



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:30 pm GMT

PDB ID : 3V0C
Title : 4.3 angstrom crystal structure of an inactive BoNT/A (E224Q/R363A/Y366F)
Authors : Gu, S.; Rumpel, S.; Zhou, J.; Strotmeier, J.; Bigalke, H.; Perry, K.; Shoemaker, C.B.; Rummel, A.; Jin, R.
Deposited on : 2011-12-07
Resolution : 4.30 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 : trunk28620
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) : recalc28949

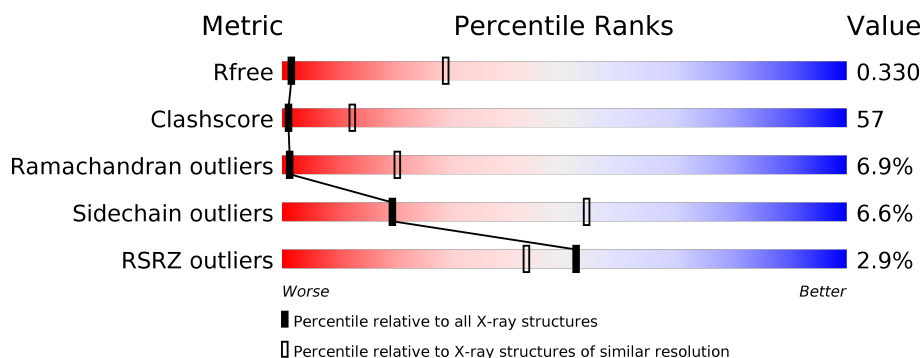
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 1002 (4.92-3.62) |
| Clashscore | 112137 | 1001 (4.92-3.68) |
| Ramachandran outliers | 110173 | 1012 (4.92-3.64) |
| Sidechain outliers | 110143 | 1021 (4.92-3.62) |
| RSRZ outliers | 101464 | 1009 (4.92-3.62) |

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 | 1312 | <div> <div>3%</div> <div>28%</div> <div>59%</div> <div>9%</div> <div>.</div> </div> |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10390 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 BoNT/A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 1277 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10389 | 6664 | 1714 | 1979 | 32 | | | |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 224 | GLN | GLU | ENGINEERED MUTATION | UNP Q7B8V4 |
| A | 363 | ALA | ARG | ENGINEERED MUTATION | UNP Q7B8V4 |
| A | 366 | PHE | TYR | ENGINEERED MUTATION | UNP Q7B8V4 |
| A | 1158 | ALA | THR | CONFLICT | UNP Q7B8V4 |
| A | 1297 | VAL | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1298 | PRO | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1299 | PRO | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1300 | THR | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1301 | PRO | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1302 | GLY | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1303 | SER | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1304 | ALA | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1305 | TRP | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1306 | SER | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1307 | HIS | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1308 | PRO | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1309 | GLN | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1310 | PHE | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1311 | GLU | - | EXPRESSION TAG | UNP Q7B8V4 |
| A | 1312 | LYS | - | EXPRESSION TAG | UNP Q7B8V4 |

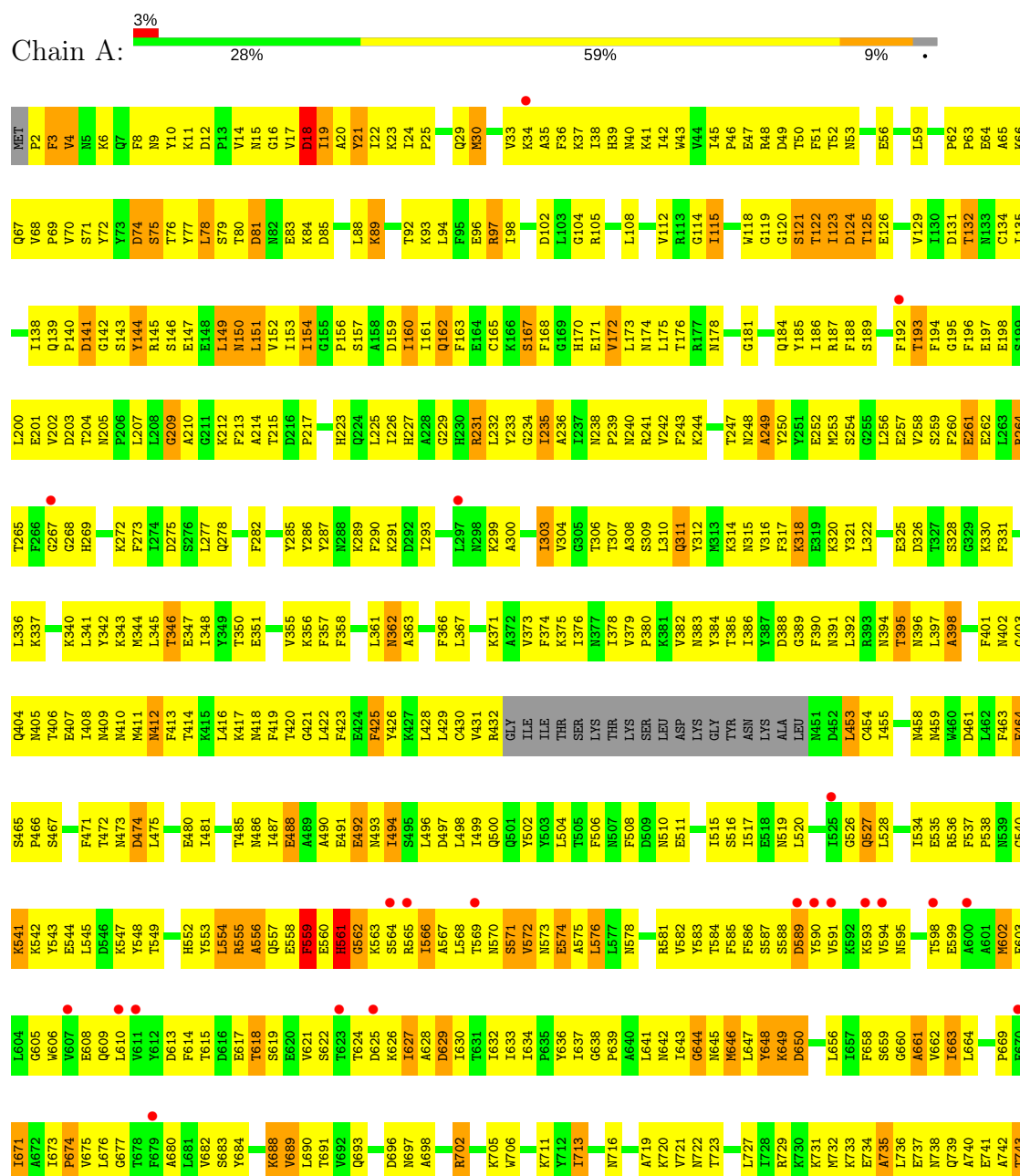
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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: BoNT/A



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Y1267 | Y1268 | R1269 | Q1270 | I1271 | E1272 | R1273 | L1276 | T1277 | L1278 | G1279 | C1280 | S1281 | W1282 | E1283 | F1284 | I1285 | P1286 | V1287 | D1288 | D1289 | G1290 | W1291 | G1292 | E1293 | L1296 | VAL | PRO | THR | PRO | GLY | SER | ALA | TRP | SER | HIS | PRO | PHE | GLU | LYS | | | | | | | | | | | | | | | | | | |
| Q1199 | E1203 | K1204 | I1205 | L1206 | L1209 | E1210 | T1211 | P1212 | L1213 | Y1214 | G1215 | N1216 | L1217 | S1218 | Q1219 | V1220 | V1221 | N1227 | D1228 | Q1229 | G1230 | I1231 | T1232 | N1233 | K1234 | C1235 | K1236 | W1237 | N1238 | L1239 | Q1240 | D1241 | N1242 | N1243 | G1244 | N1245 | I1247 | G1248 | F1249 | I1250 | G1251 | F1252 | H1253 | G1254 | F1255 | N1256 | A1259 | K1260 | L1261 | V1262 | A1263 | S1264 | W1266 | | | | |
| R1131 | G1132 | Y1133 | M1134 | Y1135 | L1136 | K1137 | G1138 | P1139 | V1143 | M1144 | T1145 | T1146 | M1147 | T1148 | Y1149 | L1150 | M1151 | L1154 | Y1155 | R1156 | K1159 | F1160 | I1161 | I1162 | K1163 | K1164 | Y1165 | A1166 | S1167 | G1168 | K1169 | K1170 | D1171 | W1172 | I1173 | V1174 | R1175 | M1176 | V1180 | Y1181 | N1182 | M1183 | V1186 | K1189 | E1190 | Y1191 | R1192 | L1193 | A1194 | T1195 | M1196 | A1197 | S1198 | | | | |
| Y1066 | I1067 | W1068 | I1069 | K1070 | Y1071 | F1072 | M1073 | L1074 | F1075 | D1076 | K1077 | E1078 | L1079 | M1080 | K1081 | E1082 | E1083 | I1084 | K1085 | D1086 | L1087 | Y1088 | D1089 | N1090 | Q1091 | I1096 | L1097 | K1098 | D1099 | F1100 | W1101 | G1102 | D1103 | Y1104 | L1105 | Q1106 | K1109 | P1110 | Y1111 | Y1112 | M1113 | L1114 | M1115 | L1116 | Y1117 | D1118 | P1119 | Y1122 | V1123 | D1124 | V1125 | W1126 | N1127 | V1128 | I1130 | | |
| S1002 | Q1003 | M1004 | I1005 | S1008 | D1009 | Y1010 | I1011 | N1012 | K1013 | Y1014 | N1015 | F1016 | T1017 | V1018 | E1019 | L1020 | N1021 | M1022 | R1023 | L1024 | Y1025 | N1026 | S1027 | K1028 | I1029 | Y1030 | I1031 | R1034 | L1035 | I1036 | K1039 | P1040 | Y1041 | S1042 | N1043 | L1044 | G1045 | N1046 | I1047 | H1048 | A1049 | S1050 | N1051 | N1052 | I1053 | M1054 | F1055 | K1056 | L1057 | C1060 | R1061 | D1062 | T1063 | H1064 | R1065 | | |
| S942 | T943 | S944 | W945 | I946 | R947 | R948 | I949 | P950 | K951 | Y952 | F953 | N954 | S955 | I956 | S957 | L958 | N959 | N960 | E961 | Y962 | T963 | I964 | I965 | N966 | C967 | M968 | E969 | N970 | N971 | S972 | G973 | K975 | Q976 | S977 | L978 | N979 | Y980 | G981 | E982 | I984 | W985 | T986 | L987 | Q988 | D989 | T990 | Q991 | E992 | I993 | Q994 | R995 | R996 | V997 | V998 | F999 | K1000 | Y1001 |
| L808 | E809 | D812 | L815 | K816 | L819 | L820 | K821 | Y822 | I823 | Y824 | D825 | N826 | R827 | G828 | T829 | L830 | I831 | Q832 | K833 | I834 | D835 | K838 | D839 | K840 | V841 | N842 | T844 | N845 | S846 | T847 | D848 | Q852 | K855 | Y856 | V857 | D858 | N859 | Q860 | R861 | L862 | L863 | S864 | T865 | F866 | Y869 | I870 | K871 | N872 | I873 | K806 | R875 | | | | | | |
| K744 | A745 | I746 | N748 | Y749 | Q750 | Y751 | N752 | Q753 | T755 | E756 | E757 | K758 | N759 | N760 | N761 | I762 | R763 | F764 | I766 | D767 | D768 | L769 | K772 | D773 | N774 | E775 | S776 | I777 | K778 | K779 | A780 | W781 | I782 | N783 | I784 | K786 | N789 | Q790 | C791 | S792 | V793 | S794 | Y795 | L796 | M797 | N798 | I801 | P802 | Y803 | K806 | R807 | | | | | | |
| T876 | L879 | N880 | L881 | Y882 | Y883 | E884 | S885 | N886 | H887 | L888 | I889 | D890 | L891 | S892 | R893 | G897 | I898 | N899 | I900 | Q901 | K902 | K903 | F906 | D907 | P908 | I909 | D910 | N911 | Q912 | Q913 | I914 | S915 | L916 | F917 | N918 | L919 | E920 | S921 | S922 | K923 | I924 | E925 | V926 | I927 | L928 | K929 | I932 | V933 | Y934 | N935 | I870 | K871 | N872 | I873 | K806 | R875 | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 31 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 167.52Å 167.52Å 158.73Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 45.11 – 4.30 45.11 – 4.30 | Depositor EDS |
| % Data completeness (in resolution range) | 99.9 (45.11-4.30) 99.9 (45.11-4.30) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.96 (at 4.28Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.7.2_869) | Depositor |
| R, R_{free} | 0.322 , 0.349 0.312 , 0.330 | Depositor DCC |
| R_{free} test set | 912 reflections (5.11%) | DCC |
| Wilson B-factor (Å ²) | 161.8 | Xtriage |
| Anisotropy | 0.203 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 241.0 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Estimated twinning fraction | 0.021 for -h,-k,l | Xtriage |
| F_o, F_c correlation | 0.83 | EDS |
| Total number of atoms | 10390 | wwPDB-VP |
| Average B, all atoms (Å ²) | 235.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 | 1.16 | 0/10610 | 0.66 | 1/14367 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|----------|------|------------------------|---------------------|
| 1 | A | 151 | LEU | CA-CB-CG | 6.20 | 129.55 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 10389 | 0 | 10255 | 1168 | 9 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| All | All | 10390 | 0 | 10255 | 1168 | 9 |

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 57.

