



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:08 am BST

PDB ID : 3ZEF  
Title : Crystal structure of Prp8:Aar2 complex: second crystal form at 3.1 Angstrom resolution  
Authors : Galej, W.P.; Oubridge, C.; Newman, A.J.; Nagai, K.  
Deposited on : 2012-12-05  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.11   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |



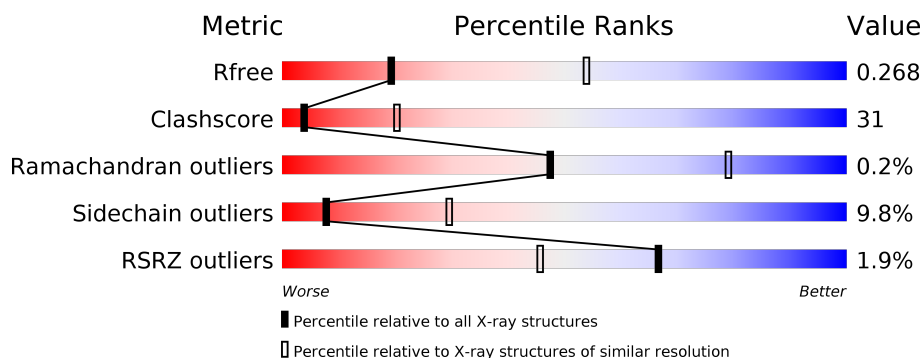
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1094 (3.10-3.10)                                      |
| Clashscore            | 141614                      | 1184 (3.10-3.10)                                      |
| Ramachandran outliers | 138981                      | 1141 (3.10-3.10)                                      |
| Sidechain outliers    | 138945                      | 1141 (3.10-3.10)                                      |
| RSRZ outliers         | 127900                      | 1067 (3.10-3.10)                                      |

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                    |
|-----|-------|--------|---|
| 1   | A     | 355    | <div> <div>2%</div> <div>75% 15% 8%</div> </div>    |
| 1   | D     | 355    | <div> <div>67% 18% 11%</div> </div>                 |
| 2   | B     | 1531   | <div> <div>2%</div> <div>52% 33% 6% 9%</div> </div> |
| 2   | E     | 1531   | <div> <div>2%</div> <div>58% 29% 5% 7%</div> </div> |



## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28285 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 A1 CISTRON-SPLICING FACTOR AAR2.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 327      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2684  | 1722 | 438 | 508 | 16 |         |         |       |
| 1   | D     | 317      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2618  | 1682 | 426 | 493 | 17 |         |         |       |

- Molecule 2 is a protein called PRE-MRNA-SPLICING FACTOR 8.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | B     | 1398     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11401 | 7329 | 1926 | 2109 | 37 |         |         |       |
| 2   | E     | 1420     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11582 | 7445 | 1958 | 2142 | 37 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

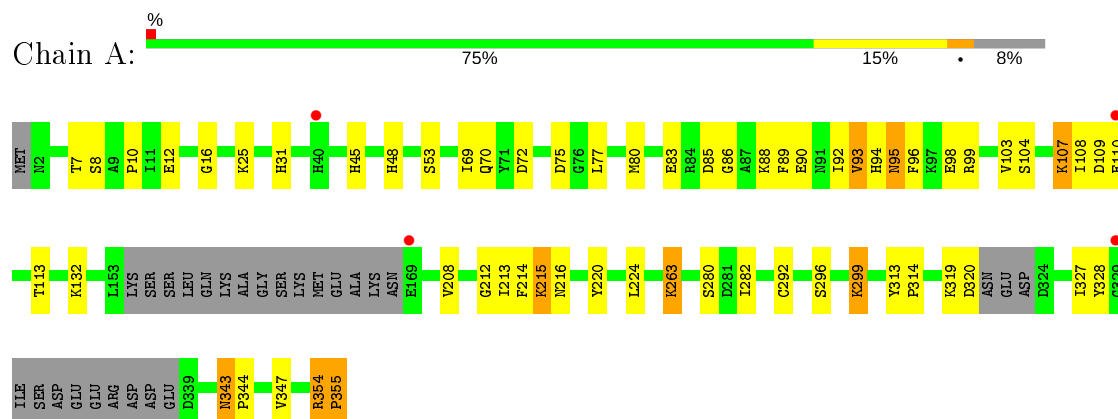
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 883     | SER      | -      | expression tag      | UNP P33334 |
| B     | 884     | GLY      | -      | expression tag      | UNP P33334 |
| B     | 1961    | ASN      | LEU    | engineered mutation | UNP P33334 |
| B     | 1999    | LEU      | ILE    | engineered mutation | UNP P33334 |
| E     | 883     | SER      | -      | expression tag      | UNP P33334 |
| E     | 884     | GLY      | -      | expression tag      | UNP P33334 |
| E     | 1961    | ASN      | LEU    | engineered mutation | UNP P33334 |
| E     | 1999    | LEU      | ILE    | engineered mutation | UNP P33334 |



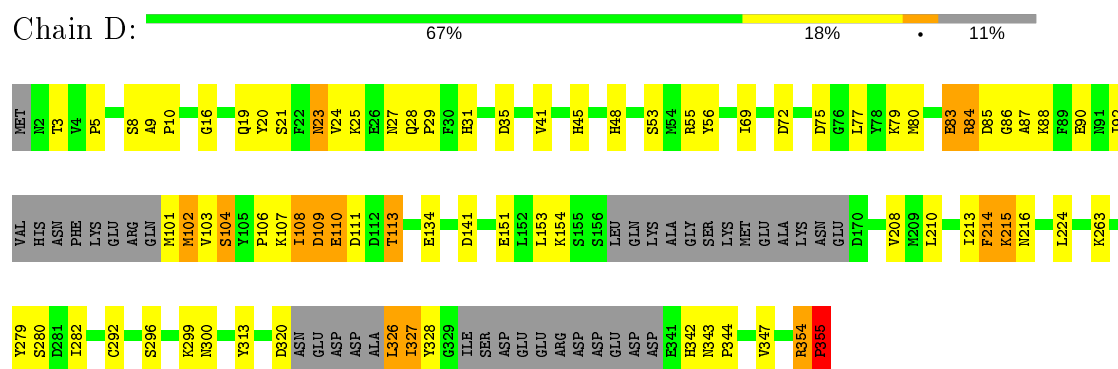
### 3 Residue-property plots

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.

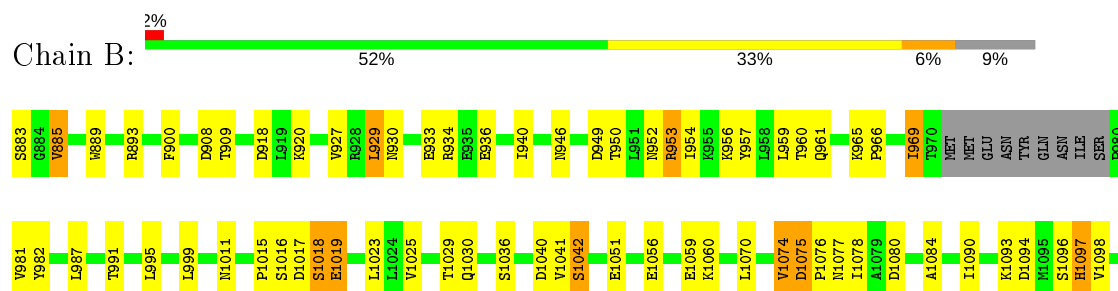
#### • Molecule 1: A1 CISTRON-SPLICING FACTOR AAR2



#### • Molecule 1: A1 CISTRON-SPLICING FACTOR AAR2



#### • Molecule 2: PRE-MRNA-SPLICING FACTOR 8



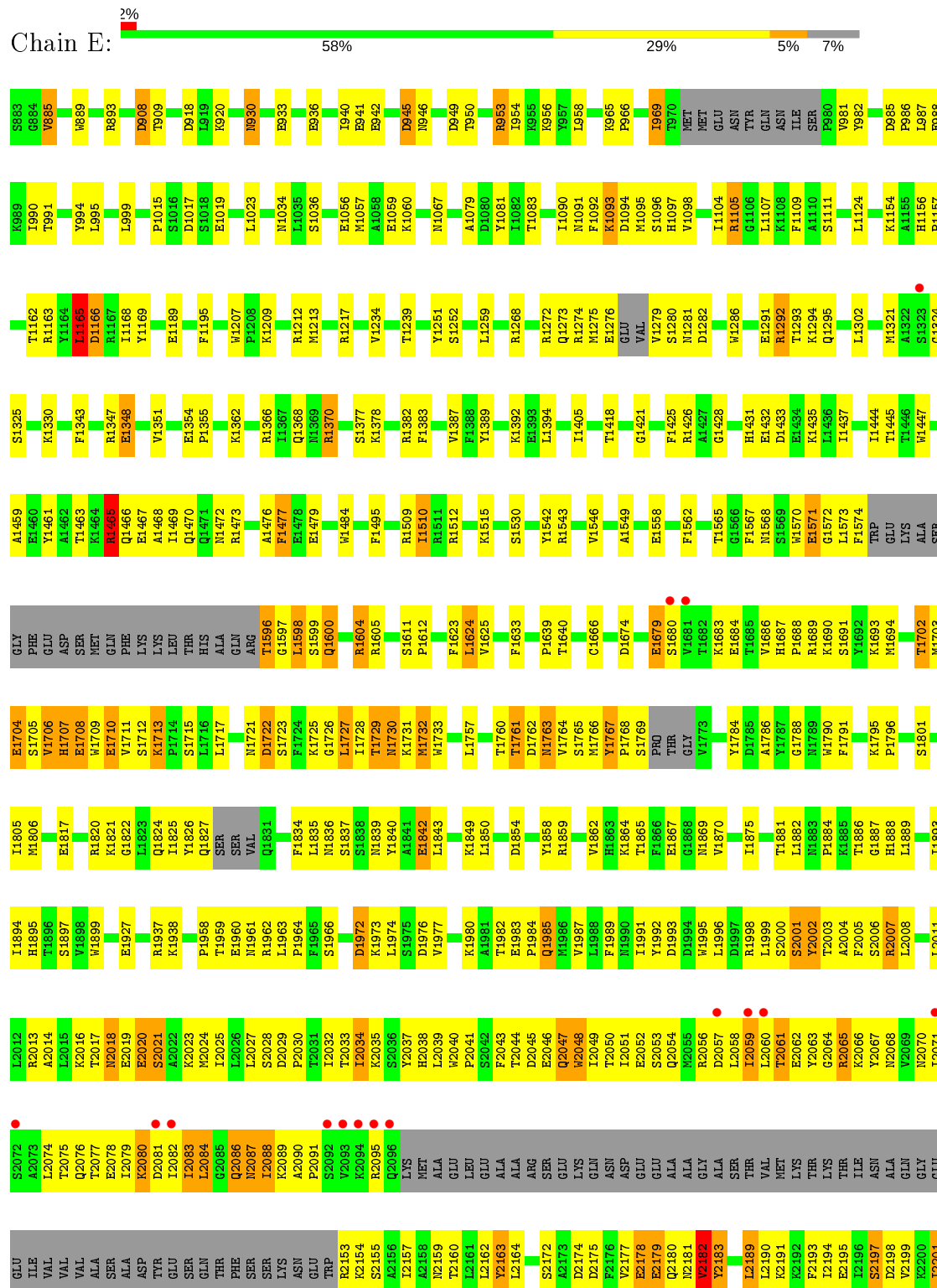


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| N2322 | N2323 | N2324 | N2325 | F2329 | F2330 | F2331 | F2332 | F2333 | F2334 | F2335 | F2336 | A2337 | Q2338 | L2340 | L2341 | S2342 | D2343 | A2344 | L2345 | G2346 | G2347 | N2348 | F2349 | L2350 | L2351 | P2352 | G2353 | G2354 | N2355 | V2356 | N2357 | N2358 | F2361 | N2362 | N2367 | Q2368 | E2369 | G2370 | N2373 | F2374 | K2375 | Y2376 | P2379 | L2380 | E2381 | F2382 | F2383 | G2384 | E2385 | N2386 | H2387 | ARG   | N2391 |       |       |       |       |       |       |       |       |       |       |       |       |       |
| L2196 | S2197 | D2198 | V2199 | K2200 | L2201 | Q2202 | V2203 | F2206 | L2207 | Y2208 | G2209 | A2270 | E2273 | V2274 | A2275 | L2276 | S2277 | P2278 | K2279 | L2280 | F2281 | A2282 | D2283 | G2284 | K2285 | L2286 | D2287 | L2288 | A2289 | D2290 | L2291 | S2292 | L2293 | F2294 | S2295 | L2296 | P2297 | Q2237 | L2238 | S2239 | N2240 | L2241 | P2242 | D2243 | L2244 | G2245 | L2246 | L2247 | P2248 | D2249 | E2250 | E2251 | G2252 | L2253 | E2254 | L2255 | L2256 | G2257 | W2258 | L2259 |       |       |       |       |       |       |
| GLU   | GLU   | ILE   | VAL   | VAL   | VAL   | ALA   | SER   | ALA   | ASP   | TYR   | GLU   | SER   | GLN   | THR   | PHE   | SER   | SER   | LYS   | N2150 | E2151 | W2152 | R2153 | K2154 | S2155 | A2156 | L2157 | A2158 | N2159 | T2160 | L2161 | L2162 | L2163 | L2164 | R2165 | G2234 | S2235 | L2166 | K2167 | D2174 | D2175 | F2176 | V2177 | E2178 | E2179 | Q2180 | N2181 | Y2182 | Y2183 | V2184 | L2185 | P2186 | K2187 | N2188 | L2189 | L2190 | K2191 | K2192 | F2193 | E2195 |       |       |       |       |       |       |       |
| N2068 | Y2069 | N2070 | L2071 | S2072 | Q2076 | T2079 | K2080 | L2081 | L2082 | L2083 | L2084 | G2085 | Q2086 | N2087 | L2088 | K2089 | A2090 | P2091 | SER   | VAL   | LYS   | ARG   | GLN   | LYS   | ALA   | GLU   | ALA   | ALA   | GLU   | LEU   | GLU   | ALA   | ALA   | ARG   | SER   | GLU   | LYS   | GLN   | ASN   | ASP   | GLU   | GLU   | ALA   | ALA   | GLY   | SER   | THR   | VAL   | MET   | LYS   | THR   | VAL   | MET   | LYS   | THR   | LYS   | L2056 | L2057 | L2058 | L2059 | L2060 | L2061 | L2062 | L2063 | G2064 | Y2067 |
| E1842 | L1843 | F1844 | N1845 | H1846 | L1847 | T1848 | K1849 | L1850 | F1851 | V1852 | L1853 | D1854 | T1855 | M1856 | L1857 | F1858 | R1859 | K1864 | T1865 | F1866 | E1867 | H1868 | L1869 | K1870 | T1875 | N1876 | F1880 | T1881 | L1882 | M1883 | P1884 | D1885 | T1886 | G1887 | H1888 | L1889 | F1890 | L1891 | K1892 | L1893 | L1894 | H1895 | S1896 | S1897 | V1898 | W1899 | ALA   | GLY   | GLN   | VAL   | GLU   | PHO   | PHE   | GLN   | L2056 | L2057 | L2058 | L2059 | L2060 | L2061 | L2062 | L2063 | G2064 | Y2067 |       |       |
| V1917 | V1921 | K1926 | E1927 | E1928 | Q1929 | P1930 | K1931 | Q1932 | L1941 | L1944 | E1945 | M1948 | R1957 | P1958 | T1959 | E1960 | N1961 | R1962 | L1963 | M1969 | D1972 | K1973 | L1974 | S1975 | D1976 | P1977 | V1978 | M1979 | K1980 | E1983 | P1984 | Q1985 | M1986 | V1987 | L1988 | F1989 | N1990 | I1991 | Y1992 | D1993 | L1994 | W1995 | L1996 | D1997 | R1904 | L1905 | S1906 | Q1907 | S2000 | Y2002 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| E1842 | L1843 | F1844 | N1845 | H1846 | L1847 | T1848 | K1849 | L1850 | F1851 | V1852 | L1853 | D1854 | T1855 | M1856 | L1857 | F1858 | R1859 | K1864 | T1865 | F1866 | E1867 | H1868 | L1869 | K1870 | T1875 | N1876 | F1880 | T1881 | L1882 | M1883 | P1884 | D1885 | T1886 | G1887 | H1888 | L1889 | F1890 | L1891 | K1892 | L1893 | L1894 | H1895 | S1896 | S1897 | V1898 | W1899 | ALA   | GLY   | GLN   | VAL   | GLU   | PHO   | PHE   | GLN   | L2056 | L2057 | L2058 | L2059 | L2060 | L2061 | L2062 | L2063 | G2064 | Y2067 |       |       |
| N2068 | Y2069 | N2070 | L2071 | S2072 | Q2076 | T2079 | K2080 | L2081 | L2082 | L2083 | L2084 | G2085 | Q2086 | N2087 | L2088 | K2089 | A2090 | P2091 | SER   | VAL   | LYS   | ARG   | GLN   | LYS   | ALA   | GLU   | ALA   | ALA   | GLU   | LEU   | GLU   | ALA   | ALA   | ARG   | SER   | GLU   | LYS   | GLN   | ASN   | ASP   | GLU   | GLU   | ALA   | ALA   | GLY   | SER   | THR   | VAL   | MET   | LYS   | THR   | VAL   | MET   | LYS   | THR   | LYS   | L2056 | L2057 | L2058 | L2059 | L2060 | L2061 | L2062 | L2063 | G2064 | Y2067 |
| GLU   | GLU   | ILE   | VAL   | VAL   | VAL   | ALA   | SER   | ALA   | ASP   | TYR   | GLU   | SER   | GLN   | THR   | PHE   | SER   | SER   | LYS   | N2150 | E2151 | W2152 | R2153 | K2154 | S2155 | A2156 | L2157 | A2158 | N2159 | T2160 | L2161 | L2162 | L2163 | L2164 | R2165 | G2234 | S2235 | L2166 | K2167 | D2174 | D2175 | F2176 | V2177 | E2178 | E2179 | Q2180 | N2181 | Y2182 | Y2183 | V2184 | L2185 | P2186 | K2187 | N2188 | L2189 | L2190 | K2191 | K2192 | F2193 | E2195 |       |       |       |       |       |       |       |
| L2196 | S2197 | D2198 | V2199 | K2200 | L2201 | Q2202 | V2203 | F2206 | L2207 | Y2208 | G2209 | A2270 | E2273 | V2274 | A2275 | L2276 | S2277 | P2278 | K2279 | L2280 | F2281 | A2282 | D2283 | G2284 | K2285 | L2286 | D2287 | L2288 | A2289 | D2290 | L2291 | S2292 | L2293 | F2294 | S2295 | L2296 | P2297 | Q2237 | L2238 | S2239 | N2240 | L2241 | P2242 | D2243 | L2244 | G2245 | L2246 | L2247 | P2248 | D2249 | E2250 | E2251 | G2252 | L2253 | E2254 | L2255 | L2256 | G2257 | W2258 | L2259 |       |       |       |       |       |       |
| H2260 | T2261 | Q2262 | T2263 | E2264 | E2265 | L2266 | K2267 | F2268 | M2269 | A2270 | E2273 | V2274 | A2275 | L2276 | S2277 | P2278 | K2279 | L2280 | F2281 | A2282 | D2283 | G2284 | K2285 | L2286 | D2287 | L2288 | A2289 | D2290 | L2291 | S2292 | L2293 | F2294 | S2295 | L2296 | P2297 | Q2237 | L2238 | S2239 | N2240 | L2241 | P2242 | D2243 | L2244 | G2245 | L2246 | L2247 | P2248 | D2249 | E2250 | E2251 | G2252 | L2253 | E2254 | L2255 | L2256 | G2257 | W2258 | L2259 |       |       |       |       |       |       |       |       |
| N2322 | N2323 | N2324 | N2325 | F2329 | F2330 | F2331 | F2332 | F2333 | F2334 | F2335 | F2336 | A2337 | Q2338 | L2340 | L2341 | S2342 | D2343 | A2344 | L2345 | G2346 | G2347 | N2348 | F2349 | L2350 | L2351 | P2352 | G2353 | G2354 | N2355 | V2356 | N2357 | N2358 | F2361 | N2362 | N2367 | Q2368 | E2369 | G2370 | N2373 | F2374 | K2375 | Y2376 | P2379 | L2380 | E2381 | F2382 | F2383 | G2384 | E2385 | N2386 | H2387 | ARG   | N2391 |       |       |       |       |       |       |       |       |       |       |       |       |       |
| L1104 | R1105 | G1106 | L1107 | F1108 | F1109 | A1110 | S1111 | I1121 | L1124 | L1125 | P1137 | S1138 | N1139 | N1140 | P1141 | N1142 | S1149 | K1150 | E1151 | V1152 | E1153 | K1154 | L1156 | P1157 | T1158 | R1159 | T1162 | D1163 | Y1164 | L1165 | D1166 | R1167 | I1168 | Y1169 | D1177 | E1180 | E1181 | D1184 | E1185 | Y1186 | L1187 | A1188 | E1189 | N1190 | P1191 | D1192 | F1195 | G1196 | S1197 | W1207 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| R1212 | M1213 | Q1218 | W1228 | R1233 | S1237 | L1238 | T1239 | Y1251 | S1252 | K1253 | Y1259 | F1260 | G1264 | R1268 | Q1273 | R1274 | M1275 | L1276 | GLU   | VAL   | VAL   | SER   | D1281 | D1282 | W1286 | D1287 | L1288 | R1292 | R1296 | L1302 | S1305 | E1308 | L1309 | K1310 | K1311 | R1317 | M1321 | G1324 | S1325 | W1327 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| I1340 | F1343 | E1348 | E1354 | P1355 | Q1368 | S1377 | F1383 | V1387 | F1388 | Y1389 | L1394 | I1405 | L1406 | R1426 | T1430 | H1431 | E1432 | D1433 | E1434 | K1435 | L1436 | I1437 | I1444 | W1447 | D1453 | T1463 | R1464 | Q1466 | E1467 | Q1471 | N1472 | R1473 | R1475 | L1476 | F1477 | E1478 | E1479 | R1486 | F1486 | A1503 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| R1506 | R1509 | I1510 | R1511 | R1512 | K1515 | R1521 | Y1542 | Y1546 | E1558 | K1563 | M1568 | S1569 | W1570 | E1571 | G1572 | L1573 | F1574 | L1575 | GLU   | LYS   | ALA   | SER   | GLY   | PHE   | GLU   | ASP   | SER   | MET   | GLN   | PHE   | LYS   | LEU   | THR   | HIS   | ALA   | Q1594 | R1595 | T1596 | G1597 | L1598 | L1599 | Q1600 | R1604 | R1605 | P1611 | P1612 | W1612 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| L1624 | V1625 | F1633 | P1639 | T1640 | I1661 | C1666 | L1673 | D1674 | Q1677 | L1678 | E1679 | K1683 | E1684 | T1685 | H1686 | H1687 | P1688 | L1689 | K1690 | S1691 | Y1692 | K1693 | M1703 | E1704 | S1705 | W1706 | H1707 | E1708 | H1709 | E1710 | K1713 | L1718 | L1719 | T1720 | D1722 | L1727 | L1728 | T1729 | N1730 | K1731 | ASN   | R1732 | W1733 | R1739 | Y1840 | A1841 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| D1747 | R1750 | Y1759 | D1762 | N1763 | V1764 | P1768 | T1771 | G1772 | Y1784 | D1785 | A1786 | F1791 | K1795 | P1796 | L1797 | M1800 | S1801 | M1802 | R1803 | T1804 | I1805 | M1806 | K1807 | D1808 | N1809 | E1817 | K1821 | G1822 | L1823 | Q1824 | L1825 | TYR   | GLN   | SER   | SER   | VAL   | GLN   | GLU   | PHO   | PHE   | GLN   | L2056 | L2057 | L2058 | L2059 | L2060 | L2061 | L2062 | L2063 | G2064 | Y2067 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| E1842 | L1843 | F1844 | N1845 | H1846 | L1847 | T1848 | K1849 | L1850 | F1851 | V1852 | L1853 | D1854 | T1855 | M1856 | L1857 | F1858 | R1859 | K1864 | T1865 | F1866 | E1867 | H1868 | L1869 | K1870 | T1875 | N1876 | F1880 | T1881 | L1882 | M1883 | P1884 | D1885 | T1886 | G1887 | H1888 | L1889 | F1890 | L1891 | K1892 | L1893 | L1894 | H1895 | S1896 | S1897 | V1898 | W1899 | ALA   | GLY   | GLN   | VAL   | GLU   | PHO   | PHE   | GLN   | L2056 | L2057 | L2058 | L2059 | L2060 | L2061 | L2062 | L2063 | G2064 | Y2067 |       |       |
| V1917 | V1921 | K1926 | E1927 | E1928 | Q1929 | P1930 | K1931 | Q1932 | L1941 | L1944 | E1945 | M1948 | R1957 | P1958 | T1959 | E1960 | N1961 | R1962 | L1963 | M1969 | D1972 | K1973 | L1974 | S1975 | D1976 | P1977 | V1978 | M1979 | K1980 | E1983 | P1984 | Q1985 | M1986 | V1987 | L1988 | F1989 | N1990 | I1991 | Y1992 | D1993 | L1994 | W1995 | L1996 | D1997 | R1904 | L1905 | S1906 | Q1907 | S2000 | Y2002 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| E1842 | L1843 | F1844 | N1845 | H1846 | L1847 | T1848 | K1849 | L1850 | F1851 | V1852 | L1853 | D1854 | T1855 | M1856 | L1857 | F1858 | R1859 | K1864 | T1865 | F1866 | E1867 | H1868 | L1869 | K1870 | T1875 | N1876 | F1880 | T1881 | L1882 | M1883 | P1884 | D1885 | T1886 | G1887 | H1888 | L1889 | F1890 | L1891 | K1892 | L1893 | L1894 | H1895 | S1896 | S1897 | V1898 | W1899 | ALA   | GLY   | GLN   | VAL   | GLU   | PHO   | PHE   | GLN   | L2056 | L2057 | L2058 | L2059 | L2060 | L2061 | L2062 | L2063 | G2064 | Y2067 |       |       |
| N2068 | Y2069 | N2070 | L2071 | S2072 | Q2076 | T2079 | K2080 | L2081 | L2082 | L2083 | L2084 | G2085 | Q2086 | N2087 | L2088 | K2089 | A2090 | P2091 | SER   | VAL   | LYS   | ARG   | GLN   | LYS   | ALA   | GLU   | ALA   | ALA   | GLU   | LEU   | GLU   | ALA   | ALA   | ARG   | SER   | GLU   | LYS   | GLN   | ASN   | ASP   | GLU   | GLU   | ALA   | ALA   | GLY   | SER   | THR   | VAL   | MET   | LYS   | THR   | VAL   | MET   | LYS   | THR   | LYS   | L2056 | L2057 | L2058 | L2059 | L2060 | L2061 | L2062 | L2063 | G2064 | Y2067 |
| GLU   | GLU   | ILE   | VAL   | VAL   | VAL   | ALA   | SER   | ALA   | ASP   | TYR   | GLU   | SER   | GLN   | THR   | PHE   | SER   | SER   | LYS   | N2150 | E2151 | W2152 | R2153 | K2154 | S2155 | A2156 | L2157 | A2158 | N2159 | T2160 | L2161 | L2162 | L2163 | L2164 | R2165 | G2234 | S2235 | L2166 | K2167 | D2174 | D2175 | F2176 | V2177 | E2178 | E2179 | Q2180 | N2181 | Y2182 | Y2183 | V2184 | L2185 | P2186 | K2187 | N2188 | L2189 | L2190 | K2191 | K2192 | F2193 | E2195 |       |       |       |       |       |       |       |
| L2196 | S2197 | D2198 | V2199 | K2200 | L2201 | Q2202 | V2203 | F2206 | L2207 | Y2208 | G2209 | A2270 | E2273 | V2274 | A2275 | L2276 | S2277 | P2278 | K2279 | L2280 | F2281 | A2282 | D2283 | G2284 | K2285 | L2286 | D2287 | L2288 | A2289 | D2290 | L2291 | S2292 | L2293 | F2294 | S2295 | L2296 | P2297 | Q2237 | L2238 | S2239 | N2240 | L2241 | P2242 | D2243 | L2244 | G2245 | L2246 | L2247 | P2248 | D2249 | E2250 | E2251 | G2252 | L2253 | E2254 | L2255 | L2256 | G2257 | W2258 | L2259 |       |       |       |       |       |       |
| H2260 | T2261 | Q2262 | T2263 | E2264 | E2265 | L2266 | K2267 | F2268 | M2269 | A2270 | E2273 | V2274 | A2275 | L2276 | S2277 | P2278 | K2279 | L2280 | F2281 | A2282 | D2283 | G2284 | K2285 | L2286 | D2287 | L2288 | A2289 | D2290 | L2291 | S2292 | L22   |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

