C | 1:A:513:LEU:HD23 | 2.38 | 0.42 |
| 1:A:582:ASP:CG | 1:A:592:LEU:HD22 | 2.40 | 0.42 |
| 1:A:613:HIS:O | 1:A:614:TYR:CG | 2.72 | 0.42 |
| 1:A:614:TYR:HD2 | 1:A:620:TRP:HB3 | 1.85 | 0.42 |
| 1:A:607:TRP:H | 1:A:620:TRP:HZ3 | 1.67 | 0.42 |
| 1:A:601:LYS:CE | 1:A:721:ALA:HB1 | 2.50 | 0.42 |
| 1:A:765:PRO:HG2 | 1:A:766:PHE:H | 1.84 | 0.42 |
| 1:A:275:ARG:NE | 1:A:843:GLN:HB2 | 2.34 | 0.42 |
| 1:A:842:PRO:CB | 1:A:856:GLU:OE1 | 2.57 | 0.42 |
| 1:A:868:ASP:HB3 | 1:A:1199:THR:CB | 2.45 | 0.42 |
| 1:A:914:THR:OG1 | 1:A:999:ASP:CG | 2.58 | 0.42 |
| 2:B:189:ALA:O | 2:B:190:LEU:C | 2.58 | 0.42 |
| 2:B:187:HIS:HA | 2:B:190:LEU:HD23 | 2.02 | 0.42 |
| 2:B:267:ALA:HB1 | 2:B:270:PRO:CD | 2.49 | 0.42 |
| 2:B:344:ARG:N | 2:B:344:ARG:NE | 2.67 | 0.42 |
| 2:B:69:LEU:C | 2:B:73:CYS:HG | 2.22 | 0.42 |
| 2:B:90:SER:C | 2:B:93:SER:HG | 2.21 | 0.42 |
| 2:C:197:LEU:CD1 | 2:C:322:LEU:HD11 | 2.49 | 0.42 |
| 2:C:213:VAL:HG23 | 2:C:235:THR:OG1 | 2.19 | 0.42 |
| 1:A:783:PRO:HG2 | 2:C:363:ARG:CD | 2.49 | 0.42 |
| 2:C:385:LEU:HA | 2:C:385:LEU:HD23 | 1.74 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:395:LEU:C | 2:C:397:GLN:N | 2.72 | 0.42 |
| 1:D:1090:GLU:HB3 | 1:D:1092:PHE:CE1 | 2.54 | 0.42 |
| 1:D:1173:LEU:HA | 1:D:1174:PRO:HD3 | 1.75 | 0.42 |
| 1:D:375:GLU:O | 1:D:378:VAL:C | 2.54 | 0.42 |
| 1:D:658:LYS:CE | 1:D:713:PRO:CB | 2.85 | 0.42 |
| 1:D:860:LEU:HA | 1:D:860:LEU:HD23 | 1.74 | 0.42 |
| 1:D:954:ILE:O | 1:D:955:TYR:CD1 | 2.73 | 0.42 |
| 2:E:379:ALA:N | 2:E:380:PRO:HD3 | 2.35 | 0.42 |
| 2:F:113:GLU:HG2 | 2:F:266:PHE:CE1 | 2.54 | 0.42 |
| 2:F:293:PHE:CE2 | 2:F:298:GLU:HB2 | 2.55 | 0.42 |
| 2:F:305:ASN:HA | 2:F:335:VAL:HG13 | 2.00 | 0.42 |
| 2:F:389:ARG:HD2 | 2:F:389:ARG:HA | 1.74 | 0.42 |
| 2:F:414:TRP:O | 2:F:415:PRO:C | 2.57 | 0.42 |
| 1:A:1030:ARG:HD2 | 1:A:1040:LYS:NZ | 2.31 | 0.42 |
| 1:A:1108:TYR:HE2 | 1:A:1112:MET:HE3 | 1.84 | 0.42 |
| 1:A:1157:ASN:C | 1:A:1161:ARG:HD2 | 2.40 | 0.42 |
| 1:A:1205:GLY:O | 1:A:1208:ARG:CB | 2.62 | 0.42 |
| 1:A:1232:GLU:CD | 1:A:1234:ARG:HH21 | 2.22 | 0.42 |
| 1:A:849:THR:HB | 1:A:852:ARG:N | 2.34 | 0.42 |
| 1:A:895:GLU:O | 1:A:898:ILE:HG12 | 2.20 | 0.42 |
| 1:A:900:ALA:CB | 1:A:915:ALA:HB1 | 2.49 | 0.42 |
| 1:A:967:MET:CG | 1:A:978:ALA:CB | 2.98 | 0.42 |
| 2:B:241:TRP:CE3 | 2:B:255:TRP:HH2 | 2.38 | 0.42 |
| 2:B:466:MET:HE3 | 2:B:471:LEU:HD13 | 2.02 | 0.42 |
| 2:C:190:LEU:O | 2:C:193:TYR:N | 2.47 | 0.42 |
| 2:C:243:THR:O | 2:C:334:CYS:HB2 | 2.20 | 0.42 |
| 2:C:306:LEU:H | 2:C:335:VAL:CB | 2.33 | 0.42 |
| 2:C:328:ARG:C | 2:C:329:LYS:HD2 | 2.40 | 0.42 |
| 2:C:344:ARG:O | 2:C:348:ALA:N | 2.53 | 0.42 |
| 2:C:69:LEU:HD13 | 2:C:354:PHE:CD2 | 2.53 | 0.42 |
| 2:C:389:ARG:HA | 2:C:389:ARG:HD2 | 1.60 | 0.42 |
| 2:C:78:PHE:CD1 | 2:C:102:LEU:CD2 | 2.99 | 0.42 |
| 1:D:121:PRO:HB3 | 1:D:1175:GLN:NE2 | 2.35 | 0.42 |
| 1:D:1212:ILE:HA | 1:D:1213:PRO:HD3 | 1.29 | 0.42 |
| 1:D:258:GLN:O | 1:D:259:ARG:CB | 2.67 | 0.42 |
| 1:D:278:ILE:N | 1:D:291:PHE:CD1 | 2.88 | 0.42 |
| 1:D:349:ASP:O | 1:D:361:ARG:CD | 2.56 | 0.42 |
| 1:D:434:TYR:OH | 1:D:436:PRO:HB3 | 2.20 | 0.42 |
| 1:D:481:GLU:O | 1:D:482:ASP:CB | 2.68 | 0.42 |
| 1:D:487:ASP:O | 1:D:491:ASP:OD1 | 2.36 | 0.42 |
| 1:D:612:LEU:HD11 | 1:D:622:TYR:HA | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:620:TRP:H | 1:D:620:TRP:HD1 | 1.64 | 0.42 |
| 1:D:649:TYR:CD2 | 1:D:652:ILE:HD13 | 2.54 | 0.42 |
| 1:D:792:LEU:O | 1:D:793:GLU:C | 2.57 | 0.42 |
| 1:D:873:GLU:HB3 | 1:D:1200:PRO:CG | 2.47 | 0.42 |
| 1:D:967:MET:HE1 | 1:D:974:THR:C | 2.40 | 0.42 |
| 2:E:461:THR:HG23 | 2:E:461:THR:O | 2.19 | 0.42 |
| 2:F:145:PHE:HD1 | 2:F:145:PHE:N | 2.17 | 0.42 |
| 2:F:216:HIS:O | 2:F:232:GLY:N | 2.31 | 0.42 |
| 2:F:245:PRO:CD | 2:F:246:ARG:H | 2.32 | 0.42 |
| 2:F:102:LEU:HG | 2:F:380:PRO:HG3 | 2.02 | 0.42 |
| 2:F:389:ARG:CZ | 2:F:390:GLY:CA | 2.96 | 0.42 |
| 1:A:1028:VAL:O | 1:A:1031:GLU:C | 2.58 | 0.42 |
| 1:A:955:TYR:HE2 | 1:A:1102:GLN:NE2 | 2.13 | 0.42 |
| 1:A:1102:GLN:O | 1:A:1106:VAL:HG23 | 2.18 | 0.42 |
| 1:A:398:GLN:O | 1:A:399:ASP:C | 2.56 | 0.42 |
| 1:A:452:TYR:CD2 | 1:A:453:GLU:N | 2.87 | 0.42 |
| 1:A:782:GLY:HA3 | 1:A:789:PRO:HD3 | 2.02 | 0.42 |
| 1:A:827:ARG:O | 1:A:831:TYR:HE1 | 2.02 | 0.42 |
| 1:A:904:ASP:HB3 | 1:A:912:GLY:CA | 2.49 | 0.42 |
| 2:B:122:ARG:CD | 2:B:124:GLN:NE2 | 2.81 | 0.42 |
| 2:B:197:LEU:HD11 | 2:B:325:ARG:HH12 | 1.84 | 0.42 |
| 2:B:185:LEU:HD11 | 2:B:238:SER:HB2 | 2.02 | 0.42 |
| 2:B:204:LEU:HG | 2:B:325:ARG:HE | 1.82 | 0.42 |
| 2:C:110:LEU:O | 2:C:113:GLU:N | 2.53 | 0.42 |
| 2:C:225:ARG:HB3 | 2:C:226:ASN:H | 1.57 | 0.42 |
| 2:C:247:THR:OG1 | 2:C:251:TRP:HB2 | 2.20 | 0.42 |
| 2:C:308:ASP:O | 2:C:312:LEU:HD11 | 2.19 | 0.42 |
| 2:C:424:SER:O | 2:C:425:LEU:C | 2.58 | 0.42 |
| 2:C:80:SER:HG | 2:C:99:PHE:C | 2.22 | 0.42 |
| 1:D:1137:VAL:CG1 | 1:D:1139:TYR:CE1 | 2.96 | 0.42 |
| 1:D:134:ASN:O | 1:D:135:LEU:C | 2.57 | 0.42 |
| 1:D:278:ILE:HG12 | 1:D:291:PHE:CD1 | 2.54 | 0.42 |
| 1:D:623:LEU:CG | 1:D:623:LEU:O | 2.55 | 0.42 |
| 1:D:716:PRO:HB2 | 1:D:717:LEU:HD23 | 2.02 | 0.42 |
| 1:D:762:VAL:HG23 | 1:D:763:GLY:N | 2.33 | 0.42 |
| 1:D:275:ARG:NH2 | 1:D:842:PRO:CA | 2.79 | 0.42 |
| 1:D:879:GLN:O | 1:D:880:ALA:HB2 | 2.20 | 0.42 |
| 1:D:898:ILE:HG12 | 1:D:899:ALA:H | 1.85 | 0.42 |
| 1:D:943:ARG:O | 1:D:946:ALA:CB | 2.64 | 0.42 |
| 2:E:293:PHE:CE1 | 2:E:351:TYR:CE2 | 3.08 | 0.42 |
| 2:E:389:ARG:CZ | 2:E:390:GLY:O | 2.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:78:PHE:CE1 | 2:E:346:MET:CE | 3.02 | 0.42 |
| 2:F:190:LEU:O | 2:F:193:TYR:N | 2.51 | 0.42 |
| 2:F:88:ARG:HD3 | 2:F:295:TRP:CE2 | 2.54 | 0.42 |
| 2:F:236:GLU:CA | 2:F:341:ASP:CB | 2.73 | 0.42 |
| 2:F:469:SER:O | 2:F:472:LYS:N | 2.52 | 0.42 |
| 1:A:1090:GLU:O | 1:A:1091:GLU:CB | 2.68 | 0.42 |
| 1:A:1113:LEU:CB | 1:A:1117:LYS:HZ2 | 2.28 | 0.42 |
| 1:A:107:LEU:O | 1:A:111:GLY:CA | 2.67 | 0.42 |
| 1:A:209:PRO:C | 1:A:210:THR:CG2 | 2.87 | 0.42 |
| 1:A:554:GLY:O | 1:A:557:GLU:CG | 2.68 | 0.42 |
| 1:A:581:ASP:CA | 1:A:583:PRO:HD2 | 2.49 | 0.42 |
| 1:A:604:ALA:CB | 1:A:717:LEU:HD13 | 2.49 | 0.42 |
| 1:A:608:ASP:HA | 1:A:779:LEU:HD22 | 1.99 | 0.42 |
| 1:A:823:ARG:O | 1:A:824:ALA:CB | 2.68 | 0.42 |
| 1:A:864:ASN:HB2 | 1:A:865:ALA:H | 1.58 | 0.42 |
| 1:A:884:TYR:O | 1:A:885:THR:HG23 | 2.19 | 0.42 |
| 1:A:892:ASP:OD1 | 1:A:892:ASP:N | 2.42 | 0.42 |
| 1:A:951:TYR:C | 1:A:955:TYR:CD1 | 2.93 | 0.42 |
| 2:B:93:SER:C | 2:B:234:LYS:HZ1 | 2.23 | 0.42 |
| 2:B:238:SER:CA | 2:B:339:ASN:ND2 | 2.83 | 0.42 |
| 2:B:392:THR:HG22 | 2:B:393:LEU:N | 2.35 | 0.42 |
| 2:B:396:ARG:CD | 2:B:418:LEU:H | 2.25 | 0.42 |
| 2:B:471:LEU:CD1 | 2:B:474:PHE:HD2 | 2.32 | 0.42 |
| 2:C:127:PRO:HD2 | 2:C:128:VAL:H | 1.81 | 0.42 |
| 2:C:322:LEU:HD22 | 2:C:324:GLY:N | 2.34 | 0.42 |
| 2:C:347:LEU:N | 2:C:347:LEU:HD12 | 2.35 | 0.42 |
| 2:C:419:GLU:HG3 | 2:C:432:TYR:OH | 2.19 | 0.42 |
| 2:B:201:ASN:HD22 | 2:C:421:MET:CE | 2.33 | 0.42 |
| 1:D:1197:CYS:C | 1:D:1204:THR:CG2 | 2.88 | 0.42 |
| 1:D:1220:ILE:O | 1:D:1223:ILE:N | 2.52 | 0.42 |
| 1:D:242:ALA:CA | 1:D:245:ILE:HG23 | 2.42 | 0.42 |
| 1:D:309:ARG:CA | 1:D:312:TRP:HB2 | 2.39 | 0.42 |
| 1:D:348:LEU:CD1 | 1:D:350:ILE:CD1 | 2.94 | 0.42 |
| 1:D:369:LEU:O | 1:D:370:GLU:C | 2.52 | 0.42 |
| 1:D:618:HIS:N | 1:D:725:PRO:HG2 | 2.35 | 0.42 |
| 1:D:818:ARG:HE | 1:D:818:ARG:HB2 | 1.62 | 0.42 |
| 1:D:829:PRO:CG | 1:D:831:TYR:CE1 | 3.02 | 0.42 |
| 2:E:310:GLU:C | 2:E:314:MET:HG3 | 2.40 | 0.42 |
| 2:E:395:LEU:HD13 | 2:E:395:LEU:O | 2.20 | 0.42 |
| 2:E:403:PHE:HA | 2:E:413:VAL:HG21 | 2.01 | 0.42 |
| 2:E:456:ARG:HG3 | 2:E:457:SER:H | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:457:SER:OG | 2:E:458:ARG:N | 2.52 | 0.42 |
| 2:E:67:GLU:HG2 | 2:E:70:LEU:HD12 | 1.97 | 0.42 |
| 2:F:183:GLU:O | 2:F:184:ASN:OD1 | 2.38 | 0.42 |
| 2:F:185:LEU:CD1 | 2:F:236:GLU:HB2 | 2.46 | 0.42 |
| 2:F:272:ASN:CA | 2:F:292:ASN:ND2 | 2.83 | 0.42 |
| 2:F:357:THR:O | 2:F:358:GLU:CB | 2.66 | 0.42 |
| 2:E:203:ARG:NH1 | 2:F:418:LEU:HD13 | 2.34 | 0.42 |
| 1:A:1022:LEU:HB3 | 1:A:1026:ARG:HH22 | 1.85 | 0.42 |
| 1:A:267:VAL:HB | 1:A:269:HIS:CE1 | 2.55 | 0.42 |
| 1:A:284:ILE:O | 1:A:284:ILE:HG22 | 2.19 | 0.42 |
| 1:A:269:HIS:O | 1:A:293:ASP:HA | 2.19 | 0.42 |
| 1:A:474:LEU:HB3 | 1:A:712:VAL:H | 1.85 | 0.42 |
| 1:A:805:HIS:CG | 1:A:806:LYS:N | 2.88 | 0.42 |
| 1:A:275:ARG:HH22 | 1:A:845:VAL:CA | 2.23 | 0.42 |
| 1:A:962:ALA:CB | 1:A:986:TYR:CZ | 2.98 | 0.42 |
| 2:B:289:LEU:CB | 2:B:300:ILE:HG13 | 2.50 | 0.42 |
| 2:B:374:LEU:H | 2:B:458:ARG:CZ | 2.20 | 0.42 |
| 2:B:424:SER:OG | 2:B:425:LEU:N | 2.52 | 0.42 |
| 2:B:435:MET:O | 2:B:437:ILE:N | 2.53 | 0.42 |
| 2:B:461:THR:OG1 | 2:B:463:LYS:HE3 | 2.20 | 0.42 |
| 2:B:466:MET:CG | 2:B:467:HIS:N | 2.80 | 0.42 |
| 2:C:241:TRP:CD1 | 2:C:243:THR:CG2 | 3.00 | 0.42 |
| 2:C:306:LEU:C | 2:C:335:VAL:HB | 2.40 | 0.42 |
| 2:C:59:ALA:N | 2:C:60:PRO:HD2 | 2.35 | 0.42 |
| 2:C:86:LEU:O | 2:C:87:SER:C | 2.58 | 0.42 |
| 1:D:1015:THR:O | 1:D:1016:GLU:HB2 | 2.19 | 0.42 |
| 1:D:285:GLN:HE22 | 1:D:1128:ARG:CB | 2.32 | 0.42 |
| 1:D:1124:ALA:HB2 | 1:D:1231:LEU:HB3 | 2.02 | 0.42 |
| 1:D:239:LEU:O | 1:D:242:ALA:N | 2.47 | 0.42 |
| 1:D:285:GLN:NE2 | 1:D:1128:ARG:CB | 2.83 | 0.42 |
| 1:D:289:MET:CE | 1:D:290:ARG:N | 2.83 | 0.42 |
| 1:D:348:LEU:HD13 | 1:D:350:ILE:CD1 | 2.48 | 0.42 |
| 1:D:387:GLU:O | 1:D:390:GLN:CG | 2.67 | 0.42 |
| 1:D:462:SER:O | 1:D:466:LEU:HD13 | 2.20 | 0.42 |
| 1:D:538:GLU:CD | 1:D:542:ASP:CG | 2.78 | 0.42 |
| 1:D:576:LEU:HD22 | 2:F:481:SER:CB | 2.49 | 0.42 |
| 1:D:666:GLN:HA | 1:D:669:MET:HG3 | 2.00 | 0.42 |
| 1:D:801:TRP:HE3 | 1:D:804:ALA:HB3 | 1.85 | 0.42 |
| 1:D:871:GLY:O | 1:D:872:SER:C | 2.57 | 0.42 |
| 1:D:955:TYR:HB3 | 1:D:1098:ASN:OD1 | 2.19 | 0.42 |
| 2:E:250:GLN:CD | 2:E:250:GLN:C | 2.78 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:109:ASN:HB2 | 2:E:378:LEU:O | 2.20 | 0.42 |
| 2:E:398:VAL:HG22 | 2:E:402:LEU:HG | 2.02 | 0.42 |
| 2:E:406:LEU:HG | 2:E:413:VAL:HG21 | 2.01 | 0.42 |
| 2:E:472:LYS:NZ | 2:E:473:ASP:OD1 | 2.53 | 0.42 |
| 2:E:95:CYS:O | 2:E:96:HIS:C | 2.58 | 0.42 |
| 2:F:263:TRP:O | 2:F:264:ARG:C | 2.58 | 0.42 |
| 2:F:442:LEU:CB | 2:F:455:LEU:HD22 | 2.49 | 0.42 |
| 1:A:1013:ASP:CG | 1:A:1014:ARG:N | 2.73 | 0.42 |
| 1:A:1219:ASP:O | 1:A:1223:ILE:CG2 | 2.65 | 0.42 |
| 1:A:204:ALA:C | 1:A:206:GLY:N | 2.72 | 0.42 |
| 1:A:290:ARG:O | 1:A:291:PHE:CD2 | 2.73 | 0.42 |
| 1:A:316:LYS:HB2 | 1:A:348:LEU:HD11 | 2.02 | 0.42 |
| 1:A:312:TRP:CZ2 | 1:A:346:ASP:O | 2.54 | 0.42 |
| 1:A:357:SER:O | 1:A:361:VAL:HG12 | 2.20 | 0.42 |
| 1:A:500:ALA:HB1 | 1:A:520:ALA:HB2 | 2.02 | 0.42 |
| 1:A:593:SER:C | 1:A:594:LEU:HD23 | 2.40 | 0.42 |
| 1:A:869:ARG:NE | 1:A:870:VAL:HG23 | 2.35 | 0.42 |
| 1:A:941:ILE:HG22 | 1:A:942:SER:O | 2.20 | 0.42 |
| 1:A:996:ARG:HD2 | 1:A:1004:LEU:HD13 | 2.01 | 0.42 |
| 2:B:118:VAL:HG21 | 2:B:239:LEU:HD22 | 2.02 | 0.42 |
| 2:B:261:GLN:OE1 | 2:B:266:PHE:CE1 | 2.73 | 0.42 |
| 2:B:107:ARG:HB2 | 2:B:346:MET:SD | 2.60 | 0.42 |
| 2:C:300:ILE:CG2 | 2:C:342:LEU:CD1 | 2.83 | 0.42 |
| 2:C:322:LEU:HD22 | 2:C:323:HIS:N | 2.35 | 0.42 |
| 2:C:325:ARG:NH2 | 2:C:327:GLY:HA2 | 2.35 | 0.42 |
| 2:C:361:PHE:C | 2:C:362:THR:HG23 | 2.40 | 0.42 |
| 2:C:433:ASP:C | 2:C:435:MET:N | 2.72 | 0.42 |
| 2:C:72:ILE:HG23 | 2:C:76:ARG:HE | 1.84 | 0.42 |
| 1:D:1015:THR:C | 1:D:1017:GLY:H | 2.23 | 0.42 |
| 1:D:1056:GLU:CA | 1:D:1059:ASN:HD21 | 2.24 | 0.42 |
| 1:D:1102:GLN:O | 1:D:1103:SER:C | 2.56 | 0.42 |
| 1:D:1151:LEU:HD21 | 1:D:1224:ILE:HB | 2.02 | 0.42 |
| 1:D:175:TRP:HZ2 | 1:D:183:GLU:HG3 | 1.79 | 0.42 |
| 1:D:278:ILE:CA | 1:D:291:PHE:CD1 | 3.03 | 0.42 |
| 1:D:380:GLY:O | 1:D:381:THR:CG2 | 2.58 | 0.42 |
| 1:D:472:GLN:O | 2:F:461:THR:CG2 | 2.68 | 0.42 |
| 1:D:525:MET:O | 1:D:526:ASP:CG | 2.57 | 0.42 |
| 1:D:544:MET:O | 1:D:548:CYS:N | 2.52 | 0.42 |
| 1:D:631:LEU:O | 1:D:633:LYS:N | 2.53 | 0.42 |
| 1:D:634:LEU:HA | 1:D:635:PRO:HD3 | 1.78 | 0.42 |
| 2:E:308:ASP:O | 2:E:309:HIS:O | 2.38 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:203:ARG:HA | 2:F:325:ARG:CG | 2.47 | 0.42 |
| 2:F:300:ILE:N | 2:F:344:ARG:HH12 | 2.18 | 0.42 |
| 2:F:374:LEU:HB2 | 2:F:379:ALA:HB2 | 2.02 | 0.42 |
| 2:F:408:GLU:O | 2:F:409:ASN:C | 2.58 | 0.42 |