All (1168) 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:A:277:LEU:HD22 | 1:A:474:ASP:HB3 | 1.24 | 1.13 |
| 1:A:872:ASN:HD21 | 1:A:874:ILE:HB | 1.12 | 1.11 |
| 1:A:948:ARG:HB3 | 1:A:1068:TRP:HB2 | 1.28 | 1.10 |
| 1:A:310:LEU:HD11 | 1:A:314:LYS:HE3 | 1.38 | 1.05 |
| 1:A:1027:SER:HB2 | 1:A:1041:ILE:HD11 | 1.37 | 1.02 |
| 1:A:969:GLU:H | 1:A:972:SER:HB3 | 1.24 | 1.02 |
| 1:A:1248:GLY:HA2 | 1:A:1268:ASN:HD21 | 1.16 | 1.02 |
| 1:A:927:ILE:HG12 | 1:A:1052:ASN:HB3 | 1.36 | 1.01 |
| 1:A:346:THR:HG22 | 1:A:347:GLU:HG3 | 1.41 | 1.01 |
| 1:A:1010:TYR:HB3 | 1:A:1015:ILE:HD11 | 1.41 | 0.99 |
| 1:A:52:THR:HG22 | 1:A:528:LEU:HD11 | 1.47 | 0.96 |
| 1:A:806:LYS:HD2 | 1:A:934:TYR:HB3 | 1.48 | 0.95 |
| 1:A:910:ASP:HB3 | 1:A:913:GLN:HE21 | 1.30 | 0.95 |
| 1:A:576:LEU:HA | 1:A:581:ARG:HB2 | 1.49 | 0.95 |
| 1:A:566:ILE:HG12 | 1:A:749:TYR:CD1 | 2.02 | 0.95 |
| 1:A:763:ASN:HB2 | 1:A:765:ASN:ND2 | 1.82 | 0.95 |
| 1:A:2:PRO:HG2 | 1:A:39:HIS:CD2 | 2.03 | 0.94 |
| 1:A:629:ASP:OD1 | 1:A:630:ILE:HG13 | 1.71 | 0.91 |
| 1:A:264:ARG:HH11 | 1:A:264:ARG:HG2 | 1.33 | 0.91 |
| 1:A:217:PRO:HG2 | 1:A:378:ILE:HD11 | 1.49 | 0.90 |
| 1:A:584:THR:HG22 | 1:A:586:PHE:H | 1.38 | 0.89 |
| 1:A:242:VAL:HG11 | 1:A:257:GLU:HB2 | 1.53 | 0.89 |
| 1:A:1027:SER:HB2 | 1:A:1041:ILE:CD1 | 2.02 | 0.89 |
| 1:A:21:TYR:HE1 | 1:A:34:LYS:HB2 | 1.36 | 0.88 |
| 1:A:418:ASN:HD21 | 1:A:420:THR:HB | 1.36 | 0.88 |
| 1:A:17:VAL:HG12 | 1:A:145:ARG:HH22 | 1.39 | 0.87 |
| 1:A:428:LEU:HB3 | 1:A:542:LYS:HA | 1.57 | 0.87 |
| 1:A:559:PHE:HB3 | 1:A:582:VAL:HG22 | 1.57 | 0.86 |
| 1:A:41:LYS:HB3 | 1:A:150:ASN:HB2 | 1.58 | 0.85 |
| 1:A:49:ASP:HB3 | 1:A:187:ARG:HE | 1.41 | 0.85 |
| 1:A:815:LEU:HD23 | 1:A:845:LEU:HD11 | 1.58 | 0.85 |
| 1:A:575:ALA:O | 1:A:581:ARG:HB2 | 1.77 | 0.85 |
| 1:A:426:TYR:CE1 | 1:A:540:GLY:HA2 | 2.11 | 0.84 |
| 1:A:984:ILE:HG12 | 1:A:998:VAL:HG22 | 1.60 | 0.84 |
| 1:A:24:ILE:HD11 | 1:A:45:ILE:HD11 | 1.59 | 0.84 |
| 1:A:556:ALA:O | 1:A:583:TYR:HB3 | 1.78 | 0.84 |
| 1:A:969:GLU:N | 1:A:972:SER:HB3 | 1.93 | 0.84 |
| 1:A:755:THR:O | 1:A:756:GLU:HB2 | 1.78 | 0.84 |
| 1:A:969:GLU:H | 1:A:972:SER:CB | 1.90 | 0.84 |
| 1:A:968:MET:HG2 | 1:A:972:SER:O | 1.78 | 0.84 |
| 1:A:968:MET:HA | 1:A:972:SER:HB3 | 1.59 | 0.83 |
| 1:A:1019:ILE:HG12 | 1:A:1029:ILE:HD12 | 1.59 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:952:TYR:HB2 | 1:A:1003:GLN:HE22 | 1.43 | 0.83 |
| 1:A:122:THR:O | 1:A:126:GLU:HB3 | 1.79 | 0.83 |
| 1:A:605:GLY:HA2 | 1:A:608:GLU:OE1 | 1.77 | 0.83 |
| 1:A:22:ILE:HD13 | 1:A:35:ALA:HB3 | 1.61 | 0.83 |
| 1:A:35:ALA:HB2 | 1:A:45:ILE:HG12 | 1.61 | 0.83 |
| 1:A:43:TRP:HD1 | 1:A:149:LEU:HD21 | 1.44 | 0.83 |
| 1:A:306:THR:HG22 | 1:A:516:SER:O | 1.78 | 0.82 |
| 1:A:1163:LYS:HB2 | 1:A:1181:TYR:HB2 | 1.61 | 0.82 |
| 1:A:872:ASN:ND2 | 1:A:874:ILE:HB | 1.93 | 0.82 |
| 1:A:789:ASN:HD21 | 1:A:861:ARG:HE | 1.26 | 0.82 |
| 1:A:872:ASN:ND2 | 1:A:874:ILE:H | 1.78 | 0.82 |
| 1:A:713:ILE:HD11 | 1:A:796:LEU:HD21 | 1.61 | 0.82 |
| 1:A:594:VAL:HG12 | 1:A:746:ILE:HG21 | 1.59 | 0.82 |
| 1:A:21:TYR:CE1 | 1:A:34:LYS:HB2 | 2.15 | 0.82 |
| 1:A:573:ASN:O | 1:A:576:LEU:HG | 1.80 | 0.82 |
| 1:A:1248:GLY:HA2 | 1:A:1268:ASN:ND2 | 1.95 | 0.82 |
| 1:A:979:ASN:O | 1:A:982:GLU:HG2 | 1.79 | 0.82 |
| 1:A:70:VAL:HG12 | 1:A:161:ILE:HD11 | 1.62 | 0.81 |
| 1:A:52:THR:CG2 | 1:A:528:LEU:HD11 | 2.09 | 0.81 |
| 1:A:927:ILE:HG12 | 1:A:1052:ASN:CB | 2.10 | 0.81 |
| 1:A:624:THR:HB | 1:A:627:ILE:HD13 | 1.62 | 0.81 |
| 1:A:397:LEU:HA | 1:A:402:ASN:HB2 | 1.60 | 0.81 |
| 1:A:487:ILE:HG23 | 1:A:488:GLU:OE1 | 1.81 | 0.81 |
| 1:A:344:MET:HE3 | 1:A:502:TYR:HD2 | 1.43 | 0.81 |
| 1:A:702:ARG:HG3 | 1:A:702:ARG:HH11 | 1.46 | 0.81 |
| 1:A:473:ASN:OD1 | 1:A:475:LEU:HD12 | 1.79 | 0.81 |
| 1:A:610:LEU:HD12 | 1:A:747:ILE:HD11 | 1.63 | 0.80 |
| 1:A:1110:PRO:HB2 | 1:A:1159:LYS:HD3 | 1.63 | 0.80 |
| 1:A:1013:ARG:HG2 | 1:A:1101:TRP:HA | 1.64 | 0.80 |
| 1:A:872:ASN:HD21 | 1:A:874:ILE:CB | 1.94 | 0.80 |
| 1:A:391:ASN:HD21 | 1:A:404:GLN:HE21 | 1.25 | 0.80 |
| 1:A:464:PHE:CE2 | 1:A:466:PRO:HG3 | 2.17 | 0.80 |
| 1:A:277:LEU:HD23 | 1:A:472:THR:HG22 | 1.62 | 0.80 |
| 1:A:763:ASN:HD22 | 1:A:765:ASN:HD21 | 1.29 | 0.80 |
| 1:A:1203:GLU:O | 1:A:1204:LYS:HD3 | 1.81 | 0.80 |
| 1:A:385:THR:HG23 | 1:A:388:ASP:H | 1.47 | 0.79 |
| 1:A:643:ILE:HG21 | 1:A:664:LEU:HD23 | 1.64 | 0.79 |
| 1:A:986:THR:HG22 | 1:A:996:ARG:HB3 | 1.63 | 0.79 |
| 1:A:929:LYS:O | 1:A:932:ILE:HG22 | 1.82 | 0.79 |
| 1:A:277:LEU:CD2 | 1:A:474:ASP:HB3 | 2.10 | 0.79 |
| 1:A:1099:ASP:HB2 | 1:A:1103:ASP:H | 1.47 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:375:LYS:HB3 | 1:A:414:THR:HB | 1.63 | 0.78 |
| 1:A:122:THR:HB | 1:A:126:GLU:OE1 | 1.84 | 0.78 |
| 1:A:18:ASP:HA | 1:A:37:LYS:HB2 | 1.65 | 0.78 |
| 1:A:344:MET:HE3 | 1:A:502:TYR:CD2 | 2.19 | 0.78 |
| 1:A:961:GLU:HB2 | 1:A:979:ASN:HD22 | 1.46 | 0.78 |
| 1:A:306:THR:HG21 | 1:A:515:ILE:HG22 | 1.66 | 0.78 |
| 1:A:798:ASN:ND2 | 1:A:893:ARG:HG3 | 1.99 | 0.77 |
| 1:A:962:TYR:H | 1:A:962:TYR:HD1 | 1.32 | 0.77 |
| 1:A:1057:LEU:H | 1:A:1057:LEU:HD12 | 1.48 | 0.77 |
| 1:A:1227:ASN:ND2 | 1:A:1229:GLN:HB3 | 2.00 | 0.77 |
| 1:A:590:TYR:O | 1:A:594:VAL:HG23 | 1.84 | 0.77 |
| 1:A:1196:ASN:O | 1:A:1199:GLN:HG3 | 1.85 | 0.76 |
| 1:A:170:HIS:CD2 | 1:A:172:VAL:H | 2.02 | 0.76 |
| 1:A:1265:ASN:HA | 1:A:1268:ASN:HD22 | 1.48 | 0.76 |
| 1:A:2:PRO:O | 1:A:39:HIS:HD2 | 1.69 | 0.76 |
| 1:A:935:ASN:HA | 1:A:1049:ALA:HB2 | 1.67 | 0.76 |
| 1:A:1233:ASN:ND2 | 1:A:1271:ILE:HG23 | 2.01 | 0.76 |
| 1:A:1211:ILE:H | 1:A:1211:ILE:HD12 | 1.51 | 0.75 |
| 1:A:985:TRP:CD2 | 1:A:1019:ILE:HG21 | 2.22 | 0.75 |
| 1:A:547:LYS:NZ | 1:A:646:MET:HB3 | 2.02 | 0.75 |
| 1:A:11:LYS:NZ | 1:A:81:ASP:HB3 | 2.01 | 0.75 |
| 1:A:935:ASN:HA | 1:A:1049:ALA:CB | 2.16 | 0.75 |
| 1:A:1020:THR:HG23 | 1:A:1078:GLU:HG3 | 1.67 | 0.75 |
| 1:A:42:ILE:HD12 | 1:A:151:LEU:HD12 | 1.68 | 0.75 |
| 1:A:873:ILE:O | 1:A:876:THR:HB | 1.85 | 0.74 |
| 1:A:987:LEU:HD12 | 1:A:1041:ILE:HD13 | 1.68 | 0.74 |
| 1:A:154:ILE:H | 1:A:154:ILE:HD12 | 1.51 | 0.74 |
| 1:A:1203:GLU:HB3 | 1:A:1262:VAL:HG11 | 1.70 | 0.74 |
| 1:A:14:VAL:HG13 | 1:A:20:ALA:HA | 1.69 | 0.74 |
| 1:A:39:HIS:ND1 | 1:A:40:ASN:N | 2.35 | 0.74 |
| 1:A:903:LYS:HB2 | 1:A:922:SER:HB3 | 1.69 | 0.74 |
| 1:A:264:ARG:NH1 | 1:A:264:ARG:HG2 | 1.98 | 0.74 |
| 1:A:634:ILE:HG22 | 1:A:637:ILE:HG13 | 1.68 | 0.74 |
| 1:A:1248:GLY:CA | 1:A:1268:ASN:HD21 | 1.98 | 0.74 |
| 1:A:952:TYR:CE2 | 1:A:980:TYR:HA | 2.23 | 0.74 |
| 1:A:713:ILE:HG12 | 1:A:801:ILE:HD13 | 1.69 | 0.73 |
| 1:A:765:ASN:HB3 | 1:A:768:ASP:HB2 | 1.69 | 0.73 |
| 1:A:417:LYS:HE3 | 1:A:419:PHE:CE1 | 2.23 | 0.73 |
| 1:A:1100:PHE:HD1 | 1:A:1283:GLU:HG2 | 1.54 | 0.73 |
| 1:A:418:ASN:ND2 | 1:A:420:THR:H | 1.86 | 0.73 |
| 1:A:584:THR:HG22 | 1:A:586:PHE:N | 2.02 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:809:GLU:HG2 | 1:A:934:TYR:CE2 | 2.23 | 0.73 |
| 1:A:641:LEU:HB2 | 1:A:643:ILE:HG12 | 1.68 | 0.73 |
| 1:A:584:THR:HG22 | 1:A:585:PHE:N | 2.01 | 0.73 |
| 1:A:984:ILE:HG23 | 1:A:998:VAL:HG22 | 1.69 | 0.73 |
| 1:A:622:SER:HB2 | 1:A:633:ILE:HB | 1.70 | 0.73 |
| 1:A:918:ASN:ND2 | 1:A:1065:ARG:HB3 | 2.03 | 0.73 |
| 1:A:102:ASP:HB2 | 1:A:357:PHE:HE2 | 1.54 | 0.73 |
| 1:A:882:ARG:HH22 | 1:A:1073:ASN:ND2 | 1.86 | 0.73 |
| 1:A:17:VAL:HG12 | 1:A:145:ARG:NH2 | 2.03 | 0.73 |
| 1:A:790:GLN:O | 1:A:794:SER:HB3 | 1.89 | 0.72 |
| 1:A:1155:TYR:CE2 | 1:A:1287:VAL:HG13 | 2.23 | 0.72 |
| 1:A:420:THR:HG22 | 1:A:420:THR:O | 1.90 | 0.72 |
| 1:A:395:THR:C | 1:A:397:LEU:H | 1.93 | 0.72 |
| 1:A:201:GLU:HG3 | 1:A:361:LEU:CD1 | 2.20 | 0.72 |
| 1:A:644:GLY:O | 1:A:647:LEU:HG | 1.90 | 0.72 |
| 1:A:167:SER:HB3 | 1:A:231:ARG:HH12 | 1.53 | 0.72 |
| 1:A:626:LYS:C | 1:A:627:ILE:HD12 | 2.10 | 0.72 |
| 1:A:210:ALA:H | 1:A:405:ASN:ND2 | 1.88 | 0.72 |
| 1:A:755:THR:OG1 | 1:A:757:GLU:HG2 | 1.89 | 0.72 |
| 1:A:429:LEU:HD23 | 1:A:543:TYR:HB2 | 1.72 | 0.71 |
| 1:A:702:ARG:O | 1:A:705:LYS:HB3 | 1.89 | 0.71 |
| 1:A:153:ILE:HD13 | 1:A:186:ILE:HB | 1.69 | 0.71 |
| 1:A:18:ASP:HA | 1:A:37:LYS:CB | 2.20 | 0.71 |
| 1:A:1011:ILE:HG21 | 1:A:1291:TRP:HZ3 | 1.54 | 0.71 |
| 1:A:306:THR:HG21 | 1:A:515:ILE:CG2 | 2.21 | 0.71 |
| 1:A:226:ILE:HD13 | 1:A:350:THR:HA | 1.73 | 0.71 |
| 1:A:946:TRP:HB2 | 1:A:1070:LYS:HB3 | 1.73 | 0.70 |
| 1:A:249:ALA:HB3 | 1:A:252:GLU:HG3 | 1.72 | 0.70 |
| 1:A:481:ILE:HD13 | 1:A:698:ALA:HA | 1.74 | 0.70 |
| 1:A:201:GLU:HG3 | 1:A:361:LEU:HD11 | 1.73 | 0.70 |
| 1:A:974:TRP:HB2 | 1:A:985:TRP:CH2 | 2.27 | 0.70 |
| 1:A:798:ASN:HD22 | 1:A:893:ARG:CG | 2.05 | 0.70 |
| 1:A:264:ARG:HH11 | 1:A:264:ARG:CG | 2.05 | 0.70 |
| 1:A:210:ALA:N | 1:A:405:ASN:ND2 | 2.40 | 0.70 |
| 1:A:598:THR:HG22 | 1:A:602:MET:O | 1.92 | 0.70 |
| 1:A:210:ALA:N | 1:A:405:ASN:HD21 | 1.90 | 0.70 |
| 1:A:1249:PHE:CE2 | 1:A:1271:ILE:HD12 | 2.27 | 0.69 |
| 1:A:1044:LEU:HD23 | 1:A:1047:ILE:HD11 | 1.74 | 0.69 |
| 1:A:990:THR:C | 1:A:992:GLU:H | 1.95 | 0.69 |
| 1:A:1193:LEU:HD11 | 1:A:1206:LEU:HD13 | 1.73 | 0.69 |
| 1:A:549:THR:H | 1:A:552:HIS:HD2 | 1.41 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:575:ALA:HB1 | 1:A:582:VAL:O | 1.92 | 0.69 |
| 1:A:184:GLN:OE1 | 1:A:231:ARG:HD3 | 1.92 | 0.69 |
| 1:A:49:ASP:CB | 1:A:187:ARG:HE | 2.05 | 0.69 |
| 1:A:757:GLU:HB2 | 1:A:760:ASN:ND2 | 2.08 | 0.69 |
| 1:A:181:GLY:HA2 | 1:A:231:ARG:O | 1.93 | 0.68 |
| 1:A:749:TYR:O | 1:A:752:ASN:HB3 | 1.92 | 0.68 |
| 1:A:1096:ILE:O | 1:A:1098:LYS:HE3 | 1.93 | 0.68 |
| 1:A:1041:ILE:O | 1:A:1041:ILE:HG22 | 1.93 | 0.68 |
| 1:A:789:ASN:ND2 | 1:A:861:ARG:HE | 1.92 | 0.68 |
| 1:A:967:CYS:SG | 1:A:1050:SER:HB2 | 2.34 | 0.68 |
| 1:A:745:ALA:O | 1:A:748:ASN:HB3 | 1.94 | 0.68 |
| 1:A:202:VAL:HG11 | 1:A:778:ASN:O | 1.93 | 0.68 |
| 1:A:1168:GLY:C | 1:A:1170:LYS:H | 1.95 | 0.68 |
| 1:A:1210:GLU:HG3 | 1:A:1212:PRO:HD2 | 1.75 | 0.68 |
| 1:A:944:SER:HB3 | 1:A:1018:THR:HG23 | 1.75 | 0.68 |
| 1:A:1227:ASN:O | 1:A:1230:GLY:N | 2.27 | 0.68 |
| 1:A:193:THR:HG21 | 1:A:215:THR:O | 1.93 | 0.68 |
| 1:A:1010:TYR:CB | 1:A:1015:ILE:HD11 | 2.19 | 0.68 |