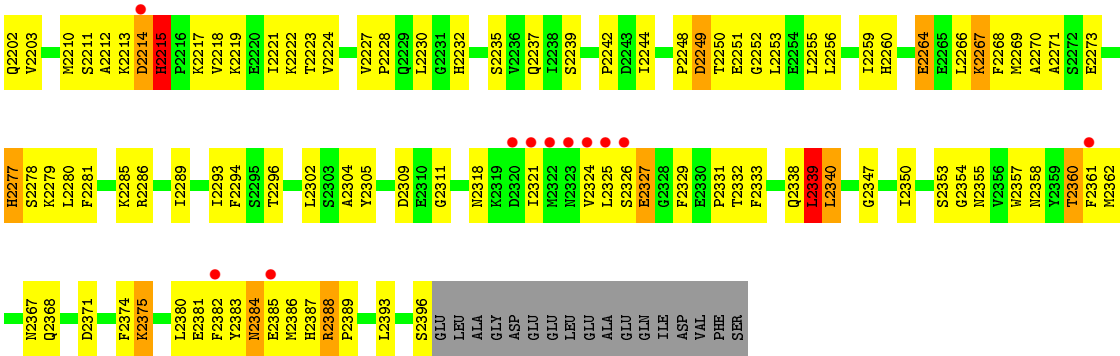


|     |
|-----|
| VAL |
| HIS |
| PHE |
| LEU |
| GLN |
| PHE |
| SER |
| GLU |
| LEU |
| ALA |
| GLY |
| ASP |
| GLU |
| GLU |
| LEU |
| GLU |
| ALA |
| GLN |
| ILE |
| ASP |
| VAL |
| PHE |
| SER |

● Molecule 2: PRE-MRNA-SPLICING FACTOR 8









## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 125.42Å 177.84Å 216.60Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 137.45 – 3.10<br>92.50 – 3.00                               | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (137.45-3.10)<br>99.8 (92.50-3.00)                     | Depositor<br>EDS |
| $R_{merge}$   | 0.16  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.69 (at 3.01Å)   | Xtriage          |
| Refinement program  | REFMAC 5.8.0016   | Depositor        |
| R, $R_{free}$   | 0.220 , 0.267<br>0.221 , 0.268                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4874 reflections (5.01%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 79.1  | Xtriage          |
| Anisotropy  | 0.449   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 67.2   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 28285   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 96.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5812e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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     | 0.55         | 0/2754         | 0.72        | 2/3725 (0.1%)   |
| 1   | D     | 0.56         | 0/2685         | 0.75        | 4/3626 (0.1%)   |
| 2   | B     | 0.59         | 1/11671 (0.0%) | 0.79        | 5/15827 (0.0%)  |
| 2   | E     | 0.58         | 3/11856 (0.0%) | 0.77        | 8/16074 (0.0%)  |
| All | All   | 0.58         | 4/28966 (0.0%) | 0.77        | 19/39252 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | D     | 0                   | 1                   |
| 2   | B     | 0                   | 6                   |
| 2   | E     | 0                   | 5                   |
| All | All   | 0                   | 14                  |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | E     | 1708 | GLU  | CD-OE1 | 8.75  | 1.35        | 1.25     |
| 2   | E     | 1571 | GLU  | CD-OE1 | 7.11  | 1.33        | 1.25     |
| 2   | B     | 1164 | TYR  | CE2-CZ | -6.19 | 1.30        | 1.38     |
| 2   | E     | 1708 | GLU  | CD-OE2 | 6.10  | 1.32        | 1.25     |

All (19) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | E     | 2339 | LEU  | CA-CB-CG  | 7.05  | 131.52      | 115.30   |
| 2   | E     | 1105 | ARG  | NE-CZ-NH1 | 6.47  | 123.54      | 120.30   |
| 1   | D     | 355  | PRO  | CA-N-CD   | -6.36 | 102.59      | 111.50   |
| 1   | A     | 354  | ARG  | C-N-CD    | 6.34  | 141.71      | 128.40   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | E     | 1465 | ARG  | NE-CZ-NH1 | 6.09  | 123.35      | 120.30   |
| 2   | E     | 1963 | LEU  | CA-CB-CG  | -6.00 | 101.50      | 115.30   |
| 1   | D     | 354  | ARG  | C-N-CD    | 5.73  | 140.43      | 128.40   |
| 2   | E     | 1165 | LEU  | CA-CB-CG  | 5.71  | 128.43      | 115.30   |
| 2   | E     | 1604 | ARG  | NE-CZ-NH1 | 5.60  | 123.10      | 120.30   |
| 2   | B     | 1988 | LEU  | CA-CB-CG  | 5.45  | 127.83      | 115.30   |
| 1   | A     | 355  | PRO  | CA-N-CD   | -5.42 | 103.91      | 111.50   |
| 2   | E     | 1105 | ARG  | NE-CZ-NH2 | -5.39 | 117.60      | 120.30   |
| 2   | B     | 1105 | ARG  | NE-CZ-NH1 | 5.38  | 122.99      | 120.30   |
| 2   | B     | 1075 | ASP  | C-N-CD    | 5.32  | 139.56      | 128.40   |
| 2   | B     | 1465 | ARG  | NE-CZ-NH1 | 5.28  | 122.94      | 120.30   |
| 2   | B     | 927  | VAL  | CB-CA-C   | -5.25 | 101.43      | 111.40   |
| 1   | D     | 41   | VAL  | N-CA-C    | -5.23 | 96.88       | 111.00   |
| 2   | E     | 2182 | VAL  | CB-CA-C   | -5.23 | 101.47      | 111.40   |
| 1   | D     | 214  | PHE  | N-CA-C    | -5.16 | 97.06       | 111.00   |

There are no chirality outliers.

All (14) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 107  | LYS  | Peptide |
| 1   | A     | 93   | VAL  | Peptide |
| 2   | B     | 1164 | TYR  | Peptide |
| 2   | B     | 1433 | ASP  | Peptide |
| 2   | B     | 1704 | GLU  | Peptide |
| 2   | B     | 2152 | TRP  | Peptide |
| 2   | B     | 2153 | ARG  | Peptide |
| 2   | B     | 2250 | THR  | Peptide |
| 1   | D     | 110  | GLU  | Peptide |
| 2   | E     | 1092 | PHE  | Peptide |
| 2   | E     | 1572 | GLY  | Peptide |
| 2   | E     | 1706 | VAL  | Peptide |
| 2   | E     | 2083 | ILE  | Peptide |
| 2   | E     | 2215 | HIS  | Peptide |

## 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     | 2684  | 0        | 2530     | 54      | 0            |
| 1   | D     | 2618  | 0        | 2494     | 81      | 0            |
| 2   | B     | 11401 | 0        | 11345    | 879     | 1            |
| 2   | E     | 11582 | 0        | 11528    | 721     | 1            |
| All | All   | 28285 | 0        | 27897    | 1719    | 1            |

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 31.