| 2:F:427:GLN:O | 2:F:430:SER:OG | 2.28 | 0.42 |
| 2:F:436:SER:O | 2:F:437:ILE:C | 2.58 | 0.42 |
| 2:F:473:ASP:O | 2:F:476:ILE:HD12 | 2.20 | 0.42 |
| 1:A:1025:LEU:O | 1:A:1026:ARG:CG | 2.63 | 0.42 |
| 1:A:955:TYR:CB | 1:A:1098:ASN:OD1 | 2.65 | 0.42 |
| 1:A:1135:ASP:N | 1:A:1136:GLU:OE2 | 2.45 | 0.42 |
| 1:A:1207:GLU:H | 1:A:1210:TYR:H | 1.66 | 0.42 |
| 1:A:199:VAL:HG21 | 1:A:277:HIS:CB | 2.50 | 0.42 |
| 1:A:213:VAL:HG13 | 1:A:397:ALA:CB | 2.44 | 0.42 |
| 1:A:394:GLN:OE1 | 1:A:395:TYR:HA | 2.20 | 0.42 |
| 1:A:607:TRP:HZ2 | 1:A:671:GLN:N | 2.18 | 0.42 |
| 1:A:608:ASP:OD2 | 1:A:614:TYR:OH | 2.29 | 0.42 |
| 2:B:182:ARG:HD3 | 2:B:214:CYS:HA | 2.02 | 0.42 |
| 2:B:128:VAL:HG12 | 2:B:209:ALA:O | 2.20 | 0.42 |
| 2:C:198:ASP:OD1 | 2:C:198:ASP:O | 2.38 | 0.42 |
| 2:C:252:LEU:CD2 | 2:C:252:LEU:C | 2.89 | 0.42 |
| 2:C:456:ARG:CG | 2:C:457:SER:N | 2.79 | 0.42 |
| 1:D:1037:GLN:H | 1:D:1037:GLN:HG2 | 1.38 | 0.42 |
| 1:D:1057:MET:CB | 1:D:1064:ILE:HD11 | 2.29 | 0.42 |
| 1:D:1103:SER:O | 1:D:1104:SER:C | 2.57 | 0.42 |
| 1:D:289:MET:HE2 | 1:D:290:ARG:N | 2.35 | 0.42 |
| 1:D:739:TYR:C | 1:D:740:ASN:CG | 2.79 | 0.42 |
| 1:D:770:PHE:CE1 | 1:D:968:GLN:CA | 3.03 | 0.42 |
| 1:D:797:MET:H | 1:D:797:MET:HG3 | 1.49 | 0.42 |
| 1:D:813:VAL:HG21 | 1:D:815:TRP:CZ2 | 2.55 | 0.42 |
| 1:D:841:LEU:HA | 1:D:842:PRO:HD3 | 1.72 | 0.42 |
| 1:D:967:MET:SD | 1:D:978:ALA:CB | 3.07 | 0.42 |
| 2:E:121:PHE:HA | 2:F:407:LEU:CD1 | 2.49 | 0.42 |
| 2:E:471:LEU:HD12 | 2:E:471:LEU:O | 2.20 | 0.42 |
| 2:E:80:SER:O | 2:E:86:LEU:HD21 | 2.20 | 0.42 |
| 2:F:184:ASN:O | 2:F:185:LEU:C | 2.58 | 0.42 |
| 2:F:275:SER:HA | 2:F:288:LYS:O | 2.20 | 0.42 |
| 1:D:546:ARG:NH2 | 2:F:408:GLU:OE1 | 2.53 | 0.42 |
| 2:F:468:ILE:C | 2:F:471:LEU:HD13 | 2.41 | 0.42 |
| 1:A:1193:VAL:HG22 | 1:A:1194:THR:H | 1.85 | 0.41 |
| 1:A:293:ASP:HB2 | 1:A:296:SER:OG | 2.20 | 0.41 |
| 1:A:373:PRO:CD | 1:A:374:ARG:H | 2.32 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:415:LEU:C | 1:A:417:ARG:N | 2.73 | 0.41 |
| 1:A:454:GLU:O | 1:A:455:LEU:C | 2.57 | 0.41 |
| 1:A:612:LEU:CD2 | 1:A:614:TYR:CA | 2.98 | 0.41 |
| 1:A:643:ALA:O | 1:A:644:GLY:C | 2.58 | 0.41 |
| 1:A:730:PRO:HG2 | 1:A:731:SER:H | 1.85 | 0.41 |
| 1:A:886:LEU:CD1 | 1:A:1189:LEU:HD21 | 2.50 | 0.41 |
| 2:B:196:CYS:O | 2:B:199:LEU:HB3 | 2.20 | 0.41 |
| 2:B:269:SER:C | 2:B:271:SER:N | 2.68 | 0.41 |
| 1:D:873:GLU:N | 1:D:1200:PRO:HD3 | 2.35 | 0.41 |
| 1:D:172:ALA:HB1 | 1:D:221:TYR:HB2 | 2.02 | 0.41 |
| 1:D:206:GLY:C | 1:D:208:CYS:H | 2.20 | 0.41 |
| 1:D:236:THR:O | 1:D:237:SER:HB3 | 2.20 | 0.41 |
| 1:D:245:ILE:HG13 | 1:D:246:PRO:CG | 2.47 | 0.41 |
| 1:D:288:ARG:NH1 | 1:D:290:ARG:HH22 | 2.18 | 0.41 |
| 1:D:420:HIS:CD2 | 1:D:1020:ILE:CG2 | 3.02 | 0.41 |
| 1:D:434:TYR:CD1 | 1:D:841:LEU:HD21 | 2.55 | 0.41 |
| 1:D:457:ARG:C | 1:D:460:LYS:NZ | 2.73 | 0.41 |
| 1:D:461:LYS:HE3 | 1:D:461:LYS:HB3 | 1.84 | 0.41 |
| 1:D:488:LEU:HD23 | 1:D:488:LEU:N | 2.34 | 0.41 |
| 1:D:669:MET:HA | 1:D:670:PRO:HA | 1.58 | 0.41 |
| 1:D:808:ILE:HD13 | 1:D:874:LEU:CD2 | 2.50 | 0.41 |
| 2:E:379:ALA:HB3 | 2:E:438:LEU:HD11 | 2.02 | 0.41 |
| 2:E:456:ARG:NH1 | 2:E:463:LYS:HE3 | 2.32 | 0.41 |
| 2:E:476:ILE:O | 2:E:480:SER:N | 2.43 | 0.41 |
| 2:F:286:GLY:CA | 2:F:303:LEU:O | 2.68 | 0.41 |
| 2:F:293:PHE:C | 2:F:295:TRP:N | 2.74 | 0.41 |
| 2:F:197:LEU:HD12 | 2:F:322:LEU:HD21 | 2.00 | 0.41 |
| 2:F:335:VAL:HG22 | 2:F:336:LEU:N | 2.35 | 0.41 |
| 2:F:239:LEU:HG | 2:F:336:LEU:CD1 | 2.50 | 0.41 |
| 2:F:383:VAL:CG2 | 2:F:384:ALA:H | 2.33 | 0.41 |
| 2:F:394:GLU:HA | 2:F:397:GLN:CD | 2.39 | 0.41 |
| 2:E:203:ARG:NH2 | 2:F:418:LEU:CD1 | 2.83 | 0.41 |
| 2:F:372:LEU:CG | 2:F:436:SER:HB2 | 2.49 | 0.41 |
| 2:F:474:PHE:CZ | 2:F:475:LEU:HD23 | 2.55 | 0.41 |
| 1:A:955:TYR:HE2 | 1:A:1102:GLN:HE21 | 1.68 | 0.41 |
| 1:A:1230:SER:HB3 | 1:A:1231:LEU:H | 1.58 | 0.41 |
| 1:A:177:ARG:O | 1:A:179:GLY:N | 2.53 | 0.41 |
| 1:A:196:VAL:HA | 1:A:267:VAL:HG12 | 2.02 | 0.41 |
| 1:A:449:GLN:HA | 1:A:452:TYR:CD1 | 2.53 | 0.41 |
| 1:A:485:LEU:O | 1:A:489:GLU:HG3 | 2.20 | 0.41 |
| 1:A:630:ASN:C | 1:A:630:ASN:ND2 | 2.74 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:784:GLY:N | 2:C:362:THR:O | 2.54 | 0.41 |
| 1:A:792:LEU:O | 1:A:796:LYS:CD | 2.67 | 0.41 |
| 1:A:906:HIS:C | 1:A:908:ALA:H | 2.23 | 0.41 |
| 2:B:259:ARG:HD2 | 2:B:262:TRP:HB2 | 2.01 | 0.41 |
| 2:B:76:ARG:NH2 | 2:B:431:LYS:HG3 | 2.35 | 0.41 |
| 2:C:102:LEU:HD11 | 2:C:435:MET:SD | 2.60 | 0.41 |
| 2:C:121:PHE:CE1 | 2:C:122:ARG:HD2 | 2.55 | 0.41 |
| 2:C:125:VAL:CG1 | 2:C:206:TYR:HD1 | 2.33 | 0.41 |
| 2:C:208:LEU:HG | 2:C:208:LEU:H | 0.84 | 0.41 |
| 2:C:208:LEU:CD1 | 2:C:240:VAL:C | 2.80 | 0.41 |
| 2:C:272:ASN:HB3 | 2:C:292:ASN:CB | 2.47 | 0.41 |
| 2:C:473:ASP:O | 2:C:477:LYS:HG3 | 2.20 | 0.41 |
| 1:D:1019:TRP:NE1 | 1:D:1020:ILE:HG22 | 2.32 | 0.41 |
| 1:D:1122:GLU:OE2 | 1:D:1122:GLU:CA | 2.68 | 0.41 |
| 1:D:1220:ILE:HB | 1:D:1221:TYR:H | 1.41 | 0.41 |
| 1:D:209:PRO:O | 1:D:210:THR:OG1 | 2.38 | 0.41 |
| 1:D:345:TRP:O | 1:D:345:TRP:CE3 | 2.73 | 0.41 |
| 1:D:444:TYR:CE2 | 1:D:877:MET:SD | 3.13 | 0.41 |
| 1:D:546:ARG:HH21 | 2:F:404:ASN:ND2 | 2.18 | 0.41 |
| 1:D:611:PRO:HG2 | 1:D:622:TYR:CE2 | 2.55 | 0.41 |
| 1:D:631:LEU:O | 1:D:633:LYS:HG3 | 2.20 | 0.41 |
| 1:D:765:PRO:HG2 | 1:D:766:PHE:CG | 2.55 | 0.41 |
| 1:D:797:MET:HB2 | 1:D:869:ARG:HH11 | 1.85 | 0.41 |
| 1:D:896:LEU:HD13 | 1:D:896:LEU:HA | 1.85 | 0.41 |
| 2:E:213:VAL:HG13 | 2:E:235:THR:HG23 | 1.96 | 0.41 |
| 2:E:389:ARG:HH21 | 2:E:391:PRO:C | 2.20 | 0.41 |
| 2:E:415:PRO:HB2 | 2:E:417:TYR:CZ | 2.55 | 0.41 |
| 2:E:476:ILE:O | 2:E:480:SER:HB3 | 2.19 | 0.41 |
| 2:F:201:ASN:O | 2:F:202:LYS:CB | 2.68 | 0.41 |
| 2:F:238:SER:HA | 2:F:338:VAL:CB | 2.49 | 0.41 |
| 2:F:299:LEU:CD2 | 2:F:299:LEU:H | 2.09 | 0.41 |
| 2:F:308:ASP:OD2 | 2:F:334:CYS:SG | 2.76 | 0.41 |
| 1:A:1010:LEU:C | 1:A:1012:VAL:H | 2.19 | 0.41 |
| 1:A:1028:VAL:HG23 | 1:A:1029:GLN:HG3 | 2.01 | 0.41 |
| 1:A:105:GLU:O | 1:A:109:LYS:HE2 | 2.20 | 0.41 |
| 1:A:1108:TYR:CE2 | 1:A:1112:MET:HE1 | 2.55 | 0.41 |
| 1:A:1128:ARG:O | 1:A:1139:TYR:HA | 2.21 | 0.41 |
| 1:A:110:HIS:C | 1:A:112:LEU:HD12 | 2.41 | 0.41 |
| 1:A:1195:MET:O | 1:A:1196:ASP:CB | 2.67 | 0.41 |
| 1:A:196:VAL:HA | 1:A:269:HIS:NE2 | 2.35 | 0.41 |
| 1:A:239:LEU:H | 1:A:239:LEU:HG | 1.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:253:ALA:CB | 1:A:256:PRO:HB3 | 2.37 | 0.41 |
| 1:A:272:SER:O | 1:A:274:ASP:N | 2.52 | 0.41 |
| 1:A:481:GLU:C | 1:A:482:ASP:OD1 | 2.59 | 0.41 |
| 1:A:620:TRP:HD1 | 1:A:749:PHE:O | 2.03 | 0.41 |
| 1:A:726:LYS:C | 1:A:727:ASP:O | 2.57 | 0.41 |
| 1:A:829:PRO:HB3 | 1:A:883:GLY:N | 2.35 | 0.41 |
| 1:A:913:CYS:O | 1:A:917:GLY:N | 2.54 | 0.41 |
| 2:C:134:LYS:HD3 | 2:C:180:LYS:HZ2 | 1.86 | 0.41 |
| 2:C:188:GLY:C | 2:C:190:LEU:N | 2.70 | 0.41 |
| 2:C:208:LEU:CD1 | 2:C:208:LEU:H | 1.98 | 0.41 |
| 2:C:222:LYS:HB2 | 2:C:223:GLN:H | 1.56 | 0.41 |
| 2:C:413:VAL:CG1 | 2:C:414:TRP:N | 2.83 | 0.41 |
| 2:C:433:ASP:C | 2:C:435:MET:H | 2.23 | 0.41 |
| 1:D:1043:VAL:HG23 | 1:D:1043:VAL:O | 2.20 | 0.41 |
| 1:D:1129:PHE:CE2 | 1:D:1139:TYR:CD2 | 3.09 | 0.41 |
| 1:D:1154:GLN:HG2 | 1:D:1179:PHE:HE2 | 1.82 | 0.41 |
| 1:D:444:TYR:CE2 | 1:D:1210:TYR:HB2 | 2.55 | 0.41 |
| 1:D:180:PRO:O | 1:D:181:GLU:CD | 2.59 | 0.41 |
| 1:D:256:PRO:HB3 | 1:D:281:GLN:CA | 2.49 | 0.41 |
| 1:D:267:VAL:CB | 1:D:269:HIS:HD2 | 2.14 | 0.41 |
| 1:D:275:ARG:NE | 1:D:842:PRO:C | 2.72 | 0.41 |
| 1:D:451:THR:HA | 1:D:454:GLU:HG3 | 2.01 | 0.41 |
| 1:D:468:ASN:O | 1:D:472:GLN:HB2 | 2.21 | 0.41 |
| 1:D:500:ALA:HB2 | 1:D:521:PRO:CD | 2.49 | 0.41 |
| 1:D:722:ARG:CG | 1:D:722:ARG:NH1 | 2.83 | 0.41 |
| 1:D:601:LYS:NZ | 1:D:722:ARG:H | 2.17 | 0.41 |
| 1:D:74:LEU:CD1 | 1:D:76:ILE:O | 2.67 | 0.41 |
| 1:D:812:MET:O | 1:D:840:ILE:CG2 | 2.58 | 0.41 |
| 1:D:79:LEU:CB | 1:D:83:LEU:HD11 | 2.46 | 0.41 |
| 2:E:203:ARG:CZ | 2:E:203:ARG:CB | 2.97 | 0.41 |
| 2:E:264:ARG:HG2 | 2:E:273:PHE:CG | 2.55 | 0.41 |
| 2:E:259:ARG:NH2 | 2:E:301:GLU:OE1 | 2.53 | 0.41 |
| 2:E:328:ARG:O | 2:E:329:LYS:HG3 | 2.20 | 0.41 |
| 2:E:87:SER:C | 2:E:89:ASP:H | 2.24 | 0.41 |
| 2:F:254:PHE:HA | 2:F:257:ARG:HD2 | 2.02 | 0.41 |
| 2:F:375:HIS:N | 2:F:378:LEU:HB2 | 2.35 | 0.41 |
| 2:F:386:ASP:O | 2:F:443:VAL:N | 2.36 | 0.41 |
| 2:F:403:PHE:CD2 | 2:F:407:LEU:HB2 | 2.54 | 0.41 |
| 2:F:426:GLU:OE2 | 2:F:426:GLU:HA | 2.20 | 0.41 |
| 2:F:468:ILE:CG2 | 2:F:469:SER:N | 2.83 | 0.41 |
| 2:F:470:LYS:O | 2:F:474:PHE:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:F:475:LEU:H | 2:F:475:LEU:HG | 1.58 | 0.41 |
| 1:A:1041:TRP:NE1 | 1:A:1043:VAL:CG2 | 2.83 | 0.41 |
| 1:A:1093:MET:HG3 | 1:A:1093:MET:H | 1.68 | 0.41 |
| 1:A:1122:GLU:C | 1:A:1123:PHE:HD1 | 2.20 | 0.41 |
| 1:A:1158:LEU:HD23 | 1:A:1158:LEU:N | 2.34 | 0.41 |
| 1:A:1233:LYS:C | 1:A:1236:GLN:NE2 | 2.73 | 0.41 |
| 1:A:175:TRP:O | 1:A:176:THR:CB | 2.68 | 0.41 |
| 1:A:259:ARG:O | 1:A:260:ASP:CB | 2.68 | 0.41 |
| 1:A:371:LYS:HB2 | 1:A:374:ARG:HD2 | 2.03 | 0.41 |
| 1:A:417:ARG:C | 1:A:419:PRO:HD3 | 2.41 | 0.41 |
| 1:A:425:ALA:O | 1:A:428:LEU:HB2 | 2.21 | 0.41 |
| 1:A:497:GLN:O | 1:A:498:LYS:CG | 2.68 | 0.41 |
| 1:A:560:PRO:O | 1:A:561:LYS:HB2 | 2.20 | 0.41 |
| 1:A:606:THR:HG22 | 1:A:614:TYR:CE2 | 2.55 | 0.41 |
| 1:A:645:VAL:CG1 | 1:A:647:CYS:O | 2.68 | 0.41 |
| 1:A:617:ARG:HB3 | 1:A:763:GLY:C | 2.41 | 0.41 |
| 1:A:441:TRP:HD1 | 1:A:877:MET:SD | 2.44 | 0.41 |
| 1:A:944:GLU:O | 1:A:948:ILE:HG12 | 2.21 | 0.41 |
| 2:B:183:GLU:C | 2:B:214:CYS:SG | 2.99 | 0.41 |
| 2:C:197:LEU:C | 2:C:199:LEU:N | 2.72 | 0.41 |
| 2:C:282:GLU:C | 2:C:284:ARG:N | 2.71 | 0.41 |
| 2:C:238:SER:HB2 | 2:C:338:VAL:HG11 | 2.01 | 0.41 |
| 2:C:432:TYR:HB3 | 2:C:437:ILE:CD1 | 2.50 | 0.41 |
| 1:A:556:THR:CG2 | 2:C:467:HIS:NE2 | 2.84 | 0.41 |
| 1:D:97:GLU:CB | 1:D:101:ARG:NH1 | 2.83 | 0.41 |
| 1:D:869:ARG:HA | 1:D:1200:PRO:HB2 | 2.02 | 0.41 |
| 1:D:247:LEU:N | 1:D:247:LEU:HD12 | 2.35 | 0.41 |
| 1:D:265:LEU:HG | 1:D:267:VAL:N | 2.35 | 0.41 |
| 1:D:387:GLU:O | 1:D:390:GLN:HG2 | 2.20 | 0.41 |
| 1:D:531:GLY:HA2 | 1:D:532:PRO:HD3 | 1.68 | 0.41 |
| 1:D:863:SER:O | 1:D:875:LYS:HE2 | 2.20 | 0.41 |
| 2:E:212:GLY:O | 2:E:235:THR:C | 2.58 | 0.41 |
| 2:E:302:THR:O | 2:E:338:VAL:HA | 2.20 | 0.41 |
| 2:E:447:THR:CG2 | 2:E:452:LEU:H | 2.32 | 0.41 |
| 2:E:455:LEU:O | 2:E:463:LYS:CA | 2.59 | 0.41 |
| 2:F:114:TRP:HB2 | 2:F:262:TRP:HZ2 | 1.77 | 0.41 |
| 2:F:193:TYR:O | 2:F:193:TYR:CD1 | 2.74 | 0.41 |
| 2:F:204:LEU:HD12 | 2:F:204:LEU:H | 1.84 | 0.41 |
| 2:F:282:GLU:C | 2:F:284:ARG:H | 2.22 | 0.41 |
| 2:F:289:LEU:O | 2:F:299:LEU:C | 2.58 | 0.41 |
| 2:F:360:SER:OG | 2:F:364:LYS:HD2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:432:TYR:O | 2:F:436:SER:N | 2.53 | 0.41 |
| 2:F:82:SER:CA | 2:F:86:LEU:CD2 | 2.77 | 0.41 |
| 1:A:139:PHE:CD2 | 1:A:1111:LEU:HG | 2.56 | 0.41 |
| 1:A:1131:ILE:HG23 | 1:A:1137:VAL:CG1 | 2.49 | 0.41 |
| 1:A:1179:PHE:CD1 | 1:A:1220:ILE:HG12 | 2.55 | 0.41 |
| 1:A:1183:VAL:O | 1:A:1217:ALA:CB | 2.68 | 0.41 |
| 1:A:1184:ASP:N | 1:A:1184:ASP:OD1 | 2.54 | 0.41 |
| 1:A:156:LEU:CD2 | 1:A:156:LEU:N | 2.83 | 0.41 |
| 1:A:255:SER:N | 1:A:256:PRO:HA | 2.35 | 0.41 |
| 1:A:345:TRP:O | 1:A:345:TRP:CD1 | 2.74 | 0.41 |
| 1:A:606:THR:HG21 | 1:A:613:HIS:N | 2.25 | 0.41 |
| 1:A:597:ARG:HB2 | 1:A:616:GLU:OE1 | 2.20 | 0.41 |
| 1:A:618:HIS:O | 1:A:762:VAL:HG21 | 2.20 | 0.41 |
| 1:A:659:HIS:HD2 | 1:A:720:THR:H | 1.67 | 0.41 |
| 1:A:667:GLN:CG | 1:A:668:LEU:N | 2.82 | 0.41 |
| 1:A:739:TYR:CA | 1:A:741:ASP:O | 2.67 | 0.41 |
| 1:A:765:PRO:HG2 | 1:A:766:PHE:N | 2.36 | 0.41 |
| 1:A:769:ASP:OD1 | 1:A:1057:MET:HE2 | 2.20 | 0.41 |
| 2:B:125:VAL:CG1 | 2:B:126:PHE:N | 2.82 | 0.41 |
| 2:B:431:LYS:HG2 | 2:B:435:MET:HG3 | 2.02 | 0.41 |
| 2:B:436:SER:C | 2:B:458:ARG:HH11 | 2.23 | 0.41 |
| 2:C:115:TRP:CD1 | 2:C:119:VAL:CG2 | 3.03 | 0.41 |
| 2:C:208:LEU:N | 2:C:208:LEU:CD1 | 2.57 | 0.41 |
| 2:C:413:VAL:HG12 | 2:C:414:TRP:H | 1.84 | 0.41 |
| 1:D:1005:VAL:O | 1:D:1006:ARG:C | 2.55 | 0.41 |
| 1:D:1132:SER:CA | 1:D:1136:GLU:O | 2.62 | 0.41 |
| 1:D:1200:PRO:HD2 | 1:D:1203:PRO:CB | 2.51 | 0.41 |
| 1:D:163:PRO:O | 1:D:165:LYS:HE3 | 2.21 | 0.41 |
| 1:D:255:SER:HB3 | 1:D:256:PRO:O | 2.18 | 0.41 |
| 1:D:269:HIS:O | 1:D:274:ASP:OD2 | 2.38 | 0.41 |