| 1:A:310:LEU:CD1 | 1:A:314:LYS:HE3 | 2.20 | 0.68 |
| 1:A:212:LYS:HE2 | 1:A:371:LYS:HB2 | 1.76 | 0.67 |
| 1:A:463:PHE:CE1 | 1:A:727:LEU:HD23 | 2.29 | 0.67 |
| 1:A:23:LYS:NZ | 1:A:23:LYS:HB2 | 2.09 | 0.67 |
| 1:A:409:ASN:OD1 | 1:A:412:ASN:HB2 | 1.94 | 0.67 |
| 1:A:426:TYR:CZ | 1:A:540:GLY:HA2 | 2.28 | 0.67 |
| 1:A:105:ARG:HG2 | 1:A:508:PHE:CE1 | 2.28 | 0.67 |
| 1:A:1023:ARG:HD3 | 1:A:1023:ARG:O | 1.95 | 0.67 |
| 1:A:585:PHE:HB3 | 1:A:639:PRO:O | 1.95 | 0.67 |
| 1:A:656:LEU:HA | 1:A:663:ILE:HD12 | 1.76 | 0.67 |
| 1:A:1241:ASP:OD2 | 1:A:1245:ASN:HB2 | 1.95 | 0.67 |
| 1:A:984:ILE:HG23 | 1:A:998:VAL:CG2 | 2.24 | 0.67 |
| 1:A:43:TRP:CD1 | 1:A:149:LEU:HD21 | 2.29 | 0.67 |
| 1:A:1099:ASP:OD2 | 1:A:1103:ASP:HB2 | 1.96 | 0.66 |
| 1:A:820:LEU:HD21 | 1:A:842:ASN:OD1 | 1.94 | 0.66 |
| 1:A:30:MET:HE2 | 1:A:33:VAL:HG23 | 1.76 | 0.66 |
| 1:A:22:ILE:HD11 | 1:A:43:TRP:CZ3 | 2.30 | 0.66 |
| 1:A:646:MET:O | 1:A:647:LEU:HD23 | 1.96 | 0.66 |
| 1:A:713:ILE:HD11 | 1:A:796:LEU:CD2 | 2.25 | 0.66 |
| 1:A:145:ARG:HA | 1:A:519:ASN:OD1 | 1.96 | 0.66 |
| 1:A:176:THR:CG2 | 1:A:236:ALA:HB3 | 2.26 | 0.66 |
| 1:A:455:ILE:CG2 | 1:A:555:ARG:HD2 | 2.26 | 0.66 |
| 1:A:275:ASP:OD2 | 1:A:472:THR:HB | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:500:GLN:HE22 | 1:A:504:LEU:HD21 | 1.60 | 0.66 |
| 1:A:830:LEU:HB2 | 1:A:834:VAL:HG13 | 1.76 | 0.66 |
| 1:A:1193:LEU:C | 1:A:1193:LEU:HD12 | 2.16 | 0.66 |
| 1:A:209:GLY:HA3 | 1:A:405:ASN:HD22 | 1.61 | 0.66 |
| 1:A:1155:TYR:CD2 | 1:A:1287:VAL:HG22 | 2.31 | 0.65 |
| 1:A:181:GLY:HA3 | 1:A:232:LEU:O | 1.97 | 0.65 |
| 1:A:839:ASP:O | 1:A:843:ASN:HB2 | 1.97 | 0.65 |
| 1:A:986:THR:HG22 | 1:A:996:ARG:CB | 2.26 | 0.65 |
| 1:A:1101:TRP:CZ3 | 1:A:1286:PRO:O | 2.49 | 0.65 |
| 1:A:643:ILE:O | 1:A:645:ASN:N | 2.28 | 0.65 |
| 1:A:671:ILE:N | 1:A:671:ILE:HD12 | 2.12 | 0.65 |
| 1:A:985:TRP:HB2 | 1:A:1019:ILE:HD13 | 1.77 | 0.65 |
| 1:A:253:MET:HG3 | 1:A:463:PHE:O | 1.97 | 0.65 |
| 1:A:485:THR:HB | 1:A:697:ASN:HD22 | 1.60 | 0.65 |
| 1:A:576:LEU:HA | 1:A:581:ARG:CB | 2.27 | 0.65 |
| 1:A:754:TYR:OH | 1:A:757:GLU:HG3 | 1.96 | 0.65 |
| 1:A:798:ASN:HD22 | 1:A:893:ARG:HG3 | 1.58 | 0.65 |
| 1:A:968:MET:CA | 1:A:972:SER:HB3 | 2.27 | 0.65 |
| 1:A:115:ILE:HG22 | 1:A:317:PHE:HE1 | 1.62 | 0.64 |
| 1:A:526:GLY:O | 1:A:527:GLN:HB2 | 1.95 | 0.64 |
| 1:A:557:GLN:O | 1:A:738:ASN:HB3 | 1.95 | 0.64 |
| 1:A:1145:THR:HG22 | 1:A:1145:THR:O | 1.96 | 0.64 |
| 1:A:22:ILE:CD1 | 1:A:35:ALA:HB3 | 2.26 | 0.64 |
| 1:A:22:ILE:HD12 | 1:A:22:ILE:N | 2.12 | 0.64 |
| 1:A:1061:ARG:HG2 | 1:A:1061:ARG:HH11 | 1.61 | 0.64 |
| 1:A:356:LYS:HD2 | 1:A:496:LEU:HD21 | 1.79 | 0.64 |
| 1:A:948:ARG:HH11 | 1:A:948:ARG:HG2 | 1.62 | 0.64 |
| 1:A:1265:ASN:HA | 1:A:1268:ASN:ND2 | 2.12 | 0.64 |
| 1:A:406:THR:HG22 | 1:A:413:PHE:CG | 2.33 | 0.64 |
| 1:A:634:ILE:HD11 | 1:A:783:ASN:HB3 | 1.79 | 0.64 |
| 1:A:634:ILE:HG12 | 1:A:784:ILE:HG12 | 1.78 | 0.64 |
| 1:A:463:PHE:CZ | 1:A:727:LEU:HD23 | 2.33 | 0.64 |
| 1:A:11:LYS:HZ1 | 1:A:81:ASP:CB | 2.11 | 0.64 |
| 1:A:882:ARG:HA | 1:A:912:ASN:HD21 | 1.61 | 0.64 |
| 1:A:1296:LEU:HD23 | 1:A:1296:LEU:H | 1.62 | 0.64 |
| 1:A:464:PHE:O | 1:A:465:SER:HB3 | 1.96 | 0.64 |
| 1:A:628:ALA:O | 1:A:629:ASP:HB2 | 1.97 | 0.64 |
| 1:A:1080:ASN:O | 1:A:1084:ILE:HG12 | 1.97 | 0.64 |
| 1:A:306:THR:HG23 | 1:A:517:ILE:HG22 | 1.80 | 0.64 |
| 1:A:1195:THR:HB | 1:A:1206:LEU:HD23 | 1.80 | 0.63 |
| 1:A:733:LYS:HB2 | 1:A:781:MET:CE | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:24:ILE:CD1 | 1:A:45:ILE:HD11 | 2.28 | 0.63 |
| 1:A:167:SER:HB3 | 1:A:231:ARG:NH1 | 2.13 | 0.63 |
| 1:A:1192:ARG:HD3 | 1:A:1219:GLN:OE1 | 1.98 | 0.63 |
| 1:A:913:GLN:HG2 | 1:A:1070:LYS:HE2 | 1.79 | 0.63 |
| 1:A:987:LEU:HD12 | 1:A:1041:ILE:CD1 | 2.28 | 0.63 |
| 1:A:336:LEU:HD12 | 1:A:336:LEU:O | 1.99 | 0.63 |
| 1:A:458:ASN:HB3 | 1:A:461:ASP:HB2 | 1.79 | 0.63 |
| 1:A:965:ILE:HD12 | 1:A:976:VAL:HG21 | 1.80 | 0.63 |
| 1:A:881:LEU:HD11 | 1:A:1072:PHE:HB3 | 1.79 | 0.63 |
| 1:A:740:ALA:O | 1:A:744:LYS:HG3 | 1.98 | 0.63 |
| 1:A:819:LEU:HD23 | 1:A:841:VAL:HB | 1.80 | 0.63 |
| 1:A:397:LEU:O | 1:A:398:ALA:HB2 | 1.98 | 0.63 |
| 1:A:744:LYS:O | 1:A:748:ASN:HB2 | 1.99 | 0.62 |
| 1:A:547:LYS:HE2 | 1:A:646:MET:SD | 2.39 | 0.62 |
| 1:A:1062:ASP:OD1 | 1:A:1064:HIS:N | 2.32 | 0.62 |
| 1:A:918:ASN:HD22 | 1:A:1065:ARG:HB3 | 1.61 | 0.62 |
| 1:A:122:THR:O | 1:A:123:ILE:HB | 1.99 | 0.62 |
| 1:A:1117:TYR:HD2 | 1:A:1252:PHE:HZ | 1.47 | 0.62 |
| 1:A:572:VAL:HG12 | 1:A:574:GLU:H | 1.64 | 0.62 |
| 1:A:161:ILE:HD12 | 1:A:194:PHE:CE2 | 2.34 | 0.62 |
| 1:A:320:LYS:HD3 | 1:A:321:TYR:CE2 | 2.35 | 0.62 |
| 1:A:115:ILE:HA | 1:A:150:ASN:HD21 | 1.64 | 0.62 |
| 1:A:53:ASN:HB3 | 1:A:56:GLU:HB2 | 1.80 | 0.62 |
| 1:A:549:THR:H | 1:A:552:HIS:CD2 | 2.18 | 0.62 |
| 1:A:98:ILE:O | 1:A:104:GLY:HA3 | 1.98 | 0.62 |
| 1:A:940:ASN:HA | 1:A:1021:ASN:O | 1.99 | 0.62 |
| 1:A:951:LYS:HG3 | 1:A:952:TYR:N | 2.14 | 0.62 |
| 1:A:1011:ILE:CG2 | 1:A:1291:TRP:HZ3 | 2.13 | 0.62 |
| 1:A:85:ASP:O | 1:A:89:LYS:HD3 | 2.00 | 0.62 |
| 1:A:1255:PHE:CD2 | 1:A:1260:LYS:HD2 | 2.35 | 0.61 |
| 1:A:223:HIS:ND1 | 1:A:351:GLU:OE1 | 2.32 | 0.61 |
| 1:A:917:PHE:O | 1:A:1057:LEU:HD13 | 2.00 | 0.61 |
| 1:A:1168:GLY:O | 1:A:1170:LYS:HG2 | 1.99 | 0.61 |
| 1:A:500:GLN:NE2 | 1:A:504:LEU:HD21 | 2.14 | 0.61 |
| 1:A:637:ILE:HD11 | 1:A:784:ILE:HG23 | 1.82 | 0.61 |
| 1:A:764:PHE:CZ | 1:A:769:LEU:HD22 | 2.34 | 0.61 |
| 1:A:556:ALA:HB2 | 1:A:576:LEU:HD23 | 1.81 | 0.61 |
| 1:A:747:ILE:HG21 | 1:A:764:PHE:CZ | 2.36 | 0.61 |
| 1:A:361:LEU:H | 1:A:404:GLN:HE22 | 1.48 | 0.61 |
| 1:A:962:TYR:CE2 | 1:A:1057:LEU:HD23 | 2.35 | 0.61 |
| 1:A:23:LYS:HB2 | 1:A:23:LYS:HZ2 | 1.64 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:789:ASN:OD1 | 1:A:861:ARG:HG2 | 2.00 | 0.61 |
| 1:A:682:VAL:HG12 | 1:A:684:TYR:CE1 | 2.35 | 0.61 |
| 1:A:731:LYS:O | 1:A:734:GLU:HB3 | 2.01 | 0.61 |
| 1:A:1101:TRP:HZ3 | 1:A:1286:PRO:O | 1.84 | 0.61 |
| 1:A:287:TYR:CE2 | 1:A:291:LYS:HD2 | 2.36 | 0.61 |
| 1:A:643:ILE:C | 1:A:645:ASN:H | 2.04 | 0.61 |
| 1:A:325:GLU:HB3 | 1:A:331:PHE:CD1 | 2.36 | 0.60 |
| 1:A:455:ILE:HG21 | 1:A:555:ARG:HD2 | 1.81 | 0.60 |
| 1:A:584:THR:HG22 | 1:A:585:PHE:H | 1.64 | 0.60 |
| 1:A:15:ASN:OD1 | 1:A:17:VAL:O | 2.19 | 0.60 |
| 1:A:306:THR:HG22 | 1:A:517:ILE:HA | 1.82 | 0.60 |
| 1:A:406:THR:O | 1:A:410:ASN:HA | 2.01 | 0.60 |
| 1:A:250:TYR:HB2 | 1:A:429:LEU:CD2 | 2.31 | 0.60 |
| 1:A:769:LEU:O | 1:A:772:LYS:HB2 | 2.01 | 0.60 |
| 1:A:618:THR:HG23 | 1:A:780:ALA:HB2 | 1.83 | 0.60 |
| 1:A:872:ASN:HD22 | 1:A:874:ILE:H | 1.47 | 0.60 |
| 1:A:135:ILE:CG2 | 1:A:149:LEU:HD12 | 2.31 | 0.60 |
| 1:A:49:ASP:OD1 | 1:A:52:THR:HB | 2.01 | 0.60 |
| 1:A:593:LYS:HD3 | 1:A:609:GLN:CD | 2.21 | 0.60 |
| 1:A:325:GLU:HB3 | 1:A:331:PHE:CE1 | 2.36 | 0.60 |
| 1:A:1128:VAL:HG11 | 1:A:1191:TYR:CE2 | 2.37 | 0.60 |
| 1:A:348:ILE:HG23 | 1:A:499:ILE:HG12 | 1.83 | 0.60 |
| 1:A:903:LYS:HG3 | 1:A:921:SER:HB2 | 1.83 | 0.60 |
| 1:A:1075:PHE:CD2 | 1:A:1079:LEU:HD11 | 2.36 | 0.59 |
| 1:A:702:ARG:NH1 | 1:A:702:ARG:HG3 | 2.17 | 0.59 |
| 1:A:961:GLU:HA | 1:A:978:LEU:O | 2.02 | 0.59 |
| 1:A:163:PHE:HA | 1:A:187:ARG:O | 2.01 | 0.59 |
| 1:A:250:TYR:HB2 | 1:A:429:LEU:HD22 | 1.84 | 0.59 |
| 1:A:52:THR:HG23 | 1:A:528:LEU:HD21 | 1.82 | 0.59 |
| 1:A:1099:ASP:HB2 | 1:A:1103:ASP:N | 2.15 | 0.59 |
| 1:A:591:VAL:HG12 | 1:A:595:ASN:HD22 | 1.66 | 0.59 |
| 1:A:852:GLN:OE1 | 1:A:855:LYS:HE3 | 2.01 | 0.59 |
| 1:A:974:TRP:HA | 1:A:986:THR:O | 2.01 | 0.59 |
| 1:A:134:CYS:HB3 | 1:A:147:GLU:O | 2.02 | 0.59 |
| 1:A:170:HIS:HD2 | 1:A:172:VAL:H | 1.45 | 0.59 |
| 1:A:249:ALA:HB3 | 1:A:252:GLU:CG | 2.32 | 0.59 |
| 1:A:336:LEU:CD1 | 1:A:340:LYS:HE3 | 2.32 | 0.59 |
| 1:A:634:ILE:CG2 | 1:A:637:ILE:HG13 | 2.31 | 0.59 |
| 1:A:872:ASN:ND2 | 1:A:874:ILE:N | 2.50 | 0.59 |
| 1:A:535:GLU:HG3 | 1:A:537:PHE:CZ | 2.37 | 0.59 |
| 1:A:961:GLU:CB | 1:A:979:ASN:HD22 | 2.13 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:923:LYS:HD3 | 1:A:1056:LYS:HD3 | 1.84 | 0.59 |
| 1:A:8:PHE:HD1 | 1:A:19:ILE:HD11 | 1.67 | 0.59 |
| 1:A:906:PHE:O | 1:A:907:ASP:C | 2.41 | 0.59 |
| 1:A:949:ILE:O | 1:A:1012:ASN:HA | 2.03 | 0.59 |
| 1:A:277:LEU:HD23 | 1:A:472:THR:CG2 | 2.30 | 0.59 |
| 1:A:802:PRO:HB3 | 1:A:932:ILE:HD11 | 1.84 | 0.59 |
| 1:A:428:LEU:O | 1:A:543:TYR:N | 2.35 | 0.59 |
| 1:A:706:TRP:CZ3 | 1:A:848:ASP:HB2 | 2.38 | 0.59 |
| 1:A:1016:PHE:CE2 | 1:A:1088:TYR:HB2 | 2.38 | 0.59 |
| 1:A:1241:ASP:CG | 1:A:1245:ASN:HB2 | 2.23 | 0.59 |
| 1:A:576:LEU:HA | 1:A:581:ARG:HD2 | 1.85 | 0.59 |
| 1:A:636:TYR:C | 1:A:639:PRO:HD2 | 2.23 | 0.59 |
| 1:A:995:GLN:OE1 | 1:A:996:ARG:N | 2.35 | 0.59 |
| 1:A:1101:TRP:CZ3 | 1:A:1288:ASP:HB2 | 2.38 | 0.58 |
| 1:A:498:LEU:O | 1:A:502:TYR:HD1 | 1.85 | 0.58 |
| 1:A:97:ARG:HG2 | 1:A:386:ILE:O | 2.03 | 0.58 |
| 1:A:934:TYR:O | 1:A:937:MET:HB2 | 2.03 | 0.58 |
| 1:A:952:TYR:CE1 | 1:A:1065:ARG:CZ | 2.86 | 0.58 |
| 1:A:1014:TRP:CH2 | 1:A:1070:LYS:HE3 | 2.38 | 0.58 |
| 1:A:1193:LEU:CD1 | 1:A:1206:LEU:HD13 | 2.33 | 0.58 |
| 1:A:566:ILE:HG12 | 1:A:749:TYR:CG | 2.39 | 0.58 |
| 1:A:658:PHE:CD1 | 1:A:889:ILE:HG21 | 2.38 | 0.58 |
| 1:A:1255:PHE:O | 1:A:1256:ASN:HB2 | 2.03 | 0.58 |
| 1:A:578:ASN:O | 1:A:581:ARG:HB3 | 2.04 | 0.58 |
| 1:A:857:VAL:O | 1:A:863:LEU:HD11 | 2.01 | 0.58 |
| 1:A:1164:LYS:HD3 | 1:A:1168:GLY:HA2 | 1.86 | 0.58 |
| 1:A:1211:ILE:HD12 | 1:A:1211:ILE:N | 2.18 | 0.58 |
| 1:A:950:PRO:O | 1:A:1065:ARG:NH2 | 2.36 | 0.58 |
| 1:A:312:TYR:CE2 | 1:A:515:ILE:HG13 | 2.39 | 0.58 |
| 1:A:584:THR:CG2 | 1:A:585:PHE:N | 2.66 | 0.58 |
| 1:A:984:ILE:HG22 | 1:A:985:TRP:N | 2.18 | 0.58 |
| 1:A:425:PHE:CZ | 1:A:537:PHE:HB2 | 2.39 | 0.58 |
| 1:A:11:LYS:HZ1 | 1:A:81:ASP:HB3 | 1.69 | 0.58 |
| 1:A:1234:LYS:O | 1:A:1236:LYS:HG3 | 2.04 | 0.58 |
| 1:A:1239:LEU:HD13 | 1:A:1240:GLN:N | 2.19 | 0.58 |
| 1:A:226:ILE:CG2 | 1:A:265:THR:HG23 | 2.34 | 0.58 |
| 1:A:455:ILE:HD12 | 1:A:552:HIS:ND1 | 2.19 | 0.58 |
| 1:A:566:ILE:HD13 | 1:A:749:TYR:HB3 | 1.86 | 0.58 |
| 1:A:764:PHE:HZ | 1:A:769:LEU:HD22 | 1.68 | 0.58 |
| 1:A:952:TYR:CD2 | 1:A:980:TYR:HA | 2.39 | 0.57 |