All (1719) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2043:PHE:CE2  | 2:B:2051:ILE:HD11 | 1.31                     | 1.63              |
| 2:B:2259:ILE:HD13 | 2:B:2291:ILE:CB   | 1.30                     | 1.60              |
| 2:B:2183:TYR:CE1  | 2:B:2219:LYS:HD3  | 1.45                     | 1.49              |
| 2:B:2183:TYR:HE1  | 2:B:2219:LYS:CD   | 1.26                     | 1.47              |
| 2:B:2236:VAL:HG22 | 2:B:2238:ILE:CD1  | 1.44                     | 1.47              |
| 2:E:2210:MET:HE1  | 2:E:2253:LEU:N    | 1.11                     | 1.43              |
| 2:E:2210:MET:HE1  | 2:E:2252:GLY:C    | 1.06                     | 1.41              |
| 2:B:2259:ILE:CD1  | 2:B:2291:ILE:HB   | 1.48                     | 1.40              |
| 2:E:2034:ILE:HD12 | 2:E:2041:PRO:N    | 1.12                     | 1.40              |
| 2:E:2210:MET:CE   | 2:E:2252:GLY:C    | 1.89                     | 1.39              |
| 2:E:2034:ILE:CD1  | 2:E:2041:PRO:CA   | 1.99                     | 1.39              |
| 2:E:2080:LYS:HD2  | 2:E:2083:ILE:CG1  | 1.49                     | 1.38              |
| 2:B:2308:THR:HG23 | 2:B:2333:PHE:O    | 1.23                     | 1.36              |
| 2:E:2304:ALA:HB2  | 2:E:2339:LEU:CD2  | 1.55                     | 1.35              |
| 2:E:2011:LEU:HD13 | 2:E:2040:TRP:CZ3  | 1.59                     | 1.34              |
| 2:E:1995:TRP:CZ3  | 2:E:2007:ARG:HG2  | 1.63                     | 1.33              |
| 2:B:2044:THR:HG23 | 2:B:2047:GLN:NE2  | 1.40                     | 1.33              |
| 2:E:2041:PRO:HB2  | 2:E:2043:PHE:CE1  | 1.61                     | 1.32              |
| 2:B:2182:VAL:HG12 | 2:B:2338:GLN:CB   | 1.59                     | 1.32              |
| 2:E:1998:ARG:CZ   | 2:E:2045:ASP:OD2  | 1.75                     | 1.31              |
| 2:B:1125:LEU:O    | 2:B:1233:ARG:NH1  | 1.62                     | 1.31              |
| 2:E:2018:ASN:ND2  | 2:E:2058:LEU:HD11 | 1.41                     | 1.30              |
| 2:B:2210:MET:CE   | 2:B:2253:LEU:HA   | 1.61                     | 1.29              |
| 2:B:2259:ILE:CD1  | 2:B:2291:ILE:CB   | 2.04                     | 1.28              |
| 2:E:2046:GLU:O    | 2:E:2049:ILE:HG22 | 1.24                     | 1.28              |
| 2:E:2210:MET:SD   | 2:E:2252:GLY:O    | 1.92                     | 1.27              |
| 2:E:1392:LYS:NZ   | 2:E:1599:SER:O    | 1.67                     | 1.27              |
| 2:E:2178:GLU:O    | 2:E:2217:LYS:NZ   | 1.68                     | 1.26              |
| 2:B:900:PHE:HB2   | 2:B:1075:ASP:OD2  | 1.09                     | 1.26              |
| 2:E:1472:ASN:O    | 2:E:2325:LEU:HB2  | 1.11                     | 1.25              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1865:THR:HB   | 2:E:1867:GLU:OE1  | 1.20                     | 1.25              |
| 2:E:2034:ILE:CD1  | 2:E:2041:PRO:N    | 1.98                     | 1.25              |
| 2:B:2259:ILE:CD1  | 2:B:2291:ILE:CG2  | 2.15                     | 1.24              |
| 2:E:2011:LEU:CD1  | 2:E:2040:TRP:CZ3  | 2.20                     | 1.24              |
| 2:E:2043:PHE:CD2  | 2:E:2051:ILE:HG13 | 1.71                     | 1.23              |
| 2:B:2043:PHE:CE2  | 2:B:2051:ILE:CD1  | 2.20                     | 1.23              |
| 2:E:2034:ILE:HD11 | 2:E:2041:PRO:CG   | 1.68                     | 1.23              |
| 2:E:2047:GLN:O    | 2:E:2050:THR:N    | 1.70                     | 1.23              |
| 2:E:2080:LYS:CD   | 2:E:2083:ILE:CD1  | 2.17                     | 1.23              |
| 2:B:2259:ILE:HD13 | 2:B:2291:ILE:CG2  | 1.68                     | 1.22              |
| 2:B:2259:ILE:HD12 | 2:B:2291:ILE:O    | 1.39                     | 1.22              |
| 2:B:2281:PHE:O    | 2:B:2286:ARG:HA   | 1.39                     | 1.22              |
| 2:B:2236:VAL:CG2  | 2:B:2238:ILE:CD1  | 2.16                     | 1.22              |
| 2:B:1604:ARG:NH2  | 2:B:1822:GLY:O    | 1.72                     | 1.22              |
| 2:E:2018:ASN:HD21 | 2:E:2058:LEU:CD1  | 1.51                     | 1.22              |
| 2:B:900:PHE:CB    | 2:B:1075:ASP:OD2  | 1.87                     | 1.21              |
| 2:E:2210:MET:CE   | 2:E:2253:LEU:N    | 1.99                     | 1.21              |
| 2:B:1993:ASP:OD2  | 2:B:2038:HIS:HB3  | 1.39                     | 1.21              |
| 2:E:2080:LYS:CD   | 2:E:2083:ILE:HD11 | 1.69                     | 1.21              |
| 2:E:2043:PHE:CE2  | 2:E:2051:ILE:HG13 | 1.74                     | 1.20              |
| 2:E:2046:GLU:O    | 2:E:2049:ILE:CG2  | 1.90                     | 1.20              |
| 2:E:2034:ILE:HD11 | 2:E:2041:PRO:HG3  | 1.19                     | 1.19              |
| 2:E:2034:ILE:HG23 | 2:E:2040:TRP:O    | 1.04                     | 1.18              |
| 2:B:1729:THR:HG21 | 2:B:1771:THR:CG2  | 1.74                     | 1.18              |
| 1:D:86:GLY:O      | 1:D:90:GLU:HB2    | 1.43                     | 1.18              |
| 2:B:2182:VAL:CG1  | 2:B:2338:GLN:HB3  | 1.74                     | 1.18              |
| 2:E:2024:MET:CE   | 2:E:2157:ILE:CG2  | 2.21                     | 1.18              |
| 1:D:19:GLN:NE2    | 1:D:110:GLU:HG2   | 1.58                     | 1.17              |
| 2:B:2358:ASN:HB3  | 2:B:2387:HIS:ND1  | 1.57                     | 1.17              |
| 2:B:1993:ASP:CG   | 2:B:2038:HIS:HB3  | 1.64                     | 1.16              |
| 2:E:2034:ILE:HD12 | 2:E:2040:TRP:C    | 1.64                     | 1.16              |
| 2:E:2034:ILE:HG23 | 2:E:2040:TRP:C    | 1.62                     | 1.16              |
| 2:B:2259:ILE:HD11 | 2:B:2291:ILE:HG22 | 1.25                     | 1.16              |
| 2:B:2281:PHE:O    | 2:B:2286:ARG:CA   | 1.93                     | 1.16              |
| 2:B:2339:LEU:HD12 | 2:B:2340:LEU:N    | 1.57                     | 1.16              |
| 2:B:1729:THR:CG2  | 2:B:1771:THR:HG21 | 1.75                     | 1.15              |
| 2:B:2357:TRP:HH2  | 2:B:2382:PHE:CE1  | 1.63                     | 1.15              |
| 2:B:2358:ASN:HB3  | 2:B:2387:HIS:CE1  | 1.82                     | 1.14              |
| 2:B:2052:GLU:O    | 2:B:2056:ARG:HG3  | 1.48                     | 1.14              |
| 2:E:2034:ILE:HD12 | 2:E:2041:PRO:CA   | 1.67                     | 1.14              |
| 2:B:2034:ILE:CG1  | 2:B:2041:PRO:HA   | 1.75                     | 1.14              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:2037:TYR:CD1  | 2:E:2038:HIS:CD2  | 2.36                     | 1.13              |
| 2:B:2224:VAL:CG1  | 2:B:2349:PHE:CZ   | 2.32                     | 1.13              |
| 2:B:2210:MET:HG3  | 2:B:2222:LYS:HD2  | 1.15                     | 1.13              |
| 2:E:1731:LYS:CE   | 2:E:1768:PRO:HB2  | 1.77                     | 1.12              |
| 2:B:1729:THR:HG21 | 2:B:1771:THR:HG21 | 1.19                     | 1.12              |
| 2:E:2034:ILE:HD13 | 2:E:2041:PRO:HA   | 1.13                     | 1.12              |
| 2:E:1472:ASN:O    | 2:E:2325:LEU:CB   | 1.96                     | 1.12              |
| 2:E:1998:ARG:NE   | 2:E:2045:ASP:OD2  | 1.84                     | 1.11              |
| 2:E:2018:ASN:HD22 | 2:E:2058:LEU:HD21 | 1.10                     | 1.11              |
| 2:B:2182:VAL:HG13 | 2:B:2338:GLN:OE1  | 1.49                     | 1.10              |
| 2:E:2034:ILE:CG2  | 2:E:2040:TRP:O    | 1.98                     | 1.10              |
| 2:E:1763:ASN:C    | 2:E:1766:MET:CE   | 2.20                     | 1.10              |
| 2:E:1865:THR:CB   | 2:E:1867:GLU:OE1  | 1.98                     | 1.10              |
| 2:B:2208:TYR:HB3  | 2:B:2253:LEU:CD2  | 1.82                     | 1.10              |
| 2:B:2236:VAL:HG22 | 2:B:2238:ILE:HD13 | 1.26                     | 1.09              |
| 2:E:2080:LYS:HD3  | 2:E:2083:ILE:HD11 | 1.10                     | 1.09              |
| 2:B:2191:LYS:O    | 2:B:2195:GLU:HG3  | 1.51                     | 1.09              |
| 2:E:1998:ARG:NH1  | 2:E:2045:ASP:OD2  | 1.86                     | 1.08              |
| 2:E:2048:TRP:O    | 2:E:2052:GLU:HB3  | 1.51                     | 1.08              |
| 2:E:2385:GLU:O    | 2:E:2388:ARG:HB2  | 1.53                     | 1.08              |
| 2:B:2224:VAL:O    | 2:B:2349:PHE:CD1  | 2.06                     | 1.08              |
| 2:B:2358:ASN:N    | 2:B:2387:HIS:HE1  | 1.51                     | 1.08              |
| 2:E:2037:TYR:HD1  | 2:E:2038:HIS:CD2  | 1.71                     | 1.08              |
| 2:B:2357:TRP:CH2  | 2:B:2382:PHE:CE1  | 2.42                     | 1.08              |
| 2:B:2339:LEU:O    | 2:B:2340:LEU:HD12 | 1.51                     | 1.08              |
| 2:E:1763:ASN:C    | 2:E:1766:MET:HE2  | 1.73                     | 1.07              |
| 2:B:2314:TRP:O    | 2:B:2318:ASN:ND2  | 1.87                     | 1.07              |
| 2:E:2080:LYS:CD   | 2:E:2083:ILE:CG1  | 2.33                     | 1.06              |
| 2:B:2183:TYR:CE1  | 2:B:2219:LYS:CD   | 2.15                     | 1.06              |
| 2:E:2080:LYS:CD   | 2:E:2083:ILE:HG13 | 1.84                     | 1.06              |
| 2:B:2208:TYR:HB3  | 2:B:2253:LEU:HD21 | 1.34                     | 1.06              |
| 2:B:2159:ASN:OD1  | 2:B:2199:VAL:HG13 | 1.56                     | 1.06              |
| 2:E:2018:ASN:ND2  | 2:E:2058:LEU:CD1  | 2.11                     | 1.05              |
| 2:B:2150:ASN:HA   | 2:B:2152:TRP:CZ3  | 1.90                     | 1.05              |
| 2:B:2210:MET:CE   | 2:B:2253:LEU:CA   | 2.34                     | 1.05              |
| 2:E:1604:ARG:NH2  | 2:E:1822:GLY:O    | 1.90                     | 1.05              |
| 2:B:2157:ILE:O    | 2:B:2160:THR:OG1  | 1.75                     | 1.05              |
| 2:E:1291:GLU:O    | 2:E:1294:LYS:HE3  | 1.55                     | 1.05              |
| 2:E:2064:GLY:O    | 2:E:2067:TYR:N    | 1.89                     | 1.05              |
| 2:B:2307:LEU:HD12 | 2:B:2308:THR:N    | 1.72                     | 1.04              |
| 2:E:2039:LEU:HB2  | 2:E:2040:TRP:NE1  | 1.71                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2043:PHE:CZ   | 2:B:2051:ILE:HD11 | 1.92                     | 1.04              |
| 2:B:2281:PHE:O    | 2:B:2286:ARG:N    | 1.90                     | 1.04              |
| 2:B:2358:ASN:H    | 2:B:2387:HIS:CE1  | 1.74                     | 1.04              |
| 2:B:2358:ASN:CB   | 2:B:2387:HIS:CE1  | 2.41                     | 1.04              |
| 2:E:2255:LEU:O    | 2:E:2285:LYS:NZ   | 1.91                     | 1.04              |
| 2:B:2034:ILE:HG12 | 2:B:2041:PRO:HA   | 1.36                     | 1.04              |
| 2:B:2210:MET:HE3  | 2:B:2253:LEU:CA   | 1.87                     | 1.03              |
| 2:B:2210:MET:SD   | 2:B:2222:LYS:HD3  | 1.99                     | 1.03              |
| 2:E:1597:GLY:HA2  | 2:E:1598:LEU:HB3  | 1.37                     | 1.03              |
| 2:E:2039:LEU:HB2  | 2:E:2040:TRP:CD1  | 1.94                     | 1.02              |
| 2:B:1859:ARG:HD2  | 2:B:1876:ASN:O    | 1.59                     | 1.02              |
| 2:B:2268:PHE:HD2  | 2:B:2331:PRO:HB3  | 1.23                     | 1.02              |
| 2:E:1465:ARG:HG2  | 2:E:1465:ARG:HH11 | 1.24                     | 1.02              |
| 2:E:2034:ILE:CD1  | 2:E:2041:PRO:HA   | 1.71                     | 1.02              |
| 2:E:2024:MET:HE3  | 2:E:2157:ILE:CG2  | 1.86                     | 1.02              |
| 2:E:1727:LEU:C    | 2:E:1728:ILE:HD13 | 1.81                     | 1.01              |
| 2:B:1885:LYS:O    | 2:B:2001:SER:OG   | 1.76                     | 1.01              |
| 2:E:2048:TRP:O    | 2:E:2052:GLU:CB   | 2.08                     | 1.01              |
| 2:B:2224:VAL:HB   | 2:B:2349:PHE:CZ   | 1.96                     | 1.00              |
| 2:E:1731:LYS:HE2  | 2:E:1768:PRO:HB2  | 1.02                     | 1.00              |
| 1:D:109:ASP:OD1   | 1:D:111:ASP:N     | 1.94                     | 1.00              |
| 2:E:2024:MET:HE1  | 2:E:2157:ILE:HG22 | 1.44                     | 1.00              |
| 2:E:2230:LEU:HD12 | 2:E:2360:THR:HA   | 1.42                     | 0.99              |
| 2:B:2350:ILE:HD13 | 2:B:2376:TYR:HA   | 1.44                     | 0.99              |
| 2:E:1995:TRP:CZ3  | 2:E:2007:ARG:CG   | 2.45                     | 0.99              |
| 2:E:1995:TRP:CH2  | 2:E:2007:ARG:HG2  | 1.96                     | 0.99              |
| 2:E:1705:SER:OG   | 2:E:1730:ASN:O    | 1.80                     | 0.99              |
| 2:E:2304:ALA:HB2  | 2:E:2339:LEU:HD23 | 1.44                     | 0.99              |
| 2:E:2353:SER:O    | 2:E:2375:LYS:NZ   | 1.95                     | 0.99              |
| 2:B:2030:PRO:O    | 2:B:2033:THR:OG1  | 1.79                     | 0.99              |
| 2:E:2041:PRO:CB   | 2:E:2043:PHE:CE1  | 2.44                     | 0.99              |
| 2:B:2037:TYR:HB2  | 2:B:2038:HIS:CD2  | 1.96                     | 0.99              |
| 2:B:2381:GLU:OE1  | 2:B:2381:GLU:N    | 1.95                     | 0.99              |
| 2:E:2304:ALA:HB2  | 2:E:2339:LEU:HD22 | 1.42                     | 0.99              |
| 2:B:2024:MET:O    | 2:B:2028:SER:HB2  | 1.63                     | 0.99              |
| 2:B:2210:MET:CG   | 2:B:2222:LYS:HD2  | 1.93                     | 0.98              |
| 2:B:2182:VAL:HA   | 2:B:2338:GLN:HB2  | 1.43                     | 0.98              |
| 2:B:2224:VAL:HG12 | 2:B:2349:PHE:CE1  | 1.97                     | 0.98              |
| 2:E:2018:ASN:HD21 | 2:E:2058:LEU:CG   | 1.76                     | 0.98              |
| 2:E:2304:ALA:CB   | 2:E:2339:LEU:CD2  | 2.41                     | 0.98              |
| 2:B:2224:VAL:HB   | 2:B:2349:PHE:CE1  | 1.99                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2294:PHE:HD2  | 2:B:2301:SER:OG   | 1.45                     | 0.98              |
| 2:B:1011:ASN:ND2  | 2:B:1142:ASN:O    | 1.97                     | 0.98              |
| 2:E:2034:ILE:CG2  | 2:E:2040:TRP:C    | 2.32                     | 0.98              |
| 2:E:2024:MET:HE1  | 2:E:2157:ILE:CG2  | 1.90                     | 0.97              |
| 2:E:2213:LYS:HA   | 2:E:2215:HIS:H    | 1.30                     | 0.97              |
| 2:B:2236:VAL:CG2  | 2:B:2238:ILE:HD11 | 1.94                     | 0.97              |
| 2:B:2358:ASN:H    | 2:B:2387:HIS:HE1  | 0.98                     | 0.97              |
| 2:E:1207:TRP:O    | 2:E:1212:ARG:NH1  | 1.96                     | 0.97              |
| 2:E:2080:LYS:HD2  | 2:E:2083:ILE:CD1  | 1.86                     | 0.97              |
| 2:E:1834:PHE:CE2  | 2:E:1960:GLU:OE2  | 2.17                     | 0.97              |
| 2:B:2236:VAL:HG22 | 2:B:2238:ILE:HD11 | 1.41                     | 0.97              |
| 2:E:1067:ASN:HD22 | 2:E:1083:THR:HG21 | 1.27                     | 0.97              |
| 2:E:2024:MET:HE3  | 2:E:2157:ILE:HG23 | 1.47                     | 0.96              |
| 1:D:327:ILE:HB    | 1:D:328:TYR:HD1   | 1.27                     | 0.96              |
| 2:B:2259:ILE:CD1  | 2:B:2291:ILE:HG22 | 1.84                     | 0.96              |
| 2:E:2154:LYS:O    | 2:E:2157:ILE:N    | 1.98                     | 0.96              |
| 2:E:1324:GLY:HA2  | 2:E:1325:SER:OG   | 1.62                     | 0.96              |
| 2:B:2224:VAL:CB   | 2:B:2349:PHE:CE1  | 2.49                     | 0.96              |
| 2:E:2034:ILE:CD1  | 2:E:2041:PRO:CG   | 2.44                     | 0.96              |
| 2:B:1568:ASN:OD1  | 2:B:1569:SER:OG   | 1.84                     | 0.95              |
| 2:E:1966:SER:OG   | 2:E:2016:LYS:HE3  | 1.66                     | 0.95              |
| 2:E:1702:THR:CG2  | 2:E:1768:PRO:HG3  | 1.97                     | 0.95              |
| 2:E:1762:ASP:OD1  | 2:E:1763:ASN:ND2  | 1.99                     | 0.95              |
| 2:B:1887:GLY:HA3  | 2:B:1992:TYR:CD2  | 2.01                     | 0.95              |
| 2:B:2210:MET:HG3  | 2:B:2222:LYS:CD   | 1.96                     | 0.95              |
| 2:B:2224:VAL:CB   | 2:B:2349:PHE:CZ   | 2.50                     | 0.95              |
| 2:E:2278:SER:O    | 2:E:2281:PHE:N    | 1.98                     | 0.95              |
| 2:B:1707:HIS:CD2  | 2:B:1708:GLU:HB2  | 2.01                     | 0.95              |
| 2:B:2034:ILE:HG12 | 2:B:2041:PRO:CA   | 1.97                     | 0.95              |
| 2:B:2230:LEU:O    | 2:B:2236:VAL:HG23 | 1.66                     | 0.95              |
| 2:E:2018:ASN:ND2  | 2:E:2058:LEU:CG   | 2.29                     | 0.95              |
| 2:B:2043:PHE:HE2  | 2:B:2051:ILE:HD11 | 1.24                     | 0.94              |
| 2:B:2357:TRP:CH2  | 2:B:2382:PHE:CD1  | 2.55                     | 0.94              |
| 1:D:151:GLU:OE2   | 1:D:154:LYS:HE3   | 1.67                     | 0.94              |
| 2:B:2210:MET:HE3  | 2:B:2253:LEU:HA   | 0.95                     | 0.94              |
| 2:E:2011:LEU:HD13 | 2:E:2040:TRP:CE3  | 2.03                     | 0.94              |
| 2:E:2041:PRO:HB2  | 2:E:2043:PHE:HE1  | 1.23                     | 0.94              |
| 2:E:1567:PHE:CZ   | 2:E:1820:ARG:NH1  | 2.36                     | 0.94              |
| 1:D:107:LYS:HB3   | 1:D:108:ILE:HG22  | 1.50                     | 0.94              |
| 2:E:1711:VAL:HG12 | 2:E:1790:TRP:O    | 1.68                     | 0.94              |
| 2:B:2310:GLU:OE1  | 2:B:2310:GLU:N    | 2.00                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1252:SER:O    | 2:B:1274:ARG:NH1  | 1.99                     | 0.93              |
| 2:E:2043:PHE:CD2  | 2:E:2051:ILE:CG1  | 2.50                     | 0.93              |
| 2:E:1826:TYR:OH   | 2:E:1938:LYS:NZ   | 1.99                     | 0.93              |
| 2:E:2011:LEU:HD13 | 2:E:2040:TRP:HZ3  | 1.23                     | 0.93              |
| 2:B:2224:VAL:CG1  | 2:B:2349:PHE:CE1  | 2.50                     | 0.93              |
| 2:E:1998:ARG:CD   | 2:E:2045:ASP:OD2  | 2.16                     | 0.93              |
| 2:E:1709:TRP:O    | 2:E:1729:THR:N    | 2.01                     | 0.93              |
| 1:A:86:GLY:O      | 1:A:90:GLU:HG2    | 1.66                     | 0.93              |
| 2:B:2011:LEU:HD13 | 2:B:2040:TRP:CZ3  | 2.04                     | 0.93              |
| 2:E:1684:GLU:OE2  | 2:E:1702:THR:OG1  | 1.85                     | 0.93              |
| 2:E:2267:LYS:O    | 2:E:2305:TYR:OH   | 1.86                     | 0.93              |
| 1:D:19:GLN:HE21   | 1:D:110:GLU:HG2   | 1.25                     | 0.93              |
| 2:B:2192:LYS:O    | 2:B:2195:GLU:N    | 2.02                     | 0.92              |
| 2:B:1993:ASP:OD2  | 2:B:2038:HIS:CB   | 2.17                     | 0.92              |
| 2:E:2034:ILE:CD1  | 2:E:2041:PRO:CB   | 2.46                     | 0.92              |
| 2:E:1731:LYS:HE2  | 2:E:1768:PRO:CB   | 1.97                     | 0.92              |
| 2:E:2210:MET:CE   | 2:E:2253:LEU:CA   | 2.47                     | 0.92              |