| 1:D:823:ARG:CD | 1:D:824:ALA:H | 2.32 | 0.41 |
| 1:D:902:LEU:HA | 1:D:902:LEU:HD12 | 1.80 | 0.41 |
| 2:E:323:HIS:O | 2:E:330:ASN:HA | 2.20 | 0.41 |
| 2:E:325:ARG:CG | 2:E:330:ASN:H | 2.34 | 0.41 |
| 2:E:341:ASP:C | 2:E:341:ASP:OD1 | 2.59 | 0.41 |
| 2:E:354:PHE:HB2 | 2:E:372:LEU:CD1 | 2.50 | 0.41 |
| 2:F:78:PHE:HD1 | 2:F:102:LEU:HD22 | 1.78 | 0.41 |
| 2:F:131:LEU:HD12 | 2:F:131:LEU:HA | 1.88 | 0.41 |
| 2:F:247:THR:HG1 | 2:F:248:SER:N | 2.19 | 0.41 |
| 2:F:460:THR:C | 2:F:461:THR:HG23 | 2.41 | 0.41 |
| 1:A:756:ASP:OD2 | 1:A:1057:MET:HG2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:879:GLN:CG | 1:A:1189:LEU:CD2 | 2.79 | 0.41 |
| 1:A:1198:LYS:O | 1:A:1199:THR:CB | 2.68 | 0.41 |
| 1:A:174:GLY:O | 1:A:220:TRP:HB2 | 2.21 | 0.41 |
| 1:A:256:PRO:CB | 1:A:281:GLN:HA | 2.46 | 0.41 |
| 1:A:439:GLN:HG3 | 1:A:836:LEU:O | 2.20 | 0.41 |
| 1:A:670:PRO:O | 1:A:671:GLN:C | 2.59 | 0.41 |
| 1:A:792:LEU:O | 1:A:796:LYS:HD3 | 2.21 | 0.41 |
| 1:A:904:ASP:OD1 | 1:A:904:ASP:N | 2.51 | 0.41 |
| 1:A:985:MET:H | 1:A:985:MET:HG3 | 1.73 | 0.41 |
| 2:B:261:GLN:CA | 2:B:264:ARG:NE | 2.70 | 0.41 |
| 2:B:471:LEU:HA | 2:B:474:PHE:HB3 | 2.01 | 0.41 |
| 2:C:393:LEU:O | 2:C:397:GLN:HB3 | 2.21 | 0.41 |
| 2:C:452:LEU:HD12 | 2:C:453:ILE:HG12 | 2.02 | 0.41 |
| 1:D:1165:ALA:HB1 | 1:D:1173:LEU:HD12 | 1.91 | 0.41 |
| 1:D:140:ARG:O | 1:D:144:GLN:CB | 2.61 | 0.41 |
| 1:D:146:GLN:HG2 | 1:D:146:GLN:H | 1.44 | 0.41 |
| 1:D:295:MET:O | 1:D:298:HIS:N | 2.54 | 0.41 |
| 1:D:203:LEU:CB | 1:D:379:LYS:O | 2.69 | 0.41 |
| 1:D:391:ASP:O | 1:D:395:TYR:CD1 | 2.74 | 0.41 |
| 1:D:522:GLY:C | 1:D:524:PRO:N | 2.74 | 0.41 |
| 1:D:495:PHE:O | 1:D:573:TYR:CZ | 2.73 | 0.41 |
| 1:D:611:PRO:CB | 1:D:612:LEU:HD13 | 2.37 | 0.41 |
| 1:D:738:PRO:C | 1:D:739:TYR:O | 2.57 | 0.41 |
| 1:D:622:TYR:HB2 | 1:D:747:CYS:O | 2.21 | 0.41 |
| 1:D:81:ARG:HD3 | 1:D:126:ARG:HA | 2.01 | 0.41 |
| 1:D:444:TYR:CD2 | 1:D:877:MET:SD | 3.14 | 0.41 |
| 1:D:950:ASN:O | 1:D:953:ARG:N | 2.53 | 0.41 |
| 2:E:106:LEU:HD12 | 2:E:109:ASN:ND2 | 2.36 | 0.41 |
| 2:E:123:GLU:O | 2:E:125:VAL:O | 2.39 | 0.41 |
| 2:E:201:ASN:OD1 | 2:F:422:GLN:CD | 2.59 | 0.41 |
| 2:E:205:PRO:HB3 | 2:E:242:PHE:C | 2.41 | 0.41 |
| 2:E:353:SER:HA | 2:E:373:LYS:O | 2.20 | 0.41 |
| 2:E:370:LYS:O | 2:E:433:ASP:CG | 2.58 | 0.41 |
| 2:E:389:ARG:N | 2:E:395:LEU:CD1 | 2.77 | 0.41 |
| 2:E:406:LEU:HG | 2:E:413:VAL:HG22 | 2.01 | 0.41 |
| 2:E:418:LEU:HD23 | 2:E:418:LEU:HA | 1.88 | 0.41 |
| 2:F:336:LEU:HD21 | 2:F:337:SER:O | 2.21 | 0.41 |
| 2:F:61:GLY:CA | 2:F:64:GLU:HG2 | 2.51 | 0.41 |
| 1:A:1125:ILE:C | 1:A:1126:ASP:OD1 | 2.59 | 0.41 |
| 1:A:211:LEU:HA | 1:A:222:SER:H | 1.86 | 0.41 |
| 1:A:276:ALA:CB | 1:A:279:ARG:HG2 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:292:LEU:HD11 | 1:A:428:LEU:CD2 | 2.51 | 0.41 |
| 1:A:412:PRO:O | 1:A:415:LEU:N | 2.53 | 0.41 |
| 1:A:456:GLN:HE21 | 1:A:798:ILE:HD11 | 1.86 | 0.41 |
| 1:A:465:ASP:OD1 | 1:A:466:LEU:N | 2.54 | 0.41 |
| 1:A:745:PRO:HD2 | 1:A:746:GLY:H | 1.85 | 0.41 |
| 1:A:78:MET:O | 1:A:79:LEU:HD23 | 2.21 | 0.41 |
| 1:A:817:PRO:CG | 1:A:818:ARG:N | 2.84 | 0.41 |
| 1:A:900:ALA:HB1 | 1:A:915:ALA:HB1 | 2.02 | 0.41 |
| 1:A:928:GLY:C | 1:A:930:ASP:N | 2.74 | 0.41 |
| 1:A:931:LEU:CD2 | 1:A:932:HIS:N | 2.77 | 0.41 |
| 2:B:473:ASP:O | 2:B:477:LYS:HE3 | 2.21 | 0.41 |
| 2:C:113:GLU:O | 2:C:116:THR:CG2 | 2.59 | 0.41 |
| 2:C:290:TYR:CD1 | 2:C:299:LEU:HD22 | 2.56 | 0.41 |
| 2:C:240:VAL:C | 2:C:336:LEU:CB | 2.83 | 0.41 |
| 2:C:344:ARG:N | 2:C:347:LEU:HD22 | 2.35 | 0.41 |
| 2:C:362:THR:O | 2:C:363:ARG:HD2 | 2.21 | 0.41 |
| 1:D:1045:ALA:HB1 | 1:D:1092:PHE:CE1 | 2.55 | 0.41 |
| 1:D:1097:VAL:O | 1:D:1098:ASN:C | 2.57 | 0.41 |
| 1:D:1193:VAL:O | 1:D:1195:MET:CE | 2.69 | 0.41 |
| 1:D:138:HIS:O | 1:D:142:LEU:CG | 2.52 | 0.41 |
| 1:D:270:ASN:C | 1:D:274:ASP:CG | 2.79 | 0.41 |
| 1:D:350:ILE:HG22 | 1:D:352:SER:CB | 2.40 | 0.41 |
| 1:D:374:ARG:NE | 1:D:392:LEU:CD2 | 2.83 | 0.41 |
| 1:D:466:LEU:N | 1:D:466:LEU:CD1 | 2.82 | 0.41 |
| 1:D:490:TRP:O | 1:D:580:LEU:CA | 2.68 | 0.41 |
| 1:D:637:GLY:O | 1:D:641:GLU:HG3 | 2.21 | 0.41 |
| 1:D:752:LEU:HB3 | 1:D:753:PRO:CB | 2.49 | 0.41 |
| 1:D:770:PHE:O | 1:D:773:LYS:HG2 | 2.20 | 0.41 |
| 1:D:897:TRP:HH2 | 1:D:1173:LEU:CD1 | 2.26 | 0.41 |
| 1:D:989:THR:C | 1:D:998:SER:OG | 2.59 | 0.41 |
| 2:E:259:ARG:NE | 2:E:301:GLU:OE1 | 2.54 | 0.41 |
| 2:E:76:ARG:HG3 | 2:E:435:MET:HG3 | 2.03 | 0.41 |
| 2:E:441:VAL:HG22 | 2:E:455:LEU:CB | 2.51 | 0.41 |
| 2:F:114:TRP:CD1 | 2:F:259:ARG:NH1 | 2.81 | 0.41 |
| 2:F:138:LEU:HA | 2:F:138:LEU:HD13 | 1.81 | 0.41 |
| 2:F:197:LEU:C | 2:F:199:LEU:N | 2.74 | 0.41 |
| 2:F:350:LEU:CD1 | 2:F:351:TYR:H | 2.32 | 0.41 |
| 2:F:446:THR:CB | 2:F:450:ASN:OD1 | 2.69 | 0.41 |
| 2:F:482:ALA:O | 2:F:483:LYS:C | 2.59 | 0.41 |
| 2:E:129:ASP:OD1 | 2:F:98:GLY:HA3 | 2.21 | 0.41 |
| 1:A:1032:THR:C | 1:A:1034:ARG:H | 2.23 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:851:THR:OG1 | 1:A:1099:TRP:CD1 | 2.69 | 0.41 |
| 1:A:1134:HIS:CB | 1:A:1136:GLU:OE2 | 2.69 | 0.41 |
| 1:A:1179:PHE:CD1 | 1:A:1220:ILE:CG2 | 2.99 | 0.41 |
| 1:A:1200:PRO:O | 1:A:1202:ASN:N | 2.53 | 0.41 |
| 1:A:1206:MET:O | 1:A:1207:GLU:CB | 2.69 | 0.41 |
| 1:A:1208:ARG:C | 1:A:1210:TYR:N | 2.70 | 0.41 |
| 1:A:1218:LEU:O | 1:A:1222:GLN:NE2 | 2.53 | 0.41 |
| 1:A:169:TRP:CD1 | 1:A:169:TRP:N | 2.88 | 0.41 |
| 1:A:226:GLN:OE1 | 1:A:229:VAL:CG2 | 2.69 | 0.41 |
| 1:A:289:MET:O | 1:A:290:ARG:HG3 | 2.20 | 0.41 |
| 1:A:143:ALA:CB | 1:A:421:PRO:HB2 | 2.50 | 0.41 |
| 1:A:441:TRP:CZ2 | 1:A:874:LEU:CB | 3.04 | 0.41 |
| 1:A:443:ARG:HG3 | 1:A:447:GLU:OE1 | 2.21 | 0.41 |
| 1:A:503:VAL:HG11 | 1:A:520:ALA:O | 2.17 | 0.41 |
| 1:A:539:PHE:CD2 | 1:A:539:PHE:O | 2.73 | 0.41 |
| 1:A:656:TYR:HA | 1:A:659:HIS:CB | 2.50 | 0.41 |
| 1:A:741:ASP:CG | 1:A:742:VAL:N | 2.72 | 0.41 |
| 1:A:811:GLN:O | 1:A:812:MET:C | 2.59 | 0.41 |
| 1:A:848:GLY:O | 1:A:849:THR:O | 2.38 | 0.41 |
| 2:B:104:VAL:HG21 | 2:C:128:VAL:C | 2.40 | 0.41 |
| 2:B:250:GLN:C | 2:B:252:LEU:N | 2.74 | 0.41 |
| 2:B:238:SER:CA | 2:B:339:ASN:HD21 | 2.33 | 0.41 |
| 2:B:474:PHE:CG | 2:B:475:LEU:N | 2.89 | 0.41 |
| 2:C:247:THR:HG1 | 2:C:251:TRP:HB2 | 1.86 | 0.41 |
| 2:C:254:PHE:O | 2:C:257:ARG:HB2 | 2.21 | 0.41 |
| 2:C:289:LEU:C | 2:C:290:TYR:CG | 2.94 | 0.41 |
| 2:C:346:MET:O | 2:C:350:LEU:HD11 | 2.20 | 0.41 |
| 2:C:397:GLN:C | 2:C:399:CYS:N | 2.73 | 0.41 |
| 2:C:413:VAL:HG12 | 2:C:415:PRO:CD | 2.51 | 0.41 |
| 1:D:1067:SER:HB3 | 1:D:1073:PRO:CG | 2.51 | 0.41 |
| 1:D:1144:GLU:HG3 | 1:D:1145:ASP:OD1 | 2.20 | 0.41 |
| 1:D:1200:PRO:HD2 | 1:D:1203:PRO:HB2 | 2.01 | 0.41 |
| 1:D:213:VAL:C | 1:D:401:TRP:CZ2 | 2.71 | 0.41 |
| 1:D:385:ILE:CG2 | 1:D:386:ARG:N | 2.83 | 0.41 |
| 1:D:399:ASP:O | 1:D:403:THR:HG22 | 2.20 | 0.41 |
| 1:D:434:TYR:O | 1:D:1130:CYS:CB | 2.58 | 0.41 |
| 1:D:498:LYS:HZ2 | 1:D:521:PRO:HB3 | 1.85 | 0.41 |
| 1:D:647:CYS:HB3 | 1:D:649:TYR:H | 1.85 | 0.41 |
| 1:D:618:HIS:CB | 1:D:725:PRO:CB | 2.98 | 0.41 |
| 1:D:944:GLU:HG2 | 1:D:947:LYS:HE3 | 2.03 | 0.41 |
| 2:E:439:PHE:CZ | 2:E:478:TYR:CZ | 3.08 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:456:ARG:HG3 | 2:E:462:MET:CA | 2.51 | 0.41 |
| 2:F:125:VAL:C | 2:F:126:PHE:CG | 2.92 | 0.41 |
| 2:F:218:VAL:HG13 | 2:F:218:VAL:O | 2.21 | 0.41 |
| 2:F:447:THR:HG23 | 2:F:448:LEU:N | 2.35 | 0.41 |
| 2:F:78:PHE:C | 2:F:79:LEU:HD22 | 2.41 | 0.41 |
| 1:A:1024:ASP:O | 1:A:1026:ARG:HG3 | 2.21 | 0.41 |
| 1:A:102:ARG:H | 1:A:102:ARG:HG2 | 1.51 | 0.41 |
| 1:A:1144:GLU:C | 1:A:1146:ARG:N | 2.74 | 0.41 |
| 1:A:1198:LYS:O | 1:A:1199:THR:HG23 | 2.20 | 0.41 |
| 1:A:1231:LEU:CD1 | 1:A:1235:SER:HB3 | 2.51 | 0.41 |
| 1:A:312:TRP:HH2 | 1:A:346:ASP:N | 2.18 | 0.41 |
| 1:A:371:LYS:HG3 | 1:A:372:GLU:HG2 | 2.02 | 0.41 |
| 1:A:411:LEU:CD1 | 1:A:411:LEU:C | 2.89 | 0.41 |
| 1:A:501:LYS:HB3 | 1:A:502:LYS:H | 1.44 | 0.41 |
| 1:A:503:VAL:C | 1:A:505:LYS:H | 2.23 | 0.41 |
| 1:A:634:LEU:HA | 1:A:638:THR:OG1 | 2.21 | 0.41 |
| 1:A:814:VAL:HG22 | 1:A:839:ALA:O | 2.21 | 0.41 |
| 1:A:875:LYS:HB3 | 1:A:1189:LEU:O | 2.21 | 0.41 |
| 1:A:880:ALA:H | 1:A:881:PRO:CD | 2.32 | 0.41 |
| 1:A:886:LEU:CD2 | 1:A:886:LEU:N | 2.68 | 0.41 |
| 1:A:993:ARG:O | 1:A:994:TRP:C | 2.58 | 0.41 |
| 2:B:186:LEU:HD23 | 2:B:186:LEU:O | 2.21 | 0.41 |
| 2:B:185:LEU:CD1 | 2:B:238:SER:HB2 | 2.50 | 0.41 |
| 2:C:184:ASN:HB3 | 2:C:187:HIS:H | 1.85 | 0.41 |
| 2:C:247:THR:HG1 | 2:C:251:TRP:CB | 2.32 | 0.41 |
| 2:C:253:ASP:HA | 2:C:256:LEU:CD2 | 2.49 | 0.41 |
| 2:C:237:ALA:N | 2:C:341:ASP:HB3 | 2.36 | 0.41 |
| 2:C:344:ARG:HG3 | 2:C:344:ARG:H | 1.58 | 0.41 |
| 2:C:354:PHE:O | 2:C:356:LEU:N | 2.54 | 0.41 |
| 2:C:358:GLU:O | 2:C:361:PHE:N | 2.45 | 0.41 |
| 2:C:72:ILE:HG23 | 2:C:76:ARG:CD | 2.51 | 0.41 |
| 1:D:1000:GLU:O | 1:D:1003:TRP:CB | 2.69 | 0.41 |
| 1:D:1067:SER:CB | 1:D:1071:ARG:HB3 | 2.50 | 0.41 |
| 1:D:1163:MET:HE2 | 1:D:1167:LYS:HG3 | 2.03 | 0.41 |
| 1:D:1108:TYR:CA | 1:D:1164:PHE:CE1 | 3.01 | 0.41 |
| 1:D:1206:MET:HG2 | 2:F:257:ARG:CZ | 2.45 | 0.41 |
| 1:D:143:ALA:HB1 | 1:D:425:ALA:HB3 | 2.03 | 0.41 |
| 1:D:297:MET:CG | 1:D:411:LEU:HD13 | 2.50 | 0.41 |
| 1:D:432:VAL:HG11 | 1:D:1128:ARG:NE | 2.06 | 0.41 |
| 1:D:482:ASP:CG | 1:D:483:PRO:HD2 | 2.42 | 0.41 |
| 1:D:482:ASP:C | 1:D:482:ASP:OD1 | 2.60 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:500:ALA:CB | 1:D:521:PRO:CD | 2.98 | 0.41 |
| 1:D:598:VAL:N | 1:D:616:GLU:OE2 | 2.53 | 0.41 |
| 1:D:666:GLN:HA | 1:D:669:MET:O | 2.19 | 0.41 |
| 1:D:720:THR:CA | 1:D:721:ALA:O | 2.69 | 0.41 |
| 1:D:992:LEU:C | 1:D:996:ARG:NE | 2.75 | 0.41 |
| 2:E:201:ASN:CB | 2:F:421:MET:SD | 3.09 | 0.41 |
| 2:E:393:LEU:O | 2:E:396:ARG:CG | 2.68 | 0.41 |
| 2:F:401:GLY:O | 2:F:402:LEU:C | 2.59 | 0.41 |
| 2:F:481:SER:O | 2:F:484:ASN:HB2 | 2.21 | 0.41 |
| 2:F:86:LEU:C | 2:F:87:SER:O | 2.59 | 0.41 |
| 1:A:1038:TRP:CZ3 | 1:A:1041:TRP:CD2 | 3.09 | 0.41 |
| 1:A:1155:ILE:HD13 | 1:A:1158:LEU:HD12 | 2.02 | 0.41 |
| 1:A:136:ASP:CB | 1:A:1163:MET:HE3 | 2.51 | 0.41 |
| 1:A:136:ASP:HB2 | 1:A:1163:MET:HE3 | 2.03 | 0.41 |
| 1:A:1166:TYR:CD2 | 1:A:1171:ASN:HA | 2.56 | 0.41 |
| 1:A:1184:ASP:HA | 1:A:1217:ALA:HB2 | 2.02 | 0.41 |
| 1:A:197:PHE:CB | 1:A:277:HIS:HD2 | 2.33 | 0.41 |
| 1:A:313:ILE:HA | 1:A:316:LYS:CG | 2.51 | 0.41 |
| 1:A:406:VAL:HG22 | 1:A:407:PHE:HD2 | 1.85 | 0.41 |
| 1:A:444:TYR:OH | 1:A:1200:PRO:CG | 2.66 | 0.41 |
| 1:A:601:LYS:HZ1 | 1:A:721:ALA:CA | 2.34 | 0.41 |
| 1:A:607:TRP:O | 1:A:610:PHE:HA | 2.21 | 0.41 |
| 1:A:645:VAL:C | 1:A:650:ARG:HD2 | 2.33 | 0.41 |
| 1:A:74:LEU:CD1 | 1:A:78:MET:N | 2.84 | 0.41 |
| 1:A:617:ARG:CD | 1:A:763:GLY:O | 2.69 | 0.41 |
| 1:A:76:ILE:HG13 | 1:A:77:GLN:N | 2.34 | 0.41 |
| 2:B:199:LEU:HD13 | 2:B:200:VAL:N | 2.35 | 0.41 |
| 2:B:389:ARG:N | 2:B:389:ARG:NE | 2.68 | 0.41 |
| 2:B:428:LEU:HD12 | 2:B:431:LYS:NZ | 2.35 | 0.41 |
| 2:C:193:TYR:O | 2:C:194:VAL:C | 2.59 | 0.41 |
| 2:C:256:LEU:HD13 | 2:C:303:LEU:HD22 | 2.02 | 0.41 |
| 1:A:556:THR:CG2 | 2:C:452:LEU:HB3 | 2.33 | 0.41 |
| 1:D:1003:TRP:CH2 | 1:D:1101:VAL:CG2 | 3.04 | 0.41 |
| 1:D:1129:PHE:CZ | 1:D:1139:TYR:CE2 | 3.09 | 0.41 |
| 1:D:1166:TYR:HA | 1:D:1169:GLY:C | 2.41 | 0.41 |
| 1:D:1171:ASN:O | 1:D:1172:ASP:OD1 | 2.39 | 0.41 |
| 1:D:282:TYR:HB2 | 1:D:841:LEU:HD11 | 2.01 | 0.41 |
| 1:D:289:MET:C | 1:D:290:ARG:HD2 | 2.41 | 0.41 |
| 1:D:515:ILE:HG12 | 1:D:568:GLY:HA3 | 2.02 | 0.41 |
| 1:D:546:ARG:O | 1:D:550:GLN:CD | 2.59 | 0.41 |
| 1:D:586:THR:O | 1:D:586:THR:HG22 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:592:LEU:O | 1:D:593:SER:C | 2.56 | 0.41 |
| 1:D:612:LEU:CD1 | 1:D:622:TYR:HA | 2.51 | 0.41 |
| 1:D:647:CYS:CB | 1:D:648:PRO:HD2 | 2.51 | 0.41 |
| 1:D:840:ILE:HG22 | 1:D:841:LEU:N | 2.36 | 0.41 |
| 1:D:913:CYS:O | 1:D:918:TRP:N | 2.54 | 0.41 |
| 1:D:914:THR:O | 1:D:914:THR:CG2 | 2.69 | 0.41 |
| 1:D:923:GLY:CA | 1:D:931:LEU:CD1 | 2.98 | 0.41 |
| 2:E:201:ASN:HB3 | 2:F:421:MET:HE1 | 2.02 | 0.41 |
| 2:E:442:LEU:HD13 | 2:E:443:VAL:CA | 2.49 | 0.41 |
| 2:F:181:LEU:O | 2:F:182:ARG:C | 2.59 | 0.41 |
| 2:F:289:LEU:HD23 | 2:F:289:LEU:HA | 1.85 | 0.41 |
| 2:F:303:LEU:C | 2:F:304:TRP:CD1 | 2.93 | 0.41 |
| 2:F:326:ASP:OD2 | 2:F:329:LYS:O | 2.39 | 0.41 |
| 2:F:336:LEU:HD23 | 2:F:337:SER:O | 2.20 | 0.41 |