| 1:A:1097:LEU:HD23 | 1:A:1236:LYS:HD2 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:242:VAL:HG13 | 1:A:258:VAL:O | 2.03 | 0.57 |
| 1:A:258:VAL:HG21 | 1:A:367:LEU:HD21 | 1.87 | 0.57 |
| 1:A:624:THR:HG21 | 1:A:633:ILE:HD12 | 1.85 | 0.57 |
| 1:A:487:ILE:CG2 | 1:A:488:GLU:N | 2.66 | 0.57 |
| 1:A:960:ASN:HD21 | 1:A:1061:ARG:H | 1.52 | 0.57 |
| 1:A:229:GLY:O | 1:A:233:TYR:HD1 | 1.88 | 0.57 |
| 1:A:542:LYS:HE2 | 1:A:544:GLU:HG3 | 1.87 | 0.57 |
| 1:A:193:THR:HG22 | 1:A:194:PHE:H | 1.70 | 0.57 |
| 1:A:2:PRO:O | 1:A:4:VAL:N | 2.37 | 0.57 |
| 1:A:866:PHE:O | 1:A:870:ILE:HG12 | 2.05 | 0.57 |
| 1:A:903:LYS:CB | 1:A:922:SER:HB3 | 2.34 | 0.57 |
| 1:A:72:TYR:CE2 | 1:A:160:ILE:HD12 | 2.39 | 0.57 |
| 1:A:861:ARG:NH2 | 1:A:862:LEU:HD21 | 2.19 | 0.57 |
| 1:A:1155:TYR:CE2 | 1:A:1287:VAL:HG22 | 2.40 | 0.57 |
| 1:A:1296:LEU:HD23 | 1:A:1296:LEU:N | 2.20 | 0.57 |
| 1:A:574:GLU:C | 1:A:576:LEU:H | 2.07 | 0.57 |
| 1:A:963:THR:O | 1:A:1057:LEU:HA | 2.04 | 0.57 |
| 1:A:1168:GLY:O | 1:A:1170:LYS:N | 2.37 | 0.56 |
| 1:A:30:MET:CE | 1:A:33:VAL:HG23 | 2.35 | 0.56 |
| 1:A:473:ASN:ND2 | 1:A:475:LEU:H | 2.03 | 0.56 |
| 1:A:669:PRO:HB3 | 1:A:720:LYS:HB3 | 1.87 | 0.56 |
| 1:A:259:SER:OG | 1:A:262:GLU:HB2 | 2.05 | 0.56 |
| 1:A:362:ASN:ND2 | 1:A:363:ALA:O | 2.38 | 0.56 |
| 1:A:395:THR:O | 1:A:397:LEU:N | 2.37 | 0.56 |
| 1:A:72:TYR:CZ | 1:A:416:LEU:HD13 | 2.40 | 0.56 |
| 1:A:480:GLU:HA | 1:A:680:ALA:HB3 | 1.86 | 0.56 |
| 1:A:80:THR:OG1 | 1:A:83:GLU:HG3 | 2.06 | 0.56 |
| 1:A:948:ARG:HB3 | 1:A:1068:TRP:CB | 2.19 | 0.56 |
| 1:A:918:ASN:OD1 | 1:A:1060:CYS:HB3 | 2.04 | 0.56 |
| 1:A:1096:ILE:HG21 | 1:A:1104:TYR:CD1 | 2.41 | 0.56 |
| 1:A:395:THR:C | 1:A:397:LEU:N | 2.58 | 0.56 |
| 1:A:1080:ASN:HD21 | 1:A:1082:LYS:HB3 | 1.69 | 0.56 |
| 1:A:1210:GLU:HB3 | 1:A:1213:ASP:OD2 | 2.05 | 0.56 |
| 1:A:195:GLY:HA3 | 1:A:374:PHE:HE1 | 1.70 | 0.56 |
| 1:A:935:ASN:OD1 | 1:A:1049:ALA:HB3 | 2.06 | 0.56 |
| 1:A:1075:PHE:CE2 | 1:A:1079:LEU:HD11 | 2.41 | 0.56 |
| 1:A:1114:LEU:HD12 | 1:A:1115:ASN:N | 2.20 | 0.56 |
| 1:A:1127:ASN:O | 1:A:1132:GLY:HA3 | 2.06 | 0.56 |
| 1:A:8:PHE:CD1 | 1:A:19:ILE:HD11 | 2.41 | 0.56 |
| 1:A:594:VAL:CG1 | 1:A:746:ILE:HG21 | 2.32 | 0.56 |
| 1:A:963:THR:HA | 1:A:977:SER:HA | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:115:ILE:HD12 | 1:A:316:VAL:HG11 | 1.86 | 0.56 |
| 1:A:1155:TYR:OH | 1:A:1291:TRP:HB3 | 2.06 | 0.56 |
| 1:A:628:ALA:O | 1:A:629:ASP:CB | 2.53 | 0.56 |
| 1:A:1227:ASN:HB3 | 1:A:1231:ILE:O | 2.06 | 0.56 |
| 1:A:733:LYS:O | 1:A:737:GLU:HG3 | 2.06 | 0.56 |
| 1:A:660:GLY:O | 1:A:662:VAL:N | 2.39 | 0.56 |
| 1:A:879:LEU:HB3 | 1:A:1074:LEU:HB3 | 1.88 | 0.56 |
| 1:A:269:HIS:O | 1:A:272:LYS:N | 2.35 | 0.56 |
| 1:A:1029:ILE:O | 1:A:1029:ILE:HG23 | 2.05 | 0.56 |
| 1:A:154:ILE:HD13 | 1:A:187:ARG:HG3 | 1.87 | 0.56 |
| 1:A:856:TYR:O | 1:A:857:VAL:HG23 | 2.06 | 0.56 |
| 1:A:1136:LEU:HD11 | 1:A:1252:PHE:CD2 | 2.41 | 0.55 |
| 1:A:337:LYS:HA | 1:A:340:LYS:HD2 | 1.88 | 0.55 |
| 1:A:573:ASN:C | 1:A:575:ALA:H | 2.10 | 0.55 |
| 1:A:575:ALA:O | 1:A:581:ARG:CB | 2.53 | 0.55 |
| 1:A:952:TYR:HB2 | 1:A:1003:GLN:NE2 | 2.18 | 0.55 |
| 1:A:1085:LYS:HE3 | 1:A:1089:ASP:OD2 | 2.06 | 0.55 |
| 1:A:1137:LYS:HG3 | 1:A:1138:GLY:H | 1.70 | 0.55 |
| 1:A:1173:ILE:HB | 1:A:1175:ARG:HH12 | 1.71 | 0.55 |
| 1:A:176:THR:HG22 | 1:A:236:ALA:HB3 | 1.88 | 0.55 |
| 1:A:951:LYS:NZ | 1:A:1151:ASN:OD1 | 2.40 | 0.55 |
| 1:A:1167:SER:HB3 | 1:A:1170:LYS:NZ | 2.21 | 0.55 |
| 1:A:643:ILE:C | 1:A:645:ASN:N | 2.58 | 0.55 |
| 1:A:1204:LYS:H | 1:A:1262:VAL:HG13 | 1.71 | 0.55 |
| 1:A:559:PHE:C | 1:A:559:PHE:CD1 | 2.79 | 0.55 |
| 1:A:972:SER:HB2 | 1:A:1048:HIS:HB2 | 1.88 | 0.55 |
| 1:A:1130:ILE:HD12 | 1:A:1131:ARG:N | 2.22 | 0.55 |
| 1:A:542:LYS:HE2 | 1:A:544:GLU:CG | 2.36 | 0.55 |
| 1:A:706:TRP:CD2 | 1:A:808:LEU:HD13 | 2.41 | 0.55 |
| 1:A:9:ASN:HB2 | 1:A:12:ASP:OD1 | 2.06 | 0.55 |
| 1:A:1211:ILE:H | 1:A:1211:ILE:CD1 | 2.18 | 0.55 |
| 1:A:1155:TYR:CZ | 1:A:1287:VAL:HA | 2.41 | 0.55 |
| 1:A:555:ARG:O | 1:A:558:GLU:HG3 | 2.07 | 0.55 |
| 1:A:702:ARG:HE | 1:A:812:ASP:CG | 2.09 | 0.55 |
| 1:A:22:ILE:CG2 | 1:A:24:ILE:HD12 | 2.37 | 0.55 |
| 1:A:888:LEU:HB3 | 1:A:900:ILE:HD11 | 1.89 | 0.55 |
| 1:A:1276:ARG:O | 1:A:1278:LEU:HG | 2.07 | 0.55 |
| 1:A:243:PHE:CZ | 1:A:273:PHE:HB3 | 2.41 | 0.55 |
| 1:A:429:LEU:O | 1:A:454:CYS:HA | 2.06 | 0.55 |
| 1:A:1022:ASN:HB2 | 1:A:1078:GLU:OE2 | 2.07 | 0.55 |
| 1:A:1013:ARG:HG3 | 1:A:1101:TRP:HD1 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1277:THR:HG22 | 1:A:1277:THR:O | 2.07 | 0.54 |
| 1:A:226:ILE:HD13 | 1:A:350:THR:CA | 2.36 | 0.54 |
| 1:A:754:TYR:OH | 1:A:757:GLU:O | 2.23 | 0.54 |
| 1:A:1020:THR:CG2 | 1:A:1078:GLU:HG3 | 2.36 | 0.54 |
| 1:A:212:LYS:CE | 1:A:371:LYS:HB2 | 2.37 | 0.54 |
| 1:A:2:PRO:HG2 | 1:A:39:HIS:NE2 | 2.22 | 0.54 |
| 1:A:458:ASN:HD22 | 1:A:459:ASN:H | 1.55 | 0.54 |
| 1:A:1034:ARG:CZ | 1:A:1036:ILE:HD11 | 2.36 | 0.54 |
| 1:A:422:LEU:HD23 | 1:A:423:PHE:CE1 | 2.42 | 0.54 |
| 1:A:48:ARG:CZ | 1:A:59:LEU:HD13 | 2.36 | 0.54 |
| 1:A:888:LEU:HD21 | 1:A:914:ILE:HD11 | 1.89 | 0.54 |
| 1:A:984:ILE:HG12 | 1:A:998:VAL:CG2 | 2.32 | 0.54 |
| 1:A:1112:TYR:CZ | 1:A:1159:LYS:HE2 | 2.42 | 0.54 |
| 1:A:322:LEU:HD12 | 1:A:341:LEU:HB2 | 1.88 | 0.54 |
| 1:A:632:ILE:HD12 | 1:A:786:LYS:HB3 | 1.89 | 0.54 |
| 1:A:815:LEU:HD23 | 1:A:845:LEU:CD1 | 2.36 | 0.54 |
| 1:A:566:ILE:CD1 | 1:A:749:TYR:HB3 | 2.37 | 0.54 |
| 1:A:115:ILE:CG2 | 1:A:317:PHE:HE1 | 2.21 | 0.54 |
| 1:A:584:THR:CG2 | 1:A:585:PHE:H | 2.21 | 0.54 |
| 1:A:669:PRO:HG3 | 1:A:721:VAL:HG22 | 1.89 | 0.54 |
| 1:A:72:TYR:CE1 | 1:A:416:LEU:HD13 | 2.43 | 0.54 |
| 1:A:1077:LYS:HE3 | 1:A:1083:GLU:OE1 | 2.08 | 0.54 |
| 1:A:178:ASN:O | 1:A:289:LYS:HB3 | 2.08 | 0.54 |
| 1:A:625:ASP:C | 1:A:627:ILE:H | 2.10 | 0.54 |
| 1:A:11:LYS:HZ2 | 1:A:81:ASP:HB3 | 1.72 | 0.54 |
| 1:A:816:LYS:O | 1:A:820:LEU:HD23 | 2.08 | 0.54 |
| 1:A:97:ARG:HD3 | 1:A:358:PHE:CE1 | 2.43 | 0.54 |
| 1:A:11:LYS:NZ | 1:A:81:ASP:CB | 2.70 | 0.54 |
| 1:A:587:SER:H | 1:A:617:GLU:CD | 2.10 | 0.54 |
| 1:A:663:ILE:O | 1:A:663:ILE:HG22 | 2.08 | 0.54 |
| 1:A:903:LYS:CG | 1:A:921:SER:HB2 | 2.38 | 0.53 |
| 1:A:309:SER:O | 1:A:312:TYR:N | 2.41 | 0.53 |
| 1:A:754:TYR:CG | 1:A:755:THR:N | 2.76 | 0.53 |
| 1:A:123:ILE:HD12 | 1:A:123:ILE:N | 2.23 | 0.53 |
| 1:A:515:ILE:HG22 | 1:A:515:ILE:O | 2.08 | 0.53 |
| 1:A:1163:LYS:HD3 | 1:A:1183:ASN:ND2 | 2.24 | 0.53 |
| 1:A:418:ASN:ND2 | 1:A:420:THR:N | 2.56 | 0.53 |
| 1:A:423:PHE:O | 1:A:426:TYR:HD2 | 1.90 | 0.53 |
| 1:A:909:ILE:HD11 | 1:A:1106:GLN:OE1 | 2.08 | 0.53 |
| 1:A:658:PHE:HD1 | 1:A:889:ILE:HG21 | 1.72 | 0.53 |
| 1:A:661:ALA:HB1 | 1:A:791:CYS:HB3 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:925:GLU:HB2 | 1:A:1054:MET:SD | 2.49 | 0.53 |
| 1:A:17:VAL:O | 1:A:18:ASP:OD1 | 2.27 | 0.53 |
| 1:A:458:ASN:ND2 | 1:A:459:ASN:N | 2.57 | 0.53 |
| 1:A:772:LYS:O | 1:A:774:ASN:N | 2.41 | 0.53 |
| 1:A:1005:ILE:O | 1:A:1151:ASN:HA | 2.09 | 0.53 |
| 1:A:1164:LYS:HD3 | 1:A:1168:GLY:CA | 2.39 | 0.53 |
| 1:A:432:ARG:N | 1:A:545:LEU:O | 2.42 | 0.53 |
| 1:A:797:MET:CE | 1:A:866:PHE:HE1 | 2.22 | 0.53 |
| 1:A:269:HIS:O | 1:A:272:LYS:HB2 | 2.09 | 0.53 |
| 1:A:318:LYS:CG | 1:A:331:PHE:CE1 | 2.92 | 0.53 |
| 1:A:52:THR:CG2 | 1:A:528:LEU:HD21 | 2.39 | 0.53 |
| 1:A:535:GLU:HG3 | 1:A:535:GLU:O | 2.09 | 0.53 |
| 1:A:824:TYR:O | 1:A:827:ARG:HG2 | 2.09 | 0.53 |
| 1:A:1116:LEU:HB2 | 1:A:1281:SER:O | 2.09 | 0.53 |
| 1:A:549:THR:N | 1:A:552:HIS:HD2 | 2.05 | 0.53 |
| 1:A:573:ASN:C | 1:A:575:ALA:N | 2.63 | 0.53 |
| 1:A:641:LEU:HD11 | 1:A:732:MET:SD | 2.49 | 0.53 |
| 1:A:816:LYS:HE3 | 1:A:842:ASN:HA | 1.89 | 0.53 |
| 1:A:1146:THR:O | 1:A:1147:ASN:HB2 | 2.09 | 0.52 |
| 1:A:1241:ASP:HB3 | 1:A:1247:ILE:HD11 | 1.91 | 0.52 |
| 1:A:594:VAL:HG12 | 1:A:746:ILE:HD13 | 1.91 | 0.52 |
| 1:A:405:ASN:CG | 1:A:408:ILE:HD13 | 2.30 | 0.52 |
| 1:A:903:LYS:HA | 1:A:903:LYS:HE2 | 1.89 | 0.52 |
| 1:A:1112:TYR:CE1 | 1:A:1159:LYS:HE2 | 2.44 | 0.52 |
| 1:A:1205:ILE:O | 1:A:1206:LEU:HB2 | 2.08 | 0.52 |
| 1:A:22:ILE:HD12 | 1:A:22:ILE:H | 1.72 | 0.52 |
| 1:A:226:ILE:HG21 | 1:A:265:THR:HG23 | 1.90 | 0.52 |
| 1:A:407:GLU:O | 1:A:410:ASN:HB2 | 2.08 | 0.52 |
| 1:A:552:HIS:O | 1:A:555:ARG:HB3 | 2.09 | 0.52 |
| 1:A:906:PHE:CE2 | 1:A:914:ILE:HG12 | 2.44 | 0.52 |
| 1:A:140:PRO:C | 1:A:142:GLY:H | 2.13 | 0.52 |
| 1:A:318:LYS:NZ | 1:A:325:GLU:HG2 | 2.25 | 0.52 |
| 1:A:348:ILE:HD13 | 1:A:494:ILE:HG23 | 1.90 | 0.52 |
| 1:A:589:ASP:OD1 | 1:A:593:LYS:HE3 | 2.10 | 0.52 |
| 1:A:947:ILE:CG2 | 1:A:1015:ILE:HB | 2.40 | 0.52 |
| 1:A:1163:LYS:HG3 | 1:A:1183:ASN:ND2 | 2.24 | 0.52 |
| 1:A:562:GLY:C | 1:A:564:SER:H | 2.13 | 0.52 |
| 1:A:1009:ASP:HA | 1:A:1013:ARG:HH11 | 1.73 | 0.52 |
| 1:A:238:ASN:HD21 | 1:A:240:ASN:HD22 | 1.58 | 0.52 |
| 1:A:684:TYR:CD2 | 1:A:690:LEU:HD23 | 2.44 | 0.52 |
| 1:A:669:PRO:HG3 | 1:A:721:VAL:CG2 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:735:ALA:O | 1:A:738:ASN:N | 2.42 | 0.52 |
| 1:A:952:TYR:HE2 | 1:A:981:GLY:H | 1.56 | 0.52 |
| 1:A:614:PHE:CD2 | 1:A:773:LEU:HD22 | 2.45 | 0.52 |
| 1:A:15:ASN:O | 1:A:17:VAL:N | 2.42 | 0.52 |
| 1:A:197:GLU:CG | 1:A:212:LYS:HG2 | 2.39 | 0.52 |
| 1:A:989:ASP:HB2 | 1:A:1046:ASN:O | 2.10 | 0.52 |
| 1:A:3:PHE:O | 1:A:4:VAL:HB | 2.10 | 0.52 |
| 1:A:267:GLY:O | 1:A:268:GLY:C | 2.48 | 0.51 |
| 1:A:872:ASN:HD22 | 1:A:874:ILE:N | 2.05 | 0.51 |
| 1:A:872:ASN:HB3 | 1:A:875:ASN:ND2 | 2.26 | 0.51 |
| 1:A:1154:LEU:O | 1:A:1156:ARG:N | 2.40 | 0.51 |
| 1:A:1163:LYS:HD3 | 1:A:1183:ASN:HD22 | 1.75 | 0.51 |
| 1:A:282:PHE:O | 1:A:285:TYR:HB3 | 2.10 | 0.51 |
| 1:A:258:VAL:HG22 | 1:A:366:PHE:HE2 | 1.74 | 0.51 |
| 1:A:46:PRO:O | 1:A:84:LYS:HD3 | 2.09 | 0.51 |
| 1:A:547:LYS:HZ3 | 1:A:646:MET:HB3 | 1.75 | 0.51 |
| 1:A:554:LEU:HA | 1:A:557:GLN:NE2 | 2.26 | 0.51 |
| 1:A:763:ASN:ND2 | 1:A:765:ASN:HD21 | 2.04 | 0.51 |
| 1:A:139:GLN:NE2 | 1:A:145:ARG:NH1 | 2.59 | 0.51 |
| 1:A:948:ARG:NH1 | 1:A:948:ARG:HG2 | 2.23 | 0.51 |
| 1:A:17:VAL:C | 1:A:19:ILE:H | 2.13 | 0.51 |
| 1:A:973:GLY:N | 1:A:988:GLN:O | 2.44 | 0.51 |