| 2:E:2034:ILE:HG21 | 2:E:2040:TRP:N    | 1.84                     | 0.92              |
| 2:E:2304:ALA:CB   | 2:E:2339:LEU:HD23 | 2.00                     | 0.92              |
| 2:E:2210:MET:HE1  | 2:E:2253:LEU:CA   | 1.99                     | 0.92              |
| 2:B:1961:ASN:OD1  | 2:B:2079:ILE:HD11 | 1.68                     | 0.92              |
| 2:E:1826:TYR:H    | 2:E:1827:GLN:HG3  | 1.35                     | 0.92              |
| 2:B:1887:GLY:HA3  | 2:B:1992:TYR:HD2  | 1.33                     | 0.92              |
| 2:B:2315:GLY:O    | 2:B:2318:ASN:N    | 2.03                     | 0.92              |
| 2:E:2210:MET:CE   | 2:E:2252:GLY:O    | 2.14                     | 0.92              |
| 2:B:2183:TYR:HE1  | 2:B:2219:LYS:HD2  | 1.34                     | 0.91              |
| 2:E:2041:PRO:CB   | 2:E:2043:PHE:HE1  | 1.80                     | 0.91              |
| 2:B:2339:LEU:CD1  | 2:B:2340:LEU:N    | 2.33                     | 0.91              |
| 2:E:2028:SER:O    | 2:E:2030:PRO:HD3  | 1.70                     | 0.91              |
| 2:E:2019:GLU:O    | 2:E:2023:LYS:HG3  | 1.68                     | 0.91              |
| 2:E:2030:PRO:HB2  | 2:E:2153:ARG:NH2  | 1.85                     | 0.91              |
| 2:B:2282:ALA:HB2  | 2:B:2316:GLU:OE2  | 1.70                     | 0.91              |
| 2:B:2034:ILE:HG13 | 2:B:2041:PRO:HA   | 1.51                     | 0.91              |
| 2:B:2286:ARG:HD3  | 2:B:2312:TYR:CZ   | 2.07                     | 0.90              |
| 2:B:2182:VAL:HG12 | 2:B:2338:GLN:HB3  | 0.92                     | 0.90              |
| 2:E:2202:GLN:HE22 | 2:E:2235:SER:CA   | 1.84                     | 0.90              |
| 2:B:2357:TRP:HH2  | 2:B:2382:PHE:CD1  | 1.87                     | 0.90              |
| 2:B:2183:TYR:HE1  | 2:B:2219:LYS:HD3  | 0.77                     | 0.90              |
| 2:B:2259:ILE:HD11 | 2:B:2291:ILE:CG2  | 1.91                     | 0.90              |
| 2:B:2182:VAL:CG1  | 2:B:2338:GLN:CB   | 2.42                     | 0.90              |
| 2:B:2237:GLN:C    | 2:B:2238:ILE:HD13 | 1.92                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2224:VAL:HG11 | 2:B:2349:PHE:HZ   | 1.35                     | 0.89              |
| 2:E:1292:ARG:HD3  | 2:E:1293:THR:HG23 | 1.54                     | 0.89              |
| 2:B:2339:LEU:CD1  | 2:B:2340:LEU:H    | 1.85                     | 0.89              |
| 2:E:2050:THR:O    | 2:E:2053:SER:OG   | 1.90                     | 0.89              |
| 2:B:1961:ASN:OD1  | 2:B:2079:ILE:CD1  | 2.20                     | 0.89              |
| 2:B:2044:THR:OG1  | 2:B:2047:GLN:HG3  | 1.72                     | 0.89              |
| 2:E:1834:PHE:HE2  | 2:E:1960:GLU:OE2  | 1.51                     | 0.89              |
| 2:E:2014:ALA:HA   | 2:E:2059:ILE:CD1  | 2.03                     | 0.89              |
| 2:B:1983:GLU:HB2  | 2:B:1984:PRO:HD2  | 1.52                     | 0.89              |
| 2:B:2236:VAL:CG2  | 2:B:2238:ILE:HD12 | 2.02                     | 0.89              |
| 2:E:2210:MET:HE1  | 2:E:2252:GLY:O    | 1.72                     | 0.89              |
| 2:B:950:THR:O     | 2:B:954:ILE:HG13  | 1.72                     | 0.89              |
| 2:B:1848:ILE:HD13 | 2:B:1928:GLU:O    | 1.72                     | 0.89              |
| 2:E:2011:LEU:HD12 | 2:E:2040:TRP:CZ3  | 2.06                     | 0.89              |
| 2:B:2182:VAL:CA   | 2:B:2338:GLN:HB2  | 2.03                     | 0.88              |
| 2:E:1324:GLY:CA   | 2:E:1325:SER:OG   | 2.21                     | 0.88              |
| 2:B:2019:GLU:O    | 2:B:2023:LYS:HG3  | 1.74                     | 0.88              |
| 2:B:2259:ILE:HD12 | 2:B:2291:ILE:C    | 1.93                     | 0.88              |
| 2:B:1594:GLN:OE1  | 2:B:1595:ARG:N    | 2.06                     | 0.88              |
| 1:D:106:PRO:O     | 1:D:107:LYS:HG2   | 1.71                     | 0.88              |
| 1:D:31:HIS:O      | 1:D:102:MET:SD    | 2.31                     | 0.88              |
| 2:E:2037:TYR:CD1  | 2:E:2038:HIS:NE2  | 2.42                     | 0.88              |
| 2:B:1016:SER:OG   | 2:B:1018:SER:OG   | 1.92                     | 0.87              |
| 2:B:2282:ALA:CB   | 2:B:2316:GLU:OE2  | 2.21                     | 0.87              |
| 2:E:2018:ASN:HD22 | 2:E:2058:LEU:CD2  | 1.86                     | 0.87              |
| 2:E:2018:ASN:ND2  | 2:E:2058:LEU:HD21 | 1.87                     | 0.87              |
| 1:A:347:VAL:HG21  | 2:B:1875:ILE:HD11 | 1.56                     | 0.87              |
| 2:E:1762:ASP:OD2  | 2:E:1764:VAL:HG22 | 1.75                     | 0.87              |
| 2:E:941:GLU:O     | 2:E:945:ASP:OD1   | 1.93                     | 0.87              |
| 2:B:1849:LYS:O    | 2:B:1850:LEU:HD23 | 1.75                     | 0.87              |
| 2:B:1015:PRO:HD2  | 2:B:1165:LEU:HD23 | 1.54                     | 0.86              |
| 2:E:1998:ARG:HD2  | 2:E:2045:ASP:OD2  | 1.74                     | 0.86              |
| 2:E:2080:LYS:HD2  | 2:E:2083:ILE:HG13 | 0.88                     | 0.86              |
| 2:B:2286:ARG:HD3  | 2:B:2312:TYR:CE2  | 2.11                     | 0.86              |
| 2:B:2358:ASN:HB3  | 2:B:2387:HIS:HD1  | 1.37                     | 0.86              |
| 2:E:1466:GLN:O    | 2:E:1469:ILE:N    | 2.09                     | 0.86              |
| 2:E:1992:TYR:OH   | 2:E:2005:PHE:HB2  | 1.76                     | 0.86              |
| 2:B:2020:GLU:OE1  | 2:B:2165:ARG:NH2  | 2.07                     | 0.86              |
| 2:B:1137:PRO:HG2  | 2:B:1140:ASN:O    | 1.76                     | 0.85              |
| 2:E:2030:PRO:HB2  | 2:E:2153:ARG:HH21 | 1.41                     | 0.85              |
| 2:E:2014:ALA:CA   | 2:E:2059:ILE:HD11 | 2.06                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:94:HIS:O      | 1:A:98:GLU:CB     | 2.24                     | 0.85              |
| 2:B:2203:VAL:CG2  | 2:B:2382:PHE:CE1  | 2.59                     | 0.85              |
| 2:B:2207:ILE:N    | 2:B:2257:GLY:O    | 2.09                     | 0.85              |
| 1:D:106:PRO:C     | 1:D:107:LYS:HG2   | 1.93                     | 0.85              |
| 2:B:1868:GLY:O    | 2:B:1870:VAL:HG23 | 1.75                     | 0.85              |
| 2:B:2182:VAL:CG1  | 2:B:2338:GLN:OE1  | 2.24                     | 0.85              |
| 2:E:1252:SER:O    | 2:E:1274:ARG:NH1  | 2.08                     | 0.85              |
| 2:E:2177:VAL:HG23 | 2:E:2180:GLN:H    | 1.41                     | 0.85              |
| 2:B:2350:ILE:HG23 | 2:B:2375:LYS:O    | 1.76                     | 0.85              |
| 2:B:2256:LEU:O    | 2:B:2288:CYS:SG   | 2.34                     | 0.85              |
| 2:E:2011:LEU:CD1  | 2:E:2040:TRP:CE3  | 2.59                     | 0.85              |
| 2:E:2037:TYR:CD1  | 2:E:2038:HIS:HD2  | 1.95                     | 0.85              |
| 2:B:2357:TRP:HH2  | 2:B:2382:PHE:HE1  | 1.18                     | 0.85              |
| 2:E:1757:LEU:O    | 2:E:1761:THR:HG23 | 1.77                     | 0.84              |
| 2:B:2034:ILE:CG1  | 2:B:2041:PRO:CA   | 2.55                     | 0.84              |
| 2:B:2178:GLU:O    | 2:B:2217:LYS:CD   | 2.24                     | 0.84              |
| 2:B:2210:MET:SD   | 2:B:2222:LYS:CD   | 2.65                     | 0.84              |
| 1:D:327:ILE:HB    | 1:D:328:TYR:CD1   | 2.12                     | 0.84              |
| 2:E:2065:ARG:NH1  | 2:E:2065:ARG:HB3  | 1.93                     | 0.84              |
| 2:B:1887:GLY:CA   | 2:B:1992:TYR:CD2  | 2.60                     | 0.84              |
| 2:B:2157:ILE:O    | 2:B:2160:THR:N    | 2.08                     | 0.84              |
| 2:B:2281:PHE:CE1  | 2:B:2288:CYS:HB2  | 2.13                     | 0.84              |
| 2:B:1994:ASP:O    | 2:B:1997:ASP:HB2  | 1.78                     | 0.84              |
| 2:B:2049:ILE:O    | 2:B:2053:SER:OG   | 1.93                     | 0.84              |
| 2:B:1686:VAL:HG11 | 2:B:1690:LYS:HD2  | 1.60                     | 0.83              |
| 2:E:1763:ASN:CA   | 2:E:1766:MET:HE2  | 2.08                     | 0.83              |
| 2:E:2174:ASP:OD1  | 2:E:2175:ASP:N    | 2.10                     | 0.83              |
| 2:B:1895:HIS:CD2  | 2:B:1896:THR:H    | 1.94                     | 0.83              |
| 2:B:2203:VAL:HG22 | 2:B:2382:PHE:HE1  | 1.43                     | 0.83              |
| 2:B:2208:TYR:CD2  | 2:B:2253:LEU:HD13 | 2.12                     | 0.83              |
| 2:B:2183:TYR:CE1  | 2:B:2219:LYS:HD2  | 2.09                     | 0.83              |
| 2:B:2294:PHE:CZ   | 2:B:2296:THR:CG2  | 2.61                     | 0.83              |
| 2:E:1712:SER:OG   | 2:E:1713:LYS:O    | 1.94                     | 0.83              |
| 2:E:1763:ASN:O    | 2:E:1766:MET:CE   | 2.25                     | 0.83              |
| 2:E:2034:ILE:HD13 | 2:E:2041:PRO:CA   | 1.80                     | 0.83              |
| 2:E:2064:GLY:O    | 2:E:2068:ASN:N    | 2.11                     | 0.83              |
| 2:E:2210:MET:HE2  | 2:E:2253:LEU:HA   | 1.59                     | 0.83              |
| 2:B:1999:LEU:HD12 | 2:B:2000:SER:H    | 1.43                     | 0.83              |
| 2:B:2182:VAL:HA   | 2:B:2338:GLN:CB   | 2.08                     | 0.83              |
| 2:B:2210:MET:CG   | 2:B:2222:LYS:CD   | 2.54                     | 0.83              |
| 2:B:2294:PHE:CZ   | 2:B:2296:THR:HG21 | 2.13                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:2034:ILE:HD12 | 2:E:2041:PRO:CD   | 2.09                     | 0.83              |
| 2:E:2381:GLU:OE1  | 2:E:2381:GLU:N    | 2.10                     | 0.83              |
| 2:B:1853:ASP:OD1  | 2:B:1855:THR:OG1  | 1.97                     | 0.82              |
| 2:B:2256:LEU:C    | 2:B:2288:CYS:SG   | 2.58                     | 0.82              |
| 2:E:2189:LEU:CD1  | 2:E:2224:VAL:HG23 | 2.09                     | 0.82              |
| 2:B:2380:LEU:HD13 | 2:B:2384:ASN:OD1  | 1.77                     | 0.82              |
| 2:E:1711:VAL:CG1  | 2:E:1790:TRP:O    | 2.28                     | 0.82              |
| 2:B:2224:VAL:C    | 2:B:2349:PHE:CE1  | 2.53                     | 0.82              |
| 2:B:2224:VAL:O    | 2:B:2349:PHE:HD1  | 1.63                     | 0.82              |
| 2:B:1848:ILE:CD1  | 2:B:1928:GLU:O    | 2.27                     | 0.82              |
| 2:B:1999:LEU:HD21 | 2:B:2003:THR:HG22 | 1.60                     | 0.82              |
| 2:E:2034:ILE:HD11 | 2:E:2041:PRO:CB   | 2.07                     | 0.82              |
| 2:B:1999:LEU:HD11 | 2:B:2003:THR:HB   | 1.60                     | 0.82              |
| 2:B:1568:ASN:OD1  | 2:B:1569:SER:N    | 2.13                     | 0.82              |
| 2:B:2339:LEU:HD12 | 2:B:2340:LEU:H    | 1.35                     | 0.82              |
| 2:E:1705:SER:OG   | 2:E:1730:ASN:CA   | 2.28                     | 0.82              |
| 2:E:1987:VAL:HG12 | 2:E:1989:PHE:CE1  | 2.15                     | 0.82              |
| 2:E:2083:ILE:HG22 | 2:E:2084:LEU:HD13 | 1.62                     | 0.81              |
| 2:E:2080:LYS:HD3  | 2:E:2083:ILE:CD1  | 1.92                     | 0.81              |
| 2:B:2192:LYS:O    | 2:B:2195:GLU:HB2  | 1.80                     | 0.81              |
| 2:E:2024:MET:CE   | 2:E:2157:ILE:HG23 | 2.01                     | 0.81              |
| 2:B:2224:VAL:HG12 | 2:B:2349:PHE:HE1  | 1.45                     | 0.81              |
| 2:E:1711:VAL:CB   | 2:E:1790:TRP:O    | 2.28                     | 0.81              |
| 2:E:2074:LEU:O    | 2:E:2075:THR:OG1  | 1.98                     | 0.81              |
| 2:B:1895:HIS:CD2  | 2:B:1896:THR:OG1  | 2.33                     | 0.81              |
| 2:B:1941:LEU:O    | 2:B:1945:GLU:HG3  | 1.81                     | 0.81              |
| 2:B:2044:THR:HG23 | 2:B:2047:GLN:CD   | 2.00                     | 0.81              |
| 2:B:2060:LEU:O    | 2:B:2063:TYR:HB3  | 1.80                     | 0.81              |
| 2:B:2224:VAL:HG11 | 2:B:2349:PHE:CZ   | 2.09                     | 0.81              |
| 2:B:2358:ASN:CA   | 2:B:2387:HIS:CE1  | 2.63                     | 0.81              |
| 2:E:1974:LEU:O    | 2:E:1977:VAL:HG22 | 1.80                     | 0.81              |
| 2:E:2177:VAL:CG2  | 2:E:2180:GLN:HB2  | 2.09                     | 0.81              |
| 2:B:2047:GLN:O    | 2:B:2051:ILE:N    | 2.13                     | 0.81              |
| 1:D:107:LYS:HB3   | 1:D:108:ILE:CG2   | 2.10                     | 0.81              |
| 2:E:1727:LEU:O    | 2:E:1728:ILE:HD13 | 1.80                     | 0.81              |
| 2:E:2018:ASN:HD21 | 2:E:2058:LEU:HD11 | 1.07                     | 0.81              |
| 1:D:210:LEU:O     | 1:D:214:PHE:O     | 1.99                     | 0.81              |
| 2:E:2030:PRO:HG2  | 2:E:2153:ARG:NE   | 1.95                     | 0.81              |
| 2:B:2182:VAL:HG12 | 2:B:2338:GLN:CG   | 2.11                     | 0.81              |
| 2:B:2198:ASP:OD1  | 2:B:2200:LYS:N    | 2.14                     | 0.81              |
| 2:B:2259:ILE:HD12 | 2:B:2291:ILE:HB   | 1.63                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2178:GLU:O    | 2:B:2217:LYS:HD3  | 1.79                     | 0.80              |
| 2:E:1849:LYS:O    | 2:E:1850:LEU:HD23 | 1.81                     | 0.80              |
| 2:B:2259:ILE:HD13 | 2:B:2291:ILE:HB   | 0.81                     | 0.80              |
| 2:E:1711:VAL:CG1  | 2:E:1791:PHE:HB3  | 2.11                     | 0.80              |
| 2:B:1707:HIS:NE2  | 2:B:1708:GLU:HB2  | 1.97                     | 0.80              |
| 2:E:2202:GLN:NE2  | 2:E:2235:SER:C    | 2.34                     | 0.80              |
| 2:B:2367:ASN:OD1  | 2:B:2370:GLY:N    | 2.15                     | 0.80              |
| 2:B:900:PHE:CA    | 2:B:1075:ASP:OD2  | 2.28                     | 0.80              |
| 2:E:2384:ASN:HD22 | 2:E:2386:MET:H    | 1.30                     | 0.80              |
| 2:B:2279:LYS:HZ3  | 2:B:2368:GLN:HE22 | 1.30                     | 0.80              |
| 2:B:2308:THR:CG2  | 2:B:2333:PHE:O    | 2.19                     | 0.80              |
| 2:E:2037:TYR:HD1  | 2:E:2038:HIS:NE2  | 1.77                     | 0.80              |
| 2:E:1995:TRP:CE2  | 2:E:2007:ARG:HD2  | 2.17                     | 0.80              |
| 2:E:2034:ILE:CD1  | 2:E:2041:PRO:CD   | 2.59                     | 0.80              |
| 2:E:2084:LEU:HD22 | 2:E:2084:LEU:O    | 1.81                     | 0.80              |
| 2:B:2044:THR:CG2  | 2:B:2047:GLN:NE2  | 2.36                     | 0.80              |
| 2:E:1995:TRP:CH2  | 2:E:2007:ARG:CG   | 2.62                     | 0.80              |
| 2:B:2358:ASN:CA   | 2:B:2387:HIS:HE1  | 1.95                     | 0.79              |
| 2:B:1843:LEU:HD11 | 2:B:1884:PRO:CG   | 2.12                     | 0.79              |
| 2:E:1987:VAL:CG1  | 2:E:1989:PHE:CE1  | 2.65                     | 0.79              |
| 2:B:1961:ASN:CG   | 2:B:2079:ILE:HD11 | 2.03                     | 0.79              |
| 2:B:1976:ASP:O    | 2:B:1980:LYS:HG3  | 1.83                     | 0.79              |
| 2:B:2176:PHE:HA   | 2:B:2338:GLN:NE2  | 1.97                     | 0.79              |
| 2:E:2065:ARG:HB3  | 2:E:2065:ARG:CZ   | 2.12                     | 0.79              |
| 2:B:2035:LYS:HD2  | 2:B:2037:TYR:CE1  | 2.17                     | 0.79              |
| 2:B:2176:PHE:HA   | 2:B:2338:GLN:HE21 | 1.47                     | 0.79              |
| 2:E:2202:GLN:NE2  | 2:E:2235:SER:CA   | 2.46                     | 0.79              |
| 1:D:75:ASP:OD2    | 1:D:79:LYS:CE     | 2.31                     | 0.79              |
| 2:B:2184:VAL:HG23 | 2:B:2219:LYS:O    | 1.83                     | 0.79              |
| 2:E:1995:TRP:CD2  | 2:E:2007:ARG:HD2  | 2.17                     | 0.79              |
| 2:E:2353:SER:HA   | 2:E:2375:LYS:CD   | 2.13                     | 0.79              |
| 2:B:1895:HIS:CD2  | 2:B:1896:THR:N    | 2.51                     | 0.78              |
| 2:B:2224:VAL:CG1  | 2:B:2349:PHE:HZ   | 1.86                     | 0.78              |
| 2:E:2384:ASN:ND2  | 2:E:2386:MET:H    | 1.81                     | 0.78              |
| 2:E:1703:MET:N    | 2:E:1732:MET:O    | 2.17                     | 0.78              |
| 2:B:2183:TYR:CD2  | 2:B:2289:ILE:HD13 | 2.19                     | 0.78              |
| 2:B:1843:LEU:HD12 | 2:B:1843:LEU:O    | 1.84                     | 0.78              |
| 2:B:2154:LYS:O    | 2:B:2157:ILE:HB   | 1.82                     | 0.78              |
| 2:E:2034:ILE:CG2  | 2:E:2040:TRP:N    | 2.47                     | 0.78              |
| 2:E:2043:PHE:HB3  | 2:E:2047:GLN:HG3  | 1.66                     | 0.78              |
| 2:B:2358:ASN:N    | 2:B:2387:HIS:CE1  | 2.39                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:55:ARG:NH2    | 1:D:279:TYR:CE1   | 2.51                     | 0.78              |
| 2:B:1111:SER:HB2  | 2:B:1510:ILE:HG12 | 1.65                     | 0.78              |
| 2:B:1348:GLU:OE1  | 2:B:1447:TRP:N    | 2.15                     | 0.78              |
| 2:E:1727:LEU:HD23 | 2:E:1728:ILE:H    | 1.49                     | 0.78              |
| 2:B:1797:LEU:O    | 2:B:1801:SER:OG   | 2.00                     | 0.77              |
| 2:B:1503:ALA:O    | 2:B:1506:ARG:NH1  | 2.17                     | 0.77              |
| 2:B:2224:VAL:O    | 2:B:2349:PHE:CE1  | 2.36                     | 0.77              |
| 2:E:2087:ASN:HD22 | 2:E:2089:LYS:H    | 1.31                     | 0.77              |
| 2:B:2236:VAL:HG21 | 2:B:2238:ILE:HD12 | 1.65                     | 0.77              |
| 2:B:2279:LYS:NZ   | 2:B:2368:GLN:NE2  | 2.33                     | 0.77              |
| 2:B:1983:GLU:HB2  | 2:B:1984:PRO:CD   | 2.14                     | 0.77              |
| 2:B:2268:PHE:CD2  | 2:B:2331:PRO:HB3  | 2.15                     | 0.77              |
| 1:D:108:ILE:HD13  | 1:D:109:ASP:H     | 1.48                     | 0.77              |
| 2:E:1562:PHE:O    | 2:E:1565:THR:OG1  | 2.02                     | 0.77              |
| 2:E:1565:THR:O    | 2:E:1820:ARG:NH2  | 2.17                     | 0.77              |
| 2:E:2078:GLU:C    | 2:E:2079:ILE:HD13 | 2.05                     | 0.77              |
| 2:E:2210:MET:CE   | 2:E:2253:LEU:HA   | 2.14                     | 0.77              |
| 2:B:2157:ILE:C    | 2:B:2160:THR:HG1  | 1.85                     | 0.77              |
| 2:B:2283:ASP:OD1  | 2:B:2284:LYS:HA   | 1.84                     | 0.77              |
| 2:E:2080:LYS:CE   | 2:E:2083:ILE:CD1  | 2.63                     | 0.77              |
| 2:E:1163:ARG:HG3  | 2:E:1168:ILE:HG22 | 1.67                     | 0.77              |
| 2:E:2201:ILE:HG21 | 2:E:2382:PHE:CZ   | 2.20                     | 0.77              |
| 2:B:1999:LEU:HD21 | 2:B:2003:THR:CG2  | 2.15                     | 0.77              |
| 2:B:2357:TRP:CH2  | 2:B:2382:PHE:HE1  | 1.95                     | 0.77              |