| 1:D:546:ARG:NH1 | 2:F:408:GLU:OE1 | 2.54 | 0.41 |
| 2:F:454:HIS:O | 2:F:455:LEU:CB | 2.49 | 0.41 |
| 2:F:458:ARG:CG | 2:F:459:ASP:N | 2.83 | 0.41 |
| 2:F:80:SER:HB2 | 2:F:98:GLY:C | 2.41 | 0.41 |
| 2:F:86:LEU:N | 2:F:86:LEU:CD1 | 2.84 | 0.41 |
| 1:A:1113:LEU:HD22 | 1:A:1139:TYR:OH | 2.20 | 0.41 |
| 1:A:1149:ALA:O | 1:A:1152:ALA:N | 2.54 | 0.41 |
| 1:A:148:LEU:HA | 1:A:148:LEU:HD23 | 1.88 | 0.41 |
| 1:A:181:GLU:CG | 1:A:182:GLY:N | 2.83 | 0.41 |
| 1:A:456:GLN:O | 1:A:457:ARG:C | 2.58 | 0.41 |
| 1:A:502:LYS:CD | 1:A:506:GLU:OE1 | 2.41 | 0.41 |
| 1:A:566:LEU:O | 1:A:567:PRO:C | 2.59 | 0.41 |
| 1:A:798:ILE:HD11 | 1:A:802:ARG:NE | 2.30 | 0.41 |
| 2:B:450:ASN:ND2 | 2:B:452:LEU:HB2 | 2.36 | 0.41 |
| 2:C:146:ARG:NE | 2:C:228:VAL:HG11 | 2.36 | 0.41 |
| 2:C:347:LEU:CD1 | 2:C:347:LEU:N | 2.82 | 0.41 |
| 1:D:1212:ILE:HG13 | 1:D:1213:PRO:HD2 | 2.03 | 0.41 |
| 1:D:157:LEU:HA | 1:D:157:LEU:HD22 | 1.83 | 0.41 |
| 1:D:274:ASP:HA | 1:D:277:HIS:HD2 | 1.85 | 0.41 |
| 1:D:420:HIS:O | 1:D:424:LEU:CG | 2.68 | 0.41 |
| 1:D:444:TYR:C | 1:D:446:ALA:N | 2.72 | 0.41 |
| 1:D:477:GLU:HG2 | 1:D:478:ARG:H | 1.86 | 0.41 |
| 1:D:500:ALA:HB1 | 1:D:520:ALA:HB3 | 2.03 | 0.41 |
| 1:D:654:SER:O | 1:D:655:LEU:C | 2.58 | 0.41 |
| 1:D:656:TYR:HA | 1:D:659:HIS:HE1 | 1.85 | 0.41 |
| 1:D:72:ASN:OD1 | 1:D:80:SER:OG | 2.31 | 0.41 |
| 1:D:865:ALA:HB2 | 1:D:872:SER:C | 2.40 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:244:PRO:HB3 | 2:F:245:PRO:HD2 | 2.02 | 0.41 |
| 2:F:251:TRP:HZ3 | 2:F:254:PHE:CD1 | 2.38 | 0.41 |
| 2:F:291:TYR:O | 2:F:297:LYS:HA | 2.21 | 0.41 |
| 2:F:342:LEU:C | 2:F:344:ARG:N | 2.62 | 0.41 |
| 2:F:348:ALA:HA | 2:F:351:TYR:HB2 | 2.02 | 0.41 |
| 2:F:365:LYS:HG3 | 2:F:366:ASN:N | 2.35 | 0.41 |
| 2:F:453:ILE:CD1 | 2:F:465:MET:HB3 | 2.36 | 0.41 |
| 1:A:1066:THR:CB | 1:A:1071:ARG:HB3 | 2.50 | 0.40 |
| 1:A:107:LEU:HA | 1:A:110:HIS:HB2 | 2.02 | 0.40 |
| 1:A:1144:GLU:O | 1:A:1145:ASP:C | 2.57 | 0.40 |
| 1:A:279:ARG:HB3 | 1:A:280:GLU:OE2 | 2.20 | 0.40 |
| 1:A:301:ILE:CD1 | 1:A:414:PHE:C | 2.90 | 0.40 |
| 1:A:513:LEU:HA | 1:A:514:PRO:HD2 | 1.61 | 0.40 |
| 1:A:576:LEU:HD12 | 1:A:577:CYS:H | 1.77 | 0.40 |
| 1:A:812:MET:O | 1:A:813:VAL:CB | 2.69 | 0.40 |
| 1:A:920:THR:O | 1:A:921:LEU:C | 2.58 | 0.40 |
| 2:B:264:ARG:O | 2:B:267:ALA:N | 2.54 | 0.40 |
| 2:B:474:PHE:CD2 | 2:B:475:LEU:HG | 2.56 | 0.40 |
| 2:C:125:VAL:HG22 | 2:C:208:LEU:CB | 2.48 | 0.40 |
| 2:C:241:TRP:CE3 | 2:C:336:LEU:CD1 | 3.02 | 0.40 |
| 2:C:291:TYR:OH | 2:C:351:TYR:HB3 | 2.21 | 0.40 |
| 2:C:393:LEU:O | 2:C:397:GLN:CB | 2.69 | 0.40 |
| 2:C:411:ILE:HG23 | 2:C:411:ILE:O | 2.20 | 0.40 |
| 1:D:1066:THR:C | 1:D:1073:PRO:HD3 | 2.41 | 0.40 |
| 1:D:174:GLY:HA2 | 1:D:220:TRP:N | 2.36 | 0.40 |
| 1:D:189:ILE:HG21 | 1:D:258:GLN:CB | 2.45 | 0.40 |
| 1:D:198:ASP:CB | 1:D:400:VAL:CG1 | 2.87 | 0.40 |
| 1:D:408:GLN:HA | 1:D:411:LEU:CD1 | 2.46 | 0.40 |
| 1:D:455:LEU:HD11 | 1:D:797:MET:SD | 2.61 | 0.40 |
| 1:D:453:GLU:C | 1:D:457:ARG:HG2 | 2.40 | 0.40 |
| 1:D:585:TRP:N | 1:D:585:TRP:HE3 | 2.18 | 0.40 |
| 1:D:849:THR:HG22 | 1:D:850:ILE:HG12 | 2.03 | 0.40 |
| 1:D:441:TRP:CG | 1:D:878:VAL:O | 2.74 | 0.40 |
| 1:D:900:ALA:HB1 | 1:D:915:ALA:CA | 2.51 | 0.40 |
| 2:E:123:GLU:O | 2:E:125:VAL:N | 2.54 | 0.40 |
| 2:E:259:ARG:HE | 2:E:301:GLU:CD | 2.23 | 0.40 |
| 2:E:319:VAL:HG23 | 2:E:332:VAL:HG21 | 2.03 | 0.40 |
| 2:E:380:PRO:O | 2:E:382:LYS:N | 2.54 | 0.40 |
| 2:F:146:ARG:NE | 2:F:228:VAL:HG11 | 2.36 | 0.40 |
| 2:F:187:HIS:O | 2:F:188:GLY:C | 2.59 | 0.40 |
| 2:F:239:LEU:O | 2:F:336:LEU:CD2 | 2.46 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:252:LEU:HD12 | 2:F:305:ASN:HB2 | 2.01 | 0.40 |
| 2:F:347:LEU:H | 2:F:347:LEU:HD13 | 1.86 | 0.40 |
| 2:F:69:LEU:HD21 | 2:F:351:TYR:HA | 2.03 | 0.40 |
| 2:F:418:LEU:O | 2:F:418:LEU:HD12 | 2.21 | 0.40 |
| 2:F:419:GLU:CG | 2:F:432:TYR:OH | 2.68 | 0.40 |
| 2:F:455:LEU:HG | 2:F:456:ARG:NH2 | 2.36 | 0.40 |
| 1:A:995:TYR:HB2 | 1:A:1004:LEU:HD11 | 2.02 | 0.40 |
| 1:A:1163:MET:O | 1:A:1164:PHE:C | 2.59 | 0.40 |
| 1:A:1177:VAL:O | 1:A:1178:ALA:C | 2.59 | 0.40 |
| 1:A:191:GLU:O | 1:A:193:ARG:NH1 | 2.54 | 0.40 |
| 1:A:260:ASP:O | 1:A:260:ASP:OD1 | 2.39 | 0.40 |
| 1:A:260:ASP:CA | 1:A:264:GLN:NE2 | 2.84 | 0.40 |
| 1:A:313:ILE:CD1 | 1:A:314:ALA:N | 2.85 | 0.40 |
| 1:A:423:THR:HB | 1:A:424:LEU:HD23 | 2.03 | 0.40 |
| 1:A:486:TRP:HA | 1:A:489:GLU:OE2 | 2.21 | 0.40 |
| 1:A:610:PHE:CB | 1:A:611:PRO:HD3 | 2.51 | 0.40 |
| 1:A:633:LYS:O | 1:A:634:LEU:CD1 | 2.70 | 0.40 |
| 1:A:78:MET:SD | 1:A:123:VAL:HG11 | 2.61 | 0.40 |
| 1:A:812:MET:CG | 1:A:813:VAL:N | 2.84 | 0.40 |
| 1:A:813:VAL:HB | 1:A:840:ILE:CG1 | 2.43 | 0.40 |
| 1:A:79:LEU:HB2 | 1:A:89:GLY:CA | 2.50 | 0.40 |
| 2:B:261:GLN:O | 2:B:265:LYS:HA | 2.21 | 0.40 |
| 2:B:481:SER:O | 2:B:484:ASN:HB2 | 2.21 | 0.40 |
| 2:C:254:PHE:N | 2:C:257:ARG:HH21 | 2.19 | 0.40 |
| 2:C:299:LEU:O | 2:C:300:ILE:C | 2.59 | 0.40 |
| 2:C:343:ASP:HB2 | 2:C:347:LEU:HD11 | 2.02 | 0.40 |
| 2:C:69:LEU:HD21 | 2:C:351:TYR:HA | 2.03 | 0.40 |
| 2:C:389:ARG:O | 2:C:392:THR:HA | 2.21 | 0.40 |
| 2:C:437:ILE:O | 2:C:437:ILE:HG13 | 2.21 | 0.40 |
| 1:D:1025:LEU:HD22 | 1:D:1091:GLU:OE2 | 2.21 | 0.40 |
| 1:D:1068:ASP:O | 1:D:1071:ARG:HG2 | 2.21 | 0.40 |
| 1:D:308:GLN:HE21 | 1:D:1091:GLU:N | 2.18 | 0.40 |
| 1:D:223:TRP:C | 1:D:227:ARG:HD2 | 2.41 | 0.40 |
| 1:D:369:LEU:HD22 | 1:D:372:GLU:HG3 | 2.03 | 0.40 |
| 1:D:453:GLU:C | 1:D:457:ARG:CG | 2.89 | 0.40 |
| 1:D:483:PRO:HA | 1:D:486:TRP:CD1 | 2.55 | 0.40 |
| 1:D:602:LEU:O | 1:D:604:ALA:N | 2.54 | 0.40 |
| 1:D:620:TRP:HE1 | 1:D:751:LYS:HB2 | 1.84 | 0.40 |
| 1:D:605:LEU:HA | 1:D:782:GLY:H | 1.86 | 0.40 |
| 1:D:894:GLN:HE22 | 1:D:1180:PHE:HE2 | 1.69 | 0.40 |
| 2:E:115:TRP:CD1 | 2:E:115:TRP:O | 2.75 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:116:THR:O | 2:E:120:VAL:N | 2.47 | 0.40 |
| 2:E:375:HIS:CG | 2:E:376:PRO:CA | 3.04 | 0.40 |
| 2:E:380:PRO:O | 2:E:382:LYS:CA | 2.68 | 0.40 |
| 2:E:386:ASP:O | 2:E:387:VAL:CG1 | 2.70 | 0.40 |
| 2:E:445:GLU:O | 2:E:446:THR:C | 2.58 | 0.40 |
| 2:E:453:ILE:O | 2:E:465:MET:HA | 2.21 | 0.40 |
| 2:F:106:LEU:HG | 2:F:346:MET:CG | 2.51 | 0.40 |
| 2:F:298:GLU:CG | 2:F:344:ARG:NH2 | 2.84 | 0.40 |
| 2:F:400:GLN:C | 2:F:400:GLN:NE2 | 2.75 | 0.40 |
| 2:F:403:PHE:CD2 | 2:F:404:ASN:N | 2.89 | 0.40 |
| 2:F:406:LEU:N | 2:F:406:LEU:HD13 | 2.36 | 0.40 |
| 2:E:126:PHE:CE2 | 2:F:414:TRP:CZ3 | 3.09 | 0.40 |
| 2:F:422:GLN:O | 2:F:423:SER:OG | 2.24 | 0.40 |
| 2:F:384:ALA:HB3 | 2:F:440:THR:HG22 | 2.04 | 0.40 |
| 2:F:441:VAL:HB | 2:F:454:HIS:O | 2.21 | 0.40 |
| 2:F:455:LEU:CA | 2:F:456:ARG:NE | 2.73 | 0.40 |
| 1:A:1170:LEU:N | 1:A:1170:LEU:HD12 | 2.37 | 0.40 |
| 1:A:174:GLY:CA | 1:A:220:TRP:HB2 | 2.50 | 0.40 |
| 1:A:258:GLN:O | 1:A:259:ARG:NH2 | 2.54 | 0.40 |
| 1:A:261:TRP:CA | 1:A:261:TRP:CE3 | 3.00 | 0.40 |
| 1:A:273:PHE:CA | 1:A:276:ALA:H | 2.33 | 0.40 |
| 1:A:352:SER:C | 1:A:358:LEU:CD2 | 2.88 | 0.40 |
| 1:A:822:PRO:O | 1:A:825:VAL:HB | 2.22 | 0.40 |
| 1:A:851:THR:O | 1:A:852:ARG:CB | 2.69 | 0.40 |
| 1:A:755:LYS:CD | 1:A:964:ARG:NH1 | 2.67 | 0.40 |
| 2:B:192:HIS:O | 2:B:193:TYR:C | 2.58 | 0.40 |
| 2:B:204:LEU:CD1 | 2:B:324:GLY:HA3 | 2.51 | 0.40 |
| 2:B:69:LEU:CA | 2:B:72:ILE:HG12 | 2.52 | 0.40 |
| 2:C:190:LEU:O | 2:C:191:GLU:C | 2.58 | 0.40 |
| 2:B:77:HIS:CB | 2:C:195:ASN:OD1 | 2.67 | 0.40 |
| 2:C:197:LEU:HD11 | 2:C:322:LEU:CD1 | 2.51 | 0.40 |
| 2:C:200:VAL:O | 2:C:201:ASN:CB | 2.69 | 0.40 |
| 2:C:406:LEU:HD11 | 2:C:472:LYS:HZ2 | 1.85 | 0.40 |
| 2:C:403:PHE:N | 2:C:406:LEU:HD22 | 2.36 | 0.40 |
| 2:C:422:GLN:O | 2:C:423:SER:OG | 2.22 | 0.40 |
| 2:C:464:GLU:O | 2:C:464:GLU:OE2 | 2.39 | 0.40 |
| 2:C:64:GLU:CG | 2:C:65:GLY:N | 2.84 | 0.40 |
| 2:C:99:PHE:N | 2:C:99:PHE:CD2 | 2.89 | 0.40 |
| 1:D:1066:THR:CG2 | 1:D:1066:THR:O | 2.69 | 0.40 |
| 1:D:851:THR:HG21 | 1:D:1102:GLN:CG | 2.51 | 0.40 |
| 1:D:1163:MET:HE2 | 1:D:1167:LYS:CG | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1224:ILE:HG12 | 1:D:1228:LYS:HA | 2.03 | 0.40 |
| 1:D:175:TRP:HA | 1:D:185:VAL:CG2 | 2.48 | 0.40 |
| 1:D:193:ARG:HD2 | 1:D:263:GLU:OE2 | 2.21 | 0.40 |
| 1:D:238:GLN:OE1 | 1:D:238:GLN:HA | 2.19 | 0.40 |
| 1:D:266:VAL:HA | 1:D:289:MET:CE | 2.52 | 0.40 |
| 1:D:350:ILE:CA | 1:D:352:SER:H | 2.33 | 0.40 |
| 1:D:484:TRP:NE1 | 1:D:488:LEU:CG | 2.84 | 0.40 |
| 1:D:597:ARG:CB | 1:D:616:GLU:CD | 2.89 | 0.40 |
| 1:D:734:HIS:HA | 1:D:752:LEU:HD11 | 2.03 | 0.40 |
| 2:E:370:LYS:O | 2:E:433:ASP:C | 2.60 | 0.40 |
| 2:F:180:LYS:O | 2:F:180:LYS:HE3 | 2.17 | 0.40 |
| 2:F:315:TYR:N | 2:F:315:TYR:CD2 | 2.89 | 0.40 |
| 2:F:350:LEU:CD1 | 2:F:351:TYR:N | 2.85 | 0.40 |
| 2:F:431:LYS:HD3 | 2:F:432:TYR:N | 2.36 | 0.40 |
| 2:F:473:ASP:O | 2:F:476:ILE:CD1 | 2.69 | 0.40 |
| 1:A:422:VAL:HG11 | 1:A:1111:LEU:HD11 | 2.03 | 0.40 |
| 1:A:175:TRP:CB | 1:A:184:ALA:C | 2.86 | 0.40 |
| 1:A:174:GLY:HA2 | 1:A:220:TRP:CB | 2.51 | 0.40 |
| 1:A:659:HIS:HD1 | 1:A:663:GLN:CG | 2.35 | 0.40 |
| 1:A:761:ASN:N | 1:A:761:ASN:OD1 | 2.54 | 0.40 |
| 1:A:851:THR:HG21 | 1:A:853:ARG:HB2 | 2.00 | 0.40 |
| 1:A:83:LEU:O | 1:A:87:ILE:O | 2.40 | 0.40 |
| 1:A:905:ALA:HA | 1:A:910:MET:HA | 2.02 | 0.40 |
| 1:A:905:ALA:HB1 | 1:A:1169:GLY:HA2 | 2.03 | 0.40 |
| 2:B:256:LEU:O | 2:B:257:ARG:C | 2.60 | 0.40 |
| 2:B:265:LYS:O | 2:B:266:PHE:CB | 2.69 | 0.40 |
| 2:B:420:THR:OG1 | 2:B:420:THR:O | 2.32 | 0.40 |
| 2:B:456:ARG:HB3 | 2:B:457:SER:H | 1.70 | 0.40 |
| 2:B:87:SER:C | 2:B:89:ASP:N | 2.73 | 0.40 |
| 2:C:335:VAL:O | 2:C:335:VAL:HG13 | 2.20 | 0.40 |
| 2:C:240:VAL:O | 2:C:336:LEU:HD13 | 2.21 | 0.40 |
| 2:C:385:LEU:HD21 | 2:C:402:LEU:CD2 | 2.39 | 0.40 |
| 2:C:399:CYS:C | 2:C:401:GLY:N | 2.69 | 0.40 |
| 2:C:476:ILE:HD13 | 2:C:477:LYS:CG | 2.50 | 0.40 |
| 2:C:82:SER:C | 2:C:86:LEU:CD1 | 2.89 | 0.40 |
| 1:D:1071:ARG:C | 1:D:1073:PRO:HD2 | 2.42 | 0.40 |
| 1:D:148:LEU:HA | 1:D:148:LEU:HD23 | 1.88 | 0.40 |
| 1:D:307:PHE:CA | 1:D:310:SER:OG | 2.67 | 0.40 |
| 1:D:421:PRO:CG | 1:D:422:VAL:H | 2.32 | 0.40 |
| 1:D:458:GLU:C | 1:D:460:LYS:CE | 2.90 | 0.40 |
| 1:D:484:TRP:CE2 | 1:D:488:LEU:HD11 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:513:LEU:H | 1:D:570:PRO:HD3 | 1.85 | 0.40 |
| 1:D:603:MET:HB3 | 1:D:605:LEU:HD23 | 2.00 | 0.40 |
| 1:D:606:THR:CG2 | 1:D:611:PRO:O | 2.69 | 0.40 |
| 1:D:614:TYR:CE2 | 1:D:620:TRP:CD2 | 3.08 | 0.40 |
| 1:D:630:ASN:ND2 | 1:D:632:ALA:N | 2.69 | 0.40 |
| 1:D:788:GLY:C | 1:D:792:LEU:HD13 | 2.42 | 0.40 |
| 1:D:950:ASN:O | 1:D:951:TYR:C | 2.58 | 0.40 |
| 2:E:370:LYS:HE3 | 2:E:370:LYS:HB3 | 1.65 | 0.40 |
| 2:F:111:ALA:O | 2:F:115:TRP:CB | 2.70 | 0.40 |
| 2:F:180:LYS:CA | 2:F:180:LYS:HE3 | 2.47 | 0.40 |
| 2:F:254:PHE:HA | 2:F:257:ARG:HD3 | 2.03 | 0.40 |
| 2:F:341:ASP:OD1 | 2:F:342:LEU:C | 2.60 | 0.40 |
| 2:F:76:ARG:CZ | 2:F:434:GLU:CD | 2.89 | 0.40 |
| 1:A:903:GLY:N | 1:A:1002:GLU:HB3 | 2.32 | 0.40 |
| 1:A:1111:LEU:HB3 | 1:A:1160:THR:HG23 | 2.03 | 0.40 |
| 1:A:181:GLU:C | 1:A:181:GLU:CD | 2.80 | 0.40 |
| 1:A:206:GLY:C | 1:A:208:CYS:H | 2.24 | 0.40 |
| 1:A:244:LEU:HD23 | 1:A:244:LEU:HA | 1.81 | 0.40 |
| 1:A:203:LEU:HD11 | 1:A:379:LYS:C | 2.34 | 0.40 |
| 1:A:526:ASP:CG | 1:A:527:GLN:N | 2.74 | 0.40 |
| 1:A:606:THR:O | 1:A:607:TRP:CD1 | 2.75 | 0.40 |
| 1:A:612:LEU:CD2 | 1:A:614:TYR:N | 2.83 | 0.40 |
| 1:A:617:ARG:O | 1:A:762:VAL:CG2 | 2.60 | 0.40 |
| 1:A:659:HIS:CD2 | 1:A:716:PRO:O | 2.75 | 0.40 |
| 2:B:185:LEU:HB3 | 2:B:214:CYS:SG | 2.61 | 0.40 |
| 2:B:306:LEU:O | 2:B:307:GLY:C | 2.58 | 0.40 |
| 2:B:375:HIS:ND1 | 2:B:378:LEU:HD13 | 2.37 | 0.40 |
| 2:B:393:LEU:O | 2:B:396:ARG:HB3 | 2.21 | 0.40 |
| 2:C:368:HIS:O | 2:C:368:HIS:CG | 2.75 | 0.40 |
| 2:C:368:HIS:O | 2:C:368:HIS:ND1 | 2.55 | 0.40 |
| 2:C:470:LYS:N | 2:C:471:LEU:HD12 | 2.36 | 0.40 |
| 1:D:1067:SER:CA | 1:D:1071:ARG:CA | 2.82 | 0.40 |
| 1:D:1200:PRO:O | 1:D:1201:SER:C | 2.59 | 0.40 |
| 1:D:197:PHE:CZ | 1:D:219:ALA:CB | 3.04 | 0.40 |
| 1:D:282:TYR:HE2 | 1:D:432:VAL:CB | 2.34 | 0.40 |
| 1:D:371:LYS:CD | 1:D:392:LEU:CD2 | 2.98 | 0.40 |
| 1:D:536:GLU:H | 1:D:536:GLU:HG2 | 1.78 | 0.40 |
| 1:D:584:ALA:HB1 | 1:D:585:TRP:CZ3 | 2.57 | 0.40 |
| 1:D:624:VAL:HB | 1:D:747:CYS:SG | 2.62 | 0.40 |
| 1:D:780:GLN:OE1 | 1:D:781:ALA:N | 2.49 | 0.40 |