| 1:A:114:GLY:O | 1:A:320:LYS:HD2 | 2.11 | 0.51 |
| 1:A:146:SER:OG | 1:A:520:LEU:N | 2.42 | 0.51 |
| 1:A:275:ASP:OD1 | 1:A:278:GLN:HG3 | 2.11 | 0.51 |
| 1:A:336:LEU:HD12 | 1:A:340:LYS:HE3 | 1.93 | 0.51 |
| 1:A:258:VAL:HG13 | 1:A:366:PHE:CE2 | 2.46 | 0.51 |
| 1:A:193:THR:OG1 | 1:A:376:ILE:HD13 | 2.11 | 0.51 |
| 1:A:649:LYS:O | 1:A:650:ASP:O | 2.28 | 0.51 |
| 1:A:1114:LEU:HD12 | 1:A:1114:LEU:C | 2.30 | 0.51 |
| 1:A:755:THR:O | 1:A:756:GLU:CB | 2.55 | 0.51 |
| 1:A:9:ASN:HB2 | 1:A:12:ASP:CG | 2.31 | 0.51 |
| 1:A:310:LEU:O | 1:A:314:LYS:HG3 | 2.11 | 0.51 |
| 1:A:614:PHE:O | 1:A:618:THR:HB | 2.10 | 0.51 |
| 1:A:547:LYS:HZ2 | 1:A:646:MET:HB3 | 1.74 | 0.51 |
| 1:A:35:ALA:CB | 1:A:45:ILE:HG12 | 2.38 | 0.50 |
| 1:A:429:LEU:CD2 | 1:A:543:TYR:HB2 | 2.39 | 0.50 |
| 1:A:972:SER:O | 1:A:973:GLY:O | 2.30 | 0.50 |
| 1:A:351:GLU:O | 1:A:355:VAL:HG23 | 2.10 | 0.50 |
| 1:A:487:ILE:HG22 | 1:A:488:GLU:N | 2.26 | 0.50 |
| 1:A:74:ASP:O | 1:A:76:THR:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:929:LYS:O | 1:A:933:VAL:HG23 | 2.12 | 0.50 |
| 1:A:1041:ILE:HG23 | 1:A:1044:LEU:HB2 | 1.92 | 0.50 |
| 1:A:1197:ALA:HB2 | 1:A:1247:ILE:CD1 | 2.42 | 0.50 |
| 1:A:1130:ILE:HD12 | 1:A:1130:ILE:C | 2.32 | 0.50 |
| 1:A:167:SER:HB2 | 1:A:184:GLN:NE2 | 2.26 | 0.50 |
| 1:A:763:ASN:HB2 | 1:A:765:ASN:HD21 | 1.73 | 0.50 |
| 1:A:962:TYR:CE1 | 1:A:978:LEU:HB2 | 2.46 | 0.50 |
| 1:A:947:ILE:O | 1:A:1014:TRP:HA | 2.11 | 0.50 |
| 1:A:36:PHE:N | 1:A:36:PHE:CD1 | 2.79 | 0.50 |
| 1:A:1161:ILE:HG22 | 1:A:1163:LYS:HD3 | 1.93 | 0.50 |
| 1:A:21:TYR:O | 1:A:138:ILE:HB | 2.12 | 0.50 |
| 1:A:1010:TYR:HB3 | 1:A:1015:ILE:CD1 | 2.29 | 0.50 |
| 1:A:1133:TYR:CD2 | 1:A:1260:LYS:NZ | 2.80 | 0.50 |
| 1:A:150:ASN:O | 1:A:232:LEU:HD21 | 2.12 | 0.50 |
| 1:A:431:VAL:HB | 1:A:453:LEU:HD23 | 1.94 | 0.50 |
| 1:A:428:LEU:HD23 | 1:A:542:LYS:HG3 | 1.92 | 0.50 |
| 1:A:70:VAL:HG12 | 1:A:71:SER:N | 2.27 | 0.50 |
| 1:A:746:ILE:HG22 | 1:A:747:ILE:N | 2.26 | 0.50 |
| 1:A:827:ARG:C | 1:A:829:THR:H | 2.14 | 0.50 |
| 1:A:1026:ASN:HB3 | 1:A:1040:PRO:HA | 1.94 | 0.50 |
| 1:A:1122:TYR:CE1 | 1:A:1137:LYS:HB3 | 2.47 | 0.50 |
| 1:A:247:THR:HG21 | 1:A:254:SER:O | 2.12 | 0.50 |
| 1:A:355:VAL:O | 1:A:355:VAL:HG12 | 2.12 | 0.50 |
| 1:A:38:ILE:O | 1:A:39:HIS:HB2 | 2.11 | 0.50 |
| 1:A:1104:TYR:CD2 | 1:A:1173:ILE:HD13 | 2.47 | 0.50 |
| 1:A:1288:ASP:O | 1:A:1290:GLY:N | 2.45 | 0.50 |
| 1:A:422:LEU:HD23 | 1:A:423:PHE:HE1 | 1.77 | 0.50 |
| 1:A:458:ASN:ND2 | 1:A:459:ASN:H | 2.10 | 0.50 |
| 1:A:481:ILE:CD1 | 1:A:698:ALA:HA | 2.40 | 0.50 |
| 1:A:624:THR:CG2 | 1:A:633:ILE:HD12 | 2.41 | 0.50 |
| 1:A:201:GLU:HG3 | 1:A:361:LEU:HD13 | 1.92 | 0.49 |
| 1:A:537:PHE:HB3 | 1:A:538:PRO:HD2 | 1.94 | 0.49 |
| 1:A:673:ILE:O | 1:A:807:ARG:NH1 | 2.45 | 0.49 |
| 1:A:920:GLU:HG3 | 1:A:920:GLU:O | 2.12 | 0.49 |
| 1:A:1236:LYS:NZ | 1:A:1282:TRP:O | 2.43 | 0.49 |
| 1:A:10:TYR:HA | 1:A:36:PHE:HZ | 1.76 | 0.49 |
| 1:A:379:VAL:N | 1:A:380:PRO:HD2 | 2.28 | 0.49 |
| 1:A:641:LEU:HD11 | 1:A:732:MET:HG2 | 1.95 | 0.49 |
| 1:A:156:PRO:HD3 | 1:A:189:SER:HB2 | 1.93 | 0.49 |
| 1:A:247:THR:HG23 | 1:A:254:SER:HA | 1.93 | 0.49 |
| 1:A:638:GLY:N | 1:A:639:PRO:HD2 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:746:ILE:O | 1:A:747:ILE:C | 2.49 | 0.49 |
| 1:A:965:ILE:O | 1:A:976:VAL:N | 2.45 | 0.49 |
| 1:A:1233:ASN:HD22 | 1:A:1271:ILE:HG23 | 1.75 | 0.49 |
| 1:A:1291:TRP:O | 1:A:1293:GLU:N | 2.46 | 0.49 |
| 1:A:235:ILE:O | 1:A:235:ILE:HG23 | 2.12 | 0.49 |
| 1:A:114:GLY:O | 1:A:320:LYS:CE | 2.60 | 0.49 |
| 1:A:394:ASN:O | 1:A:395:THR:C | 2.51 | 0.49 |
| 1:A:571:SER:OG | 1:A:572:VAL:N | 2.44 | 0.49 |
| 1:A:743:THR:O | 1:A:743:THR:CG2 | 2.61 | 0.49 |
| 1:A:1209:LEU:CD1 | 1:A:1217:LEU:HD12 | 2.43 | 0.49 |
| 1:A:1255:PHE:HD2 | 1:A:1260:LYS:HD2 | 1.76 | 0.49 |
| 1:A:318:LYS:HG3 | 1:A:331:PHE:HE1 | 1.77 | 0.49 |
| 1:A:380:PRO:HG2 | 1:A:383:ASN:HB2 | 1.95 | 0.49 |
| 1:A:647:LEU:O | 1:A:648:TYR:C | 2.51 | 0.49 |
| 1:A:79:SER:N | 1:A:83:GLU:OE1 | 2.45 | 0.49 |
| 1:A:269:HIS:HE1 | 1:A:859:ASN:HD22 | 1.59 | 0.49 |
| 1:A:72:TYR:CD2 | 1:A:160:ILE:HD12 | 2.48 | 0.49 |
| 1:A:872:ASN:ND2 | 1:A:874:ILE:CB | 2.64 | 0.49 |
| 1:A:986:THR:HG21 | 1:A:996:ARG:NH2 | 2.27 | 0.49 |
| 1:A:1241:ASP:OD1 | 1:A:1241:ASP:C | 2.51 | 0.49 |
| 1:A:22:ILE:HD13 | 1:A:35:ALA:CB | 2.37 | 0.49 |
| 1:A:961:GLU:CA | 1:A:979:ASN:HD22 | 2.26 | 0.49 |
| 1:A:962:TYR:CD2 | 1:A:1057:LEU:HD23 | 2.48 | 0.49 |
| 1:A:172:VAL:HG12 | 1:A:172:VAL:O | 2.12 | 0.49 |
| 1:A:209:GLY:HA3 | 1:A:213:PHE:CZ | 2.48 | 0.49 |
| 1:A:243:PHE:HD1 | 1:A:260:PHE:HE1 | 1.59 | 0.49 |
| 1:A:378:ILE:HG23 | 1:A:384:TYR:CD1 | 2.48 | 0.49 |
| 1:A:583:TYR:CG | 1:A:584:THR:N | 2.80 | 0.49 |
| 1:A:540:GLY:O | 1:A:541:LYS:C | 2.50 | 0.49 |
| 1:A:733:LYS:HB2 | 1:A:781:MET:HE1 | 1.95 | 0.49 |
| 1:A:526:GLY:O | 1:A:527:GLN:CB | 2.61 | 0.48 |
| 1:A:559:PHE:HB3 | 1:A:582:VAL:CG2 | 2.37 | 0.48 |
| 1:A:966:ASN:HD22 | 1:A:975:LYS:HG3 | 1.78 | 0.48 |
| 1:A:954:ASN:O | 1:A:1148:ILE:HD13 | 2.13 | 0.48 |
| 1:A:1105:LEU:HD21 | 1:A:1162:ILE:CD1 | 2.43 | 0.48 |
| 1:A:1109:LYS:NZ | 1:A:1286:PRO:CB | 2.76 | 0.48 |
| 1:A:3:PHE:HA | 1:A:96:GLU:OE1 | 2.12 | 0.48 |
| 1:A:702:ARG:NH1 | 1:A:702:ARG:CG | 2.76 | 0.48 |
| 1:A:966:ASN:HA | 1:A:975:LYS:HB2 | 1.95 | 0.48 |
| 1:A:1111:TYR:CD1 | 1:A:1286:PRO:HB3 | 2.47 | 0.48 |
| 1:A:45:ILE:HG22 | 1:A:47:GLU:HG2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1171:ASP:OD2 | 1:A:1173:ILE:HB | 2.13 | 0.48 |
| 1:A:1173:ILE:HB | 1:A:1175:ARG:NH1 | 2.28 | 0.48 |
| 1:A:135:ILE:HG21 | 1:A:149:LEU:HD12 | 1.94 | 0.48 |
| 1:A:384:TYR:HA | 1:A:389:GLY:O | 2.12 | 0.48 |
| 1:A:306:THR:CG2 | 1:A:517:ILE:HG22 | 2.42 | 0.48 |
| 1:A:1027:SER:CB | 1:A:1041:ILE:HD11 | 2.24 | 0.48 |
| 1:A:555:ARG:HA | 1:A:555:ARG:HE | 1.78 | 0.48 |
| 1:A:647:LEU:O | 1:A:649:LYS:N | 2.46 | 0.48 |
| 1:A:974:TRP:H | 1:A:987:LEU:HA | 1.77 | 0.48 |
| 1:A:17:VAL:O | 1:A:19:ILE:N | 2.46 | 0.48 |
| 1:A:609:GLN:HG2 | 1:A:613:ASP:OD2 | 2.14 | 0.48 |
| 1:A:621:VAL:CG1 | 1:A:632:ILE:HG23 | 2.44 | 0.48 |
| 1:A:1117:TYR:C | 1:A:1119:PRO:HD3 | 2.34 | 0.48 |
| 1:A:1137:LYS:HG3 | 1:A:1138:GLY:N | 2.28 | 0.48 |
| 1:A:214:ALA:CB | 1:A:413:PHE:CE1 | 2.97 | 0.48 |
| 1:A:641:LEU:HB2 | 1:A:643:ILE:CG1 | 2.39 | 0.48 |
| 1:A:676:LEU:CD1 | 1:A:808:LEU:HD23 | 2.44 | 0.48 |
| 1:A:118:TRP:CD1 | 1:A:317:PHE:HZ | 2.31 | 0.48 |
| 1:A:1253:HIS:O | 1:A:1259:ALA:HA | 2.14 | 0.48 |
| 1:A:210:ALA:H | 1:A:405:ASN:HD21 | 1.51 | 0.48 |
| 1:A:171:GLU:HG2 | 1:A:172:VAL:CG2 | 2.43 | 0.48 |
| 1:A:311:GLN:NE2 | 1:A:312:TYR:N | 2.61 | 0.48 |
| 1:A:559:PHE:O | 1:A:559:PHE:CD1 | 2.67 | 0.48 |
| 1:A:903:LYS:HB2 | 1:A:922:SER:CB | 2.41 | 0.48 |
| 1:A:1135:TYR:N | 1:A:1135:TYR:CD1 | 2.81 | 0.48 |
| 1:A:760:ASN:O | 1:A:761:ASN:CB | 2.62 | 0.48 |
| 1:A:144:TYR:C | 1:A:144:TYR:CD1 | 2.87 | 0.47 |
| 1:A:22:ILE:HG21 | 1:A:24:ILE:HD12 | 1.96 | 0.47 |
| 1:A:33:VAL:HG12 | 1:A:34:LYS:N | 2.29 | 0.47 |
| 1:A:970:ASN:O | 1:A:971:ASN:HB2 | 2.13 | 0.47 |
| 1:A:1113:MET:CE | 1:A:1160:PHE:HB2 | 2.44 | 0.47 |
| 1:A:1104:TYR:HB3 | 1:A:1173:ILE:HG23 | 1.96 | 0.47 |
| 1:A:1199:GLN:NE2 | 1:A:1204:LYS:HA | 2.29 | 0.47 |
| 1:A:569:THR:O | 1:A:595:ASN:ND2 | 2.45 | 0.47 |
| 1:A:796:LEU:CD2 | 1:A:801:ILE:HG12 | 2.44 | 0.47 |
| 1:A:838:LYS:NZ | 1:A:838:LYS:HB3 | 2.29 | 0.47 |
| 1:A:225:LEU:C | 1:A:227:HIS:N | 2.68 | 0.47 |
| 1:A:304:VAL:HG23 | 1:A:304:VAL:O | 2.14 | 0.47 |
| 1:A:455:ILE:CD1 | 1:A:552:HIS:ND1 | 2.78 | 0.47 |
| 1:A:702:ARG:C | 1:A:702:ARG:HD2 | 2.35 | 0.47 |
| 1:A:874:ILE:C | 1:A:876:THR:H | 2.17 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1100:PHE:CD1 | 1:A:1283:GLU:HG2 | 2.43 | 0.47 |
| 1:A:1296:LEU:CD2 | 1:A:1296:LEU:H | 2.27 | 0.47 |
| 1:A:420:THR:O | 1:A:421:GLY:C | 2.51 | 0.47 |
| 1:A:974:TRP:HB2 | 1:A:985:TRP:CZ2 | 2.50 | 0.47 |
| 1:A:1009:ASP:HA | 1:A:1013:ARG:NH1 | 2.29 | 0.47 |
| 1:A:1269:ARG:NH1 | 1:A:1273:ARG:HH11 | 2.11 | 0.47 |
| 1:A:135:ILE:HG23 | 1:A:149:LEU:HD12 | 1.96 | 0.47 |
| 1:A:757:GLU:HB2 | 1:A:760:ASN:HD22 | 1.76 | 0.47 |
| 1:A:997:VAL:HG11 | 1:A:1027:SER:O | 2.14 | 0.47 |
| 1:A:1193:LEU:HD12 | 1:A:1194:ALA:N | 2.28 | 0.47 |
| 1:A:93:LYS:NZ | 1:A:378:ILE:O | 2.34 | 0.47 |
| 1:A:671:ILE:HG22 | 1:A:673:ILE:HD11 | 1.97 | 0.47 |
| 1:A:705:LYS:HD3 | 1:A:705:LYS:O | 2.15 | 0.47 |
| 1:A:944:SER:HA | 1:A:1017:VAL:O | 2.15 | 0.47 |
| 1:A:149:LEU:HD13 | 1:A:152:VAL:CG2 | 2.45 | 0.47 |
| 1:A:248:ASN:O | 1:A:249:ALA:HB2 | 2.14 | 0.47 |
| 1:A:974:TRP:CE3 | 1:A:985:TRP:CZ3 | 3.02 | 0.47 |
| 1:A:1010:TYR:HD2 | 1:A:1015:ILE:CD1 | 2.28 | 0.47 |
| 1:A:212:LYS:HE2 | 1:A:371:LYS:CB | 2.43 | 0.47 |
| 1:A:299:LYS:HB2 | 1:A:299:LYS:HE3 | 1.74 | 0.47 |
| 1:A:217:PRO:CG | 1:A:378:ILE:HD11 | 2.33 | 0.47 |
| 1:A:660:GLY:C | 1:A:662:VAL:H | 2.18 | 0.47 |
| 1:A:554:LEU:HD11 | 1:A:734:GLU:HG2 | 1.97 | 0.47 |
| 1:A:802:PRO:CB | 1:A:932:ILE:HD11 | 2.45 | 0.47 |
| 1:A:968:MET:HA | 1:A:972:SER:CB | 2.39 | 0.47 |
| 1:A:145:ARG:O | 1:A:145:ARG:HG3 | 2.15 | 0.47 |
| 1:A:197:GLU:HG2 | 1:A:212:LYS:HG2 | 1.96 | 0.47 |
| 1:A:627:ILE:HD12 | 1:A:627:ILE:N | 2.30 | 0.47 |
| 1:A:92:THR:HG22 | 1:A:93:LYS:N | 2.29 | 0.47 |
| 1:A:947:ILE:HG22 | 1:A:1015:ILE:HB | 1.97 | 0.47 |
| 1:A:948:ARG:HA | 1:A:1013:ARG:O | 2.15 | 0.47 |
| 1:A:1041:ILE:C | 1:A:1043:ASN:H | 2.18 | 0.47 |
| 1:A:1205:ILE:O | 1:A:1261:LEU:O | 2.33 | 0.47 |
| 1:A:420:THR:CG2 | 1:A:420:THR:O | 2.59 | 0.47 |
| 1:A:168:PHE:HA | 1:A:528:LEU:HA | 1.96 | 0.47 |
| 1:A:574:GLU:HA | 1:A:574:GLU:OE1 | 2.15 | 0.47 |
| 1:A:574:GLU:CD | 1:A:574:GLU:N | 2.66 | 0.47 |
| 1:A:576:LEU:CA | 1:A:581:ARG:HB2 | 2.35 | 0.47 |
| 1:A:585:PHE:CE1 | 1:A:586:PHE:CE1 | 3.03 | 0.47 |
| 1:A:663:ILE:CG2 | 1:A:663:ILE:O | 2.62 | 0.47 |
| 1:A:702:ARG:O | 1:A:702:ARG:HD2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:987:LEU:CD1 | 1:A:1041:ILE:HD13 | 2.43 | 0.46 |
| 1:A:1014:TRP:HD1 | 1:A:1102:GLY:HA3 | 1.80 | 0.46 |
| 1:A:1096:ILE:HD12 | 1:A:1104:TYR:CE1 | 2.50 | 0.46 |
| 1:A:1124:ASP:HB2 | 1:A:1137:LYS:HB2 | 1.97 | 0.46 |