| 2:E:2087:ASN:HD22 | 2:E:2089:LYS:N    | 1.83                     | 0.77              |
| 2:B:2294:PHE:HD2  | 2:B:2301:SER:HG   | 0.78                     | 0.76              |
| 2:B:2247:LEU:HD12 | 2:B:2248:PRO:CD   | 2.16                     | 0.76              |
| 2:E:2201:ILE:HG21 | 2:E:2382:PHE:HZ   | 1.49                     | 0.76              |
| 2:B:2281:PHE:C    | 2:B:2286:ARG:HA   | 2.04                     | 0.76              |
| 2:B:2286:ARG:CD   | 2:B:2312:TYR:CE2  | 2.68                     | 0.76              |
| 2:E:1111:SER:HB2  | 2:E:1510:ILE:HG12 | 1.66                     | 0.76              |
| 2:E:2057:ASP:O    | 2:E:2061:THR:N    | 2.17                     | 0.76              |
| 2:B:2244:ILE:O    | 2:B:2250:THR:HG21 | 1.85                     | 0.76              |
| 1:A:344:PRO:HB3   | 2:B:1858:TYR:CE1  | 2.21                     | 0.76              |
| 2:B:2280:LEU:HD12 | 2:B:2281:PHE:CE2  | 2.21                     | 0.76              |
| 2:E:1348:GLU:OE1  | 2:E:1447:TRP:N    | 2.19                     | 0.76              |
| 2:E:2039:LEU:C    | 2:E:2040:TRP:CD1  | 2.59                     | 0.76              |
| 2:E:2018:ASN:ND2  | 2:E:2058:LEU:CD2  | 2.44                     | 0.76              |
| 2:E:2080:LYS:HE3  | 2:E:2083:ILE:HD12 | 1.68                     | 0.76              |
| 2:E:2210:MET:HE2  | 2:E:2253:LEU:CA   | 2.16                     | 0.76              |
| 1:A:292:CYS:O     | 1:A:296:SER:OG    | 2.03                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1729:THR:HG22 | 2:B:1771:THR:HG21 | 1.67                     | 0.75              |
| 2:B:1843:LEU:O    | 2:B:1849:LYS:HE3  | 1.86                     | 0.75              |
| 2:B:1605:ARG:NH2  | 2:B:1824:GLN:OE1  | 2.17                     | 0.75              |
| 2:B:2177:VAL:H    | 2:B:2338:GLN:NE2  | 1.84                     | 0.75              |
| 2:B:1477:PHE:CD2  | 2:B:1495:PHE:CD2  | 2.73                     | 0.75              |
| 2:B:2227:VAL:O    | 2:B:2229:GLN:HG2  | 1.87                     | 0.75              |
| 2:B:2309:ASP:HA   | 2:B:2312:TYR:HB2  | 1.66                     | 0.75              |
| 1:D:292:CYS:O     | 1:D:296:SER:OG    | 2.04                     | 0.75              |
| 2:E:1995:TRP:CH2  | 2:E:2007:ARG:CD   | 2.69                     | 0.75              |
| 2:E:2189:LEU:HD13 | 2:E:2224:VAL:HG23 | 1.66                     | 0.75              |
| 2:E:1292:ARG:HD3  | 2:E:1293:THR:CG2  | 2.16                     | 0.75              |
| 2:B:1207:TRP:O    | 2:B:1212:ARG:NH1  | 2.19                     | 0.75              |
| 2:E:2041:PRO:CG   | 2:E:2043:PHE:HE1  | 1.98                     | 0.75              |
| 2:B:1287:ASP:OD2  | 2:B:1296:ARG:NH2  | 2.18                     | 0.75              |
| 2:B:2183:TYR:CD1  | 2:B:2219:LYS:HD3  | 2.20                     | 0.75              |
| 2:E:1702:THR:HG21 | 2:E:1768:PRO:HG3  | 1.66                     | 0.75              |
| 2:E:1964:PRO:HG3  | 2:E:2013:ARG:NH1  | 2.02                     | 0.75              |
| 2:E:1324:GLY:HA2  | 2:E:1325:SER:CB   | 2.16                     | 0.75              |
| 2:E:1093:LYS:HG3  | 2:E:1094:ASP:OD1  | 1.87                     | 0.74              |
| 2:E:1570:TRP:O    | 2:E:1571:GLU:CD   | 2.25                     | 0.74              |
| 2:B:1895:HIS:HD2  | 2:B:1896:THR:H    | 1.32                     | 0.74              |
| 2:E:2047:GLN:O    | 2:E:2050:THR:CA   | 2.34                     | 0.74              |
| 1:A:212:GLY:O     | 1:A:215:LYS:NZ    | 2.19                     | 0.74              |
| 2:B:1859:ARG:CD   | 2:B:1876:ASN:O    | 2.35                     | 0.74              |
| 2:B:2232:HIS:N    | 2:B:2235:SER:O    | 2.20                     | 0.74              |
| 2:B:2236:VAL:CG1  | 2:B:2238:ILE:HD11 | 2.17                     | 0.74              |
| 2:E:1995:TRP:CE3  | 2:E:2007:ARG:HD2  | 2.22                     | 0.74              |
| 2:E:2157:ILE:O    | 2:E:2160:THR:CB   | 2.34                     | 0.74              |
| 2:E:2227:VAL:CG1  | 2:E:2239:SER:OG   | 2.35                     | 0.74              |
| 2:B:2203:VAL:HG22 | 2:B:2382:PHE:CE1  | 2.20                     | 0.74              |
| 2:E:1570:TRP:O    | 2:E:1571:GLU:OE2  | 2.04                     | 0.74              |
| 2:E:2034:ILE:HG21 | 2:E:2040:TRP:CA   | 2.17                     | 0.74              |
| 2:E:2066:LYS:HB2  | 2:E:2067:TYR:CD1  | 2.21                     | 0.74              |
| 2:B:2210:MET:HE1  | 2:B:2253:LEU:CA   | 2.16                     | 0.74              |
| 2:E:2041:PRO:HB2  | 2:E:2043:PHE:CD1  | 2.23                     | 0.74              |
| 2:E:2162:LEU:CD1  | 2:E:2194:ILE:O    | 2.36                     | 0.74              |
| 2:E:1418:THR:OG1  | 2:E:1421:GLY:O    | 2.05                     | 0.74              |
| 2:B:1999:LEU:HG   | 2:B:2000:SER:O    | 1.87                     | 0.74              |
| 2:B:2309:ASP:OD1  | 2:B:2309:ASP:N    | 2.18                     | 0.74              |
| 2:B:2185:LEU:HG   | 2:B:2186:PRO:N    | 2.00                     | 0.73              |
| 2:B:1932:GLN:OE1  | 2:B:1957:ARG:NH1  | 2.21                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1834:PHE:CD1  | 2:E:1958:PRO:HG2  | 2.23                     | 0.73              |
| 2:E:1597:GLY:CA   | 2:E:1598:LEU:HB3  | 2.18                     | 0.73              |
| 2:B:2238:ILE:HD13 | 2:B:2238:ILE:N    | 2.03                     | 0.73              |
| 2:E:2230:LEU:CD1  | 2:E:2360:THR:HA   | 2.17                     | 0.73              |
| 2:B:2309:ASP:HA   | 2:B:2312:TYR:HD2  | 1.54                     | 0.73              |
| 2:E:2047:GLN:C    | 2:E:2050:THR:H    | 1.92                     | 0.73              |
| 2:B:2034:ILE:HG12 | 2:B:2040:TRP:C    | 2.09                     | 0.73              |
| 2:B:2209:GLY:HA3  | 2:B:2256:LEU:HD21 | 1.70                     | 0.73              |
| 2:E:2202:GLN:HE22 | 2:E:2235:SER:HA   | 1.53                     | 0.73              |
| 2:E:1705:SER:OG   | 2:E:1730:ASN:C    | 2.27                     | 0.73              |
| 2:E:1987:VAL:HG11 | 2:E:1989:PHE:CZ   | 2.23                     | 0.73              |
| 2:B:1993:ASP:OD1  | 2:B:2038:HIS:HB3  | 1.88                     | 0.73              |
| 1:A:88:LYS:O      | 1:A:92:ILE:HD13   | 1.89                     | 0.72              |
| 2:B:2306:ASN:N    | 2:B:2335:THR:O    | 2.17                     | 0.72              |
| 2:E:1733:TRP:CE2  | 2:E:1767:TYR:HD2  | 2.07                     | 0.72              |
| 2:E:2024:MET:CE   | 2:E:2157:ILE:HG21 | 2.18                     | 0.72              |
| 2:E:2177:VAL:HG21 | 2:E:2180:GLN:HG3  | 1.70                     | 0.72              |
| 2:B:1679:GLU:N    | 2:B:1704:GLU:O    | 2.22                     | 0.72              |
| 2:B:2045:ASP:N    | 2:B:2045:ASP:OD1  | 2.21                     | 0.72              |
| 2:E:1973:LYS:O    | 2:E:1977:VAL:HG13 | 1.89                     | 0.72              |
| 1:D:75:ASP:OD2    | 1:D:79:LYS:NZ     | 2.23                     | 0.72              |
| 2:E:2277:HIS:HD1  | 2:E:2281:PHE:HD2  | 1.35                     | 0.72              |
| 2:E:1711:VAL:HG12 | 2:E:1791:PHE:HB3  | 1.70                     | 0.72              |
| 2:E:2021:SER:O    | 2:E:2024:MET:N    | 2.22                     | 0.72              |
| 2:E:2084:LEU:H    | 2:E:2084:LEU:HD13 | 1.55                     | 0.72              |
| 2:E:1428:GLY:N    | 2:E:1433:ASP:OD2  | 2.19                     | 0.72              |
| 2:B:2011:LEU:HD13 | 2:B:2040:TRP:CE3  | 2.24                     | 0.72              |
| 2:B:2037:TYR:HB2  | 2:B:2038:HIS:HD2  | 1.55                     | 0.72              |
| 2:B:2230:LEU:HD23 | 2:B:2237:GLN:HG3  | 1.72                     | 0.72              |
| 1:D:19:GLN:NE2    | 1:D:110:GLU:CG    | 2.49                     | 0.72              |
| 2:B:2034:ILE:HG12 | 2:B:2040:TRP:O    | 1.88                     | 0.72              |
| 2:E:2178:GLU:C    | 2:E:2217:LYS:HZ2  | 1.87                     | 0.72              |
| 2:B:2046:GLU:O    | 2:B:2049:ILE:HG22 | 1.89                     | 0.71              |
| 2:B:2165:ARG:O    | 2:B:2300:VAL:HG13 | 1.90                     | 0.71              |
| 2:B:1308:GLU:OE2  | 2:B:1311:LYS:HE3  | 1.90                     | 0.71              |
| 2:B:2247:LEU:HG   | 2:B:2375:LYS:HA   | 1.72                     | 0.71              |
| 2:B:2279:LYS:HZ3  | 2:B:2368:GLN:NE2  | 1.87                     | 0.71              |
| 2:E:2162:LEU:HD13 | 2:E:2194:ILE:O    | 1.89                     | 0.71              |
| 2:B:1996:LEU:HA   | 2:B:1999:LEU:O    | 1.89                     | 0.71              |
| 2:E:2017:THR:HG22 | 2:E:2018:ASN:OD1  | 1.91                     | 0.71              |
| 2:E:2048:TRP:O    | 2:E:2052:GLU:HB2  | 1.91                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:2014:ALA:HA   | 2:E:2059:ILE:HD11 | 1.68                     | 0.71              |
| 1:D:19:GLN:HE22   | 1:D:110:GLU:HG2   | 1.52                     | 0.71              |
| 2:E:2043:PHE:CE2  | 2:E:2051:ILE:CG1  | 2.64                     | 0.71              |
| 2:B:1983:GLU:HG3  | 2:B:1985:GLN:HE21 | 1.56                     | 0.71              |
| 2:B:2159:ASN:OD1  | 2:B:2199:VAL:CG1  | 2.37                     | 0.71              |
| 2:E:1291:GLU:O    | 2:E:1294:LYS:CE   | 2.37                     | 0.71              |
| 2:E:1465:ARG:NH1  | 2:E:1465:ARG:HG2  | 1.97                     | 0.71              |
| 2:E:1763:ASN:CA   | 2:E:1766:MET:CE   | 2.68                     | 0.71              |
| 2:B:1731:LYS:HE3  | 2:B:1768:PRO:HB2  | 1.73                     | 0.70              |
| 2:B:1927:GLU:OE1  | 2:B:1927:GLU:N    | 2.24                     | 0.70              |
| 2:B:1180:GLU:O    | 2:B:1184:ASP:OD1  | 2.09                     | 0.70              |
| 2:B:2207:ILE:HB   | 2:B:2221:ILE:HG23 | 1.71                     | 0.70              |
| 2:E:2210:MET:SD   | 2:E:2252:GLY:C    | 2.57                     | 0.70              |
| 2:B:2247:LEU:HD12 | 2:B:2248:PRO:HD2  | 1.73                     | 0.70              |
| 2:E:1679:GLU:HB2  | 2:E:1706:VAL:HG13 | 1.74                     | 0.70              |
| 2:B:1729:THR:HG21 | 2:B:1771:THR:HG23 | 1.73                     | 0.70              |
| 2:B:2048:TRP:O    | 2:B:2052:GLU:HG3  | 1.92                     | 0.70              |
| 1:D:48:HIS:CD2    | 1:D:53:SER:OG     | 2.45                     | 0.70              |
| 2:B:2044:THR:OG1  | 2:B:2047:GLN:CG   | 2.39                     | 0.70              |
| 2:B:1974:LEU:O    | 2:B:1977:VAL:HG12 | 1.91                     | 0.70              |
| 2:B:2188:ASN:HD21 | 2:B:2346:THR:HB   | 1.56                     | 0.70              |
| 2:B:2230:LEU:HB3  | 2:B:2237:GLN:CG   | 2.22                     | 0.70              |
| 2:B:2307:LEU:HD12 | 2:B:2308:THR:H    | 1.55                     | 0.70              |
| 2:B:2224:VAL:HG12 | 2:B:2349:PHE:CZ   | 2.17                     | 0.70              |
| 2:E:1093:LYS:CG   | 2:E:1094:ASP:HA   | 2.21                     | 0.70              |
| 2:B:2236:VAL:HG13 | 2:B:2238:ILE:HD11 | 1.73                     | 0.70              |
| 2:E:1731:LYS:CE   | 2:E:1768:PRO:CB   | 2.64                     | 0.70              |
| 2:E:2024:MET:HE3  | 2:E:2157:ILE:HG21 | 1.74                     | 0.70              |
| 2:B:1704:GLU:HG3  | 2:B:1730:ASN:O    | 1.92                     | 0.70              |
| 2:E:1763:ASN:O    | 2:E:1766:MET:HE1  | 1.91                     | 0.70              |
| 2:E:1995:TRP:CZ2  | 2:E:2007:ARG:HD2  | 2.27                     | 0.70              |
| 2:B:1687:HIS:ND1  | 2:B:1688:PRO:HD2  | 2.06                     | 0.69              |
| 2:B:2044:THR:HG23 | 2:B:2047:GLN:HE21 | 1.50                     | 0.69              |
| 2:E:2030:PRO:HG2  | 2:E:2153:ARG:CZ   | 2.21                     | 0.69              |
| 2:E:1093:LYS:HG3  | 2:E:1094:ASP:HA   | 1.74                     | 0.69              |
| 2:E:1687:HIS:ND1  | 2:E:1688:PRO:HD2  | 2.07                     | 0.69              |
| 2:B:1722:ASP:OD1  | 2:B:1722:ASP:N    | 2.26                     | 0.69              |
| 2:E:1711:VAL:HB   | 2:E:1790:TRP:O    | 1.92                     | 0.69              |
| 2:B:2314:TRP:O    | 2:B:2317:GLU:HB2  | 1.93                     | 0.69              |
| 2:B:2223:THR:HG23 | 2:B:2348:ASN:O    | 1.92                     | 0.69              |
| 2:E:2213:LYS:HA   | 2:E:2215:HIS:N    | 2.05                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:2084:LEU:CD1  | 2:E:2084:LEU:H    | 2.05                     | 0.69              |
| 2:B:954:ILE:HG23  | 2:B:991:THR:HG22  | 1.73                     | 0.69              |
| 2:E:1705:SER:HG   | 2:E:1730:ASN:C    | 1.93                     | 0.69              |
| 2:E:1763:ASN:HA   | 2:E:1766:MET:HE2  | 1.75                     | 0.69              |
| 2:E:2157:ILE:O    | 2:E:2160:THR:HB   | 1.92                     | 0.69              |
| 2:B:1017:ASP:HA   | 2:B:1509:ARG:HG3  | 1.75                     | 0.69              |
| 2:B:2281:PHE:CD1  | 2:B:2288:CYS:HB2  | 2.27                     | 0.69              |
| 2:E:1274:ARG:O    | 2:E:1276:GLU:HB3  | 1.93                     | 0.69              |
| 2:B:2152:TRP:HA   | 2:B:2154:LYS:N    | 2.07                     | 0.69              |
| 2:B:2210:MET:HE2  | 2:B:2252:GLY:O    | 1.93                     | 0.69              |
| 2:E:2327:GLU:HA   | 2:E:2327:GLU:OE1  | 1.93                     | 0.69              |
| 2:B:2182:VAL:CG1  | 2:B:2338:GLN:CD   | 2.62                     | 0.69              |
| 2:B:2207:ILE:HG22 | 2:B:2224:VAL:HG22 | 1.75                     | 0.69              |
| 2:B:2286:ARG:HD3  | 2:B:2312:TYR:CE1  | 2.28                     | 0.69              |
| 2:E:1472:ASN:C    | 2:E:2325:LEU:HB2  | 2.09                     | 0.69              |
| 2:E:2201:ILE:CG2  | 2:E:2382:PHE:CZ   | 2.76                     | 0.69              |
| 2:B:2268:PHE:HD2  | 2:B:2331:PRO:CB   | 2.03                     | 0.68              |
| 2:B:1475:LEU:HD12 | 2:B:1479:GLU:OE2  | 1.94                     | 0.68              |
| 2:B:1704:GLU:HG2  | 2:B:1705:SER:H    | 1.58                     | 0.68              |
| 2:B:2294:PHE:CZ   | 2:B:2296:THR:HG23 | 2.29                     | 0.68              |
| 2:E:1705:SER:OG   | 2:E:1730:ASN:HA   | 1.92                     | 0.68              |
| 2:B:2350:ILE:HD11 | 2:B:2376:TYR:CD1  | 2.29                     | 0.68              |
| 2:E:2189:LEU:HD13 | 2:E:2224:VAL:CG2  | 2.23                     | 0.68              |
| 2:B:1961:ASN:CG   | 2:B:2079:ILE:CD1  | 2.63                     | 0.68              |
| 2:B:2198:ASP:OD1  | 2:B:2199:VAL:N    | 2.27                     | 0.68              |
| 2:B:2339:LEU:HD12 | 2:B:2340:LEU:O    | 1.94                     | 0.68              |
| 2:B:1192:ASP:OD2  | 2:B:1195:PHE:HA   | 1.94                     | 0.67              |
| 2:B:1163:ARG:HG3  | 2:B:1168:ILE:HG22 | 1.77                     | 0.67              |
| 2:E:1763:ASN:HA   | 2:E:1766:MET:CE   | 2.24                     | 0.67              |
| 2:E:2018:ASN:HD21 | 2:E:2058:LEU:HG   | 1.57                     | 0.67              |
| 2:B:1880:PHE:CE2  | 2:B:1889:LEU:HD11 | 2.30                     | 0.67              |
| 2:B:1858:TYR:HB2  | 2:B:1899:TRP:CZ2  | 2.29                     | 0.67              |
| 2:B:2309:ASP:HA   | 2:B:2312:TYR:CD2  | 2.29                     | 0.67              |
| 2:E:1573:LEU:HD22 | 2:E:1826:TYR:HD2  | 1.60                     | 0.67              |
| 2:E:1834:PHE:CD2  | 2:E:1960:GLU:HG2  | 2.28                     | 0.67              |
| 2:E:2385:GLU:O    | 2:E:2388:ARG:CB   | 2.36                     | 0.67              |
| 2:E:1976:ASP:O    | 2:E:1980:LYS:HG2  | 1.94                     | 0.67              |
| 2:E:1995:TRP:CZ3  | 2:E:2007:ARG:HD2  | 2.29                     | 0.67              |
| 2:E:2179:GLU:O    | 2:E:2217:LYS:HD3  | 1.93                     | 0.67              |
| 2:B:1188:ALA:O    | 2:B:1191:PRO:HD3  | 1.95                     | 0.67              |
| 2:B:2044:THR:N    | 2:B:2047:GLN:OE1  | 2.27                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:2056:ARG:O    | 2:E:2060:LEU:HG   | 1.94                     | 0.67              |
| 2:B:1686:VAL:HG11 | 2:B:1690:LYS:CD   | 2.25                     | 0.67              |
| 2:E:1727:LEU:CD2  | 2:E:1728:ILE:H    | 2.06                     | 0.67              |
| 2:B:2192:LYS:O    | 2:B:2195:GLU:CB   | 2.43                     | 0.67              |
| 2:E:1707:HIS:HB3  | 2:E:1730:ASN:HB3  | 1.76                     | 0.67              |
| 1:D:110:GLU:HB2   | 1:D:113:THR:H     | 1.59                     | 0.67              |
| 2:B:1187:LEU:O    | 2:B:1191:PRO:HG3  | 1.95                     | 0.66              |
| 1:D:347:VAL:HG21  | 2:E:1875:ILE:HD11 | 1.76                     | 0.66              |
| 2:E:1017:ASP:HA   | 2:E:1509:ARG:HG3  | 1.76                     | 0.66              |
| 2:E:2049:ILE:O    | 2:E:2053:SER:N    | 2.28                     | 0.66              |
| 2:B:1987:VAL:HG12 | 2:B:1989:PHE:CE2  | 2.29                     | 0.66              |
| 2:B:2277:HIS:HB3  | 2:B:2307:LEU:HD23 | 1.75                     | 0.66              |
| 2:B:2343:ASP:HB3  | 2:B:2344:ARG:NH2  | 2.11                     | 0.66              |
| 2:E:2025:ILE:HG23 | 2:E:2054:GLN:NE2  | 2.10                     | 0.66              |
| 1:D:327:ILE:HD12  | 1:D:327:ILE:H     | 1.59                     | 0.66              |
| 2:E:1995:TRP:CH2  | 2:E:2007:ARG:HD2  | 2.31                     | 0.66              |
| 2:B:1040:ASP:OD1  | 2:B:1042:SER:OG   | 2.13                     | 0.66              |
| 2:E:2014:ALA:HB2  | 2:E:2059:ILE:HD11 | 1.78                     | 0.66              |
| 2:B:2178:GLU:O    | 2:B:2217:LYS:CE   | 2.43                     | 0.66              |
| 2:E:1597:GLY:CA   | 2:E:1599:SER:H    | 2.08                     | 0.66              |
| 2:B:2192:LYS:HA   | 2:B:2195:GLU:HB2  | 1.78                     | 0.66              |
| 2:B:2277:HIS:NE2  | 2:B:2288:CYS:O    | 2.28                     | 0.66              |
| 2:B:909:THR:OG1   | 2:B:2175:ASP:OD1  | 2.13                     | 0.66              |
| 2:E:2202:GLN:NE2  | 2:E:2235:SER:N    | 2.43                     | 0.66              |
| 2:B:1886:THR:OG1  | 2:B:1888:HIS:CE1  | 2.48                     | 0.66              |
| 2:B:946:ASN:HB3   | 2:B:949:ASP:OD2   | 1.96                     | 0.66              |
| 2:E:2039:LEU:CB   | 2:E:2040:TRP:CD1  | 2.77                     | 0.66              |
| 2:E:2014:ALA:CB   | 2:E:2059:ILE:HD11 | 2.26                     | 0.66              |
| 2:B:2306:ASN:OD1  | 2:B:2337:ALA:HB2  | 1.95                     | 0.66              |
| 2:B:2259:ILE:HD12 | 2:B:2291:ILE:CB   | 2.17                     | 0.66              |