| 1:D:848:GLY:O | 1:D:855:VAL:HG22 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:851:THR:C | 1:D:853:ARG:H | 2.23 | 0.40 |
| 1:D:910:MET:C | 1:D:910:MET:SD | 3.00 | 0.40 |
| 1:D:933:SER:O | 1:D:935:THR:N | 2.54 | 0.40 |
| 2:E:280:ASP:N | 2:E:304:TRP:CH2 | 2.90 | 0.40 |
| 2:E:403:PHE:HA | 2:E:413:VAL:HG11 | 2.04 | 0.40 |
| 2:E:428:LEU:C | 2:E:431:LYS:H | 2.25 | 0.40 |
| 2:E:474:PHE:O | 2:E:475:LEU:C | 2.60 | 0.40 |
| 2:E:78:PHE:CE1 | 2:E:350:LEU:CD1 | 3.04 | 0.40 |
| 2:F:406:LEU:HD13 | 2:F:406:LEU:H | 1.87 | 0.40 |
| 2:F:381:ILE:CB | 2:F:437:ILE:HG22 | 2.52 | 0.40 |

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 1:A:673:ALA:O | 2:F:318:ASN:O[2_734] | 1.91 | 0.29 |
| 1:A:673:ALA:C | 2:F:318:ASN:O[2_734] | 1.98 | 0.22 |
| 1:A:1034:ARG:NE | 2:F:450:ASN:ND2[1_545] | 2.04 | 0.16 |
| 1:A:994:TRP:NE1 | 1:D:522:GLY:N[1_545] | 2.06 | 0.14 |
| 1:D:1232:GLU:OE2 | 2:F:223:GLN:OE1[2_844] | 2.11 | 0.09 |
| 2:C:450:ASN:ND2 | 1:D:1034:ARG:NH2[1_445] | 2.12 | 0.08 |
| 1:A:518:ALA:O | 1:D:993:ARG:O[1_445] | 2.13 | 0.07 |
| 1:A:727:ASP:OD1 | 1:D:133:ASP:O[1_445] | 2.16 | 0.04 |
| 1:A:133:ASP:OD1 | 1:D:727:ASP:OD2[1_545] | 2.19 | 0.01 |
| 1:A:993:ARG:NH2 | 1:D:520:ALA:O[1_545] | 2.19 | 0.01 |

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 | 1085/1172 (93%) | 629 (58%) | 254 (23%) | 202 (19%) | 0 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-----------|-------------|---|
| 1 | D | 1086/1172 (93%) | 645 (59%) | 234 (22%) | 207 (19%) | 0 | 0 |
| 2 | B | 349/427 (82%) | 205 (59%) | 94 (27%) | 50 (14%) | 0 | 1 |
| 2 | C | 394/427 (92%) | 254 (64%) | 84 (21%) | 56 (14%) | 0 | 1 |
| 2 | E | 349/427 (82%) | 219 (63%) | 79 (23%) | 51 (15%) | 0 | 1 |
| 2 | F | 394/427 (92%) | 251 (64%) | 93 (24%) | 50 (13%) | 0 | 2 |
| All | All | 3657/4052 (90%) | 2203 (60%) | 838 (23%) | 616 (17%) | 0 | 1 |

All (616) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 72 | ASN |
| 1 | A | 76 | ILE |
| 1 | A | 96 | GLY |
| 1 | A | 163 | PRO |
| 1 | A | 169 | TRP |
| 1 | A | 170 | ALA |
| 1 | A | 176 | THR |
| 1 | A | 184 | ALA |
| 1 | A | 185 | VAL |
| 1 | A | 189 | ILE |
| 1 | A | 205 | GLU |
| 1 | A | 211 | LEU |
| 1 | A | 216 | SER |
| 1 | A | 217 | PRO |
| 1 | A | 231 | GLU |
| 1 | A | 232 | ARG |
| 1 | A | 234 | SER |
| 1 | A | 240 | SER |
| 1 | A | 253 | ALA |
| 1 | A | 255 | SER |
| 1 | A | 271 | VAL |
| 1 | A | 273 | PHE |
| 1 | A | 287 | SER |
| 1 | A | 348 | LEU |
| 1 | A | 353 | VAL |
| 1 | A | 354 | ASN |
| 1 | A | 355 | SER |
| 1 | A | 369 | PRO |
| 1 | A | 372 | GLU |
| 1 | A | 378 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 419 | PRO |
| 1 | A | 436 | PRO |
| 1 | A | 437 | VAL |
| 1 | A | 463 | LEU |
| 1 | A | 482 | ASP |
| 1 | A | 499 | LYS |
| 1 | A | 500 | ALA |
| 1 | A | 503 | VAL |
| 1 | A | 527 | GLN |
| 1 | A | 540 | GLN |
| 1 | A | 559 | LEU |
| 1 | A | 573 | TYR |
| 1 | A | 583 | PRO |
| 1 | A | 588 | GLY |
| 1 | A | 589 | PRO |
| 1 | A | 598 | VAL |
| 1 | A | 610 | PHE |
| 1 | A | 611 | PRO |
| 1 | A | 612 | LEU |
| 1 | A | 614 | TYR |
| 1 | A | 626 | GLY |
| 1 | A | 628 | ARG |
| 1 | A | 634 | LEU |
| 1 | A | 635 | PRO |
| 1 | A | 712 | VAL |
| 1 | A | 727 | ASP |
| 1 | A | 728 | THR |
| 1 | A | 731 | SER |
| 1 | A | 738 | PRO |
| 1 | A | 744 | ILE |
| 1 | A | 758 | ASN |
| 1 | A | 768 | LYS |
| 1 | A | 869 | ARG |
| 1 | A | 880 | ALA |
| 1 | A | 900 | ALA |
| 1 | A | 915 | ALA |
| 1 | A | 920 | THR |
| 1 | A | 927 | ARG |
| 1 | A | 939 | VAL |
| 1 | A | 959 | GLN |
| 1 | A | 1020 | ILE |
| 1 | A | 1032 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1034 | ARG |
| 1 | A | 1059 | ASN |
| 1 | A | 1069 | ILE |
| 1 | A | 1070 | PRO |
| 1 | A | 1125 | ILE |
| 1 | A | 1131 | ILE |
| 1 | A | 1170 | LEU |
| 1 | A | 1171 | ASN |
| 1 | A | 1192 | GLU |
| 1 | A | 1193 | VAL |
| 1 | A | 1200 | PRO |
| 1 | A | 1206 | MET |
| 1 | A | 1208 | ARG |
| 1 | A | 1213 | PRO |
| 1 | A | 1214 | GLN |
| 1 | A | 1219 | ASP |
| 1 | A | 1236 | GLN |
| 2 | B | 77 | HIS |
| 2 | B | 79 | LEU |
| 2 | B | 101 | PRO |
| 2 | B | 123 | GLU |
| 2 | B | 205 | PRO |
| 2 | B | 216 | HIS |
| 2 | B | 217 | PRO |
| 2 | B | 246 | ARG |
| 2 | B | 258 | HIS |
| 2 | B | 262 | TRP |
| 2 | B | 280 | ASP |
| 2 | B | 281 | GLU |
| 2 | B | 284 | ARG |
| 2 | B | 285 | LYS |
| 2 | B | 323 | HIS |
| 2 | B | 376 | PRO |
| 2 | B | 391 | PRO |
| 2 | B | 437 | ILE |
| 2 | C | 83 | LYS |
| 2 | C | 122 | ARG |
| 2 | C | 134 | LYS |
| 2 | C | 145 | PHE |
| 2 | C | 178 | SER |
| 2 | C | 204 | LEU |
| 2 | C | 205 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 223 | GLN |
| 2 | C | 257 | ARG |
| 2 | C | 319 | VAL |
| 2 | C | 342 | LEU |
| 2 | C | 352 | ASP |
| 2 | C | 353 | SER |
| 2 | C | 356 | LEU |
| 2 | C | 398 | VAL |
| 2 | C | 415 | PRO |
| 2 | C | 438 | LEU |
| 2 | C | 449 | GLU |
| 2 | C | 452 | LEU |
| 2 | C | 456 | ARG |
| 2 | C | 460 | THR |
| 1 | D | 73 | PRO |
| 1 | D | 81 | ARG |
| 1 | D | 116 | PRO |
| 1 | D | 163 | PRO |
| 1 | D | 167 | PRO |
| 1 | D | 168 | ALA |
| 1 | D | 171 | TRP |
| 1 | D | 173 | GLU |
| 1 | D | 193 | ARG |
| 1 | D | 205 | GLU |
| 1 | D | 211 | LEU |
| 1 | D | 212 | ALA |
| 1 | D | 213 | VAL |
| 1 | D | 219 | ALA |
| 1 | D | 221 | TYR |
| 1 | D | 234 | SER |
| 1 | D | 248 | GLU |
| 1 | D | 249 | VAL |
| 1 | D | 255 | SER |
| 1 | D | 303 | GLY |
| 1 | D | 350 | ILE |
| 1 | D | 364 | VAL |
| 1 | D | 368 | PRO |
| 1 | D | 372 | GLU |
| 1 | D | 378 | VAL |
| 1 | D | 419 | PRO |
| 1 | D | 433 | SER |
| 1 | D | 482 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 492 | LEU |
| 1 | D | 504 | LYS |
| 1 | D | 511 | SER |
| 1 | D | 517 | GLY |
| 1 | D | 521 | PRO |
| 1 | D | 523 | ASP |
| 1 | D | 530 | LEU |
| 1 | D | 540 | GLN |
| 1 | D | 559 | LEU |
| 1 | D | 577 | CYS |
| 1 | D | 589 | PRO |
| 1 | D | 597 | ARG |
| 1 | D | 598 | VAL |
| 1 | D | 599 | THR |
| 1 | D | 610 | PHE |
| 1 | D | 611 | PRO |
| 1 | D | 612 | LEU |
| 1 | D | 614 | TYR |
| 1 | D | 628 | ARG |
| 1 | D | 643 | ALA |
| 1 | D | 646 | VAL |
| 1 | D | 647 | CYS |
| 1 | D | 710 | ALA |
| 1 | D | 712 | VAL |
| 1 | D | 713 | PRO |
| 1 | D | 727 | ASP |
| 1 | D | 728 | THR |
| 1 | D | 735 | GLY |
| 1 | D | 736 | ASN |
| 1 | D | 742 | VAL |
| 1 | D | 744 | ILE |
| 1 | D | 753 | PRO |
| 1 | D | 762 | VAL |
| 1 | D | 776 | ASP |
| 1 | D | 781 | ALA |
| 1 | D | 783 | PRO |
| 1 | D | 787 | SER |
| 1 | D | 829 | PRO |
| 1 | D | 869 | ARG |
| 1 | D | 890 | ASP |
| 1 | D | 891 | VAL |
| 1 | D | 913 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 925 | LYS |
| 1 | D | 939 | VAL |
| 1 | D | 956 | GLY |
| 1 | D | 959 | GLN |
| 1 | D | 974 | THR |
| 1 | D | 992 | LEU |
| 1 | D | 1027 | LYS |
| 1 | D | 1069 | ILE |
| 1 | D | 1073 | PRO |
| 1 | D | 1174 | PRO |
| 1 | D | 1176 | SER |
| 1 | D | 1180 | PHE |
| 1 | D | 1203 | PRO |
| 1 | D | 1232 | GLU |
| 1 | D | 1236 | GLN |
| 2 | E | 70 | LEU |
| 2 | E | 87 | SER |
| 2 | E | 239 | LEU |
| 2 | E | 248 | SER |
| 2 | E | 281 | GLU |
| 2 | E | 294 | PRO |
| 2 | E | 309 | HIS |
| 2 | E | 314 | MET |
| 2 | E | 316 | PRO |
| 2 | E | 319 | VAL |
| 2 | E | 323 | HIS |
| 2 | E | 330 | ASN |
| 2 | E | 331 | VAL |
| 2 | E | 375 | HIS |
| 2 | E | 376 | PRO |
| 2 | E | 384 | ALA |
| 2 | E | 385 | LEU |
| 2 | E | 420 | THR |
| 2 | E | 432 | TYR |
| 2 | E | 449 | GLU |
| 2 | F | 83 | LYS |
| 2 | F | 87 | SER |
| 2 | F | 134 | LYS |
| 2 | F | 139 | LEU |
| 2 | F | 145 | PHE |
| 2 | F | 178 | SER |
| 2 | F | 223 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | F | 319 | VAL |
| 2 | F | 341 | ASP |
| 2 | F | 352 | ASP |
| 2 | F | 356 | LEU |
| 2 | F | 360 | SER |
| 2 | F | 365 | LYS |
| 2 | F | 389 | ARG |
| 2 | F | 415 | PRO |
| 2 | F | 453 | ILE |
| 2 | F | 456 | ARG |
| 2 | F | 460 | THR |
| 1 | A | 73 | PRO |
| 1 | A | 84 | HIS |
| 1 | A | 132 | GLY |
| 1 | A | 171 | TRP |
| 1 | A | 238 | GLN |
| 1 | A | 262 | GLN |
| 1 | A | 283 | LEU |
| 1 | A | 292 | LEU |
| 1 | A | 371 | LYS |
| 1 | A | 383 | LYS |
| 1 | A | 470 | ALA |
| 1 | A | 507 | PRO |
| 1 | A | 508 | ALA |
| 1 | A | 517 | GLY |
| 1 | A | 561 | LYS |
| 1 | A | 576 | LEU |
| 1 | A | 596 | MET |
| 1 | A | 607 | TRP |
| 1 | A | 613 | HIS |
| 1 | A | 617 | ARG |
| 1 | A | 639 | THR |
| 1 | A | 659 | HIS |
| 1 | A | 719 | LEU |
| 1 | A | 735 | GLY |
| 1 | A | 762 | VAL |
| 1 | A | 813 | VAL |
| 1 | A | 864 | ASN |
| 1 | A | 923 | GLY |
| 1 | A | 940 | GLY |
| 1 | A | 1018 | GLY |
| 1 | A | 1021 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1052 | GLY |
| 1 | A | 1094 | THR |
| 1 | A | 1122 | GLU |
| 1 | A | 1145 | ASP |
| 1 | A | 1228 | LYS |
| 1 | A | 1232 | GLU |
| 2 | B | 88 | ARG |
| 2 | B | 117 | SER |
| 2 | B | 179 | GLY |
| 2 | B | 265 | LYS |
| 2 | B | 282 | GLU |
| 2 | B | 309 | HIS |
| 2 | B | 312 | LEU |
| 2 | B | 343 | ASP |
| 2 | B | 353 | SER |
| 2 | B | 354 | PHE |
| 2 | B | 377 | CYS |
| 2 | B | 410 | GLY |
| 2 | B | 436 | SER |
| 2 | B | 441 | VAL |
| 2 | B | 469 | SER |
| 2 | C | 88 | ARG |
| 2 | C | 248 | SER |
| 2 | C | 300 | ILE |
| 2 | C | 321 | LYS |
| 2 | C | 328 | ARG |
| 2 | C | 340 | GLY |
| 2 | C | 351 | TYR |
| 2 | C | 445 | GLU |
| 2 | C | 451 | GLY |
| 2 | C | 453 | ILE |
| 2 | C | 458 | ARG |
| 1 | D | 78 | MET |
| 1 | D | 130 | LEU |
| 1 | D | 174 | GLY |
| 1 | D | 218 | SER |
| 1 | D | 220 | TRP |
| 1 | D | 223 | TRP |
| 1 | D | 292 | LEU |
| 1 | D | 371 | LYS |
| 1 | D | 392 | LEU |
| 1 | D | 421 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 469 | ASP |
| 1 | D | 510 | ALA |
| 1 | D | 519 | GLY |
| 1 | D | 525 | MET |
| 1 | D | 529 | ASP |
| 1 | D | 588 | GLY |
| 1 | D | 609 | GLY |
| 1 | D | 624 | VAL |
| 1 | D | 656 | TYR |
| 1 | D | 758 | ASN |
| 1 | D | 802 | ARG |
| 1 | D | 810 | SER |
| 1 | D | 855 | VAL |
| 1 | D | 868 | ASP |
| 1 | D | 877 | MET |
| 1 | D | 880 | ALA |
| 1 | D | 920 | THR |
| 1 | D | 940 | GLY |
| 1 | D | 1000 | GLU |
| 1 | D | 1021 | SER |
| 1 | D | 1025 | LEU |
| 1 | D | 1034 | ARG |
| 1 | D | 1042 | GLU |
| 1 | D | 1062 | GLU |
| 1 | D | 1066 | THR |
| 1 | D | 1068 | ASP |
| 1 | D | 1171 | ASN |
| 1 | D | 1172 | ASP |
| 1 | D | 1193 | VAL |
| 1 | D | 1220 | ILE |
| 1 | D | 1238 | GLY |
| 2 | E | 82 | SER |
| 2 | E | 85 | GLN |
| 2 | E | 94 | GLY |
| 2 | E | 116 | THR |
| 2 | E | 117 | SER |
| 2 | E | 231 | ILE |
| 2 | E | 264 | ARG |
| 2 | E | 298 | GLU |
| 2 | E | 311 | LEU |
| 2 | E | 401 | GLY |
| 2 | E | 405 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | E | 408 | GLU |
| 2 | E | 469 | SER |
| 2 | F | 122 | ARG |
| 2 | F | 125 | VAL |
| 2 | F | 182 | ARG |
| 2 | F | 200 | VAL |
| 2 | F | 220 | ASP |
| 2 | F | 257 | ARG |
| 2 | F | 300 | ILE |
| 2 | F | 342 | LEU |
| 2 | F | 353 | SER |
| 2 | F | 438 | LEU |
| 2 | F | 455 | LEU |
| 1 | A | 123 | VAL |
| 1 | A | 233 | TYR |
| 1 | A | 239 | LEU |
| 1 | A | 393 | MET |
| 1 | A | 570 | PRO |
| 1 | A | 587 | PRO |
| 1 | A | 716 | PRO |
| 1 | A | 726 | LYS |
| 1 | A | 763 | GLY |
| 1 | A | 777 | GLY |
| 1 | A | 787 | SER |
| 1 | A | 805 | HIS |
| 1 | A | 922 | GLN |
| 1 | A | 990 | LYS |
| 1 | A | 1000 | GLU |
| 1 | A | 1037 | GLN |
| 1 | A | 1038 | TRP |
| 1 | A | 1042 | GLU |
| 1 | A | 1071 | ARG |
| 1 | A | 1095 | SER |
| 1 | A | 1195 | MET |
| 1 | A | 1212 | ILE |
| 2 | B | 75 | ARG |
| 2 | B | 199 | LEU |
| 2 | B | 247 | THR |
| 2 | B | 267 | ALA |
| 2 | B | 283 | GLY |
| 2 | B | 349 | TYR |
| 2 | C | 137 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 220 | ASP |
| 2 | C | 368 | HIS |
| 2 | C | 423 | SER |
| 2 | C | 425 | LEU |
| 2 | C | 448 | LEU |
| 1 | D | 84 | HIS |
| 1 | D | 183 | GLU |
| 1 | D | 254 | SER |
| 1 | D | 278 | ILE |
| 1 | D | 306 | SER |
| 1 | D | 470 | ALA |
| 1 | D | 527 | GLN |
| 1 | D | 560 | PRO |
| 1 | D | 578 | PRO |
| 1 | D | 579 | ARG |
| 1 | D | 627 | ARG |
| 1 | D | 719 | LEU |
| 1 | D | 731 | SER |
| 1 | D | 811 | GLN |
| 1 | D | 876 | ALA |
| 1 | D | 1020 | ILE |
| 1 | D | 1026 | ARG |
| 1 | D | 1037 | GLN |
| 1 | D | 1040 | LYS |
| 1 | D | 1094 | THR |
| 1 | D | 1128 | ARG |
| 1 | D | 1162 | CYS |
| 1 | D | 1181 | SER |