| 1:A:171:GLU:HG2 | 1:A:172:VAL:HG23 | 1.97 | 0.46 |
| 1:A:18:ASP:HA | 1:A:37:LYS:HB3 | 1.97 | 0.46 |
| 1:A:105:ARG:NH1 | 1:A:508:PHE:CZ | 2.83 | 0.46 |
| 1:A:742:ALA:C | 1:A:744:LYS:H | 2.18 | 0.46 |
| 1:A:757:GLU:CB | 1:A:760:ASN:ND2 | 2.78 | 0.46 |
| 1:A:1233:ASN:OD1 | 1:A:1235:CYS:N | 2.43 | 0.46 |
| 1:A:1288:ASP:C | 1:A:1290:GLY:H | 2.18 | 0.46 |
| 1:A:195:GLY:HA3 | 1:A:374:PHE:CE1 | 2.49 | 0.46 |
| 1:A:761:ASN:C | 1:A:763:ASN:H | 2.16 | 0.46 |
| 1:A:674:PRO:C | 1:A:807:ARG:NH1 | 2.69 | 0.46 |
| 1:A:954:ASN:HB3 | 1:A:956:ILE:HG13 | 1.97 | 0.46 |
| 1:A:167:SER:HB2 | 1:A:184:GLN:HE22 | 1.81 | 0.46 |
| 1:A:227:HIS:CE1 | 1:A:261:GLU:OE1 | 2.68 | 0.46 |
| 1:A:346:THR:HG22 | 1:A:347:GLU:N | 2.30 | 0.46 |
| 1:A:553:TYR:CD2 | 1:A:642:ASN:HB2 | 2.51 | 0.46 |
| 1:A:915:GLN:HB2 | 1:A:1068:TRP:CZ3 | 2.50 | 0.46 |
| 1:A:21:TYR:HA | 1:A:21:TYR:HD1 | 1.68 | 0.46 |
| 1:A:729:ARG:HH22 | 1:A:789:ASN:ND2 | 2.12 | 0.46 |
| 1:A:757:GLU:CB | 1:A:760:ASN:HD22 | 2.28 | 0.46 |
| 1:A:943:THR:CG2 | 1:A:1019:ILE:HB | 2.46 | 0.46 |
| 1:A:1041:ILE:O | 1:A:1041:ILE:CG2 | 2.62 | 0.46 |
| 1:A:1018:THR:HG21 | 1:A:1084:ILE:HD12 | 1.97 | 0.46 |
| 1:A:1111:TYR:CE1 | 1:A:1286:PRO:HB3 | 2.50 | 0.46 |
| 1:A:29:GLN:N | 1:A:29:GLN:CD | 2.68 | 0.46 |
| 1:A:2:PRO:HA | 1:A:108:LEU:HD13 | 1.98 | 0.46 |
| 1:A:6:LYS:HD2 | 1:A:18:ASP:OD2 | 2.16 | 0.46 |
| 1:A:1028:LYS:HB3 | 1:A:1035:LEU:CD1 | 2.46 | 0.46 |
| 1:A:161:ILE:HB | 1:A:194:PHE:CZ | 2.51 | 0.46 |
| 1:A:119:GLY:O | 1:A:121:SER:N | 2.48 | 0.46 |
| 1:A:397:LEU:O | 1:A:398:ALA:CB | 2.62 | 0.46 |
| 1:A:671:ILE:HD13 | 1:A:803:TYR:CD2 | 2.50 | 0.46 |
| 1:A:719:ALA:HA | 1:A:723:THR:HG23 | 1.98 | 0.46 |
| 1:A:1080:ASN:OD1 | 1:A:1083:GLU:HG3 | 2.16 | 0.46 |
| 1:A:139:GLN:CD | 1:A:145:ARG:NH1 | 2.69 | 0.46 |
| 1:A:24:ILE:CD1 | 1:A:45:ILE:CD1 | 2.94 | 0.46 |
| 1:A:535:GLU:O | 1:A:536:ARG:C | 2.54 | 0.46 |
| 1:A:65:ALA:O | 1:A:536:ARG:NH2 | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:643:ILE:CG2 | 1:A:664:LEU:HD23 | 2.40 | 0.46 |
| 1:A:1205:ILE:HA | 1:A:1262:VAL:HG22 | 1.98 | 0.46 |
| 1:A:318:LYS:HG3 | 1:A:331:PHE:CE1 | 2.51 | 0.46 |
| 1:A:534:ILE:HG22 | 1:A:534:ILE:O | 2.15 | 0.46 |
| 1:A:586:PHE:HB3 | 1:A:617:GLU:OE2 | 2.15 | 0.46 |
| 1:A:696:ASP:OD1 | 1:A:840:LYS:NZ | 2.41 | 0.46 |
| 1:A:757:GLU:O | 1:A:757:GLU:HG3 | 2.16 | 0.46 |
| 1:A:965:ILE:HB | 1:A:976:VAL:HG23 | 1.97 | 0.46 |
| 1:A:984:ILE:CG2 | 1:A:998:VAL:HG22 | 2.44 | 0.46 |
| 1:A:105:ARG:HG2 | 1:A:508:PHE:HE1 | 1.78 | 0.46 |
| 1:A:1062:ASP:C | 1:A:1062:ASP:OD1 | 2.54 | 0.46 |
| 1:A:1199:GLN:HE22 | 1:A:1204:LYS:HB3 | 1.80 | 0.46 |
| 1:A:207:LEU:HD21 | 1:A:775:GLU:OE2 | 2.16 | 0.46 |
| 1:A:706:TRP:CE3 | 1:A:808:LEU:HD13 | 2.51 | 0.46 |
| 1:A:964:ILE:HG13 | 1:A:965:ILE:N | 2.31 | 0.46 |
| 1:A:1099:ASP:N | 1:A:1103:ASP:O | 2.47 | 0.45 |
| 1:A:1143:VAL:HG12 | 1:A:1149:TYR:HE1 | 1.81 | 0.45 |
| 1:A:115:ILE:HG22 | 1:A:317:PHE:CE1 | 2.48 | 0.45 |
| 1:A:318:LYS:HG2 | 1:A:331:PHE:CE1 | 2.51 | 0.45 |
| 1:A:326:ASP:OD1 | 1:A:328:SER:N | 2.49 | 0.45 |
| 1:A:492:GLU:C | 1:A:494:ILE:H | 2.18 | 0.45 |
| 1:A:566:ILE:HG23 | 1:A:749:TYR:CB | 2.46 | 0.45 |
| 1:A:39:HIS:HE1 | 1:A:511:GLU:OE2 | 1.97 | 0.45 |
| 1:A:3:PHE:O | 1:A:96:GLU:OE2 | 2.35 | 0.45 |
| 1:A:48:ARG:NH1 | 1:A:77:TYR:HB3 | 2.32 | 0.45 |
| 1:A:1197:ALA:HB2 | 1:A:1247:ILE:HD13 | 1.98 | 0.45 |
| 1:A:1203:GLU:HB3 | 1:A:1262:VAL:CG1 | 2.44 | 0.45 |
| 1:A:1238:ASN:HA | 1:A:1249:PHE:HA | 1.97 | 0.45 |
| 1:A:62:PRO:HG2 | 1:A:64:GLU:O | 2.16 | 0.45 |
| 1:A:798:ASN:HD22 | 1:A:893:ARG:HG2 | 1.81 | 0.45 |
| 1:A:315:ASN:O | 1:A:318:LYS:HB3 | 2.16 | 0.45 |
| 1:A:390:PHE:O | 1:A:392:LEU:N | 2.48 | 0.45 |
| 1:A:674:PRO:C | 1:A:807:ARG:HH11 | 2.19 | 0.45 |
| 1:A:1109:LYS:HA | 1:A:1110:PRO:HD2 | 1.79 | 0.45 |
| 1:A:123:ILE:O | 1:A:124:ASP:C | 2.53 | 0.45 |
| 1:A:1268:ASN:O | 1:A:1272:GLU:HG3 | 2.16 | 0.45 |
| 1:A:458:ASN:HD22 | 1:A:459:ASN:N | 2.13 | 0.45 |
| 1:A:661:ALA:CB | 1:A:791:CYS:HB3 | 2.46 | 0.45 |
| 1:A:906:PHE:HD2 | 1:A:911:LYS:O | 2.00 | 0.45 |
| 1:A:102:ASP:HB2 | 1:A:357:PHE:CE2 | 2.44 | 0.45 |
| 1:A:1100:PHE:CB | 1:A:1285:ILE:HG12 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:671:ILE:HD13 | 1:A:803:TYR:HD2 | 1.82 | 0.45 |
| 1:A:683:SER:HA | 1:A:822:TYR:OH | 2.17 | 0.45 |
| 1:A:566:ILE:HG23 | 1:A:749:TYR:CG | 2.51 | 0.45 |
| 1:A:764:PHE:CD1 | 1:A:764:PHE:O | 2.70 | 0.45 |
| 1:A:943:THR:HG22 | 1:A:1019:ILE:HB | 1.99 | 0.45 |
| 1:A:1186:VAL:N | 1:A:1189:LYS:O | 2.49 | 0.45 |
| 1:A:14:VAL:HA | 1:A:19:ILE:HG22 | 1.99 | 0.45 |
| 1:A:144:TYR:OH | 1:A:520:LEU:O | 2.27 | 0.45 |
| 1:A:606:TRP:O | 1:A:609:GLN:HB3 | 2.16 | 0.45 |
| 1:A:610:LEU:HD12 | 1:A:747:ILE:CD1 | 2.41 | 0.45 |
| 1:A:74:ASP:O | 1:A:75:SER:C | 2.55 | 0.45 |
| 1:A:1012:ASN:CG | 1:A:1012:ASN:O | 2.53 | 0.45 |
| 1:A:1130:ILE:HG23 | 1:A:1209:LEU:HD22 | 1.99 | 0.45 |
| 1:A:1161:ILE:HG22 | 1:A:1163:LYS:CD | 2.47 | 0.45 |
| 1:A:289:LYS:HD3 | 1:A:289:LYS:HA | 1.71 | 0.45 |
| 1:A:598:THR:HG23 | 1:A:602:MET:CE | 2.46 | 0.45 |
| 1:A:998:VAL:CG1 | 1:A:999:PHE:N | 2.80 | 0.45 |
| 1:A:1008:SER:O | 1:A:1013:ARG:NH1 | 2.50 | 0.45 |
| 1:A:143:SER:O | 1:A:144:TYR:HB3 | 2.16 | 0.45 |
| 1:A:567:ALA:O | 1:A:746:ILE:HG12 | 2.17 | 0.45 |
| 1:A:574:GLU:C | 1:A:576:LEU:N | 2.70 | 0.45 |
| 1:A:599:GLU:O | 1:A:602:MET:O | 2.35 | 0.45 |
| 1:A:593:LYS:NZ | 1:A:613:ASP:OD2 | 2.40 | 0.45 |
| 1:A:70:VAL:CG1 | 1:A:71:SER:N | 2.80 | 0.45 |
| 1:A:999:PHE:CG | 1:A:1031:ILE:HG13 | 2.52 | 0.45 |
| 1:A:1109:LYS:NZ | 1:A:1286:PRO:HB3 | 2.32 | 0.45 |
| 1:A:455:ILE:HD12 | 1:A:552:HIS:HA | 1.99 | 0.45 |
| 1:A:487:ILE:HG23 | 1:A:488:GLU:CD | 2.37 | 0.45 |
| 1:A:984:ILE:CG1 | 1:A:998:VAL:HG22 | 2.39 | 0.45 |
| 1:A:985:TRP:CG | 1:A:1019:ILE:HG21 | 2.51 | 0.44 |
| 1:A:952:TYR:CD1 | 1:A:1065:ARG:CZ | 3.00 | 0.44 |
| 1:A:306:THR:CG2 | 1:A:517:ILE:HA | 2.47 | 0.44 |
| 1:A:737:GLU:O | 1:A:741:GLU:HB2 | 2.16 | 0.44 |
| 1:A:869:TYR:CD1 | 1:A:869:TYR:C | 2.91 | 0.44 |
| 1:A:902:SER:O | 1:A:903:LYS:HE2 | 2.17 | 0.44 |
| 1:A:935:ASN:C | 1:A:937:MET:H | 2.20 | 0.44 |
| 1:A:979:ASN:O | 1:A:980:TYR:C | 2.55 | 0.44 |
| 1:A:1168:GLY:C | 1:A:1170:LYS:N | 2.64 | 0.44 |
| 1:A:1269:ARG:CZ | 1:A:1270:GLN:NE2 | 2.80 | 0.44 |
| 1:A:2:PRO:O | 1:A:39:HIS:CD2 | 2.60 | 0.44 |
| 1:A:581:ARG:O | 1:A:581:ARG:HG3 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:760:ASN:O | 1:A:761:ASN:HB2 | 2.17 | 0.44 |
| 1:A:883:TYR:H | 1:A:912:ASN:CG | 2.21 | 0.44 |
| 1:A:1104:TYR:CD2 | 1:A:1173:ILE:CD1 | 3.00 | 0.44 |
| 1:A:1288:ASP:C | 1:A:1290:GLY:N | 2.68 | 0.44 |
| 1:A:425:PHE:HZ | 1:A:537:PHE:HB2 | 1.80 | 0.44 |
| 1:A:719:ALA:HA | 1:A:723:THR:CG2 | 2.46 | 0.44 |
| 1:A:36:PHE:CZ | 1:A:88:LEU:HD22 | 2.52 | 0.44 |
| 1:A:955:SER:HA | 1:A:958:LEU:HG | 1.99 | 0.44 |
| 1:A:1029:ILE:HG23 | 1:A:1036:ILE:HB | 1.98 | 0.44 |
| 1:A:1146:THR:HG22 | 1:A:1147:ASN:ND2 | 2.33 | 0.44 |
| 1:A:122:THR:CB | 1:A:126:GLU:OE1 | 2.61 | 0.44 |
| 1:A:227:HIS:ND1 | 1:A:261:GLU:OE1 | 2.50 | 0.44 |
| 1:A:318:LYS:CG | 1:A:331:PHE:HE1 | 2.31 | 0.44 |
| 1:A:431:VAL:HG11 | 1:A:548:TYR:CE1 | 2.53 | 0.44 |
| 1:A:632:ILE:CD1 | 1:A:786:LYS:HD3 | 2.47 | 0.44 |
| 1:A:153:ILE:CD1 | 1:A:186:ILE:HB | 2.42 | 0.44 |
| 1:A:238:ASN:OD1 | 1:A:239:PRO:HD2 | 2.16 | 0.44 |
| 1:A:659:SER:HB2 | 1:A:663:ILE:HG13 | 1.98 | 0.44 |
| 1:A:688:LYS:O | 1:A:689:VAL:C | 2.55 | 0.44 |
| 1:A:964:ILE:HG13 | 1:A:965:ILE:HG13 | 2.00 | 0.44 |
| 1:A:1012:ASN:O | 1:A:1101:TRP:CD1 | 2.70 | 0.44 |
| 1:A:923:LYS:HB2 | 1:A:1056:LYS:HB2 | 1.99 | 0.44 |
| 1:A:2:PRO:HD3 | 1:A:108:LEU:HD22 | 2.00 | 0.44 |
| 1:A:1163:LYS:CD | 1:A:1183:ASN:ND2 | 2.80 | 0.44 |
| 1:A:11:LYS:HZ1 | 1:A:81:ASP:CG | 2.19 | 0.44 |
| 1:A:504:LEU:C | 1:A:506:PHE:H | 2.21 | 0.44 |
| 1:A:455:ILE:HG23 | 1:A:555:ARG:HD2 | 1.98 | 0.44 |
| 1:A:764:PHE:CE2 | 1:A:766:ILE:HG12 | 2.52 | 0.44 |
| 1:A:269:HIS:CE1 | 1:A:859:ASN:HD22 | 2.36 | 0.44 |
| 1:A:1180:VAL:HG22 | 1:A:1221:VAL:O | 2.18 | 0.44 |
| 1:A:1206:LEU:HD11 | 1:A:1250:ILE:HG12 | 2.00 | 0.44 |
| 1:A:42:ILE:CD1 | 1:A:151:LEU:HB3 | 2.48 | 0.44 |
| 1:A:603:PHE:O | 1:A:606:TRP:HB3 | 2.17 | 0.44 |
| 1:A:621:VAL:HG11 | 1:A:632:ILE:HG23 | 1.98 | 0.44 |
| 1:A:742:ALA:C | 1:A:744:LYS:N | 2.71 | 0.44 |
| 1:A:1057:LEU:N | 1:A:1057:LEU:HD12 | 2.23 | 0.44 |
| 1:A:948:ARG:CB | 1:A:1068:TRP:HB2 | 2.20 | 0.44 |
| 1:A:1211:ILE:HB | 1:A:1212:PRO:HD3 | 1.99 | 0.44 |
| 1:A:430:CYS:HA | 1:A:454:CYS:HA | 2.00 | 0.44 |
| 1:A:485:THR:HG22 | 1:A:486:ASN:N | 2.33 | 0.44 |
| 1:A:610:LEU:CD1 | 1:A:747:ILE:HD11 | 2.41 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:754:TYR:CD1 | 1:A:755:THR:N | 2.78 | 0.44 |
| 1:A:843:ASN:O | 1:A:846:SER:OG | 2.34 | 0.44 |
| 1:A:1194:ALA:O | 1:A:1206:LEU:HA | 2.18 | 0.44 |
| 1:A:1199:GLN:NE2 | 1:A:1204:LYS:HB3 | 2.32 | 0.44 |
| 1:A:198:GLU:OE2 | 1:A:200:LEU:HB2 | 2.18 | 0.44 |
| 1:A:202:VAL:HA | 1:A:205:ASN:O | 2.18 | 0.44 |
| 1:A:22:ILE:CD1 | 1:A:22:ILE:N | 2.79 | 0.44 |
| 1:A:403:GLY:HA2 | 1:A:409:ASN:HD22 | 1.83 | 0.44 |
| 1:A:417:LYS:HE3 | 1:A:419:PHE:CZ | 2.53 | 0.44 |
| 1:A:458:ASN:HB3 | 1:A:461:ASP:CB | 2.45 | 0.44 |
| 1:A:844:THR:O | 1:A:846:SER:N | 2.40 | 0.44 |
| 1:A:891:LEU:HD23 | 1:A:891:LEU:HA | 1.81 | 0.44 |
| 1:A:949:ILE:HG22 | 1:A:950:PRO:O | 2.17 | 0.44 |
| 1:A:990:THR:C | 1:A:992:GLU:N | 2.65 | 0.44 |
| 1:A:176:THR:CG2 | 1:A:176:THR:O | 2.65 | 0.43 |
| 1:A:167:SER:CB | 1:A:184:GLN:HE22 | 2.31 | 0.43 |
| 1:A:195:GLY:HA2 | 1:A:213:PHE:O | 2.18 | 0.43 |
| 1:A:234:GLY:O | 1:A:235:ILE:HD12 | 2.17 | 0.43 |
| 1:A:97:ARG:NH1 | 1:A:358:PHE:CD1 | 2.86 | 0.43 |
| 1:A:515:ILE:HA | 1:A:515:ILE:HD13 | 1.82 | 0.43 |
| 1:A:549:THR:HG23 | 1:A:552:HIS:CD2 | 2.53 | 0.43 |
| 1:A:575:ALA:O | 1:A:581:ARG:CA | 2.66 | 0.43 |
| 1:A:763:ASN:HB2 | 1:A:765:ASN:HD22 | 1.75 | 0.43 |
| 1:A:859:ASN:HD21 | 1:A:861:ARG:HH12 | 1.66 | 0.43 |
| 1:A:991:GLN:O | 1:A:993:ILE:N | 2.50 | 0.43 |
| 1:A:1025:ASN:HB3 | 1:A:1026:ASN:H | 1.50 | 0.43 |
| 1:A:1144:MET:HB3 | 1:A:1150:LEU:HD13 | 2.00 | 0.43 |
| 1:A:192:PHE:HA | 1:A:374:PHE:O | 2.18 | 0.43 |