| 2:E:1987:VAL:CG1  | 2:E:1989:PHE:CZ   | 2.79                     | 0.66              |
| 2:E:2159:ASN:ND2  | 2:E:2197:SER:O    | 2.29                     | 0.66              |
| 2:B:1727:LEU:HD23 | 2:B:1728:ILE:H    | 1.59                     | 0.66              |
| 2:B:2208:TYR:CB   | 2:B:2253:LEU:HD21 | 2.22                     | 0.66              |
| 2:B:2379:PRO:O    | 2:B:2380:LEU:HD23 | 1.96                     | 0.66              |
| 2:B:2230:LEU:O    | 2:B:2237:GLN:N    | 2.27                     | 0.65              |
| 1:D:84:ARG:HG3    | 1:D:84:ARG:HH11   | 1.60                     | 0.65              |
| 2:E:2221:ILE:HD13 | 2:E:2256:LEU:HD12 | 1.76                     | 0.65              |
| 2:E:1711:VAL:HG12 | 2:E:1790:TRP:C    | 2.17                     | 0.65              |
| 2:E:2381:GLU:CD   | 2:E:2381:GLU:H    | 1.99                     | 0.65              |
| 1:A:319:LYS:O     | 1:A:320:ASP:OD1   | 2.14                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1186:TYR:HB2  | 2:B:1228:TRP:CE3  | 2.30                     | 0.65              |
| 2:B:2203:VAL:CG2  | 2:B:2382:PHE:HE1  | 2.00                     | 0.65              |
| 2:B:2177:VAL:O    | 2:B:2180:GLN:O    | 2.14                     | 0.65              |
| 2:B:2260:HIS:CD2  | 2:B:2290:ASP:OD1  | 2.50                     | 0.65              |
| 2:B:2087:ASN:HB3  | 2:B:2089:LYS:HG3  | 1.78                     | 0.65              |
| 2:B:2368:GLN:HB3  | 2:B:2369:GLU:OE2  | 1.95                     | 0.65              |
| 2:B:2182:VAL:CA   | 2:B:2338:GLN:CB   | 2.71                     | 0.65              |
| 1:D:25:LYS:O      | 1:D:28:GLN:N      | 2.30                     | 0.65              |
| 2:E:2087:ASN:C    | 2:E:2088:ILE:HG12 | 2.16                     | 0.65              |
| 2:B:2259:ILE:CD1  | 2:B:2291:ILE:C    | 2.63                     | 0.65              |
| 2:E:1709:TRP:O    | 2:E:1728:ILE:HA   | 1.97                     | 0.65              |
| 2:E:1097:HIS:HD2  | 2:E:1098:VAL:O    | 1.80                     | 0.65              |
| 2:E:1763:ASN:C    | 2:E:1766:MET:HE1  | 2.17                     | 0.65              |
| 2:E:2034:ILE:CG2  | 2:E:2040:TRP:CA   | 2.73                     | 0.65              |
| 1:A:327:ILE:HG23  | 2:B:1340:ILE:HD11 | 1.79                     | 0.65              |
| 2:E:1886:THR:HB   | 2:E:1888:HIS:CE1  | 2.32                     | 0.65              |
| 2:E:1995:TRP:CZ3  | 2:E:2007:ARG:CD   | 2.80                     | 0.64              |
| 2:B:1598:LEU:HD22 | 2:B:1598:LEU:O    | 1.97                     | 0.64              |
| 2:B:2182:VAL:CB   | 2:B:2338:GLN:HB3  | 2.25                     | 0.64              |
| 2:E:1836:ASN:HB2  | 2:E:1839:ASN:OD1  | 1.98                     | 0.64              |
| 2:B:2192:LYS:O    | 2:B:2195:GLU:CA   | 2.44                     | 0.64              |
| 2:E:2080:LYS:CE   | 2:E:2083:ILE:HD12 | 2.25                     | 0.64              |
| 2:E:2178:GLU:O    | 2:E:2217:LYS:CE   | 2.46                     | 0.64              |
| 2:E:2037:TYR:CE1  | 2:E:2038:HIS:NE2  | 2.66                     | 0.64              |
| 2:B:2203:VAL:HG21 | 2:B:2382:PHE:CE1  | 2.32                     | 0.64              |
| 2:B:1605:ARG:NE   | 2:B:1824:GLN:OE1  | 2.30                     | 0.64              |
| 2:B:1162:THR:HG22 | 2:B:1169:TYR:HB2  | 1.79                     | 0.64              |
| 2:B:2044:THR:H    | 2:B:2047:GLN:CD   | 2.01                     | 0.64              |
| 2:E:1763:ASN:ND2  | 2:E:1763:ASN:H    | 1.93                     | 0.64              |
| 2:E:1867:GLU:H    | 2:E:1867:GLU:CD   | 2.01                     | 0.64              |
| 1:D:108:ILE:HD13  | 1:D:109:ASP:N     | 2.12                     | 0.64              |
| 2:B:2007:ARG:HG2  | 2:B:2052:GLU:OE2  | 1.98                     | 0.63              |
| 2:B:1961:ASN:OD1  | 2:B:2079:ILE:HD12 | 1.96                     | 0.63              |
| 2:B:2339:LEU:CD1  | 2:B:2340:LEU:O    | 2.46                     | 0.63              |
| 2:B:2035:LYS:HB3  | 2:B:2037:TYR:HD1  | 1.62                     | 0.63              |
| 2:B:1149:SER:OG   | 2:B:1152:VAL:HG12 | 1.97                     | 0.63              |
| 2:B:2230:LEU:HB3  | 2:B:2237:GLN:HG3  | 1.79                     | 0.63              |
| 1:D:134:GLU:N     | 1:D:134:GLU:OE1   | 2.22                     | 0.63              |
| 2:E:2384:ASN:HD22 | 2:E:2385:GLU:N    | 1.96                     | 0.63              |
| 2:B:1105:ARG:HG3  | 2:B:1105:ARG:HH11 | 1.62                     | 0.63              |
| 2:B:2208:TYR:HB3  | 2:B:2253:LEU:CD1  | 2.29                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1091:ASN:HB3  | 2:E:1093:LYS:CE   | 2.28                     | 0.63              |
| 2:E:2277:HIS:ND1  | 2:E:2281:PHE:CD2  | 2.66                     | 0.63              |
| 2:B:1999:LEU:HD12 | 2:B:2000:SER:N    | 2.12                     | 0.63              |
| 2:B:1886:THR:OG1  | 2:B:1888:HIS:ND1  | 2.32                     | 0.63              |
| 2:B:1999:LEU:HD11 | 2:B:2003:THR:CB   | 2.28                     | 0.63              |
| 2:B:2159:ASN:ND2  | 2:B:2198:ASP:HA   | 2.13                     | 0.63              |
| 2:E:2177:VAL:HG22 | 2:E:2180:GLN:HB2  | 1.80                     | 0.63              |
| 2:E:1961:ASN:OD1  | 2:E:2079:ILE:HD12 | 1.98                     | 0.62              |
| 2:E:1972:ASP:OD1  | 2:E:1972:ASP:N    | 2.32                     | 0.62              |
| 2:E:1995:TRP:CZ2  | 2:E:2007:ARG:CD   | 2.82                     | 0.62              |
| 2:B:2177:VAL:H    | 2:B:2338:GLN:HE22 | 1.47                     | 0.62              |
| 2:B:2247:LEU:HD12 | 2:B:2248:PRO:HD3  | 1.82                     | 0.62              |
| 2:E:1887:GLY:HA3  | 2:E:1992:TYR:CD2  | 2.34                     | 0.62              |
| 2:B:2037:TYR:C    | 2:B:2038:HIS:HD2  | 2.03                     | 0.62              |
| 1:D:110:GLU:HB3   | 1:D:113:THR:OG1   | 1.99                     | 0.62              |
| 2:E:1573:LEU:HD22 | 2:E:1826:TYR:CD2  | 2.33                     | 0.62              |
| 2:B:1477:PHE:CE2  | 2:B:1495:PHE:HD2  | 2.17                     | 0.62              |
| 2:E:1707:HIS:HB2  | 2:E:1708:GLU:HG3  | 1.79                     | 0.62              |
| 1:A:94:HIS:O      | 1:A:98:GLU:N      | 2.28                     | 0.62              |
| 2:B:2153:ARG:HH11 | 2:B:2153:ARG:CG   | 2.12                     | 0.62              |
| 2:B:2206:PHE:O    | 2:B:2224:VAL:HA   | 2.00                     | 0.62              |
| 1:D:109:ASP:O     | 1:D:110:GLU:HB2   | 1.99                     | 0.62              |
| 2:E:1826:TYR:N    | 2:E:1827:GLN:HG3  | 2.11                     | 0.62              |
| 2:E:1834:PHE:CE1  | 2:E:1958:PRO:HG2  | 2.35                     | 0.62              |
| 2:E:1991:ILE:CG2  | 2:E:2008:LEU:HD22 | 2.29                     | 0.62              |
| 2:E:2090:ALA:HB1  | 2:E:2091:PRO:HD2  | 1.82                     | 0.62              |
| 2:E:950:THR:O     | 2:E:954:ILE:HG13  | 2.00                     | 0.62              |
| 2:B:2286:ARG:CD   | 2:B:2312:TYR:CD2  | 2.83                     | 0.62              |
| 2:B:918:ASP:OD1   | 2:B:1515:LYS:NZ   | 2.27                     | 0.62              |
| 2:E:1162:THR:HG22 | 2:E:1169:TYR:HB2  | 1.82                     | 0.62              |
| 2:B:1324:GLY:HA2  | 2:B:1325:SER:CB   | 2.29                     | 0.61              |
| 2:B:1983:GLU:CB   | 2:B:1984:PRO:HD2  | 2.27                     | 0.61              |
| 2:B:2294:PHE:HZ   | 2:B:2296:THR:HG21 | 1.63                     | 0.61              |
| 2:E:1839:ASN:O    | 2:E:1842:GLU:HG3  | 2.00                     | 0.61              |
| 2:B:2046:GLU:O    | 2:B:2050:THR:N    | 2.33                     | 0.61              |
| 2:E:2157:ILE:O    | 2:E:2160:THR:OG1  | 2.18                     | 0.61              |
| 2:B:2278:SER:OG   | 2:B:2316:GLU:HG3  | 2.00                     | 0.61              |
| 1:D:83:GLU:HA     | 1:D:83:GLU:OE1    | 1.99                     | 0.61              |
| 2:E:1834:PHE:CD2  | 2:E:1960:GLU:CG   | 2.84                     | 0.61              |
| 2:B:2043:PHE:CD2  | 2:B:2051:ILE:CD1  | 2.82                     | 0.61              |
| 2:B:2286:ARG:HD3  | 2:B:2312:TYR:CD2  | 2.35                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1853:ASP:OD1  | 2:B:1855:THR:N    | 2.19                     | 0.61              |
| 2:E:2039:LEU:HB2  | 2:E:2040:TRP:HE1  | 1.59                     | 0.61              |
| 2:B:2185:LEU:O    | 2:B:2341:LEU:HA   | 2.00                     | 0.61              |
| 2:B:2224:VAL:C    | 2:B:2349:PHE:HE1  | 2.04                     | 0.61              |
| 2:E:2028:SER:O    | 2:E:2030:PRO:CD   | 2.46                     | 0.61              |
| 2:E:2353:SER:HA   | 2:E:2375:LYS:HD3  | 1.82                     | 0.61              |
| 2:B:2011:LEU:HD13 | 2:B:2040:TRP:CH2  | 2.35                     | 0.61              |
| 2:E:1709:TRP:N    | 2:E:1729:THR:O    | 2.32                     | 0.61              |
| 2:E:2084:LEU:N    | 2:E:2084:LEU:HD13 | 2.14                     | 0.61              |
| 2:B:1759:TYR:HA   | 2:B:1762:ASP:HB2  | 1.82                     | 0.61              |
| 2:B:2154:LYS:O    | 2:B:2157:ILE:HD13 | 2.01                     | 0.61              |
| 2:E:1324:GLY:CA   | 2:E:1325:SER:CB   | 2.76                     | 0.60              |
| 2:E:1710:GLU:OE2  | 2:E:1725:LYS:HA   | 2.01                     | 0.60              |
| 2:E:1966:SER:OG   | 2:E:2016:LYS:CE   | 2.46                     | 0.60              |
| 2:E:2177:VAL:HG21 | 2:E:2180:GLN:CG   | 2.31                     | 0.60              |
| 2:E:2358:ASN:HB3  | 2:E:2387:HIS:ND1  | 2.15                     | 0.60              |
| 2:B:1137:PRO:CG   | 2:B:1140:ASN:O    | 2.48                     | 0.60              |
| 2:B:2305:TYR:HB3  | 2:B:2334:SER:HB3  | 1.82                     | 0.60              |
| 1:A:354:ARG:HB2   | 1:A:355:PRO:HD3   | 1.83                     | 0.60              |
| 2:B:1849:LYS:C    | 2:B:1850:LEU:HD23 | 2.22                     | 0.60              |
| 2:E:1056:GLU:O    | 2:E:1060:LYS:HG2  | 2.01                     | 0.60              |
| 2:B:1823:LEU:O    | 2:B:1824:GLN:HB2  | 2.01                     | 0.60              |
| 2:B:1858:TYR:HB2  | 2:B:1899:TRP:CH2  | 2.37                     | 0.60              |
| 2:E:2304:ALA:CB   | 2:E:2339:LEU:HD22 | 2.20                     | 0.60              |
| 2:B:2152:TRP:HA   | 2:B:2154:LYS:H    | 1.67                     | 0.60              |
| 2:B:2277:HIS:HB3  | 2:B:2307:LEU:CD2  | 2.31                     | 0.60              |
| 2:E:2177:VAL:CG2  | 2:E:2180:GLN:CB   | 2.80                     | 0.60              |
| 2:E:2214:ASP:OD1  | 2:E:2214:ASP:N    | 2.34                     | 0.60              |
| 2:B:1030:GLN:HE22 | 2:B:1288:LEU:HA   | 1.64                     | 0.60              |
| 2:B:1705:SER:HB2  | 2:B:1730:ASN:O    | 2.00                     | 0.60              |
| 2:E:1467:GLU:OE1  | 2:E:1470:GLN:NE2  | 2.35                     | 0.60              |
| 2:E:1468:ALA:HB1  | 2:E:1473:ARG:O    | 2.02                     | 0.60              |
| 2:B:2236:VAL:HG21 | 2:B:2238:ILE:CD1  | 2.16                     | 0.60              |
| 1:D:342:HIS:O     | 1:D:343:ASN:ND2   | 2.31                     | 0.60              |
| 2:E:1999:LEU:HD11 | 2:E:2004:ALA:HB2  | 1.84                     | 0.60              |
| 2:B:2227:VAL:HG12 | 2:B:2239:SER:HB3  | 1.84                     | 0.60              |
| 2:E:1476:ALA:HB3  | 2:E:1479:GLU:HG3  | 1.84                     | 0.60              |
| 2:E:1639:PRO:C    | 2:E:1640:THR:HG23 | 2.22                     | 0.60              |
| 2:E:1706:VAL:O    | 2:E:1706:VAL:HG23 | 2.01                     | 0.60              |
| 2:B:2182:VAL:HG12 | 2:B:2338:GLN:CD   | 2.21                     | 0.59              |
| 2:B:2034:ILE:HG12 | 2:B:2041:PRO:N    | 2.18                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2309:ASP:O    | 2:B:2312:TYR:HB2  | 2.02                     | 0.59              |
| 1:A:319:LYS:N     | 1:A:319:LYS:HD2   | 2.18                     | 0.59              |
| 1:A:95:ASN:O      | 1:A:99:ARG:CB     | 2.51                     | 0.59              |
| 2:B:900:PHE:N     | 2:B:1075:ASP:OD2  | 2.35                     | 0.59              |
| 2:B:2353:SER:O    | 2:B:2375:LYS:NZ   | 2.30                     | 0.59              |
| 1:A:314:PRO:HB2   | 1:A:319:LYS:HB2   | 1.84                     | 0.59              |
| 2:B:1747:ASP:CG   | 2:B:1750:ARG:HG3  | 2.23                     | 0.59              |
| 2:B:1840:TYR:HH   | 2:B:2005:PHE:HD2  | 1.50                     | 0.59              |
| 2:E:1731:LYS:NZ   | 2:E:1768:PRO:HB2  | 2.17                     | 0.59              |
| 1:A:86:GLY:O      | 1:A:90:GLU:CG     | 2.46                     | 0.59              |
| 2:B:2268:PHE:HA   | 2:B:2305:TYR:CE2  | 2.37                     | 0.59              |
| 2:E:1702:THR:CG2  | 2:E:1768:PRO:CG   | 2.77                     | 0.59              |
| 2:E:1761:THR:O    | 2:E:1761:THR:OG1  | 2.21                     | 0.59              |
| 2:B:2269:MET:HE3  | 2:B:2273:GLU:HB3  | 1.82                     | 0.59              |
| 2:B:2309:ASP:O    | 2:B:2313:GLN:N    | 2.34                     | 0.59              |
| 2:E:2080:LYS:CE   | 2:E:2083:ILE:HD11 | 2.30                     | 0.59              |
| 2:B:1070:LEU:O    | 2:B:1074:VAL:HG22 | 2.03                     | 0.59              |
| 2:B:1843:LEU:HD11 | 2:B:1884:PRO:HG2  | 1.84                     | 0.59              |
| 2:B:1887:GLY:O    | 2:B:1991:ILE:HG22 | 2.03                     | 0.59              |
| 2:E:2353:SER:HA   | 2:E:2375:LYS:HD2  | 1.84                     | 0.59              |
| 2:B:1324:GLY:HA2  | 2:B:1325:SER:OG   | 2.03                     | 0.59              |
| 2:B:1733:TRP:NE1  | 2:B:1771:THR:O    | 2.35                     | 0.59              |
| 2:B:2209:GLY:N    | 2:B:2254:GLU:O    | 2.35                     | 0.59              |
| 2:B:2302:LEU:HD12 | 2:B:2302:LEU:N    | 2.18                     | 0.59              |
| 2:B:2350:ILE:HG23 | 2:B:2375:LYS:C    | 2.23                     | 0.59              |
| 2:E:1034:ASN:OD1  | 2:E:1291:GLU:N    | 2.27                     | 0.59              |
| 2:E:1067:ASN:HD22 | 2:E:1083:THR:CG2  | 2.11                     | 0.59              |
| 2:B:1453:ASP:OD2  | 2:B:1486:ARG:HD2  | 2.03                     | 0.58              |
| 2:B:1690:LYS:HA   | 2:B:1693:LYS:HG3  | 1.85                     | 0.58              |
| 2:B:2230:LEU:O    | 2:B:2236:VAL:CG2  | 2.47                     | 0.58              |
| 2:E:1893:ILE:HG12 | 2:E:1985:GLN:O    | 2.03                     | 0.58              |
| 2:E:2039:LEU:C    | 2:E:2040:TRP:CG   | 2.76                     | 0.58              |
| 2:B:2041:PRO:HG2  | 2:B:2043:PHE:CD1  | 2.38                     | 0.58              |
| 2:B:2227:VAL:CG1  | 2:B:2239:SER:HB3  | 2.34                     | 0.58              |
| 2:B:2265:GLU:O    | 2:B:2266:LEU:HD23 | 2.03                     | 0.58              |
| 2:E:889:TRP:O     | 2:E:893:ARG:HG2   | 2.04                     | 0.58              |
| 2:E:1015:PRO:HD2  | 2:E:1165:LEU:HD23 | 1.85                     | 0.58              |
| 1:A:214:PHE:O     | 1:A:215:LYS:HB2   | 2.04                     | 0.58              |
| 2:B:1687:HIS:HE1  | 2:B:1689:ARG:HG3  | 1.68                     | 0.58              |
| 2:E:2267:LYS:O    | 2:E:2305:TYR:CZ   | 2.56                     | 0.58              |
| 2:B:1727:LEU:CD2  | 2:B:1728:ILE:H    | 2.15                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2183:TYR:HD2  | 2:B:2289:ILE:HD13 | 1.67                     | 0.58              |
| 2:E:2268:PHE:CD2  | 2:E:2331:PRO:HB3  | 2.38                     | 0.58              |
| 2:E:1999:LEU:HD13 | 2:E:2003:THR:HB   | 1.85                     | 0.58              |
| 2:B:1983:GLU:CB   | 2:B:1984:PRO:CD   | 2.80                     | 0.58              |
| 2:B:2221:ILE:HD13 | 2:B:2256:LEU:HD12 | 1.85                     | 0.58              |
| 2:B:1476:ALA:O    | 2:B:1479:GLU:HB2  | 2.03                     | 0.58              |
| 2:B:1731:LYS:O    | 2:B:1771:THR:OG1  | 2.21                     | 0.58              |
| 2:B:2053:SER:HA   | 2:B:2056:ARG:HD2  | 1.86                     | 0.58              |
| 2:B:1025:VAL:O    | 2:B:1029:THR:HG23 | 2.04                     | 0.58              |
| 2:B:1056:GLU:O    | 2:B:1060:LYS:HG2  | 2.03                     | 0.58              |
| 2:B:2038:HIS:N    | 2:B:2038:HIS:CD2  | 2.72                     | 0.58              |
| 2:E:1091:ASN:HB3  | 2:E:1093:LYS:HE3  | 1.84                     | 0.58              |
| 1:D:344:PRO:HB3   | 2:E:1858:TYR:CE2  | 2.39                     | 0.57              |
| 2:B:1186:TYR:HB2  | 2:B:1228:TRP:CZ3  | 2.39                     | 0.57              |
| 2:E:1709:TRP:HB2  | 2:E:1729:THR:O    | 2.04                     | 0.57              |
| 2:E:1834:PHE:O    | 2:E:1839:ASN:ND2  | 2.34                     | 0.57              |
| 2:E:2041:PRO:CG   | 2:E:2043:PHE:CE1  | 2.80                     | 0.57              |
| 2:E:2066:LYS:HB2  | 2:E:2067:TYR:HD1  | 1.69                     | 0.57              |
| 2:E:2304:ALA:HB2  | 2:E:2339:LEU:HD21 | 1.73                     | 0.57              |
| 2:E:1704:GLU:HA   | 2:E:1704:GLU:OE1  | 2.05                     | 0.57              |
| 2:B:2268:PHE:O    | 2:B:2268:PHE:HD1  | 1.88                     | 0.57              |
| 2:E:2021:SER:O    | 2:E:2024:MET:CB   | 2.53                     | 0.57              |
| 2:B:1019:GLU:HB2  | 2:B:1023:LEU:HD23 | 1.87                     | 0.57              |
| 2:B:2309:ASP:CA   | 2:B:2312:TYR:HB2  | 2.35                     | 0.57              |
| 1:D:8:SER:OG      | 1:D:10:PRO:HD3    | 2.04                     | 0.57              |
| 2:E:1251:TYR:OH   | 2:E:1274:ARG:HD3  | 2.05                     | 0.57              |
| 2:E:1826:TYR:HA   | 2:E:1827:GLN:HB2  | 1.86                     | 0.57              |
| 2:E:2162:LEU:HD21 | 2:E:2199:VAL:HG12 | 1.86                     | 0.57              |
| 2:B:1015:PRO:CD   | 2:B:1165:LEU:HD23 | 2.29                     | 0.57              |
| 1:A:327:ILE:HG23  | 2:B:1340:ILE:CD1  | 2.34                     | 0.57              |
| 2:B:2185:LEU:HG   | 2:B:2186:PRO:CD   | 2.33                     | 0.57              |
| 2:B:2194:ILE:HA   | 2:B:2197:SER:OG   | 2.04                     | 0.57              |
| 2:B:1639:PRO:C    | 2:B:1640:THR:HG23 | 2.25                     | 0.57              |
| 2:B:2259:ILE:CD1  | 2:B:2291:ILE:O    | 2.33                     | 0.57              |
| 1:A:8:SER:OG      | 1:A:10:PRO:HD3    | 2.05                     | 0.57              |
| 2:B:1251:TYR:OH   | 2:B:1274:ARG:HD3  | 2.04                     | 0.57              |
| 2:B:2152:TRP:CA   | 2:B:2154:LYS:H    | 2.18                     | 0.57              |