| 1 | D | 1191 | LYS |
| 1 | D | 1196 | ASP |
| 2 | E | 203 | ARG |
| 2 | E | 328 | ARG |
| 2 | E | 382 | LYS |
| 2 | F | 137 | PRO |
| 2 | F | 328 | ARG |
| 2 | F | 403 | PHE |
| 2 | F | 436 | SER |
| 2 | F | 452 | LEU |
| 2 | F | 484 | ASN |
| 1 | A | 162 | LEU |
| 1 | A | 397 | ALA |
| 1 | A | 412 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 501 | LYS |
| 1 | A | 577 | CYS |
| 1 | A | 633 | LYS |
| 1 | A | 722 | ARG |
| 1 | A | 742 | VAL |
| 1 | A | 802 | ARG |
| 1 | A | 817 | PRO |
| 1 | A | 868 | ASP |
| 1 | A | 973 | LEU |
| 1 | A | 1043 | VAL |
| 1 | A | 1068 | ASP |
| 1 | A | 1129 | PHE |
| 1 | A | 1167 | LYS |
| 1 | A | 1199 | THR |
| 2 | B | 214 | CYS |
| 2 | C | 140 | PRO |
| 2 | C | 182 | ARG |
| 2 | C | 189 | ALA |
| 2 | C | 200 | VAL |
| 2 | C | 226 | ASN |
| 2 | C | 270 | PRO |
| 2 | C | 299 | LEU |
| 2 | C | 392 | THR |
| 2 | C | 419 | GLU |
| 2 | C | 478 | TYR |
| 2 | C | 484 | ASN |
| 1 | D | 97 | GLU |
| 1 | D | 119 | PRO |
| 1 | D | 165 | LYS |
| 1 | D | 179 | GLY |
| 1 | D | 210 | THR |
| 1 | D | 259 | ARG |
| 1 | D | 271 | VAL |
| 1 | D | 287 | SER |
| 1 | D | 500 | ALA |
| 1 | D | 520 | ALA |
| 1 | D | 625 | PRO |
| 1 | D | 632 | ALA |
| 1 | D | 655 | LEU |
| 1 | D | 672 | GLU |
| 1 | D | 715 | GLN |
| 1 | D | 723 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 730 | PRO |
| 1 | D | 922 | GLN |
| 1 | D | 995 | TYR |
| 1 | D | 1035 | LYS |
| 1 | D | 1108 | TYR |
| 1 | D | 1134 | HIS |
| 1 | D | 1192 | GLU |
| 2 | E | 77 | HIS |
| 2 | E | 88 | ARG |
| 2 | E | 121 | PHE |
| 2 | E | 215 | PHE |
| 2 | E | 240 | VAL |
| 2 | E | 285 | LYS |
| 2 | E | 292 | ASN |
| 2 | F | 77 | HIS |
| 2 | F | 140 | PRO |
| 2 | F | 217 | PRO |
| 2 | F | 248 | SER |
| 2 | F | 280 | ASP |
| 2 | F | 423 | SER |
| 2 | F | 451 | GLY |
| 2 | F | 478 | TYR |
| 1 | A | 71 | HIS |
| 1 | A | 248 | GLU |
| 1 | A | 380 | GLY |
| 1 | A | 421 | PRO |
| 1 | A | 462 | SER |
| 1 | A | 464 | MET |
| 1 | A | 506 | GLU |
| 1 | A | 568 | GLY |
| 1 | A | 625 | PRO |
| 1 | A | 646 | VAL |
| 1 | A | 660 | CYS |
| 1 | A | 717 | LEU |
| 1 | A | 830 | ASP |
| 1 | A | 908 | ALA |
| 1 | A | 910 | MET |
| 1 | A | 1062 | GLU |
| 1 | A | 1092 | PHE |
| 1 | A | 1182 | ALA |
| 2 | B | 201 | ASN |
| 2 | B | 316 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 413 | VAL |
| 2 | B | 484 | ASN |
| 2 | C | 110 | LEU |
| 2 | C | 124 | GLN |
| 2 | C | 280 | ASP |
| 2 | C | 389 | ARG |
| 1 | D | 169 | TRP |
| 1 | D | 177 | ARG |
| 1 | D | 184 | ALA |
| 1 | D | 191 | GLU |
| 1 | D | 279 | ARG |
| 1 | D | 405 | GLU |
| 1 | D | 477 | GLU |
| 1 | D | 562 | ARG |
| 1 | D | 633 | LYS |
| 1 | D | 780 | GLN |
| 1 | D | 882 | PRO |
| 1 | D | 941 | ILE |
| 1 | D | 1118 | TRP |
| 1 | D | 1122 | GLU |
| 2 | E | 210 | GLN |
| 2 | E | 272 | ASN |
| 2 | E | 280 | ASP |
| 2 | E | 372 | LEU |
| 2 | E | 423 | SER |
| 2 | F | 121 | PHE |
| 2 | F | 130 | ALA |
| 2 | F | 138 | LEU |
| 2 | F | 351 | TYR |
| 1 | A | 857 | PRO |
| 1 | A | 1093 | MET |
| 1 | A | 1207 | GLU |
| 2 | B | 270 | PRO |
| 2 | B | 297 | LYS |
| 2 | C | 125 | VAL |
| 1 | D | 128 | PRO |
| 1 | D | 569 | HIS |
| 1 | D | 572 | TRP |
| 1 | D | 853 | ARG |
| 1 | D | 1103 | SER |
| 1 | A | 128 | PRO |
| 1 | A | 215 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 645 | VAL |
| 1 | D | 166 | PRO |
| 1 | D | 411 | LEU |
| 1 | D | 881 | PRO |
| 1 | D | 1205 | GLY |
| 2 | F | 204 | LEU |
| 1 | A | 87 | ILE |
| 1 | A | 871 | GLY |
| 1 | A | 878 | VAL |
| 1 | A | 1010 | LEU |
| 1 | A | 1127 | GLY |
| 2 | B | 327 | GLY |
| 1 | D | 267 | VAL |
| 1 | D | 406 | VAL |
| 1 | D | 436 | PRO |
| 1 | D | 563 | PRO |
| 1 | D | 1155 | ILE |
| 1 | D | 1211 | GLY |
| 2 | F | 128 | VAL |
| 1 | A | 366 | VAL |
| 1 | A | 432 | VAL |
| 1 | A | 515 | ILE |
| 1 | A | 715 | GLN |
| 2 | B | 307 | GLY |
| 2 | B | 380 | PRO |
| 2 | C | 120 | VAL |
| 2 | C | 414 | TRP |
| 1 | D | 1137 | VAL |
| 2 | F | 414 | TRP |
| 1 | A | 560 | PRO |
| 1 | A | 621 | GLY |
| 1 | A | 855 | VAL |
| 2 | B | 213 | VAL |
| 1 | D | 435 | LEU |
| 1 | D | 817 | PRO |
| 2 | E | 135 | PRO |
| 2 | E | 179 | GLY |
| 2 | E | 200 | VAL |
| 1 | D | 648 | PRO |
| 1 | A | 753 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1 | A | 918/988 (93%) | 611 (67%) | 307 (33%) | 0 | 0 |
| 1 | D | 919/988 (93%) | 584 (64%) | 335 (36%) | 0 | 0 |
| 2 | B | 317/380 (83%) | 259 (82%) | 58 (18%) | 2 | 9 |
| 2 | C | 350/380 (92%) | 260 (74%) | 90 (26%) | 0 | 2 |
| 2 | E | 317/380 (83%) | 270 (85%) | 47 (15%) | 3 | 16 |
| 2 | F | 350/380 (92%) | 245 (70%) | 105 (30%) | 0 | 1 |
| All | All | 3171/3496 (91%) | 2229 (70%) | 942 (30%) | 0 | 1 |

All (942) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 70 | ARG |
| 1 | A | 78 | MET |
| 1 | A | 83 | LEU |
| 1 | A | 90 | GLN |
| 1 | A | 93 | GLU |
| 1 | A | 94 | MET |
| 1 | A | 97 | GLU |
| 1 | A | 101 | ARG |
| 1 | A | 102 | ARG |
| 1 | A | 107 | LEU |
| 1 | A | 109 | LYS |
| 1 | A | 120 | LEU |
| 1 | A | 125 | LEU |
| 1 | A | 128 | PRO |
| 1 | A | 131 | TYR |
| 1 | A | 135 | LEU |
| 1 | A | 138 | HIS |
| 1 | A | 141 | LEU |
| 1 | A | 146 | GLN |
| 1 | A | 156 | LEU |
| 1 | A | 157 | LEU |
| 1 | A | 161 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 169 | TRP |
| 1 | A | 177 | ARG |
| 1 | A | 183 | GLU |
| 1 | A | 187 | VAL |
| 1 | A | 190 | PRO |
| 1 | A | 193 | ARG |
| 1 | A | 195 | LEU |
| 1 | A | 197 | PHE |
| 1 | A | 202 | CYS |
| 1 | A | 208 | CYS |
| 1 | A | 216 | SER |
| 1 | A | 217 | PRO |
| 1 | A | 220 | TRP |
| 1 | A | 223 | TRP |
| 1 | A | 224 | CYS |
| 1 | A | 226 | GLN |
| 1 | A | 227 | ARG |
| 1 | A | 228 | LEU |
| 1 | A | 235 | TRP |
| 1 | A | 236 | THR |
| 1 | A | 246 | PRO |
| 1 | A | 247 | LEU |
| 1 | A | 248 | GLU |
| 1 | A | 259 | ARG |
| 1 | A | 260 | ASP |
| 1 | A | 261 | TRP |
| 1 | A | 262 | GLN |
| 1 | A | 263 | GLU |
| 1 | A | 265 | LEU |
| 1 | A | 267 | VAL |
| 1 | A | 270 | ASN |
| 1 | A | 272 | SER |
| 1 | A | 275 | ARG |
| 1 | A | 279 | ARG |
| 1 | A | 288 | ARG |
| 1 | A | 293 | ASP |
| 1 | A | 294 | THR |
| 1 | A | 298 | HIS |
| 1 | A | 307 | PHE |
| 1 | A | 308 | GLN |
| 1 | A | 311 | LEU |
| 1 | A | 312 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 346 | ASP |
| 1 | A | 350 | ILE |
| 1 | A | 351 | SER |
| 1 | A | 352 | SER |
| 1 | A | 354 | ASN |
| 1 | A | 356 | ASN |
| 1 | A | 358 | LEU |
| 1 | A | 361 | VAL |
| 1 | A | 364 | LEU |
| 1 | A | 365 | TYR |
| 1 | A | 369 | PRO |
| 1 | A | 372 | GLU |
| 1 | A | 374 | ARG |
| 1 | A | 376 | LEU |
| 1 | A | 377 | PHE |
| 1 | A | 379 | LYS |
| 1 | A | 384 | ASP |
| 1 | A | 386 | ARG |
| 1 | A | 388 | ASN |
| 1 | A | 389 | PHE |
| 1 | A | 393 | MET |
| 1 | A | 394 | GLN |
| 1 | A | 398 | GLN |
| 1 | A | 403 | THR |
| 1 | A | 406 | VAL |
| 1 | A | 415 | LEU |
| 1 | A | 416 | GLU |
| 1 | A | 417 | ARG |
| 1 | A | 424 | LEU |
| 1 | A | 429 | GLU |
| 1 | A | 430 | MET |
| 1 | A | 436 | PRO |
| 1 | A | 441 | TRP |
| 1 | A | 442 | GLU |
| 1 | A | 445 | LEU |
| 1 | A | 451 | THR |
| 1 | A | 453 | GLU |
| 1 | A | 457 | ARG |
| 1 | A | 460 | LYS |
| 1 | A | 463 | LEU |
| 1 | A | 465 | ASP |
| 1 | A | 466 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 473 | LEU |
| 1 | A | 474 | LEU |
| 1 | A | 477 | GLU |
| 1 | A | 481 | GLU |
| 1 | A | 482 | ASP |
| 1 | A | 484 | TRP |
| 1 | A | 485 | LEU |
| 1 | A | 487 | ASP |
| 1 | A | 490 | TRP |
| 1 | A | 491 | ASP |
| 1 | A | 496 | LYS |
| 1 | A | 498 | LYS |
| 1 | A | 502 | LYS |
| 1 | A | 512 | LYS |
| 1 | A | 524 | PRO |
| 1 | A | 526 | ASP |
| 1 | A | 527 | GLN |
| 1 | A | 528 | GLU |
| 1 | A | 535 | GLU |
| 1 | A | 536 | GLU |
| 1 | A | 549 | LEU |
| 1 | A | 557 | GLU |
| 1 | A | 558 | LEU |
| 1 | A | 559 | LEU |
| 1 | A | 560 | PRO |
| 1 | A | 561 | LYS |
| 1 | A | 564 | GLN |
| 1 | A | 567 | PRO |
| 1 | A | 569 | HIS |
| 1 | A | 572 | TRP |
| 1 | A | 576 | LEU |
| 1 | A | 577 | CYS |
| 1 | A | 579 | ARG |
| 1 | A | 583 | PRO |
| 1 | A | 585 | TRP |
| 1 | A | 586 | THR |
| 1 | A | 587 | PRO |
| 1 | A | 591 | LEU |
| 1 | A | 592 | LEU |
| 1 | A | 594 | LEU |
| 1 | A | 595 | GLN |
| 1 | A | 596 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 597 | ARG |
| 1 | A | 601 | LYS |
| 1 | A | 607 | TRP |
| 1 | A | 608 | ASP |
| 1 | A | 610 | PHE |
| 1 | A | 611 | PRO |
| 1 | A | 612 | LEU |
| 1 | A | 618 | HIS |
| 1 | A | 620 | TRP |
| 1 | A | 624 | VAL |
| 1 | A | 627 | ARG |
| 1 | A | 628 | ARG |
| 1 | A | 630 | ASN |
| 1 | A | 631 | LEU |
| 1 | A | 633 | LYS |
| 1 | A | 636 | THR |
| 1 | A | 639 | THR |
| 1 | A | 640 | LEU |
| 1 | A | 655 | LEU |
| 1 | A | 659 | HIS |
| 1 | A | 660 | CYS |
| 1 | A | 661 | LEU |
| 1 | A | 662 | GLU |
| 1 | A | 666 | GLN |
| 1 | A | 668 | LEU |
| 1 | A | 672 | GLU |
| 1 | A | 712 | VAL |
| 1 | A | 719 | LEU |
| 1 | A | 727 | ASP |
| 1 | A | 733 | HIS |
| 1 | A | 734 | HIS |
| 1 | A | 736 | ASN |
| 1 | A | 738 | PRO |
| 1 | A | 741 | ASP |
| 1 | A | 744 | ILE |
| 1 | A | 748 | TRP |
| 1 | A | 752 | LEU |
| 1 | A | 754 | HIS |
| 1 | A | 755 | LYS |
| 1 | A | 756 | ASP |
| 1 | A | 758 | ASN |
| 1 | A | 760 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 771 | LEU |
| 1 | A | 776 | ASP |
| 1 | A | 778 | THR |
| 1 | A | 779 | LEU |
| 1 | A | 792 | LEU |
| 1 | A | 795 | ASN |
| 1 | A | 798 | ILE |
| 1 | A | 803 | ASN |
| 1 | A | 805 | HIS |
| 1 | A | 810 | SER |
| 1 | A | 812 | MET |
| 1 | A | 813 | VAL |
| 1 | A | 817 | PRO |
| 1 | A | 823 | ARG |
| 1 | A | 826 | ILE |
| 1 | A | 827 | ARG |
| 1 | A | 831 | TYR |
| 1 | A | 833 | GLU |
| 1 | A | 840 | ILE |
| 1 | A | 850 | ILE |
| 1 | A | 851 | THR |
| 1 | A | 853 | ARG |
| 1 | A | 858 | THR |
| 1 | A | 864 | ASN |
| 1 | A | 866 | ARG |
| 1 | A | 877 | MET |
| 1 | A | 879 | GLN |
| 1 | A | 884 | TYR |
| 1 | A | 885 | THR |
| 1 | A | 886 | LEU |
| 1 | A | 891 | VAL |
| 1 | A | 892 | ASP |
| 1 | A | 894 | GLN |
| 1 | A | 898 | ILE |
| 1 | A | 904 | ASP |
| 1 | A | 906 | HIS |
| 1 | A | 910 | MET |
| 1 | A | 911 | HIS |
| 1 | A | 913 | CYS |
| 1 | A | 916 | PHE |
| 1 | A | 919 | MET |
| 1 | A | 921 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 922 | GLN |
| 1 | A | 927 | ARG |
| 1 | A | 930 | ASP |
| 1 | A | 931 | LEU |
| 1 | A | 933 | SER |
| 1 | A | 941 | ILE |
| 1 | A | 948 | ILE |
| 1 | A | 949 | PHE |
| 1 | A | 954 | ILE |
| 1 | A | 961 | PHE |
| 1 | A | 966 | LEU |
| 1 | A | 989 | THR |
| 1 | A | 992 | LEU |
| 1 | A | 997 | LEU |
| 1 | A | 1003 | TRP |
| 1 | A | 1006 | ARG |
| 1 | A | 1008 | LEU |
| 1 | A | 1011 | PRO |
| 1 | A | 1014 | ARG |
| 1 | A | 1015 | THR |
| 1 | A | 1016 | GLU |
| 1 | A | 1028 | VAL |
| 1 | A | 1029 | GLN |
| 1 | A | 1031 | GLU |
| 1 | A | 1041 | TRP |
| 1 | A | 1044 | VAL |
| 1 | A | 1047 | ARG |
| 1 | A | 1056 | GLU |
| 1 | A | 1066 | THR |
| 1 | A | 1069 | ILE |
| 1 | A | 1102 | GLN |
| 1 | A | 1109 | LEU |
| 1 | A | 1112 | MET |
| 1 | A | 1113 | LEU |
| 1 | A | 1116 | MET |
| 1 | A | 1125 | ILE |
| 1 | A | 1126 | ASP |
| 1 | A | 1130 | CYS |
| 1 | A | 1133 | ILE |
| 1 | A | 1138 | ARG |
| 1 | A | 1140 | LEU |
| 1 | A | 1145 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1148 | ARG |
| 1 | A | 1153 | LEU |
| 1 | A | 1154 | GLN |
| 1 | A | 1156 | THR |
| 1 | A | 1160 | THR |
| 1 | A | 1166 | TYR |
| 1 | A | 1170 | LEU |
| 1 | A | 1171 | ASN |
| 1 | A | 1172 | ASP |
| 1 | A | 1177 | VAL |
| 1 | A | 1180 | PHE |
| 1 | A | 1191 | LYS |
| 1 | A | 1193 | VAL |
| 1 | A | 1197 | CYS |
| 1 | A | 1198 | LYS |
| 1 | A | 1202 | ASN |
| 1 | A | 1206 | MET |
| 1 | A | 1209 | ARG |
| 1 | A | 1210 | TYR |
| 1 | A | 1213 | PRO |
| 1 | A | 1214 | GLN |
| 1 | A | 1218 | LEU |
| 1 | A | 1219 | ASP |
| 1 | A | 1220 | ILE |
| 1 | A | 1223 | ILE |
| 1 | A | 1224 | ILE |
| 1 | A | 1225 | GLU |
| 1 | A | 1226 | LEU |
| 1 | A | 1227 | THR |
| 1 | A | 1231 | LEU |
| 1 | A | 1233 | LYS |
| 1 | A | 1236 | GLN |
| 1 | A | 1237 | PRO |
| 2 | B | 74 | GLN |
| 2 | B | 77 | HIS |
| 2 | B | 78 | PHE |
| 2 | B | 83 | LYS |
| 2 | B | 84 | GLN |
| 2 | B | 86 | LEU |
| 2 | B | 89 | ASP |
| 2 | B | 96 | HIS |