| 1:A:591:VAL:HG12 | 1:A:595:ASN:ND2 | 2.32 | 0.43 |
| 1:A:748:ASN:O | 1:A:749:TYR:C | 2.56 | 0.43 |
| 1:A:1113:MET:HE3 | 1:A:1160:PHE:HB2 | 2.01 | 0.43 |
| 1:A:119:GLY:C | 1:A:121:SER:N | 2.70 | 0.43 |
| 1:A:1233:ASN:OD1 | 1:A:1235:CYS:HB2 | 2.18 | 0.43 |
| 1:A:1267:TYR:O | 1:A:1268:ASN:C | 2.57 | 0.43 |
| 1:A:126:GLU:OE2 | 1:A:304:VAL:CG1 | 2.66 | 0.43 |
| 1:A:159:ASP:C | 1:A:159:ASP:OD1 | 2.57 | 0.43 |
| 1:A:15:ASN:C | 1:A:17:VAL:H | 2.20 | 0.43 |
| 1:A:24:ILE:HG23 | 1:A:25:PRO:N | 2.33 | 0.43 |
| 1:A:67:GLN:HB3 | 1:A:425:PHE:CD2 | 2.53 | 0.43 |
| 1:A:562:GLY:O | 1:A:564:SER:N | 2.51 | 0.43 |
| 1:A:772:LYS:C | 1:A:774:ASN:N | 2.70 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:907:ASP:O | 1:A:911:LYS:HG2 | 2.17 | 0.43 |
| 1:A:243:PHE:HD1 | 1:A:260:PHE:CE1 | 2.36 | 0.43 |
| 1:A:408:ILE:C | 1:A:410:ASN:H | 2.22 | 0.43 |
| 1:A:309:SER:C | 1:A:311:GLN:N | 2.69 | 0.43 |
| 1:A:105:ARG:NH1 | 1:A:508:PHE:CE1 | 2.86 | 0.43 |
| 1:A:981:GLY:HA2 | 1:A:1001:TYR:CZ | 2.54 | 0.43 |
| 1:A:1034:ARG:NH1 | 1:A:1036:ILE:CD1 | 2.81 | 0.43 |
| 1:A:1199:GLN:HE22 | 1:A:1204:LYS:CA | 2.31 | 0.43 |
| 1:A:203:ASP:OD1 | 1:A:204:THR:N | 2.52 | 0.43 |
| 1:A:346:THR:CG2 | 1:A:347:GLU:HG3 | 2.29 | 0.43 |
| 1:A:411:MET:HG3 | 1:A:411:MET:O | 2.19 | 0.43 |
| 1:A:429:LEU:O | 1:A:552:HIS:HE1 | 2.02 | 0.43 |
| 1:A:1087:LEU:O | 1:A:1091:GLN:HG3 | 2.18 | 0.43 |
| 1:A:310:LEU:HD13 | 1:A:314:LYS:HG3 | 2.00 | 0.43 |
| 1:A:778:ASN:O | 1:A:782:ILE:HG13 | 2.18 | 0.43 |
| 1:A:162:GLN:HE21 | 1:A:162:GLN:HB3 | 1.56 | 0.43 |
| 1:A:320:LYS:HD3 | 1:A:321:TYR:CZ | 2.53 | 0.43 |
| 1:A:540:GLY:O | 1:A:541:LYS:O | 2.37 | 0.43 |
| 1:A:648:TYR:O | 1:A:649:LYS:O | 2.36 | 0.43 |
| 1:A:566:ILE:HG12 | 1:A:749:TYR:HB3 | 2.00 | 0.43 |
| 1:A:722:ASN:ND2 | 1:A:792:SER:OG | 2.52 | 0.43 |
| 1:A:809:GLU:HG2 | 1:A:934:TYR:CD2 | 2.53 | 0.43 |
| 1:A:874:ILE:HD13 | 1:A:874:ILE:HA | 1.73 | 0.43 |
| 1:A:1010:TYR:CD1 | 1:A:1010:TYR:N | 2.86 | 0.43 |
| 1:A:1061:ARG:CG | 1:A:1061:ARG:HH11 | 2.27 | 0.43 |
| 1:A:388:ASP:HB3 | 1:A:391:ASN:O | 2.18 | 0.43 |
| 1:A:473:ASN:OD1 | 1:A:475:LEU:CD1 | 2.60 | 0.43 |
| 1:A:585:PHE:HZ | 1:A:736:LEU:HD23 | 1.84 | 0.43 |
| 1:A:1070:LYS:HG2 | 1:A:1071:TYR:CG | 2.53 | 0.43 |
| 1:A:1125:VAL:HG22 | 1:A:1134:MET:SD | 2.59 | 0.43 |
| 1:A:995:GLN:NE2 | 1:A:1039:LYS:HB3 | 2.34 | 0.43 |
| 1:A:1242:ASN:C | 1:A:1244:GLY:H | 2.22 | 0.42 |
| 1:A:491:GLU:OE2 | 1:A:711:LYS:HD2 | 2.19 | 0.42 |
| 1:A:558:GLU:O | 1:A:559:PHE:CG | 2.72 | 0.42 |
| 1:A:716:ASN:OD1 | 1:A:720:LYS:HE3 | 2.19 | 0.42 |
| 1:A:1026:ASN:ND2 | 1:A:1028:LYS:HE2 | 2.34 | 0.42 |
| 1:A:1099:ASP:C | 1:A:1101:TRP:N | 2.71 | 0.42 |
| 1:A:132:THR:O | 1:A:132:THR:HG23 | 2.17 | 0.42 |
| 1:A:196:PHE:CZ | 1:A:362:ASN:HA | 2.54 | 0.42 |
| 1:A:464:PHE:O | 1:A:465:SER:CB | 2.65 | 0.42 |
| 1:A:343:LYS:HD3 | 1:A:502:TYR:OH | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:571:SER:O | 1:A:572:VAL:HB | 2.19 | 0.42 |
| 1:A:634:ILE:N | 1:A:634:ILE:HD12 | 2.34 | 0.42 |
| 1:A:885:SER:OG | 1:A:886:ASN:N | 2.52 | 0.42 |
| 1:A:973:GLY:HA2 | 1:A:988:GLN:H | 1.83 | 0.42 |
| 1:A:22:ILE:HG22 | 1:A:24:ILE:HD12 | 2.00 | 0.42 |
| 1:A:459:ASN:C | 1:A:461:ASP:H | 2.21 | 0.42 |
| 1:A:584:THR:HG21 | 1:A:586:PHE:HB2 | 2.01 | 0.42 |
| 1:A:471:PHE:CE2 | 1:A:720:LYS:HE2 | 2.54 | 0.42 |
| 1:A:879:LEU:HD23 | 1:A:1072:PHE:HE2 | 1.83 | 0.42 |
| 1:A:913:GLN:OE1 | 1:A:1014:TRP:CZ2 | 2.72 | 0.42 |
| 1:A:115:ILE:HD12 | 1:A:316:VAL:CG1 | 2.50 | 0.42 |
| 1:A:1221:VAL:CG2 | 1:A:1239:LEU:HD23 | 2.49 | 0.42 |
| 1:A:194:PHE:N | 1:A:194:PHE:CD1 | 2.87 | 0.42 |
| 1:A:244:LYS:HB2 | 1:A:467:SER:OG | 2.20 | 0.42 |
| 1:A:235:ILE:HD11 | 1:A:286:TYR:HB3 | 2.01 | 0.42 |
| 1:A:459:ASN:O | 1:A:461:ASP:N | 2.45 | 0.42 |
| 1:A:711:LYS:HB2 | 1:A:856:TYR:CE2 | 2.54 | 0.42 |
| 1:A:729:ARG:HH22 | 1:A:789:ASN:HD22 | 1.66 | 0.42 |
| 1:A:869:TYR:HD1 | 1:A:870:ILE:HD13 | 1.84 | 0.42 |
| 1:A:874:ILE:C | 1:A:876:THR:N | 2.73 | 0.42 |
| 1:A:917:PHE:O | 1:A:1057:LEU:CD1 | 2.67 | 0.42 |
| 1:A:969:GLU:O | 1:A:970:ASN:HB3 | 2.17 | 0.42 |
| 1:A:923:LYS:CD | 1:A:1056:LYS:HD3 | 2.50 | 0.42 |
| 1:A:325:GLU:HA | 1:A:330:LYS:O | 2.20 | 0.42 |
| 1:A:535:GLU:OE2 | 1:A:537:PHE:CE2 | 2.73 | 0.42 |
| 1:A:559:PHE:HE2 | 1:A:742:ALA:HA | 1.84 | 0.42 |
| 1:A:662:VAL:C | 1:A:664:LEU:H | 2.22 | 0.42 |
| 1:A:1023:ARG:HD3 | 1:A:1023:ARG:C | 2.38 | 0.42 |
| 1:A:915:GLN:HB2 | 1:A:1068:TRP:CE3 | 2.54 | 0.42 |
| 1:A:1221:VAL:HG23 | 1:A:1239:LEU:HD23 | 2.02 | 0.42 |
| 1:A:357:PHE:N | 1:A:357:PHE:CD1 | 2.87 | 0.42 |
| 1:A:374:PHE:CE2 | 1:A:406:THR:HG21 | 2.53 | 0.42 |
| 1:A:491:GLU:O | 1:A:492:GLU:C | 2.58 | 0.42 |
| 1:A:494:ILE:HD12 | 1:A:494:ILE:N | 2.35 | 0.42 |
| 1:A:758:GLU:C | 1:A:760:ASN:H | 2.22 | 0.42 |
| 1:A:761:ASN:C | 1:A:763:ASN:N | 2.73 | 0.42 |
| 1:A:882:ARG:HB3 | 1:A:912:ASN:OD1 | 2.19 | 0.42 |
| 1:A:1163:LYS:CG | 1:A:1183:ASN:ND2 | 2.83 | 0.42 |
| 1:A:170:HIS:HD2 | 1:A:173:LEU:N | 2.18 | 0.42 |
| 1:A:40:ASN:O | 1:A:112:VAL:HG23 | 2.20 | 0.42 |
| 1:A:68:VAL:CG1 | 1:A:69:PRO:HD2 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1061:ARG:NH1 | 1:A:1061:ARG:HG2 | 2.32 | 0.42 |
| 1:A:1062:ASP:OD1 | 1:A:1063:THR:N | 2.53 | 0.42 |
| 1:A:1115:ASN:HB2 | 1:A:1282:TRP:CZ3 | 2.55 | 0.42 |
| 1:A:1209:LEU:HD11 | 1:A:1217:LEU:HD12 | 2.01 | 0.42 |
| 1:A:1235:CYS:HA | 1:A:1280:CYS:O | 2.19 | 0.42 |
| 1:A:125:THR:O | 1:A:300:ALA:HA | 2.20 | 0.42 |
| 1:A:430:CYS:HA | 1:A:453:LEU:O | 2.20 | 0.42 |
| 1:A:487:ILE:O | 1:A:488:GLU:O | 2.37 | 0.42 |
| 1:A:498:LEU:HG | 1:A:502:TYR:CE1 | 2.55 | 0.42 |
| 1:A:638:GLY:O | 1:A:642:ASN:CA | 2.68 | 0.42 |
| 1:A:675:VAL:HA | 1:A:807:ARG:HD2 | 2.02 | 0.42 |
| 1:A:1128:VAL:CG1 | 1:A:1129:GLY:N | 2.83 | 0.42 |
| 1:A:1155:TYR:N | 1:A:1155:TYR:CD1 | 2.87 | 0.42 |
| 1:A:1166:ALA:O | 1:A:1167:SER:HB2 | 2.20 | 0.42 |
| 1:A:1252:PHE:O | 1:A:1253:HIS:HB2 | 2.19 | 0.42 |
| 1:A:154:ILE:HD12 | 1:A:186:ILE:O | 2.19 | 0.42 |
| 1:A:198:GLU:CD | 1:A:201:GLU:HG2 | 2.40 | 0.42 |
| 1:A:114:GLY:O | 1:A:320:LYS:CD | 2.68 | 0.42 |
| 1:A:405:ASN:OD1 | 1:A:407:GLU:N | 2.51 | 0.42 |
| 1:A:638:GLY:N | 1:A:639:PRO:CD | 2.83 | 0.42 |
| 1:A:659:SER:HB2 | 1:A:663:ILE:CD1 | 2.49 | 0.42 |
| 1:A:660:GLY:C | 1:A:662:VAL:N | 2.73 | 0.42 |
| 1:A:641:LEU:CD1 | 1:A:732:MET:SD | 3.08 | 0.42 |
| 1:A:779:LYS:HA | 1:A:782:ILE:HD12 | 2.02 | 0.42 |
| 1:A:927:ILE:HA | 1:A:1052:ASN:HB3 | 2.02 | 0.42 |
| 1:A:1061:ARG:NH1 | 1:A:1061:ARG:CG | 2.82 | 0.42 |
| 1:A:170:HIS:CG | 1:A:173:LEU:HB2 | 2.55 | 0.42 |
| 1:A:373:VAL:HG12 | 1:A:374:PHE:N | 2.35 | 0.42 |
| 1:A:568:LEU:HB3 | 1:A:595:ASN:OD1 | 2.19 | 0.42 |
| 1:A:74:ASP:OD1 | 1:A:74:ASP:O | 2.38 | 0.42 |
| 1:A:907:ASP:O | 1:A:911:LYS:HA | 2.20 | 0.42 |
| 1:A:910:ASP:C | 1:A:912:ASN:H | 2.24 | 0.42 |
| 1:A:961:GLU:HB2 | 1:A:979:ASN:ND2 | 2.23 | 0.42 |
| 1:A:1144:MET:HB3 | 1:A:1150:LEU:CD1 | 2.50 | 0.41 |
| 1:A:149:LEU:CD2 | 1:A:150:ASN:H | 2.33 | 0.41 |
| 1:A:303:ILE:HG22 | 1:A:310:LEU:HB2 | 2.02 | 0.41 |
| 1:A:502:TYR:O | 1:A:506:PHE:HB2 | 2.20 | 0.41 |
| 1:A:566:ILE:CG1 | 1:A:749:TYR:HB3 | 2.50 | 0.41 |
| 1:A:588:SER:O | 1:A:591:VAL:N | 2.53 | 0.41 |
| 1:A:684:TYR:CD1 | 1:A:684:TYR:N | 2.87 | 0.41 |
| 1:A:794:SER:O | 1:A:798:ASN:OD1 | 2.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:862:LEU:O | 1:A:865:THR:HB | 2.20 | 0.41 |
| 1:A:163:PHE:CD1 | 1:A:188:PHE:HA | 2.55 | 0.41 |
| 1:A:217:PRO:HG2 | 1:A:378:ILE:CD1 | 2.35 | 0.41 |
| 1:A:290:PHE:O | 1:A:293:ILE:N | 2.53 | 0.41 |
| 1:A:309:SER:O | 1:A:312:TYR:HB3 | 2.19 | 0.41 |
| 1:A:322:LEU:HD23 | 1:A:322:LEU:HA | 1.83 | 0.41 |
| 1:A:565:ARG:O | 1:A:566:ILE:C | 2.58 | 0.41 |
| 1:A:585:PHE:CE1 | 1:A:586:PHE:HE1 | 2.37 | 0.41 |
| 1:A:797:MET:CE | 1:A:866:PHE:CE1 | 3.01 | 0.41 |
| 1:A:965:ILE:HD12 | 1:A:976:VAL:CG2 | 2.48 | 0.41 |
| 1:A:1227:ASN:HD21 | 1:A:1229:GLN:HB3 | 1.80 | 0.41 |
| 1:A:265:THR:O | 1:A:265:THR:HG22 | 2.20 | 0.41 |
| 1:A:385:THR:HG23 | 1:A:388:ASP:N | 2.24 | 0.41 |
| 1:A:560:GLU:O | 1:A:561:HIS:C | 2.59 | 0.41 |
| 1:A:66:LYS:HE2 | 1:A:68:VAL:HG21 | 2.02 | 0.41 |
| 1:A:919:LEU:C | 1:A:921:SER:H | 2.21 | 0.41 |
| 1:A:1026:ASN:N | 1:A:1026:ASN:OD1 | 2.53 | 0.41 |
| 1:A:927:ILE:HG23 | 1:A:1051:ASN:ND2 | 2.35 | 0.41 |
| 1:A:22:ILE:CD1 | 1:A:22:ILE:H | 2.32 | 0.41 |
| 1:A:430:CYS:HB2 | 1:A:544:GLU:HA | 2.02 | 0.41 |
| 1:A:742:ALA:O | 1:A:745:ALA:N | 2.48 | 0.41 |
| 1:A:801:ILE:HB | 1:A:802:PRO:HD3 | 2.01 | 0.41 |
| 1:A:897:LYS:HG3 | 1:A:899:ASN:OD1 | 2.20 | 0.41 |
| 1:A:1241:ASP:O | 1:A:1241:ASP:OD1 | 2.39 | 0.41 |
| 1:A:70:VAL:CG1 | 1:A:161:ILE:HD11 | 2.42 | 0.41 |
| 1:A:174:ASN:C | 1:A:176:THR:H | 2.24 | 0.41 |
| 1:A:23:LYS:NZ | 1:A:23:LYS:CB | 2.81 | 0.41 |
| 1:A:638:GLY:HA2 | 1:A:643:ILE:HB | 2.02 | 0.41 |
| 1:A:662:VAL:O | 1:A:664:LEU:N | 2.53 | 0.41 |
| 1:A:473:ASN:HD21 | 1:A:674:PRO:HG3 | 1.86 | 0.41 |
| 1:A:684:TYR:HD2 | 1:A:690:LEU:HD23 | 1.85 | 0.41 |
| 1:A:819:LEU:O | 1:A:823:ILE:HG13 | 2.21 | 0.41 |
| 1:A:884:GLU:HG3 | 1:A:891:LEU:HD11 | 2.02 | 0.41 |
| 1:A:941:PHE:O | 1:A:1021:ASN:HB2 | 2.20 | 0.41 |
| 1:A:942:SER:HA | 1:A:1019:ILE:O | 2.20 | 0.41 |
| 1:A:119:GLY:C | 1:A:121:SER:H | 2.23 | 0.41 |
| 1:A:131:ASP:N | 1:A:131:ASP:OD1 | 2.53 | 0.41 |
| 1:A:342:TYR:O | 1:A:346:THR:HB | 2.19 | 0.41 |
| 1:A:93:LYS:NZ | 1:A:384:TYR:O | 2.53 | 0.41 |
| 1:A:763:ASN:C | 1:A:765:ASN:N | 2.72 | 0.41 |
| 1:A:93:LYS:HE2 | 1:A:384:TYR:HD1 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1267:TYR:CD2 | 1:A:1280:CYS:SG | 3.14 | 0.41 |
| 1:A:205:ASN:ND2 | 1:A:401:PHE:HE2 | 2.18 | 0.41 |
| 1:A:303:ILE:O | 1:A:303:ILE:HG12 | 2.19 | 0.41 |
| 1:A:588:SER:O | 1:A:591:VAL:HG23 | 2.20 | 0.41 |
| 1:A:757:GLU:CG | 1:A:760:ASN:ND2 | 2.84 | 0.41 |
| 1:A:765:ASN:CB | 1:A:768:ASP:HB2 | 2.45 | 0.41 |
| 1:A:772:LYS:O | 1:A:773:LEU:C | 2.59 | 0.41 |
| 1:A:824:TYR:C | 1:A:826:ASN:H | 2.24 | 0.41 |
| 1:A:919:LEU:HD23 | 1:A:919:LEU:N | 2.36 | 0.41 |
| 1:A:903:LYS:HB2 | 1:A:922:SER:CA | 2.51 | 0.41 |
| 1:A:996:ARG:O | 1:A:1039:LYS:HD2 | 2.20 | 0.41 |
| 1:A:1018:THR:HG21 | 1:A:1084:ILE:CD1 | 2.51 | 0.41 |