| 2:B:2221:ILE:HD13 | 2:B:2256:LEU:CD1  | 2.35                     | 0.57              |
| 2:B:889:TRP:O     | 2:B:893:ARG:HG2   | 2.05                     | 0.57              |
| 1:D:87:ALA:O      | 1:D:90:GLU:HB3    | 2.04                     | 0.57              |
| 2:E:1324:GLY:HA3  | 2:E:1325:SER:OG   | 2.02                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1721:ASN:OD1  | 2:E:1722:ASP:N    | 2.38                     | 0.57              |
| 2:B:1477:PHE:CE2  | 2:B:1495:PHE:CD2  | 2.93                     | 0.57              |
| 2:B:2228:PRO:O    | 2:B:2239:SER:HB3  | 2.05                     | 0.57              |
| 2:E:1687:HIS:HE1  | 2:E:1689:ARG:HG3  | 1.69                     | 0.57              |
| 2:B:2046:GLU:O    | 2:B:2049:ILE:N    | 2.38                     | 0.56              |
| 2:E:2018:ASN:CG   | 2:E:2058:LEU:HD11 | 2.20                     | 0.56              |
| 2:B:1977:VAL:HG13 | 2:B:1978:VAL:N    | 2.19                     | 0.56              |
| 2:B:1976:ASP:OD1  | 2:B:1980:LYS:HG3  | 2.05                     | 0.56              |
| 2:B:2191:LYS:C    | 2:B:2195:GLU:HG3  | 2.25                     | 0.56              |
| 2:B:2307:LEU:HD11 | 2:B:2311:GLY:HA3  | 1.88                     | 0.56              |
| 2:E:2358:ASN:H    | 2:E:2387:HIS:CE1  | 2.22                     | 0.56              |
| 2:E:930:ASN:HD22  | 2:E:933:GLU:HB2   | 1.70                     | 0.56              |
| 2:B:2281:PHE:CE1  | 2:B:2288:CYS:CB   | 2.87                     | 0.56              |
| 2:E:1468:ALA:O    | 2:E:1472:ASN:N    | 2.38                     | 0.56              |
| 2:E:1687:HIS:CE1  | 2:E:1688:PRO:HD2  | 2.41                     | 0.56              |
| 2:E:1826:TYR:OH   | 2:E:1938:LYS:CE   | 2.53                     | 0.56              |
| 2:B:1887:GLY:HA2  | 2:B:1992:TYR:CE2  | 2.40                     | 0.56              |
| 2:B:2035:LYS:HD2  | 2:B:2037:TYR:HE1  | 1.68                     | 0.56              |
| 2:B:2060:LEU:O    | 2:B:2064:GLY:N    | 2.38                     | 0.56              |
| 2:B:2210:MET:CE   | 2:B:2253:LEU:N    | 2.69                     | 0.56              |
| 2:E:2277:HIS:CE1  | 2:E:2281:PHE:CD2  | 2.94                     | 0.56              |
| 2:B:1075:ASP:OD1  | 2:B:1076:PRO:HD2  | 2.05                     | 0.56              |
| 2:B:1264:GLY:O    | 2:B:1305:SER:OG   | 2.24                     | 0.56              |
| 2:B:1605:ARG:CZ   | 2:B:1824:GLN:OE1  | 2.53                     | 0.56              |
| 2:B:1995:TRP:HH2  | 2:B:2011:LEU:HD11 | 1.71                     | 0.56              |
| 2:E:1431:HIS:C    | 2:E:1433:ASP:H    | 2.07                     | 0.56              |
| 2:E:2162:LEU:HD12 | 2:E:2194:ILE:O    | 2.06                     | 0.56              |
| 1:A:108:ILE:HG22  | 1:A:109:ASP:O     | 2.04                     | 0.56              |
| 2:B:2208:TYR:CB   | 2:B:2253:LEU:HD11 | 2.35                     | 0.56              |
| 2:B:2315:GLY:C    | 2:B:2318:ASN:H    | 2.08                     | 0.56              |
| 2:B:2235:SER:HB3  | 2:B:2322:MET:HA   | 1.88                     | 0.56              |
| 2:E:1973:LYS:HE3  | 2:E:2038:HIS:O    | 2.06                     | 0.56              |
| 2:E:2182:VAL:HG12 | 2:E:2338:GLN:CB   | 2.36                     | 0.56              |
| 2:B:2037:TYR:CB   | 2:B:2038:HIS:CD2  | 2.79                     | 0.56              |
| 2:B:2208:TYR:HB3  | 2:B:2253:LEU:HD22 | 1.84                     | 0.56              |
| 2:B:2282:ALA:HB1  | 2:B:2316:GLU:OE2  | 2.03                     | 0.56              |
| 2:E:1711:VAL:HG12 | 2:E:1791:PHE:CA   | 2.36                     | 0.56              |
| 2:E:1711:VAL:HG12 | 2:E:1791:PHE:CB   | 2.34                     | 0.56              |
| 2:E:2210:MET:HE1  | 2:E:2252:GLY:CA   | 2.22                     | 0.56              |
| 2:B:2024:MET:SD   | 2:B:2157:ILE:HG22 | 2.46                     | 0.56              |
| 2:E:1826:TYR:CZ   | 2:E:1938:LYS:NZ   | 2.72                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2043:PHE:CD2  | 2:B:2047:GLN:OE1  | 2.59                     | 0.55              |
| 2:B:2247:LEU:CG   | 2:B:2375:LYS:HA   | 2.35                     | 0.55              |
| 2:B:2258:TRP:HD1  | 2:B:2258:TRP:H    | 1.52                     | 0.55              |
| 2:B:2003:THR:O    | 2:B:2006:SER:N    | 2.38                     | 0.55              |
| 2:B:2358:ASN:CB   | 2:B:2387:HIS:ND1  | 2.47                     | 0.55              |
| 1:A:31:HIS:HB3    | 1:A:96:PHE:CD2    | 2.41                     | 0.55              |
| 2:E:1293:THR:O    | 2:E:1295:GLN:N    | 2.39                     | 0.55              |
| 2:B:1598:LEU:HD13 | 2:B:1598:LEU:C    | 2.26                     | 0.55              |
| 2:E:1731:LYS:NZ   | 2:E:1768:PRO:CB   | 2.68                     | 0.55              |
| 2:E:2178:GLU:O    | 2:E:2217:LYS:CD   | 2.55                     | 0.55              |
| 1:A:85:ASP:OD1    | 1:A:88:LYS:N      | 2.22                     | 0.55              |
| 2:B:1687:HIS:CE1  | 2:B:1688:PRO:HD2  | 2.41                     | 0.55              |
| 2:B:1887:GLY:CA   | 2:B:1992:TYR:CE2  | 2.90                     | 0.55              |
| 2:E:1293:THR:OG1  | 2:E:1293:THR:O    | 2.24                     | 0.55              |
| 2:E:2025:ILE:HG23 | 2:E:2054:GLN:CD   | 2.26                     | 0.55              |
| 2:E:2087:ASN:HD22 | 2:E:2088:ILE:N    | 2.04                     | 0.55              |
| 2:E:2213:LYS:CA   | 2:E:2215:HIS:H    | 2.12                     | 0.55              |
| 2:B:1795:LYS:HB3  | 2:B:1796:PRO:HD3  | 1.89                     | 0.55              |
| 2:B:2183:TYR:HD1  | 2:B:2219:LYS:HB2  | 1.71                     | 0.55              |
| 2:E:1998:ARG:HD2  | 2:E:2045:ASP:CG   | 2.27                     | 0.55              |
| 2:E:2278:SER:OG   | 2:E:2279:LYS:N    | 2.39                     | 0.55              |
| 2:E:1259:LEU:HD23 | 2:E:1268:ARG:HG3  | 1.89                     | 0.55              |
| 2:B:1866:PHE:H    | 2:B:1866:PHE:HD1  | 1.53                     | 0.55              |
| 2:B:1895:HIS:NE2  | 2:B:1896:THR:OG1  | 2.38                     | 0.55              |
| 2:B:2037:TYR:CB   | 2:B:2038:HIS:HD2  | 2.15                     | 0.55              |
| 1:D:69:ILE:HD13   | 1:D:80:MET:HA     | 1.89                     | 0.55              |
| 1:A:48:HIS:CE1    | 1:A:53:SER:HG     | 2.25                     | 0.55              |
| 2:B:2017:THR:CG2  | 2:B:2062:GLU:HG3  | 2.37                     | 0.55              |
| 2:B:2024:MET:SD   | 2:B:2157:ILE:CG2  | 2.95                     | 0.55              |
| 2:E:1991:ILE:HG23 | 2:E:2008:LEU:HD22 | 1.89                     | 0.55              |
| 2:E:2232:HIS:HE1  | 2:E:2237:GLN:HE21 | 1.55                     | 0.55              |
| 2:B:2208:TYR:CG   | 2:B:2253:LEU:HD13 | 2.42                     | 0.55              |
| 2:E:2193:PHE:CZ   | 2:E:2203:VAL:HG12 | 2.42                     | 0.55              |
| 2:E:2244:ILE:O    | 2:E:2250:THR:HG21 | 2.06                     | 0.55              |
| 2:B:2002:TYR:CD1  | 2:B:2002:TYR:C    | 2.80                     | 0.54              |
| 2:B:1679:GLU:HB3  | 2:B:1704:GLU:O    | 2.07                     | 0.54              |
| 2:B:1733:TRP:CE2  | 2:B:1772:GLY:HA3  | 2.41                     | 0.54              |
| 2:B:2037:TYR:C    | 2:B:2038:HIS:CD2  | 2.80                     | 0.54              |
| 2:B:2386:MET:HE2  | 2:B:2387:HIS:N    | 2.22                     | 0.54              |
| 2:E:2034:ILE:CD1  | 2:E:2040:TRP:C    | 2.58                     | 0.54              |
| 2:B:2061:THR:O    | 2:B:2064:GLY:N    | 2.41                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2182:VAL:N    | 2:B:2338:GLN:HB2  | 2.22                     | 0.54              |
| 2:B:1704:GLU:CG   | 2:B:1705:SER:H    | 2.20                     | 0.54              |
| 2:B:2037:TYR:N    | 2:B:2037:TYR:CD1  | 2.76                     | 0.54              |
| 2:B:2183:TYR:HD1  | 2:B:2219:LYS:CB   | 2.20                     | 0.54              |
| 2:B:2209:GLY:HA3  | 2:B:2256:LEU:CD2  | 2.35                     | 0.54              |
| 2:B:2259:ILE:CD1  | 2:B:2291:ILE:CA   | 2.84                     | 0.54              |
| 2:B:2262:GLN:N    | 2:B:2293:ILE:O    | 2.41                     | 0.54              |
| 2:B:2382:PHE:HB3  | 2:B:2383:TYR:HD1  | 1.72                     | 0.54              |
| 2:B:934:ARG:HG2   | 2:B:934:ARG:HH11  | 1.73                     | 0.54              |
| 2:E:1598:LEU:HD22 | 2:E:1598:LEU:C    | 2.28                     | 0.54              |
| 2:E:2179:GLU:HG2  | 2:E:2180:GLN:N    | 2.22                     | 0.54              |
| 2:B:2192:LYS:HA   | 2:B:2195:GLU:CG   | 2.37                     | 0.54              |
| 2:E:1710:GLU:HA   | 2:E:1728:ILE:HA   | 1.90                     | 0.54              |
| 1:A:347:VAL:HG21  | 2:B:1875:ILE:CD1  | 2.33                     | 0.54              |
| 2:B:1259:LEU:HD23 | 2:B:1268:ARG:HG3  | 1.90                     | 0.54              |
| 2:B:2192:LYS:CA   | 2:B:2195:GLU:HB2  | 2.37                     | 0.54              |
| 2:E:1624:LEU:HD23 | 2:E:1625:VAL:N    | 2.22                     | 0.54              |
| 1:A:12:GLU:HG3    | 1:A:25:LYS:HA     | 1.89                     | 0.54              |
| 2:B:885:VAL:HG21  | 2:B:1124:LEU:HD21 | 1.90                     | 0.54              |
| 1:D:35:ASP:OD2    | 1:D:104:SER:OG    | 2.25                     | 0.54              |
| 2:E:1466:GLN:O    | 2:E:1469:ILE:HB   | 2.07                     | 0.54              |
| 2:E:1825:ILE:O    | 2:E:1826:TYR:HB3  | 2.08                     | 0.54              |
| 2:B:1139:ASN:H    | 2:B:1139:ASN:ND2  | 2.05                     | 0.54              |
| 2:B:2208:TYR:HB3  | 2:B:2253:LEU:HD11 | 1.90                     | 0.54              |
| 2:E:2079:ILE:HD13 | 2:E:2079:ILE:N    | 2.23                     | 0.54              |
| 2:B:1598:LEU:H    | 2:B:1598:LEU:HD12 | 1.72                     | 0.54              |
| 2:B:2050:THR:HA   | 2:B:2053:SER:OG   | 2.06                     | 0.54              |
| 2:B:2209:GLY:O    | 2:B:2254:GLU:O    | 2.25                     | 0.54              |
| 2:B:2358:ASN:O    | 2:B:2387:HIS:ND1  | 2.41                     | 0.54              |
| 1:D:354:ARG:HB2   | 1:D:355:PRO:HD3   | 1.89                     | 0.54              |
| 2:E:1292:ARG:HG2  | 2:E:1292:ARG:HH11 | 1.72                     | 0.54              |
| 2:B:1801:SER:O    | 2:B:1805:ILE:HG23 | 2.08                     | 0.54              |
| 2:B:1882:LEU:CD1  | 2:B:1991:ILE:HG21 | 2.37                     | 0.54              |
| 2:B:1070:LEU:O    | 2:B:1074:VAL:CG2  | 2.56                     | 0.53              |
| 2:B:1961:ASN:HA   | 2:B:2079:ILE:HD12 | 1.89                     | 0.53              |
| 2:B:2007:ARG:HG2  | 2:B:2052:GLU:CD   | 2.28                     | 0.53              |
| 2:B:2210:MET:HE2  | 2:B:2252:GLY:C    | 2.27                     | 0.53              |
| 2:B:2278:SER:HB3  | 2:B:2316:GLU:CG   | 2.38                     | 0.53              |
| 2:B:2188:ASN:ND2  | 2:B:2346:THR:HB   | 2.20                     | 0.53              |
| 2:B:1190:ASN:N    | 2:B:1191:PRO:HD3  | 2.22                     | 0.53              |
| 2:B:1866:PHE:N    | 2:B:1866:PHE:CD1  | 2.76                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2296:THR:O    | 2:B:2297:PRO:C    | 2.44                     | 0.53              |
| 2:B:2386:MET:HE2  | 2:B:2387:HIS:H    | 1.73                     | 0.53              |
| 2:E:1702:THR:HG23 | 2:E:1768:PRO:HG3  | 1.85                     | 0.53              |
| 2:E:1899:TRP:CE3  | 2:E:1899:TRP:HA   | 2.43                     | 0.53              |
| 2:B:2007:ARG:NE   | 2:B:2052:GLU:OE2  | 2.41                     | 0.53              |
| 2:B:2184:VAL:O    | 2:B:2221:ILE:HG12 | 2.08                     | 0.53              |
| 2:B:2256:LEU:C    | 2:B:2288:CYS:HG   | 2.03                     | 0.53              |
| 1:A:208:VAL:O     | 1:A:213:ILE:HD12  | 2.08                     | 0.53              |
| 1:D:347:VAL:HG21  | 2:E:1875:ILE:CD1  | 2.38                     | 0.53              |
| 2:B:2202:GLN:HG2  | 2:B:2261:THR:O    | 2.09                     | 0.53              |
| 2:E:1259:LEU:CD2  | 2:E:1268:ARG:HG3  | 2.38                     | 0.53              |
| 2:E:1801:SER:O    | 2:E:1805:ILE:HG12 | 2.09                     | 0.53              |
| 2:E:2202:GLN:NE2  | 2:E:2235:SER:O    | 2.37                     | 0.53              |
| 2:B:2233:VAL:HG23 | 2:B:2234:GLY:N    | 2.24                     | 0.53              |
| 2:B:950:THR:O     | 2:B:954:ILE:N     | 2.40                     | 0.53              |
| 2:E:2227:VAL:HG13 | 2:E:2228:PRO:HD2  | 1.91                     | 0.53              |
| 1:A:109:ASP:OD2   | 1:A:113:THR:OG1   | 2.27                     | 0.53              |
| 1:D:109:ASP:OD1   | 1:D:110:GLU:N     | 2.42                     | 0.53              |
| 2:B:2035:LYS:HB3  | 2:B:2037:TYR:CD1  | 2.43                     | 0.53              |
| 2:E:2003:THR:O    | 2:E:2006:SER:N    | 2.42                     | 0.53              |
| 2:B:1624:LEU:HD23 | 2:B:1624:LEU:C    | 2.29                     | 0.53              |
| 2:B:2185:LEU:O    | 2:B:2342:SER:N    | 2.37                     | 0.53              |
| 2:B:2202:GLN:CG   | 2:B:2261:THR:O    | 2.57                     | 0.53              |
| 1:A:69:ILE:HD13   | 1:A:80:MET:HA     | 1.90                     | 0.53              |
| 2:B:1598:LEU:H    | 2:B:1598:LEU:CD1  | 2.21                     | 0.53              |
| 2:B:2339:LEU:C    | 2:B:2339:LEU:HD12 | 2.26                     | 0.53              |
| 2:B:2339:LEU:HD13 | 2:B:2340:LEU:H    | 1.68                     | 0.53              |
| 2:E:1104:ILE:CG2  | 2:E:1107:LEU:HD13 | 2.39                     | 0.53              |
| 2:E:2384:ASN:ND2  | 2:E:2385:GLU:N    | 2.57                     | 0.53              |
| 2:B:1259:LEU:CD2  | 2:B:1268:ARG:HG3  | 2.39                     | 0.52              |
| 2:B:2339:LEU:C    | 2:B:2340:LEU:HD12 | 2.24                     | 0.52              |
| 1:A:214:PHE:CE1   | 1:A:220:TYR:HA    | 2.44                     | 0.52              |
| 2:B:1107:LEU:HD23 | 2:B:1109:PHE:CE1  | 2.44                     | 0.52              |
| 2:B:2273:GLU:OE2  | 2:B:2290:ASP:OD2  | 2.26                     | 0.52              |
| 2:B:2294:PHE:CD2  | 2:B:2301:SER:OG   | 2.36                     | 0.52              |
| 2:B:1466:GLN:OE1  | 2:B:1466:GLN:HA   | 2.08                     | 0.52              |
| 2:B:1719:GLU:HA   | 2:B:1719:GLU:OE1  | 2.09                     | 0.52              |
| 2:B:2350:ILE:HD13 | 2:B:2376:TYR:CA   | 2.30                     | 0.52              |
| 2:E:1279:VAL:HG12 | 2:E:1280:SER:O    | 2.09                     | 0.52              |
| 2:E:2024:MET:O    | 2:E:2027:LEU:N    | 2.42                     | 0.52              |
| 2:B:1383:PHE:HE2  | 2:B:1387:VAL:HG21 | 1.75                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1599:SER:C    | 2:B:1600:GLN:HG2  | 2.29                     | 0.52              |
| 2:B:2223:THR:OG1  | 2:B:2348:ASN:OD1  | 2.08                     | 0.52              |
| 2:B:1721:ASN:CB   | 2:E:1463:THR:HB   | 2.39                     | 0.52              |
| 2:E:2014:ALA:HA   | 2:E:2059:ILE:HD12 | 1.87                     | 0.52              |
| 2:E:1966:SER:HG   | 2:E:2016:LYS:HE3  | 1.72                     | 0.52              |
| 2:E:2083:ILE:HG22 | 2:E:2084:LEU:CD1  | 2.38                     | 0.52              |
| 2:E:2043:PHE:HA   | 2:E:2047:GLN:OE1  | 2.10                     | 0.52              |
| 2:B:1104:ILE:CG2  | 2:B:1107:LEU:HD13 | 2.39                     | 0.52              |
| 2:B:2183:TYR:CE2  | 2:B:2289:ILE:HD13 | 2.44                     | 0.52              |
| 2:E:1324:GLY:HA2  | 2:E:1325:SER:HG   | 1.71                     | 0.52              |
| 2:E:1864:LYS:HG3  | 2:E:1870:VAL:HG22 | 1.90                     | 0.52              |
| 2:E:2182:VAL:HG12 | 2:E:2338:GLN:HB2  | 1.91                     | 0.52              |
| 2:E:2267:LYS:O    | 2:E:2305:TYR:CE1  | 2.63                     | 0.52              |
| 2:E:1767:TYR:CD1  | 2:E:1767:TYR:N    | 2.77                     | 0.52              |
| 2:E:2060:LEU:O    | 2:E:2063:TYR:HB3  | 2.09                     | 0.52              |
| 2:B:1848:ILE:O    | 2:B:1930:PRO:HA   | 2.09                     | 0.52              |
| 2:B:2060:LEU:O    | 2:B:2063:TYR:CB   | 2.53                     | 0.52              |
| 2:B:2280:LEU:CD1  | 2:B:2281:PHE:CE2  | 2.91                     | 0.52              |
| 1:D:106:PRO:C     | 1:D:107:LYS:CG    | 2.72                     | 0.52              |
| 1:D:88:LYS:O      | 1:D:92:ILE:HG13   | 2.10                     | 0.52              |
| 2:E:1286:TRP:CE2  | 2:E:1302:LEU:HD11 | 2.45                     | 0.52              |
| 2:E:1666:CYS:SG   | 2:E:1683:LYS:HE3  | 2.50                     | 0.52              |
| 2:E:2384:ASN:HD22 | 2:E:2386:MET:N    | 2.02                     | 0.52              |
| 2:E:918:ASP:OD1   | 2:E:1515:LYS:NZ   | 2.39                     | 0.52              |
| 2:B:1595:ARG:HG3  | 2:B:1596:THR:N    | 2.24                     | 0.52              |
| 2:B:2357:TRP:CH2  | 2:B:2382:PHE:HD1  | 2.22                     | 0.52              |
| 2:E:1212:ARG:HG2  | 2:E:1212:ARG:HH11 | 1.74                     | 0.52              |
| 2:B:2233:VAL:CG2  | 2:B:2234:GLY:N    | 2.73                     | 0.52              |
| 2:E:2074:LEU:C    | 2:E:2075:THR:HG1  | 2.09                     | 0.52              |
| 1:A:296:SER:O     | 1:A:299:LYS:HG2   | 2.10                     | 0.51              |
| 2:B:1093:LYS:HE2  | 2:B:1094:ASP:OD1  | 2.10                     | 0.51              |
| 2:E:2011:LEU:O    | 2:E:2014:ALA:HB3  | 2.09                     | 0.51              |
| 2:E:2302:LEU:HD12 | 2:E:2302:LEU:N    | 2.24                     | 0.51              |
| 2:B:2035:LYS:CD   | 2:B:2037:TYR:HE1  | 2.22                     | 0.51              |
| 2:B:2152:TRP:HA   | 2:B:2153:ARG:C    | 2.29                     | 0.51              |
| 2:B:2182:VAL:HG13 | 2:B:2338:GLN:CD   | 2.23                     | 0.51              |
| 2:B:2286:ARG:HD2  | 2:B:2312:TYR:CE2  | 2.45                     | 0.51              |
| 2:E:1093:LYS:CD   | 2:E:1094:ASP:HA   | 2.41                     | 0.51              |
| 1:D:20:TYR:CZ     | 1:D:106:PRO:HG2   | 2.44                     | 0.51              |
| 2:E:1107:LEU:HD23 | 2:E:1109:PHE:CE1  | 2.45                     | 0.51              |
| 2:B:2162:LEU:HD23 | 2:B:2165:ARG:NE   | 2.24                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2189:LEU:HD21 | 2:B:2347:GLY:CA   | 2.40                     | 0.51              |
| 2:E:1763:ASN:HD22 | 2:E:1763:ASN:H    | 1.58                     | 0.51              |
| 2:E:1991:ILE:HG21 | 2:E:2008:LEU:HD22 | 1.92                     | 0.51              |