| 2 | B | 101 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 105 | GLU |
| 2 | B | 109 | ASN |
| 2 | B | 122 | ARG |
| 2 | B | 123 | GLU |
| 2 | B | 184 | ASN |
| 2 | B | 203 | ARG |
| 2 | B | 205 | PRO |
| 2 | B | 208 | LEU |
| 2 | B | 210 | GLN |
| 2 | B | 230 | SER |
| 2 | B | 231 | ILE |
| 2 | B | 234 | LYS |
| 2 | B | 236 | GLU |
| 2 | B | 242 | PHE |
| 2 | B | 246 | ARG |
| 2 | B | 251 | TRP |
| 2 | B | 254 | PHE |
| 2 | B | 260 | LEU |
| 2 | B | 262 | TRP |
| 2 | B | 264 | ARG |
| 2 | B | 272 | ASN |
| 2 | B | 281 | GLU |
| 2 | B | 284 | ARG |
| 2 | B | 298 | GLU |
| 2 | B | 304 | TRP |
| 2 | B | 309 | HIS |
| 2 | B | 311 | LEU |
| 2 | B | 312 | LEU |
| 2 | B | 313 | HIS |
| 2 | B | 316 | PRO |
| 2 | B | 318 | ASN |
| 2 | B | 325 | ARG |
| 2 | B | 331 | VAL |
| 2 | B | 344 | ARG |
| 2 | B | 346 | MET |
| 2 | B | 347 | LEU |
| 2 | B | 349 | TYR |
| 2 | B | 351 | TYR |
| 2 | B | 352 | ASP |
| 2 | B | 377 | CYS |
| 2 | B | 380 | PRO |
| 2 | B | 414 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 417 | TYR |
| 2 | B | 429 | TYR |
| 2 | B | 431 | LYS |
| 2 | B | 441 | VAL |
| 2 | B | 453 | ILE |
| 2 | B | 454 | HIS |
| 2 | B | 472 | LYS |
| 2 | C | 88 | ARG |
| 2 | C | 89 | ASP |
| 2 | C | 91 | LEU |
| 2 | C | 92 | LEU |
| 2 | C | 99 | PHE |
| 2 | C | 116 | THR |
| 2 | C | 117 | SER |
| 2 | C | 118 | VAL |
| 2 | C | 120 | VAL |
| 2 | C | 124 | GLN |
| 2 | C | 125 | VAL |
| 2 | C | 128 | VAL |
| 2 | C | 131 | LEU |
| 2 | C | 132 | HIS |
| 2 | C | 133 | HIS |
| 2 | C | 180 | LYS |
| 2 | C | 186 | LEU |
| 2 | C | 193 | TYR |
| 2 | C | 197 | LEU |
| 2 | C | 198 | ASP |
| 2 | C | 199 | LEU |
| 2 | C | 205 | PRO |
| 2 | C | 206 | TYR |
| 2 | C | 208 | LEU |
| 2 | C | 210 | GLN |
| 2 | C | 214 | CYS |
| 2 | C | 215 | PHE |
| 2 | C | 224 | ILE |
| 2 | C | 226 | ASN |
| 2 | C | 230 | SER |
| 2 | C | 236 | GLU |
| 2 | C | 244 | PRO |
| 2 | C | 245 | PRO |
| 2 | C | 246 | ARG |
| 2 | C | 247 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 251 | TRP |
| 2 | C | 254 | PHE |
| 2 | C | 256 | LEU |
| 2 | C | 280 | ASP |
| 2 | C | 285 | LYS |
| 2 | C | 298 | GLU |
| 2 | C | 299 | LEU |
| 2 | C | 308 | ASP |
| 2 | C | 309 | HIS |
| 2 | C | 310 | GLU |
| 2 | C | 312 | LEU |
| 2 | C | 320 | SER |
| 2 | C | 321 | LYS |
| 2 | C | 322 | LEU |
| 2 | C | 325 | ARG |
| 2 | C | 328 | ARG |
| 2 | C | 330 | ASN |
| 2 | C | 337 | SER |
| 2 | C | 341 | ASP |
| 2 | C | 342 | LEU |
| 2 | C | 350 | LEU |
| 2 | C | 351 | TYR |
| 2 | C | 357 | THR |
| 2 | C | 363 | ARG |
| 2 | C | 364 | LYS |
| 2 | C | 367 | LEU |
| 2 | C | 369 | ARG |
| 2 | C | 385 | LEU |
| 2 | C | 387 | VAL |
| 2 | C | 389 | ARG |
| 2 | C | 394 | GLU |
| 2 | C | 395 | LEU |
| 2 | C | 396 | ARG |
| 2 | C | 399 | CYS |
| 2 | C | 400 | GLN |
| 2 | C | 402 | LEU |
| 2 | C | 403 | PHE |
| 2 | C | 406 | LEU |
| 2 | C | 407 | LEU |
| 2 | C | 417 | TYR |
| 2 | C | 431 | LYS |
| 2 | C | 435 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 439 | PHE |
| 2 | C | 448 | LEU |
| 2 | C | 456 | ARG |
| 2 | C | 457 | SER |
| 2 | C | 458 | ARG |
| 2 | C | 464 | GLU |
| 2 | C | 468 | ILE |
| 2 | C | 471 | LEU |
| 2 | C | 474 | PHE |
| 2 | C | 475 | LEU |
| 2 | C | 476 | ILE |
| 2 | C | 483 | LYS |
| 2 | C | 485 | VAL |
| 1 | D | 70 | ARG |
| 1 | D | 77 | GLN |
| 1 | D | 78 | MET |
| 1 | D | 79 | LEU |
| 1 | D | 81 | ARG |
| 1 | D | 83 | LEU |
| 1 | D | 85 | GLU |
| 1 | D | 86 | GLN |
| 1 | D | 87 | ILE |
| 1 | D | 97 | GLU |
| 1 | D | 101 | ARG |
| 1 | D | 104 | VAL |
| 1 | D | 107 | LEU |
| 1 | D | 113 | TRP |
| 1 | D | 120 | LEU |
| 1 | D | 122 | ASP |
| 1 | D | 125 | LEU |
| 1 | D | 127 | LEU |
| 1 | D | 130 | LEU |
| 1 | D | 133 | ASP |
| 1 | D | 135 | LEU |
| 1 | D | 140 | ARG |
| 1 | D | 144 | GLN |
| 1 | D | 145 | LYS |
| 1 | D | 146 | GLN |
| 1 | D | 157 | LEU |
| 1 | D | 161 | GLN |
| 1 | D | 162 | LEU |
| 1 | D | 169 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 175 | TRP |
| 1 | D | 176 | THR |
| 1 | D | 177 | ARG |
| 1 | D | 181 | GLU |
| 1 | D | 185 | VAL |
| 1 | D | 189 | ILE |
| 1 | D | 193 | ARG |
| 1 | D | 196 | VAL |
| 1 | D | 201 | VAL |
| 1 | D | 203 | LEU |
| 1 | D | 205 | GLU |
| 1 | D | 208 | CYS |
| 1 | D | 216 | SER |
| 1 | D | 217 | PRO |
| 1 | D | 218 | SER |
| 1 | D | 220 | TRP |
| 1 | D | 223 | TRP |
| 1 | D | 224 | CYS |
| 1 | D | 225 | SER |
| 1 | D | 227 | ARG |
| 1 | D | 228 | LEU |
| 1 | D | 232 | ARG |
| 1 | D | 236 | THR |
| 1 | D | 238 | GLN |
| 1 | D | 239 | LEU |
| 1 | D | 243 | ASP |
| 1 | D | 247 | LEU |
| 1 | D | 256 | PRO |
| 1 | D | 258 | GLN |
| 1 | D | 259 | ARG |
| 1 | D | 260 | ASP |
| 1 | D | 265 | LEU |
| 1 | D | 267 | VAL |
| 1 | D | 269 | HIS |
| 1 | D | 284 | ILE |
| 1 | D | 285 | GLN |
| 1 | D | 288 | ARG |
| 1 | D | 289 | MET |
| 1 | D | 293 | ASP |
| 1 | D | 298 | HIS |
| 1 | D | 301 | ILE |
| 1 | D | 305 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 307 | PHE |
| 1 | D | 308 | GLN |
| 1 | D | 313 | ILE |
| 1 | D | 316 | LYS |
| 1 | D | 317 | GLN |
| 1 | D | 347 | TRP |
| 1 | D | 348 | LEU |
| 1 | D | 352 | SER |
| 1 | D | 362 | LEU |
| 1 | D | 371 | LYS |
| 1 | D | 374 | ARG |
| 1 | D | 379 | LYS |
| 1 | D | 384 | ASP |
| 1 | D | 386 | ARG |
| 1 | D | 389 | PHE |
| 1 | D | 390 | GLN |
| 1 | D | 391 | ASP |
| 1 | D | 394 | GLN |
| 1 | D | 395 | TYR |
| 1 | D | 403 | THR |
| 1 | D | 405 | GLU |
| 1 | D | 407 | PHE |
| 1 | D | 411 | LEU |
| 1 | D | 415 | LEU |
| 1 | D | 416 | GLU |
| 1 | D | 417 | ARG |
| 1 | D | 419 | PRO |
| 1 | D | 420 | HIS |
| 1 | D | 424 | LEU |
| 1 | D | 428 | LEU |
| 1 | D | 429 | GLU |
| 1 | D | 430 | MET |
| 1 | D | 435 | LEU |
| 1 | D | 436 | PRO |
| 1 | D | 438 | ASN |
| 1 | D | 439 | GLN |
| 1 | D | 441 | TRP |
| 1 | D | 442 | GLU |
| 1 | D | 445 | LEU |
| 1 | D | 447 | GLU |
| 1 | D | 457 | ARG |
| 1 | D | 460 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 461 | LYS |
| 1 | D | 466 | LEU |
| 1 | D | 469 | ASP |
| 1 | D | 471 | CYS |
| 1 | D | 474 | LEU |
| 1 | D | 479 | TYR |
| 1 | D | 484 | TRP |
| 1 | D | 491 | ASP |
| 1 | D | 493 | GLN |
| 1 | D | 494 | GLU |
| 1 | D | 496 | LYS |
| 1 | D | 499 | LYS |
| 1 | D | 501 | LYS |
| 1 | D | 503 | VAL |
| 1 | D | 504 | LYS |
| 1 | D | 524 | PRO |
| 1 | D | 527 | GLN |
| 1 | D | 530 | LEU |
| 1 | D | 542 | ASP |
| 1 | D | 543 | VAL |
| 1 | D | 550 | GLN |
| 1 | D | 551 | LYS |
| 1 | D | 557 | GLU |
| 1 | D | 558 | LEU |
| 1 | D | 560 | PRO |
| 1 | D | 564 | GLN |
| 1 | D | 565 | HIS |
| 1 | D | 576 | LEU |
| 1 | D | 581 | ASP |
| 1 | D | 585 | TRP |
| 1 | D | 592 | LEU |
| 1 | D | 594 | LEU |
| 1 | D | 595 | GLN |
| 1 | D | 597 | ARG |
| 1 | D | 601 | LYS |
| 1 | D | 602 | LEU |
| 1 | D | 606 | THR |
| 1 | D | 608 | ASP |
| 1 | D | 612 | LEU |
| 1 | D | 615 | SER |
| 1 | D | 617 | ARG |
| 1 | D | 618 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 620 | TRP |
| 1 | D | 627 | ARG |
| 1 | D | 630 | ASN |
| 1 | D | 631 | LEU |
| 1 | D | 638 | THR |
| 1 | D | 645 | VAL |
| 1 | D | 647 | CYS |
| 1 | D | 649 | TYR |
| 1 | D | 653 | GLU |
| 1 | D | 654 | SER |
| 1 | D | 660 | CYS |
| 1 | D | 661 | LEU |
| 1 | D | 666 | GLN |
| 1 | D | 667 | GLN |
| 1 | D | 668 | LEU |
| 1 | D | 713 | PRO |
| 1 | D | 716 | PRO |
| 1 | D | 717 | LEU |
| 1 | D | 719 | LEU |
| 1 | D | 722 | ARG |
| 1 | D | 733 | HIS |
| 1 | D | 736 | ASN |
| 1 | D | 740 | ASN |
| 1 | D | 742 | VAL |
| 1 | D | 744 | ILE |
| 1 | D | 745 | PRO |
| 1 | D | 748 | TRP |
| 1 | D | 753 | PRO |
| 1 | D | 754 | HIS |
| 1 | D | 755 | LYS |
| 1 | D | 756 | ASP |
| 1 | D | 758 | ASN |
| 1 | D | 760 | CYS |
| 1 | D | 761 | ASN |
| 1 | D | 768 | LYS |
| 1 | D | 773 | LYS |
| 1 | D | 776 | ASP |
| 1 | D | 778 | THR |
| 1 | D | 779 | LEU |
| 1 | D | 780 | GLN |
| 1 | D | 795 | ASN |
| 1 | D | 797 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 801 | TRP |
| 1 | D | 802 | ARG |
| 1 | D | 805 | HIS |
| 1 | D | 807 | ARG |
| 1 | D | 809 | SER |
| 1 | D | 812 | MET |
| 1 | D | 813 | VAL |
| 1 | D | 819 | SER |
| 1 | D | 821 | LEU |
| 1 | D | 823 | ARG |
| 1 | D | 826 | ILE |
| 1 | D | 827 | ARG |
| 1 | D | 829 | PRO |
| 1 | D | 831 | TYR |
| 1 | D | 841 | LEU |
| 1 | D | 843 | GLN |
| 1 | D | 844 | VAL |
| 1 | D | 846 | THR |
| 1 | D | 850 | ILE |
| 1 | D | 858 | THR |
| 1 | D | 863 | SER |
| 1 | D | 864 | ASN |
| 1 | D | 872 | SER |
| 1 | D | 874 | LEU |
| 1 | D | 878 | VAL |
| 1 | D | 879 | GLN |
| 1 | D | 885 | THR |
| 1 | D | 886 | LEU |
| 1 | D | 892 | ASP |
| 1 | D | 895 | GLU |
| 1 | D | 896 | LEU |
| 1 | D | 898 | ILE |
| 1 | D | 904 | ASP |
| 1 | D | 906 | HIS |
| 1 | D | 907 | PHE |
| 1 | D | 910 | MET |
| 1 | D | 916 | PHE |
| 1 | D | 919 | MET |
| 1 | D | 921 | LEU |
| 1 | D | 922 | GLN |
| 1 | D | 929 | THR |
| 1 | D | 930 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 932 | HIS |
| 1 | D | 933 | SER |
| 1 | D | 934 | LYS |
| 1 | D | 948 | ILE |
| 1 | D | 955 | TYR |
| 1 | D | 961 | PHE |
| 1 | D | 963 | GLU |
| 1 | D | 967 | MET |
| 1 | D | 983 | GLN |
| 1 | D | 989 | THR |
| 1 | D | 992 | LEU |
| 1 | D | 993 | ARG |
| 1 | D | 994 | TRP |
| 1 | D | 995 | TYR |
| 1 | D | 996 | ARG |
| 1 | D | 997 | LEU |
| 1 | D | 1006 | ARG |
| 1 | D | 1008 | LEU |
| 1 | D | 1014 | ARG |
| 1 | D | 1020 | ILE |
| 1 | D | 1022 | LEU |
| 1 | D | 1023 | GLN |
| 1 | D | 1025 | LEU |
| 1 | D | 1026 | ARG |
| 1 | D | 1030 | ARG |
| 1 | D | 1034 | ARG |
| 1 | D | 1036 | SER |
| 1 | D | 1037 | GLN |
| 1 | D | 1038 | TRP |
| 1 | D | 1041 | TRP |
| 1 | D | 1043 | VAL |
| 1 | D | 1047 | ARG |
| 1 | D | 1055 | SER |
| 1 | D | 1056 | GLU |
| 1 | D | 1057 | MET |
| 1 | D | 1058 | PHE |
| 1 | D | 1060 | LYS |
| 1 | D | 1061 | LEU |
| 1 | D | 1066 | THR |
| 1 | D | 1067 | SER |
| 1 | D | 1068 | ASP |
| 1 | D | 1070 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 1071 | ARG |
| 1 | D | 1072 | THR |
| 1 | D | 1073 | PRO |
| 1 | D | 1099 | TRP |
| 1 | D | 1104 | SER |
| 1 | D | 1109 | LEU |
| 1 | D | 1113 | LEU |
| 1 | D | 1121 | GLU |
| 1 | D | 1122 | GLU |
| 1 | D | 1126 | ASP |
| 1 | D | 1130 | CYS |
| 1 | D | 1131 | ILE |
| 1 | D | 1132 | SER |
| 1 | D | 1133 | ILE |
| 1 | D | 1134 | HIS |
| 1 | D | 1135 | ASP |
| 1 | D | 1136 | GLU |
| 1 | D | 1138 | ARG |
| 1 | D | 1140 | LEU |
| 1 | D | 1146 | ARG |
| 1 | D | 1148 | ARG |
| 1 | D | 1153 | LEU |
| 1 | D | 1158 | LEU |
| 1 | D | 1163 | MET |
| 1 | D | 1164 | PHE |
| 1 | D | 1166 | TYR |
| 1 | D | 1171 | ASN |
| 1 | D | 1172 | ASP |
| 1 | D | 1175 | GLN |
| 1 | D | 1180 | PHE |
| 1 | D | 1181 | SER |
| 1 | D | 1184 | ASP |
| 1 | D | 1187 | ARG |
| 1 | D | 1191 | LYS |
| 1 | D | 1192 | GLU |
| 1 | D | 1195 | MET |
| 1 | D | 1197 | CYS |
| 1 | D | 1200 | PRO |
| 1 | D | 1203 | PRO |
| 1 | D | 1204 | THR |
| 1 | D | 1206 | MET |
| 1 | D | 1207 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 1208 | ARG |
| 1 | D | 1210 | TYR |
| 1 | D | 1212 | ILE |
| 1 | D | 1218 | LEU |
| 1 | D | 1219 | ASP |
| 1 | D | 1221 | TYR |
| 1 | D | 1223 | ILE |
| 1 | D | 1224 | ILE |
| 1 | D | 1225 | GLU |
| 1 | D | 1226 | LEU |
| 1 | D | 1227 | THR |
| 1 | D | 1230 | SER |
| 2 | E | 67 | GLU |
| 2 | E | 86 | LEU |
| 2 | E | 88 | ARG |
| 2 | E | 107 | ARG |
| 2 | E | 108 | LYS |
| 2 | E | 116 | THR |
| 2 | E | 120 | VAL |
| 2 | E | 122 | ARG |
| 2 | E | 123 | GLU |
| 2 | E | 131 | LEU |
| 2 | E | 191 | GLU |
| 2 | E | 202 | LYS |
| 2 | E | 211 | ILE |
| 2 | E | 213 | VAL |
| 2 | E | 250 | GLN |
| 2 | E | 255 | TRP |
| 2 | E | 276 | SER |
| 2 | E | 277 | ASP |
| 2 | E | 278 | CYS |
| 2 | E | 293 | PHE |
| 2 | E | 294 | PRO |
| 2 | E | 295 | TRP |
| 2 | E | 315 | TYR |
| 2 | E | 328 | ARG |
| 2 | E | 329 | LYS |
| 2 | E | 336 | LEU |
| 2 | E | 352 | ASP |
| 2 | E | 353 | SER |
| 2 | E | 378 | LEU |
| 2 | E | 385 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E | 389 | ARG |
| 2 | E | 394 | GLU |
| 2 | E | 397 | GLN |
| 2 | E | 417 | TYR |
| 2 | E | 422 | GLN |
| 2 | E | 425 | LEU |
| 2 | E | 426 | GLU |
| 2 | E | 428 | LEU |
| 2 | E | 432 | TYR |
| 2 | E | 437 | ILE |
| 2 | E | 445 | GLU |