| 1:A:1138:GLY:HA3 | 1:A:1139:PRO:HD2 | 1.73 | 0.41 |
| 1:A:250:TYR:HB2 | 1:A:429:LEU:HD21 | 2.01 | 0.41 |
| 1:A:3:PHE:O | 1:A:96:GLU:CD | 2.58 | 0.41 |
| 1:A:566:ILE:HG12 | 1:A:749:TYR:HD1 | 1.74 | 0.41 |
| 1:A:594:VAL:HG12 | 1:A:746:ILE:CD1 | 2.50 | 0.41 |
| 1:A:758:GLU:O | 1:A:759:LYS:HB2 | 2.21 | 0.41 |
| 1:A:88:LEU:HD12 | 1:A:88:LEU:HA | 1.82 | 0.41 |
| 1:A:1029:ILE:O | 1:A:1029:ILE:CG2 | 2.67 | 0.41 |
| 1:A:1065:ARG:HD2 | 1:A:1065:ARG:HA | 1.85 | 0.41 |
| 1:A:25:PRO:HD2 | 1:A:185:TYR:OH | 2.20 | 0.41 |
| 1:A:193:THR:CG2 | 1:A:215:THR:O | 2.65 | 0.41 |
| 1:A:554:LEU:HD23 | 1:A:641:LEU:CD2 | 2.51 | 0.41 |
| 1:A:289:LYS:O | 1:A:293:ILE:HG12 | 2.21 | 0.41 |
| 1:A:691:THR:C | 1:A:693:GLN:N | 2.75 | 0.41 |
| 1:A:975:LYS:O | 1:A:975:LYS:HD3 | 2.20 | 0.41 |
| 1:A:1022:ASN:HD22 | 1:A:1025:ASN:N | 2.19 | 0.41 |
| 1:A:494:ILE:HG22 | 1:A:494:ILE:O | 2.21 | 0.41 |
| 1:A:754:TYR:OH | 1:A:757:GLU:CG | 2.65 | 0.41 |
| 1:A:747:ILE:CG2 | 1:A:764:PHE:CZ | 3.02 | 0.41 |
| 1:A:950:PRO:CD | 1:A:1066:TYR:O | 2.69 | 0.41 |
| 1:A:141:ASP:OD2 | 1:A:143:SER:OG | 2.40 | 0.40 |
| 1:A:553:TYR:CG | 1:A:642:ASN:HB2 | 2.56 | 0.40 |
| 1:A:761:ASN:O | 1:A:763:ASN:N | 2.42 | 0.40 |
| 1:A:1077:LYS:HE2 | 1:A:1079:LEU:HD23 | 2.03 | 0.40 |
| 1:A:1137:LYS:CG | 1:A:1138:GLY:H | 2.34 | 0.40 |
| 1:A:583:TYR:O | 1:A:739:GLN:NE2 | 2.53 | 0.40 |
| 1:A:619:SER:O | 1:A:621:VAL:HG23 | 2.20 | 0.40 |
| 1:A:740:ALA:HB2 | 1:A:777:ILE:HD11 | 2.03 | 0.40 |
| 1:A:78:LEU:H | 1:A:83:GLU:CD | 2.24 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1193:LEU:CD1 | 1:A:1193:LEU:C | 2.87 | 0.40 |
| 1:A:1198:SER:O | 1:A:1199:GLN:O | 2.38 | 0.40 |
| 1:A:192:PHE:CZ | 1:A:375:LYS:NZ | 2.78 | 0.40 |
| 1:A:226:ILE:O | 1:A:226:ILE:HG22 | 2.20 | 0.40 |
| 1:A:336:LEU:HD11 | 1:A:340:LYS:HE3 | 2.03 | 0.40 |
| 1:A:392:LEU:HB2 | 1:A:395:THR:OG1 | 2.22 | 0.40 |
| 1:A:426:TYR:C | 1:A:426:TYR:CD1 | 2.94 | 0.40 |
| 1:A:492:GLU:O | 1:A:494:ILE:N | 2.51 | 0.40 |
| 1:A:506:PHE:HB3 | 1:A:508:PHE:CE2 | 2.57 | 0.40 |
| 1:A:568:LEU:HA | 1:A:595:ASN:OD1 | 2.21 | 0.40 |
| 1:A:690:LEU:HA | 1:A:690:LEU:HD12 | 1.80 | 0.40 |
| 1:A:94:LEU:O | 1:A:98:ILE:HG13 | 2.20 | 0.40 |
| 1:A:1269:ARG:CZ | 1:A:1270:GLN:HE22 | 2.35 | 0.40 |
| 1:A:497:ASP:O | 1:A:500:GLN:HB3 | 2.22 | 0.40 |
| 1:A:471:PHE:CE2 | 1:A:720:LYS:CE | 3.05 | 0.40 |
| 1:A:1030:TYR:CE1 | 1:A:1035:LEU:HB2 | 2.57 | 0.40 |
| 1:A:962:TYR:HE2 | 1:A:1057:LEU:HD23 | 1.81 | 0.40 |
| 1:A:815:LEU:O | 1:A:819:LEU:HB2 | 2.21 | 0.40 |
| 1:A:880:ASN:ND2 | 1:A:880:ASN:C | 2.74 | 0.40 |

All (9) 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:486:ASN:OD1 | 1:A:1273:ARG:NH2[6_555] | 1.12 | 1.08 |
| 1:A:63:PRO:O | 1:A:309:SER:N[3_564] | 1.82 | 0.38 |
| 1:A:486:ASN:CG | 1:A:1273:ARG:NH2[6_555] | 1.90 | 0.30 |
| 1:A:693:GLN:NE2 | 1:A:1276:ARG:CB[6_555] | 1.96 | 0.24 |
| 1:A:697:ASN:ND2 | 1:A:1276:ARG:NH2[6_555] | 2.00 | 0.20 |
| 1:A:486:ASN:OD1 | 1:A:1273:ARG:CZ[6_555] | 2.02 | 0.18 |
| 1:A:64:GLU:CG | 1:A:307:THR:O[3_564] | 2.07 | 0.13 |
| 1:A:693:GLN:NE2 | 1:A:1276:ARG:CG[6_555] | 2.17 | 0.03 |
| 1:A:63:PRO:O | 1:A:308:ALA:CA[3_564] | 2.18 | 0.02 |

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | A | 1273/1312 (97%) | 1008 (79%) | 177 (14%) | 88 (7%) | 1 | 20 |

All (88) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 121 | SER |
| 1 | A | 398 | ALA |
| 1 | A | 488 | GLU |
| 1 | A | 541 | LYS |
| 1 | A | 559 | PHE |
| 1 | A | 561 | HIS |
| 1 | A | 566 | ILE |
| 1 | A | 571 | SER |
| 1 | A | 629 | ASP |
| 1 | A | 649 | LYS |
| 1 | A | 650 | ASP |
| 1 | A | 831 | ILE |
| 1 | A | 973 | GLY |
| 1 | A | 974 | TRP |
| 1 | A | 992 | GLU |
| 1 | A | 1146 | THR |
| 1 | A | 1199 | GLN |
| 1 | A | 1245 | ASN |
| 1 | A | 1273 | ARG |
| 1 | A | 16 | GLY |
| 1 | A | 18 | ASP |
| 1 | A | 75 | SER |
| 1 | A | 123 | ILE |
| 1 | A | 160 | ILE |
| 1 | A | 209 | GLY |
| 1 | A | 256 | LEU |
| 1 | A | 396 | ASN |
| 1 | A | 464 | PHE |
| 1 | A | 490 | ALA |
| 1 | A | 492 | GLU |
| 1 | A | 493 | ASN |
| 1 | A | 510 | ASN |
| 1 | A | 527 | GLN |
| 1 | A | 556 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 563 | LYS |
| 1 | A | 572 | VAL |
| 1 | A | 644 | GLY |
| 1 | A | 648 | TYR |
| 1 | A | 661 | ALA |
| 1 | A | 763 | ASN |
| 1 | A | 773 | LEU |
| 1 | A | 980 | TYR |
| 1 | A | 1138 | GLY |
| 1 | A | 1176 | ASN |
| 1 | A | 1292 | GLY |
| 1 | A | 3 | PHE |
| 1 | A | 30 | MET |
| 1 | A | 115 | ILE |
| 1 | A | 124 | ASP |
| 1 | A | 157 | SER |
| 1 | A | 249 | ALA |
| 1 | A | 562 | GLY |
| 1 | A | 689 | VAL |
| 1 | A | 859 | ASN |
| 1 | A | 891 | LEU |
| 1 | A | 911 | LYS |
| 1 | A | 1155 | TYR |
| 1 | A | 1206 | LEU |
| 1 | A | 1216 | ASN |
| 1 | A | 1289 | ASP |
| 1 | A | 19 | ILE |
| 1 | A | 125 | THR |
| 1 | A | 453 | LEU |
| 1 | A | 646 | MET |
| 1 | A | 663 | ILE |
| 1 | A | 688 | LYS |
| 1 | A | 761 | ASN |
| 1 | A | 762 | ILE |
| 1 | A | 845 | LEU |
| 1 | A | 848 | ASP |
| 1 | A | 885 | SER |
| 1 | A | 1145 | THR |
| 1 | A | 4 | VAL |
| 1 | A | 74 | ASP |
| 1 | A | 141 | ASP |
| 1 | A | 175 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 395 | THR |
| 1 | A | 735 | ALA |
| 1 | A | 825 | ASP |
| 1 | A | 1165 | TYR |
| 1 | A | 1169 | ASN |
| 1 | A | 674 | PRO |
| 1 | A | 677 | GLY |
| 1 | A | 120 | GLY |
| 1 | A | 746 | ILE |
| 1 | A | 494 | ILE |
| 1 | A | 172 | VAL |
| 1 | A | 627 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 1 | A | 1158/1190 (97%) | 1082 (93%) | 76 (7%) | 19 54 |

All (76) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 18 | ASP |
| 1 | A | 21 | TYR |
| 1 | A | 50 | THR |
| 1 | A | 51 | PHE |
| 1 | A | 78 | LEU |
| 1 | A | 81 | ASP |
| 1 | A | 89 | LYS |
| 1 | A | 97 | ARG |
| 1 | A | 122 | THR |
| 1 | A | 129 | VAL |
| 1 | A | 132 | THR |
| 1 | A | 144 | TYR |
| 1 | A | 149 | LEU |
| 1 | A | 150 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 154 | ILE |
| 1 | A | 162 | GLN |
| 1 | A | 165 | CYS |
| 1 | A | 167 | SER |
| 1 | A | 193 | THR |
| 1 | A | 231 | ARG |
| 1 | A | 235 | ILE |
| 1 | A | 241 | ARG |
| 1 | A | 261 | GLU |
| 1 | A | 264 | ARG |
| 1 | A | 303 | ILE |
| 1 | A | 311 | GLN |
| 1 | A | 318 | LYS |
| 1 | A | 345 | LEU |
| 1 | A | 346 | THR |
| 1 | A | 362 | ASN |
| 1 | A | 382 | VAL |
| 1 | A | 412 | ASN |
| 1 | A | 425 | PHE |
| 1 | A | 474 | ASP |
| 1 | A | 554 | LEU |
| 1 | A | 555 | ARG |
| 1 | A | 559 | PHE |
| 1 | A | 561 | HIS |
| 1 | A | 570 | ASN |
| 1 | A | 574 | GLU |
| 1 | A | 576 | LEU |
| 1 | A | 589 | ASP |
| 1 | A | 602 | MET |
| 1 | A | 615 | THR |
| 1 | A | 618 | THR |
| 1 | A | 671 | ILE |
| 1 | A | 702 | ARG |
| 1 | A | 713 | ILE |
| 1 | A | 743 | THR |
| 1 | A | 750 | GLN |
| 1 | A | 763 | ASN |
| 1 | A | 796 | LEU |
| 1 | A | 812 | ASP |
| 1 | A | 825 | ASP |
| 1 | A | 833 | GLN |
| 1 | A | 834 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 835 | ASP |
| 1 | A | 843 | ASN |
| 1 | A | 872 | ASN |
| 1 | A | 874 | ILE |
| 1 | A | 880 | ASN |
| 1 | A | 881 | LEU |
| 1 | A | 912 | ASN |
| 1 | A | 918 | ASN |
| 1 | A | 962 | TYR |
| 1 | A | 974 | TRP |
| 1 | A | 975 | LYS |
| 1 | A | 1018 | THR |
| 1 | A | 1022 | ASN |
| 1 | A | 1026 | ASN |
| 1 | A | 1057 | LEU |
| 1 | A | 1077 | LYS |
| 1 | A | 1114 | LEU |
| 1 | A | 1193 | LEU |
| 1 | A | 1243 | ASN |
| 1 | A | 1277 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 39 | HIS |
| 1 | A | 150 | ASN |
| 1 | A | 162 | GLN |
| 1 | A | 170 | HIS |
| 1 | A | 205 | ASN |
| 1 | A | 227 | HIS |
| 1 | A | 240 | ASN |
| 1 | A | 269 | HIS |
| 1 | A | 311 | GLN |
| 1 | A | 315 | ASN |
| 1 | A | 362 | ASN |
| 1 | A | 377 | ASN |
| 1 | A | 402 | ASN |
| 1 | A | 404 | GLN |
| 1 | A | 418 | ASN |
| 1 | A | 458 | ASN |
| 1 | A | 500 | GLN |
| 1 | A | 552 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 557 | GLN |
| 1 | A | 645 | ASN |
| 1 | A | 697 | ASN |
| 1 | A | 722 | ASN |
| 1 | A | 760 | ASN |
| 1 | A | 765 | ASN |
| 1 | A | 789 | ASN |
| 1 | A | 872 | ASN |
| 1 | A | 880 | ASN |
| 1 | A | 913 | GLN |
| 1 | A | 915 | GLN |
| 1 | A | 960 | ASN |
| 1 | A | 966 | ASN |
| 1 | A | 971 | ASN |
| 1 | A | 979 | ASN |
| 1 | A | 988 | GLN |
| 1 | A | 1003 | GLN |
| 1 | A | 1012 | ASN |
| 1 | A | 1022 | ASN |
| 1 | A | 1026 | ASN |
| 1 | A | 1073 | ASN |
| 1 | A | 1120 | ASN |
| 1 | A | 1126 | ASN |
| 1 | A | 1147 | ASN |
| 1 | A | 1199 | GLN |
| 1 | A | 1243 | ASN |
| 1 | A | 1254 | GLN |
| 1 | A | 1268 | ASN |
| 1 | A | 1270 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 | 1277/1312 (97%) | 0.14 | 37 (2%) 52 43 | 119, 222, 356, 750 | 0 |

All (37) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 590 | TYR | 5.5 |
| 1 | A | 569 | THR | 5.1 |
| 1 | A | 594 | VAL | 4.6 |
| 1 | A | 625 | ASP | 4.3 |
| 1 | A | 1044 | LEU | 4.1 |
| 1 | A | 564 | SER | 3.5 |
| 1 | A | 610 | LEU | 3.5 |
| 1 | A | 1219 | GLN | 3.5 |
| 1 | A | 600 | ALA | 3.4 |
| 1 | A | 1264 | SER | 3.2 |
| 1 | A | 611 | VAL | 3.1 |
| 1 | A | 593 | LYS | 3.1 |
| 1 | A | 1229 | GLN | 3.0 |
| 1 | A | 589 | ASP | 2.9 |
| 1 | A | 591 | VAL | 2.8 |
| 1 | A | 1249 | PHE | 2.8 |
| 1 | A | 679 | PHE | 2.8 |
| 1 | A | 607 | VAL | 2.7 |
| 1 | A | 623 | THR | 2.7 |
| 1 | A | 525 | ILE | 2.6 |
| 1 | A | 756 | GLU | 2.6 |
| 1 | A | 598 | THR | 2.5 |
| 1 | A | 762 | ILE | 2.4 |
| 1 | A | 1166 | ALA | 2.4 |
| 1 | A | 1167 | SER | 2.4 |
| 1 | A | 990 | THR | 2.3 |
| 1 | A | 297 | LEU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 670 | GLU | 2.2 |
| 1 | A | 763 | ASN | 2.2 |
| 1 | A | 565 | ARG | 2.2 |
| 1 | A | 1214 | VAL | 2.2 |
| 1 | A | 951 | LYS | 2.2 |
| 1 | A | 1296 | LEU | 2.1 |
| 1 | A | 1197 | ALA | 2.1 |
| 1 | A | 267 | GLY | 2.0 |
| 1 | A | 192 | PHE | 2.0 |
| 1 | A | 34 | LYS | 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](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 2 | ZN | A | 1313 | 1/1 | 0.92 | 0.46 | - | 147,147,147,147 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.