| 2 | E | 446 | THR |
| 2 | E | 447 | THR |
| 2 | E | 449 | GLU |
| 2 | E | 455 | LEU |
| 2 | E | 467 | HIS |
| 2 | E | 483 | LYS |
| 2 | F | 86 | LEU |
| 2 | F | 88 | ARG |
| 2 | F | 89 | ASP |
| 2 | F | 91 | LEU |
| 2 | F | 92 | LEU |
| 2 | F | 95 | CYS |
| 2 | F | 99 | PHE |
| 2 | F | 116 | THR |
| 2 | F | 117 | SER |
| 2 | F | 118 | VAL |
| 2 | F | 120 | VAL |
| 2 | F | 125 | VAL |
| 2 | F | 128 | VAL |
| 2 | F | 131 | LEU |
| 2 | F | 132 | HIS |
| 2 | F | 133 | HIS |
| 2 | F | 142 | ASP |
| 2 | F | 145 | PHE |
| 2 | F | 180 | LYS |
| 2 | F | 186 | LEU |
| 2 | F | 193 | TYR |
| 2 | F | 195 | ASN |
| 2 | F | 197 | LEU |
| 2 | F | 198 | ASP |
| 2 | F | 199 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 204 | LEU |
| 2 | F | 208 | LEU |
| 2 | F | 210 | GLN |
| 2 | F | 214 | CYS |
| 2 | F | 215 | PHE |
| 2 | F | 223 | GLN |
| 2 | F | 226 | ASN |
| 2 | F | 230 | SER |
| 2 | F | 231 | ILE |
| 2 | F | 236 | GLU |
| 2 | F | 238 | SER |
| 2 | F | 244 | PRO |
| 2 | F | 245 | PRO |
| 2 | F | 246 | ARG |
| 2 | F | 247 | THR |
| 2 | F | 251 | TRP |
| 2 | F | 253 | ASP |
| 2 | F | 254 | PHE |
| 2 | F | 256 | LEU |
| 2 | F | 279 | GLN |
| 2 | F | 280 | ASP |
| 2 | F | 281 | GLU |
| 2 | F | 285 | LYS |
| 2 | F | 298 | GLU |
| 2 | F | 299 | LEU |
| 2 | F | 308 | ASP |
| 2 | F | 309 | HIS |
| 2 | F | 310 | GLU |
| 2 | F | 320 | SER |
| 2 | F | 321 | LYS |
| 2 | F | 322 | LEU |
| 2 | F | 325 | ARG |
| 2 | F | 328 | ARG |
| 2 | F | 330 | ASN |
| 2 | F | 331 | VAL |
| 2 | F | 337 | SER |
| 2 | F | 339 | ASN |
| 2 | F | 341 | ASP |
| 2 | F | 342 | LEU |
| 2 | F | 347 | LEU |
| 2 | F | 350 | LEU |
| 2 | F | 351 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 357 | THR |
| 2 | F | 364 | LYS |
| 2 | F | 367 | LEU |
| 2 | F | 369 | ARG |
| 2 | F | 387 | VAL |
| 2 | F | 389 | ARG |
| 2 | F | 394 | GLU |
| 2 | F | 395 | LEU |
| 2 | F | 396 | ARG |
| 2 | F | 400 | GLN |
| 2 | F | 402 | LEU |
| 2 | F | 403 | PHE |
| 2 | F | 406 | LEU |
| 2 | F | 407 | LEU |
| 2 | F | 412 | SER |
| 2 | F | 417 | TYR |
| 2 | F | 421 | MET |
| 2 | F | 427 | GLN |
| 2 | F | 431 | LYS |
| 2 | F | 435 | MET |
| 2 | F | 439 | PHE |
| 2 | F | 446 | THR |
| 2 | F | 450 | ASN |
| 2 | F | 452 | LEU |
| 2 | F | 453 | ILE |
| 2 | F | 455 | LEU |
| 2 | F | 456 | ARG |
| 2 | F | 458 | ARG |
| 2 | F | 459 | ASP |
| 2 | F | 461 | THR |
| 2 | F | 462 | MET |
| 2 | F | 464 | GLU |
| 2 | F | 471 | LEU |
| 2 | F | 474 | PHE |
| 2 | F | 475 | LEU |
| 2 | F | 476 | ILE |
| 2 | F | 483 | LYS |
| 2 | F | 485 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 110 | HIS |
| 1 | A | 155 | ASN |
| 1 | A | 238 | GLN |
| 1 | A | 264 | GLN |
| 1 | A | 308 | GLN |
| 1 | A | 388 | ASN |
| 1 | A | 390 | GLN |
| 1 | A | 438 | ASN |
| 1 | A | 468 | ASN |
| 1 | A | 564 | GLN |
| 1 | A | 565 | HIS |
| 1 | A | 630 | ASN |
| 1 | A | 663 | GLN |
| 1 | A | 666 | GLN |
| 1 | A | 729 | GLN |
| 1 | A | 736 | ASN |
| 1 | A | 758 | ASN |
| 1 | A | 795 | ASN |
| 1 | A | 879 | GLN |
| 1 | A | 922 | GLN |
| 1 | A | 970 | ASN |
| 1 | A | 976 | GLN |
| 1 | A | 1023 | GLN |
| 1 | A | 1029 | GLN |
| 1 | A | 1037 | GLN |
| 1 | A | 1059 | ASN |
| 1 | A | 1202 | ASN |
| 1 | A | 1214 | GLN |
| 1 | A | 1222 | GLN |
| 1 | A | 1236 | GLN |
| 2 | B | 74 | GLN |
| 2 | B | 84 | GLN |
| 2 | B | 96 | HIS |
| 2 | B | 109 | ASN |
| 2 | B | 124 | GLN |
| 2 | B | 195 | ASN |
| 2 | B | 201 | ASN |
| 2 | B | 250 | GLN |
| 2 | B | 261 | GLN |
| 2 | B | 287 | ASN |
| 2 | B | 292 | ASN |
| 2 | B | 305 | ASN |
| 2 | B | 313 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 318 | ASN |
| 2 | B | 323 | HIS |
| 2 | B | 422 | GLN |
| 2 | B | 427 | GLN |
| 2 | C | 74 | GLN |
| 2 | C | 109 | ASN |
| 2 | C | 124 | GLN |
| 2 | C | 187 | HIS |
| 2 | C | 279 | GLN |
| 2 | C | 292 | ASN |
| 2 | C | 454 | HIS |
| 1 | D | 71 | HIS |
| 1 | D | 86 | GLN |
| 1 | D | 106 | HIS |
| 1 | D | 110 | HIS |
| 1 | D | 115 | GLN |
| 1 | D | 138 | HIS |
| 1 | D | 155 | ASN |
| 1 | D | 258 | GLN |
| 1 | D | 277 | HIS |
| 1 | D | 281 | GLN |
| 1 | D | 298 | HIS |
| 1 | D | 317 | GLN |
| 1 | D | 394 | GLN |
| 1 | D | 404 | HIS |
| 1 | D | 438 | ASN |
| 1 | D | 439 | GLN |
| 1 | D | 440 | ASN |
| 1 | D | 456 | GLN |
| 1 | D | 472 | GLN |
| 1 | D | 493 | GLN |
| 1 | D | 527 | GLN |
| 1 | D | 630 | ASN |
| 1 | D | 663 | GLN |
| 1 | D | 671 | GLN |
| 1 | D | 733 | HIS |
| 1 | D | 736 | ASN |
| 1 | D | 795 | ASN |
| 1 | D | 811 | GLN |
| 1 | D | 970 | ASN |
| 1 | D | 976 | GLN |
| 1 | D | 983 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 1037 | GLN |
| 1 | D | 1059 | ASN |
| 1 | D | 1134 | HIS |
| 1 | D | 1175 | GLN |
| 1 | D | 1236 | GLN |
| 2 | E | 84 | GLN |
| 2 | E | 96 | HIS |
| 2 | E | 124 | GLN |
| 2 | E | 184 | ASN |
| 2 | E | 210 | GLN |
| 2 | E | 216 | HIS |
| 2 | E | 249 | ASN |
| 2 | E | 250 | GLN |
| 2 | E | 272 | ASN |
| 2 | E | 292 | ASN |
| 2 | E | 318 | ASN |
| 2 | E | 323 | HIS |
| 2 | E | 339 | ASN |
| 2 | E | 400 | GLN |
| 2 | E | 422 | GLN |
| 2 | E | 427 | GLN |
| 2 | E | 450 | ASN |
| 2 | E | 454 | HIS |
| 2 | F | 74 | GLN |
| 2 | F | 84 | GLN |
| 2 | F | 187 | HIS |
| 2 | F | 192 | HIS |
| 2 | F | 279 | GLN |
| 2 | F | 292 | ASN |
| 2 | F | 339 | ASN |
| 2 | F | 400 | GLN |
| 2 | F | 404 | ASN |
| 2 | F | 409 | ASN |
| 2 | F | 454 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|--------|
| 1 | A | 1093/1172 (93%) | 0.20 | 58 (5%) | 27 | 17 | 27, 80, 112, 124 | 0 |
| 1 | D | 1094/1172 (93%) | 0.12 | 47 (4%) | 36 | 25 | 27, 81, 113, 124 | 0 |
| 2 | B | 355/427 (83%) | 0.40 | 29 (8%) | 12 | 9 | 81, 111, 129, 141 | 0 |
| 2 | C | 396/427 (92%) | 0.28 | 19 (4%) | 31 | 21 | 42, 85, 113, 127 | 1 (0%) |
| 2 | E | 355/427 (83%) | 0.38 | 30 (8%) | 11 | 8 | 64, 108, 129, 144 | 0 |
| 2 | F | 396/427 (92%) | 0.17 | 21 (5%) | 27 | 17 | 42, 87, 114, 128 | 0 |
| All | All | 3689/4052 (91%) | 0.22 | 204 (5%) | 26 | 17 | 27, 88, 120, 144 | 1 (0%) |

All (204) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 267 | ALA | 7.4 |
| 1 | D | 583 | PRO | 6.8 |
| 2 | F | 327 | GLY | 6.7 |
| 1 | D | 277 | HIS | 6.1 |
| 1 | A | 563 | PRO | 6.1 |
| 2 | E | 334 | CYS | 6.0 |
| 2 | E | 335 | VAL | 6.0 |
| 2 | E | 305 | ASN | 5.9 |
| 1 | A | 748 | TRP | 5.7 |
| 1 | D | 1003 | TRP | 5.5 |
| 1 | A | 750 | PHE | 5.4 |
| 1 | A | 272 | SER | 5.0 |
| 2 | B | 179 | GLY | 5.0 |
| 1 | D | 582 | ASP | 4.9 |
| 1 | D | 866 | ARG | 4.8 |
| 1 | A | 281 | GLN | 4.6 |
| 1 | A | 723 | GLY | 4.5 |
| 2 | C | 386 | ASP | 4.5 |
| 2 | E | 299 | LEU | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 582 | ASP | 4.4 |
| 2 | B | 241 | TRP | 4.4 |
| 1 | D | 918 | TRP | 4.3 |
| 1 | A | 654 | SER | 4.3 |
| 1 | D | 1063 | SER | 4.0 |
| 1 | A | 91 | GLY | 3.9 |
| 2 | F | 178 | SER | 3.9 |
| 1 | D | 723 | GLY | 3.9 |
| 1 | A | 152 | GLU | 3.9 |
| 1 | D | 591 | LEU | 3.8 |
| 1 | D | 1239 | PRO | 3.8 |
| 2 | B | 180 | LYS | 3.7 |
| 1 | D | 221 | TYR | 3.7 |
| 2 | E | 336 | LEU | 3.6 |
| 1 | A | 241 | PRO | 3.5 |
| 2 | F | 423 | SER | 3.5 |
| 1 | A | 233 | TYR | 3.5 |
| 2 | B | 335 | VAL | 3.5 |
| 2 | E | 284 | ARG | 3.5 |
| 1 | A | 592 | LEU | 3.5 |
| 1 | D | 590 | SER | 3.4 |
| 2 | C | 137 | PRO | 3.4 |
| 2 | E | 136 | GLY | 3.4 |
| 1 | A | 277 | HIS | 3.4 |
| 2 | E | 204 | LEU | 3.4 |
| 1 | A | 1063 | SER | 3.4 |
| 2 | B | 243 | THR | 3.3 |
| 1 | A | 265 | LEU | 3.3 |
| 1 | A | 235 | TRP | 3.3 |
| 1 | A | 538 | GLU | 3.3 |
| 1 | D | 1090 | GLU | 3.3 |
| 1 | D | 178 | TYR | 3.3 |
| 1 | D | 90 | GLN | 3.2 |
| 1 | A | 590 | SER | 3.2 |
| 2 | B | 131 | LEU | 3.2 |
| 1 | D | 219 | ALA | 3.2 |
| 2 | C | 449 | GLU | 3.2 |
| 2 | B | 200 | VAL | 3.2 |
| 1 | D | 89 | GLY | 3.2 |
| 2 | B | 428 | LEU | 3.1 |
| 2 | E | 438 | LEU | 3.1 |
| 2 | F | 419 | GLU | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 558 | LEU | 3.1 |
| 2 | B | 462 | MET | 3.1 |
| 1 | A | 219 | ALA | 3.1 |
| 1 | A | 537 | GLU | 3.1 |
| 1 | A | 1054 | GLU | 3.0 |
| 2 | E | 245 | PRO | 3.0 |
| 1 | D | 195 | LEU | 3.0 |
| 1 | D | 721 | ALA | 3.0 |
| 1 | A | 1185 | ILE | 3.0 |
| 2 | B | 250 | GLN | 3.0 |
| 2 | E | 454 | HIS | 3.0 |
| 1 | D | 758 | ASN | 2.9 |
| 2 | E | 133 | HIS | 2.9 |
| 1 | D | 617 | ARG | 2.9 |
| 2 | E | 388 | GLY | 2.9 |
| 2 | E | 243 | THR | 2.9 |
| 1 | A | 94 | MET | 2.9 |
| 2 | C | 324 | GLY | 2.9 |
| 2 | E | 137 | PRO | 2.9 |
| 1 | D | 520 | ALA | 2.9 |
| 2 | B | 205 | PRO | 2.8 |
| 2 | F | 422 | GLN | 2.8 |
| 2 | F | 341 | ASP | 2.8 |
| 2 | E | 275 | SER | 2.8 |
| 1 | A | 1064 | ILE | 2.8 |
| 2 | B | 456 | ARG | 2.8 |
| 1 | D | 1045 | ALA | 2.8 |
| 1 | D | 1212 | ILE | 2.8 |
| 1 | D | 753 | PRO | 2.8 |
| 1 | D | 519 | GLY | 2.7 |
| 2 | B | 130 | ALA | 2.7 |
| 2 | E | 179 | GLY | 2.7 |
| 2 | B | 334 | CYS | 2.7 |
| 1 | A | 164 | PRO | 2.7 |
| 1 | A | 753 | PRO | 2.7 |
| 1 | D | 929 | THR | 2.7 |
| 2 | C | 178 | SER | 2.7 |
| 1 | D | 197 | PHE | 2.7 |
| 1 | A | 710 | ALA | 2.7 |
| 1 | A | 197 | PHE | 2.7 |
| 2 | F | 78 | PHE | 2.7 |
| 1 | D | 235 | TRP | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | D | 368 | PRO | 2.6 |
| 1 | A | 1093 | MET | 2.6 |
| 2 | B | 445 | GLU | 2.6 |
| 1 | A | 264 | GLN | 2.6 |
| 2 | B | 427 | GLN | 2.6 |
| 1 | A | 758 | ASN | 2.6 |
| 2 | B | 133 | HIS | 2.6 |
| 2 | B | 336 | LEU | 2.6 |
| 2 | C | 442 | LEU | 2.6 |
| 2 | B | 328 | ARG | 2.6 |
| 1 | D | 500 | ALA | 2.6 |
| 1 | D | 283 | LEU | 2.6 |
| 2 | E | 267 | ALA | 2.6 |
| 1 | D | 1012 | VAL | 2.6 |
| 2 | F | 244 | PRO | 2.6 |
| 1 | A | 867 | PRO | 2.5 |
| 2 | B | 300 | ILE | 2.5 |
| 2 | C | 454 | HIS | 2.5 |
| 2 | C | 385 | LEU | 2.5 |
| 1 | A | 841 | LEU | 2.5 |
| 2 | F | 390 | GLY | 2.5 |
| 2 | F | 224 | ILE | 2.5 |
| 1 | D | 641 | GLU | 2.5 |
| 2 | C | 333 | PRO | 2.5 |
| 2 | F | 85 | GLN | 2.5 |
| 1 | D | 234 | SER | 2.5 |
| 1 | A | 199 | VAL | 2.4 |
| 1 | D | 1008 | LEU | 2.4 |
| 2 | C | 77 | HIS | 2.4 |
| 2 | E | 306 | LEU | 2.4 |
| 1 | D | 585 | TRP | 2.4 |
| 1 | A | 918 | TRP | 2.4 |
| 1 | A | 1126 | ASP | 2.4 |
| 2 | E | 198 | ASP | 2.4 |
| 1 | A | 956 | GLY | 2.4 |
| 1 | A | 237 | SER | 2.4 |
| 2 | B | 372 | LEU | 2.4 |
| 1 | A | 273 | PHE | 2.4 |
| 1 | A | 614 | TYR | 2.4 |
| 2 | C | 219 | PHE | 2.3 |
| 1 | A | 1090 | GLU | 2.3 |
| 1 | D | 363 | TYR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | F | 204 | LEU | 2.3 |
| 1 | A | 559 | LEU | 2.3 |
| 1 | A | 591 | LEU | 2.3 |
| 2 | B | 291 | TYR | 2.3 |
| 2 | E | 203 | ARG | 2.3 |
| 1 | A | 1048 | ALA | 2.3 |
| 2 | C | 59 | ALA | 2.3 |
| 1 | D | 615 | SER | 2.3 |
| 2 | C | 439 | PHE | 2.3 |
| 2 | E | 349 | TYR | 2.3 |
| 1 | D | 150 | TYR | 2.3 |
| 1 | A | 266 | VAL | 2.3 |
| 2 | F | 411 | ILE | 2.2 |
| 2 | E | 429 | TYR | 2.2 |
| 1 | A | 1003 | TRP | 2.2 |
| 2 | C | 444 | THR | 2.2 |
| 2 | B | 258 | HIS | 2.2 |
| 2 | E | 483 | LYS | 2.2 |
| 1 | D | 673 | ALA | 2.2 |
| 2 | E | 117 | SER | 2.2 |
| 2 | F | 386 | ASP | 2.2 |
| 1 | A | 208 | CYS | 2.2 |
| 2 | C | 278 | CYS | 2.2 |
| 1 | A | 866 | ARG | 2.2 |
| 2 | F | 129 | ASP | 2.2 |
| 1 | A | 239 | LEU | 2.2 |
| 1 | D | 94 | MET | 2.2 |
| 1 | A | 560 | PRO | 2.2 |
| 1 | D | 228 | LEU | 2.1 |
| 2 | E | 417 | TYR | 2.1 |
| 2 | B | 444 | THR | 2.1 |
| 2 | C | 289 | LEU | 2.1 |
| 2 | E | 485 | VAL | 2.1 |
| 1 | A | 1233 | LYS | 2.1 |
| 2 | C | 244 | PRO | 2.1 |
| 2 | F | 333 | PRO | 2.1 |
| 2 | C | 264 | ARG | 2.1 |
| 1 | D | 1126 | ASP | 2.1 |
| 1 | D | 748 | TRP | 2.1 |
| 1 | A | 206 | GLY | 2.1 |
| 2 | E | 121 | PHE | 2.1 |
| 1 | A | 943 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 587 | PRO | 2.1 |
| 1 | A | 155 | ASN | 2.1 |
| 2 | F | 308 | ASP | 2.1 |
| 1 | A | 583 | PRO | 2.1 |
| 2 | F | 382 | LYS | 2.1 |
| 2 | F | 278 | CYS | 2.0 |
| 2 | B | 110 | LEU | 2.0 |
| 2 | F | 134 | LYS | 2.0 |
| 1 | D | 995 | TYR | 2.0 |
| 2 | B | 137 | PRO | 2.0 |
| 2 | C | 298 | GLU | 2.0 |
| 2 | E | 415 | PRO | 2.0 |
| 2 | B | 292 | ASN | 2.0 |
| 2 | B | 404 | ASN | 2.0 |
| 1 | A | 501 | LYS | 2.0 |
| 2 | E | 396 | ARG | 2.0 |
| 2 | F | 122 | ARG | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.