| 2:E:2062:GLU:OE2  | 2:E:2065:ARG:NH2  | 2.34                     | 0.51              |
| 2:E:2064:GLY:O    | 2:E:2067:TYR:CA   | 2.58                     | 0.51              |
| 2:E:2361:PHE:CZ   | 2:E:2383:TYR:CE1  | 2.98                     | 0.51              |
| 2:E:1097:HIS:CD2  | 2:E:1098:VAL:O    | 2.63                     | 0.51              |
| 2:E:1899:TRP:HE3  | 2:E:1899:TRP:HA   | 1.75                     | 0.51              |
| 2:B:959:LEU:HD12  | 2:B:1077:ASN:OD1  | 2.11                     | 0.51              |
| 2:E:1767:TYR:N    | 2:E:1767:TYR:HD1  | 2.09                     | 0.51              |
| 2:B:1041:VAL:HG21 | 2:B:1253:LYS:HA   | 1.91                     | 0.51              |
| 2:B:2037:TYR:HB2  | 2:B:2038:HIS:NE2  | 2.26                     | 0.51              |
| 2:B:2017:THR:HG23 | 2:B:2062:GLU:OE2  | 2.11                     | 0.51              |
| 2:E:1843:LEU:HD22 | 2:E:1884:PRO:HG3  | 1.93                     | 0.51              |
| 2:E:2357:TRP:H    | 2:E:2387:HIS:CE1  | 2.28                     | 0.51              |
| 2:B:2155:SER:O    | 2:B:2156:ALA:HB3  | 2.10                     | 0.51              |
| 2:E:1292:ARG:NH1  | 2:E:1292:ARG:HG2  | 2.26                     | 0.51              |
| 2:E:920:LYS:HG3   | 2:E:940:ILE:HG21  | 1.92                     | 0.51              |
| 2:B:1029:THR:HG22 | 2:B:1260:PHE:CZ   | 2.46                     | 0.51              |
| 2:B:1105:ARG:HG3  | 2:B:1105:ARG:NH1  | 2.25                     | 0.51              |
| 2:B:1029:THR:HG22 | 2:B:1260:PHE:HZ   | 1.75                     | 0.51              |
| 2:B:2019:GLU:OE2  | 2:B:2167:LYS:NZ   | 2.44                     | 0.51              |
| 2:B:2210:MET:HE1  | 2:B:2253:LEU:CB   | 2.40                     | 0.51              |
| 2:E:2050:THR:HA   | 2:E:2053:SER:HB3  | 1.93                     | 0.51              |
| 2:E:2025:ILE:CG2  | 2:E:2054:GLN:CD   | 2.79                     | 0.51              |
| 2:E:1472:ASN:C    | 2:E:2325:LEU:CB   | 2.75                     | 0.51              |
| 2:B:1687:HIS:CE1  | 2:B:1689:ARG:HG3  | 2.46                     | 0.50              |
| 2:B:2208:TYR:CB   | 2:B:2253:LEU:CD1  | 2.88                     | 0.50              |
| 2:E:2041:PRO:HG2  | 2:E:2043:PHE:CE1  | 2.46                     | 0.50              |
| 2:E:2049:ILE:O    | 2:E:2053:SER:HB3  | 2.11                     | 0.50              |
| 2:B:1075:ASP:HB3  | 2:B:1078:ILE:HD12 | 1.93                     | 0.50              |
| 2:B:1317:ARG:O    | 2:B:1321:MET:HB2  | 2.12                     | 0.50              |
| 2:B:1661:ILE:HG23 | 2:B:1805:ILE:CD1  | 2.41                     | 0.50              |
| 2:B:2157:ILE:HA   | 2:B:2160:THR:OG1  | 2.10                     | 0.50              |
| 2:B:2236:VAL:CB   | 2:B:2238:ILE:HD11 | 2.41                     | 0.50              |
| 2:E:1605:ARG:NH2  | 2:E:1824:GLN:OE1  | 2.44                     | 0.50              |
| 2:E:2034:ILE:CG2  | 2:E:2040:TRP:H    | 2.22                     | 0.50              |
| 2:B:1999:LEU:CD1  | 2:B:2003:THR:HB   | 2.36                     | 0.50              |
| 2:B:2194:ILE:O    | 2:B:2197:SER:OG   | 2.28                     | 0.50              |
| 2:B:2350:ILE:CD1  | 2:B:2376:TYR:HA   | 2.31                     | 0.50              |
| 2:E:1599:SER:C    | 2:E:1600:GLN:HG2  | 2.31                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2183:TYR:OH   | 2:B:2219:LYS:NZ   | 2.37                     | 0.50              |
| 2:B:2247:LEU:CD1  | 2:B:2248:PRO:HD3  | 2.41                     | 0.50              |
| 1:D:55:ARG:NH2    | 1:D:279:TYR:CZ    | 2.79                     | 0.50              |
| 2:E:1057:MET:CE   | 2:E:1166:ASP:HB2  | 2.41                     | 0.50              |
| 2:E:1687:HIS:CE1  | 2:E:1689:ARG:HG3  | 2.46                     | 0.50              |
| 2:E:2227:VAL:HG13 | 2:E:2239:SER:OG   | 2.10                     | 0.50              |
| 2:E:1343:PHE:HB3  | 2:E:1444:ILE:CD1  | 2.40                     | 0.50              |
| 2:E:1795:LYS:HB3  | 2:E:1796:PRO:HD3  | 1.94                     | 0.50              |
| 2:B:1854:ASP:HA   | 2:B:1857:VAL:HG23 | 1.94                     | 0.50              |
| 2:B:2157:ILE:CA   | 2:B:2160:THR:OG1  | 2.60                     | 0.50              |
| 2:B:2162:LEU:CD2  | 2:B:2165:ARG:NE   | 2.74                     | 0.50              |
| 2:E:1983:GLU:HB2  | 2:E:1984:PRO:HD2  | 1.94                     | 0.50              |
| 2:E:2040:TRP:N    | 2:E:2040:TRP:CD1  | 2.80                     | 0.50              |
| 2:E:885:VAL:HG21  | 2:E:1124:LEU:HD21 | 1.94                     | 0.50              |
| 1:A:327:ILE:HB    | 1:A:328:TYR:CD2   | 2.47                     | 0.50              |
| 2:B:1969:MET:O    | 2:B:1975:SER:OG   | 2.30                     | 0.50              |
| 2:B:2032:ILE:CD1  | 2:B:2047:GLN:HE22 | 2.24                     | 0.50              |
| 2:B:2350:ILE:CD1  | 2:B:2376:TYR:CD1  | 2.95                     | 0.50              |
| 2:E:2018:ASN:ND2  | 2:E:2058:LEU:HG   | 2.17                     | 0.50              |
| 1:D:153:LEU:C     | 1:D:153:LEU:HD23  | 2.32                     | 0.50              |
| 1:D:280:SER:HB2   | 1:D:313:TYR:CE1   | 2.47                     | 0.50              |
| 2:E:1764:VAL:N    | 2:E:1766:MET:HE2  | 2.24                     | 0.50              |
| 1:A:215:LYS:O     | 1:A:216:ASN:OD1   | 2.29                     | 0.50              |
| 2:B:1036:SER:HB3  | 2:B:1154:LYS:HE2  | 1.93                     | 0.50              |
| 2:B:2278:SER:CB   | 2:B:2316:GLU:HG3  | 2.42                     | 0.50              |
| 2:E:945:ASP:N     | 2:E:945:ASP:OD1   | 2.45                     | 0.50              |
| 1:D:19:GLN:HE22   | 1:D:110:GLU:CG    | 2.18                     | 0.49              |
| 2:E:1854:ASP:OD1  | 2:E:1937:ARG:HD3  | 2.11                     | 0.49              |
| 2:E:2051:ILE:N    | 2:E:2051:ILE:HD13 | 2.27                     | 0.49              |
| 2:E:2083:ILE:HG22 | 2:E:2084:LEU:H    | 1.77                     | 0.49              |
| 2:E:2177:VAL:CG2  | 2:E:2180:GLN:HG3  | 2.42                     | 0.49              |
| 2:E:2311:GLY:HA2  | 2:E:2333:PHE:CD1  | 2.46                     | 0.49              |
| 2:E:2182:VAL:HA   | 2:E:2338:GLN:HB2  | 1.92                     | 0.49              |
| 2:B:1666:CYS:SG   | 2:B:1683:LYS:HE3  | 2.52                     | 0.49              |
| 2:B:1890:PHE:HB3  | 2:B:1986:MET:SD   | 2.52                     | 0.49              |
| 2:B:2182:VAL:O    | 2:B:2182:VAL:HG23 | 2.11                     | 0.49              |
| 2:B:969:ILE:HA    | 2:B:981:VAL:O     | 2.12                     | 0.49              |
| 2:E:1015:PRO:CD   | 2:E:1165:LEU:HD23 | 2.42                     | 0.49              |
| 2:E:1705:SER:OG   | 2:E:1730:ASN:CB   | 2.60                     | 0.49              |
| 2:E:2064:GLY:C    | 2:E:2067:TYR:H    | 2.11                     | 0.49              |
| 2:E:2083:ILE:HG22 | 2:E:2084:LEU:N    | 2.27                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:280:SER:HB2   | 1:A:313:TYR:CE1   | 2.48                     | 0.49              |
| 2:B:1604:ARG:HH22 | 2:B:1822:GLY:C    | 2.14                     | 0.49              |
| 2:B:2192:LYS:HA   | 2:B:2195:GLU:CB   | 2.41                     | 0.49              |
| 1:D:151:GLU:OE2   | 1:D:154:LYS:CE    | 2.49                     | 0.49              |
| 2:B:1015:PRO:CD   | 2:B:1165:LEU:CD2  | 2.90                     | 0.49              |
| 2:B:2041:PRO:CG   | 2:B:2043:PHE:CE1  | 2.96                     | 0.49              |
| 2:B:2052:GLU:O    | 2:B:2056:ARG:CG   | 2.40                     | 0.49              |
| 1:D:77:LEU:C      | 1:D:77:LEU:HD12   | 2.33                     | 0.49              |
| 2:E:1711:VAL:CA   | 2:E:1790:TRP:O    | 2.60                     | 0.49              |
| 2:E:2201:ILE:HG22 | 2:E:2382:PHE:CZ   | 2.48                     | 0.49              |
| 2:E:988:GLU:O     | 2:E:991:THR:HG22  | 2.12                     | 0.49              |
| 2:B:1463:THR:O    | 2:B:1467:GLU:HG2  | 2.12                     | 0.49              |
| 2:B:2208:TYR:C    | 2:B:2253:LEU:HD21 | 2.33                     | 0.49              |
| 2:B:2247:LEU:CD1  | 2:B:2375:LYS:HA   | 2.42                     | 0.49              |
| 2:E:1394:LEU:HD23 | 2:E:1570:TRP:CZ2  | 2.47                     | 0.49              |
| 2:E:2163:TYR:CE1  | 2:E:2164:LEU:CD2  | 2.96                     | 0.49              |
| 2:B:2055:MET:O    | 2:B:2058:LEU:N    | 2.45                     | 0.49              |
| 2:B:2153:ARG:HA   | 2:B:2155:SER:O    | 2.12                     | 0.49              |
| 1:D:326:LEU:HG    | 1:D:326:LEU:O     | 2.13                     | 0.49              |
| 1:D:88:LYS:NZ     | 1:D:92:ILE:HD11   | 2.27                     | 0.49              |
| 2:E:1766:MET:C    | 2:E:1767:TYR:HD1  | 2.16                     | 0.49              |
| 1:A:72:ASP:OD2    | 1:A:75:ASP:HB2    | 2.13                     | 0.49              |
| 1:A:83:GLU:CG     | 1:A:89:PHE:HB2    | 2.42                     | 0.49              |
| 2:B:1687:HIS:ND1  | 2:B:1688:PRO:CD   | 2.76                     | 0.49              |
| 2:B:2064:GLY:O    | 2:B:2068:ASN:N    | 2.45                     | 0.49              |
| 1:D:110:GLU:O     | 1:D:111:ASP:CB    | 2.60                     | 0.49              |
| 2:E:1036:SER:HB3  | 2:E:1154:LYS:HE2  | 1.95                     | 0.49              |
| 2:E:1383:PHE:HE2  | 2:E:1387:VAL:HG21 | 1.75                     | 0.49              |
| 2:E:1368:GLN:NE2  | 2:E:1389:TYR:OH   | 2.44                     | 0.49              |
| 2:B:1097:HIS:ND1  | 2:B:1098:VAL:N    | 2.60                     | 0.49              |
| 2:B:1137:PRO:CD   | 2:B:1140:ASN:O    | 2.61                     | 0.49              |
| 2:B:1324:GLY:CA   | 2:B:1325:SER:CB   | 2.91                     | 0.49              |
| 2:B:2284:LYS:HE2  | 2:B:2285:LYS:CA   | 2.42                     | 0.49              |
| 2:B:2182:VAL:CB   | 2:B:2338:GLN:CB   | 2.89                     | 0.49              |
| 2:B:2183:TYR:N    | 2:B:2338:GLN:O    | 2.40                     | 0.49              |
| 2:E:1461:TYR:O    | 2:E:1465:ARG:N    | 2.44                     | 0.49              |
| 2:E:2177:VAL:HG23 | 2:E:2180:GLN:N    | 2.19                     | 0.49              |
| 2:E:2251:GLU:N    | 2:E:2251:GLU:OE1  | 2.46                     | 0.49              |
| 2:B:1624:LEU:HD21 | 2:B:1633:PHE:CD1  | 2.48                     | 0.49              |
| 2:B:930:ASN:N     | 2:B:933:GLU:OE1   | 2.46                     | 0.49              |
| 2:B:920:LYS:HG3   | 2:B:940:ILE:HG21  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1808:ALA:O    | 2:B:1809:ASN:C    | 2.51                     | 0.49              |
| 2:B:1993:ASP:CG   | 2:B:2038:HIS:CB   | 2.58                     | 0.49              |
| 2:B:2381:GLU:CD   | 2:B:2381:GLU:H    | 2.00                     | 0.49              |
| 2:E:2087:ASN:ND2  | 2:E:2088:ILE:N    | 2.61                     | 0.49              |
| 2:B:1465:ARG:HG3  | 2:B:1465:ARG:NH1  | 2.28                     | 0.48              |
| 2:B:1729:THR:CG2  | 2:B:1771:THR:CG2  | 2.54                     | 0.48              |
| 2:B:2044:THR:H    | 2:B:2047:GLN:NE2  | 2.11                     | 0.48              |
| 2:B:2259:ILE:HD12 | 2:B:2291:ILE:CA   | 2.42                     | 0.48              |
| 2:B:2259:ILE:HD13 | 2:B:2291:ILE:HG21 | 1.82                     | 0.48              |
| 2:B:2379:PRO:C    | 2:B:2380:LEU:HD23 | 2.33                     | 0.48              |
| 2:E:2163:TYR:CD1  | 2:E:2164:LEU:N    | 2.81                     | 0.48              |
| 2:E:2384:ASN:C    | 2:E:2384:ASN:HD22 | 2.16                     | 0.48              |
| 2:B:2282:ALA:O    | 2:B:2286:ARG:HG2  | 2.14                     | 0.48              |
| 2:E:1733:TRP:CE2  | 2:E:1767:TYR:CD2  | 2.97                     | 0.48              |
| 2:E:2163:TYR:CE1  | 2:E:2164:LEU:HD23 | 2.48                     | 0.48              |
| 2:E:2177:VAL:CG2  | 2:E:2180:GLN:CG   | 2.91                     | 0.48              |
| 2:E:2183:TYR:CD1  | 2:E:2289:ILE:HD13 | 2.48                     | 0.48              |
| 2:B:2342:SER:HG   | 2:B:2344:ARG:H    | 1.59                     | 0.48              |
| 2:B:2208:TYR:OH   | 2:B:2244:ILE:HG23 | 2.13                     | 0.48              |
| 2:B:2307:LEU:C    | 2:B:2307:LEU:HD12 | 2.28                     | 0.48              |
| 2:E:1209:LYS:HG2  | 2:E:1212:ARG:NH2  | 2.27                     | 0.48              |
| 2:E:2269:MET:HE3  | 2:E:2273:GLU:HB3  | 1.95                     | 0.48              |
| 2:E:2270:ALA:HB1  | 2:E:2324:VAL:HA   | 1.95                     | 0.48              |
| 2:B:1432:GLU:O    | 2:B:1433:ASP:CB   | 2.61                     | 0.48              |
| 2:B:2044:THR:O    | 2:B:2048:TRP:CD1  | 2.66                     | 0.48              |
| 2:B:2284:LYS:HE3  | 2:B:2284:LYS:C    | 2.34                     | 0.48              |
| 1:D:224:LEU:C     | 1:D:224:LEU:HD23  | 2.33                     | 0.48              |
| 2:E:1709:TRP:O    | 2:E:1728:ILE:CA   | 2.62                     | 0.48              |
| 2:E:2183:TYR:CE1  | 2:E:2289:ILE:HG21 | 2.48                     | 0.48              |
| 2:B:2280:LEU:HD12 | 2:B:2281:PHE:CD2  | 2.49                     | 0.48              |
| 2:B:2386:MET:CE   | 2:B:2387:HIS:N    | 2.76                     | 0.48              |
| 2:B:930:ASN:O     | 2:B:934:ARG:HB2   | 2.14                     | 0.48              |
| 2:B:2210:MET:CE   | 2:B:2252:GLY:C    | 2.82                     | 0.48              |
| 2:E:1343:PHE:HB3  | 2:E:1444:ILE:HD13 | 1.96                     | 0.48              |
| 2:E:1762:ASP:CG   | 2:E:1763:ASN:N    | 2.66                     | 0.48              |
| 2:E:2271:ALA:HA   | 2:E:2329:PHE:CE1  | 2.48                     | 0.48              |
| 1:A:77:LEU:C      | 1:A:77:LEU:HD12   | 2.33                     | 0.48              |
| 1:A:77:LEU:O      | 1:A:77:LEU:HD12   | 2.14                     | 0.48              |
| 2:B:1687:HIS:CG   | 2:B:1688:PRO:HD2  | 2.49                     | 0.48              |
| 2:B:1899:TRP:HB3  | 2:B:1905:LEU:HD21 | 1.95                     | 0.48              |
| 2:B:2278:SER:HB3  | 2:B:2316:GLU:HG2  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2384:ASN:HD22 | 2:B:2385:GLU:N    | 2.11                     | 0.48              |
| 1:D:280:SER:CB    | 1:D:313:TYR:CE1   | 2.97                     | 0.48              |
| 2:E:1865:THR:OG1  | 2:E:1867:GLU:OE1  | 2.31                     | 0.48              |
| 2:E:2019:GLU:HG2  | 2:E:2019:GLU:O    | 2.14                     | 0.48              |
| 2:B:1164:TYR:O    | 2:B:1167:ARG:N    | 2.42                     | 0.48              |
| 2:B:1188:ALA:O    | 2:B:1191:PRO:CD   | 2.62                     | 0.48              |
| 2:B:1368:GLN:NE2  | 2:B:1389:TYR:OH   | 2.47                     | 0.48              |
| 2:B:1959:THR:OG1  | 2:B:1960:GLU:N    | 2.47                     | 0.48              |
| 2:B:2183:TYR:HE2  | 2:B:2289:ILE:HG21 | 1.79                     | 0.48              |
| 2:B:2307:LEU:CD1  | 2:B:2308:THR:O    | 2.62                     | 0.48              |
| 2:B:2358:ASN:CB   | 2:B:2387:HIS:HE1  | 2.04                     | 0.48              |
| 2:E:2037:TYR:C    | 2:E:2038:HIS:CD2  | 2.88                     | 0.48              |
| 2:E:2066:LYS:HB2  | 2:E:2067:TYR:CE1  | 2.49                     | 0.48              |
| 1:A:108:ILE:N     | 1:A:108:ILE:HD12  | 2.29                     | 0.47              |
| 2:B:1041:VAL:HG23 | 2:B:1041:VAL:O    | 2.13                     | 0.47              |
| 2:B:1570:TRP:O    | 2:B:1571:GLU:HG3  | 2.14                     | 0.47              |
| 2:B:2177:VAL:N    | 2:B:2338:GLN:NE2  | 2.59                     | 0.47              |
| 2:B:936:GLU:O     | 2:B:940:ILE:CD1   | 2.61                     | 0.47              |
| 2:E:2268:PHE:C    | 2:E:2268:PHE:CD1  | 2.87                     | 0.47              |
| 2:B:1759:TYR:O    | 2:B:1762:ASP:CB   | 2.62                     | 0.47              |
| 2:B:2186:PRO:HG3  | 2:B:2345:ILE:HD12 | 1.95                     | 0.47              |
| 2:B:2267:LYS:O    | 2:B:2305:TYR:HE2  | 1.96                     | 0.47              |
| 2:E:2277:HIS:O    | 2:E:2281:PHE:HD2  | 1.96                     | 0.47              |
| 2:B:1895:HIS:CD2  | 2:B:1896:THR:HG1  | 2.26                     | 0.47              |
| 2:B:2294:PHE:CE1  | 2:B:2296:THR:HG23 | 2.48                     | 0.47              |
| 2:B:2350:ILE:HD11 | 2:B:2376:TYR:CE1  | 2.49                     | 0.47              |
| 2:B:1394:LEU:HD23 | 2:B:1570:TRP:CZ2  | 2.49                     | 0.47              |
| 2:B:1558:GLU:CD   | 2:B:1563:LYS:HZ1  | 2.17                     | 0.47              |
| 2:B:1624:LEU:HD23 | 2:B:1625:VAL:N    | 2.30                     | 0.47              |
| 2:B:1677:GLN:OE1  | 2:B:1706:VAL:HG11 | 2.15                     | 0.47              |
| 2:B:2058:LEU:O    | 2:B:2059:ILE:C    | 2.52                     | 0.47              |
| 2:B:1189:GLU:C    | 2:B:1191:PRO:HD3  | 2.35                     | 0.47              |
| 2:B:2025:ILE:HG22 | 2:B:2025:ILE:O    | 2.12                     | 0.47              |
| 2:B:2268:PHE:CE2  | 2:B:2331:PRO:HG3  | 2.49                     | 0.47              |
| 1:D:108:ILE:H     | 1:D:108:ILE:HD13  | 1.78                     | 0.47              |
| 2:E:936:GLU:O     | 2:E:940:ILE:CD1   | 2.61                     | 0.47              |
| 2:B:2302:LEU:CD1  | 2:B:2302:LEU:N    | 2.77                     | 0.47              |
| 2:B:953:ARG:HG3   | 2:B:953:ARG:HH11  | 1.79                     | 0.47              |
| 2:E:1472:ASN:HB3  | 2:E:2325:LEU:O    | 2.14                     | 0.47              |
| 2:E:1791:PHE:CD1  | 2:E:1791:PHE:C    | 2.87                     | 0.47              |
| 2:E:2053:SER:OG   | 2:E:2054:GLN:N    | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1075:ASP:CB   | 2:B:1078:ILE:HD12 | 2.45                     | 0.47              |
| 2:B:1097:HIS:ND1  | 2:B:1098:VAL:O    | 2.48                     | 0.47              |
| 2:B:2163:TYR:CD1  | 2:B:2164:LEU:N    | 2.83                     | 0.47              |
| 2:B:2192:LYS:O    | 2:B:2196:ILE:N    | 2.46                     | 0.47              |
| 2:B:2215:HIS:HB3  | 2:B:2218:VAL:HB   | 1.97                     | 0.47              |
| 2:B:2230:LEU:CD2  | 2:B:2237:GLN:HG3  | 2.44                     | 0.47              |
| 2:B:2306:ASN:HB2  | 2:B:2335:THR:OG1  | 2.14                     | 0.47              |
| 2:E:1686:VAL:HG11 | 2:E:1690:LYS:HD2  | 1.95                     | 0.47              |
| 2:E:1886:THR:CB   | 2:E:1888:HIS:CE1  | 2.96                     | 0.47              |
| 2:E:2004:ALA:O    | 2:E:2007:ARG:HB3  | 2.14                     | 0.47              |
| 2:B:2247:LEU:HA   | 2:B:2247:LEU:HD13 | 1.74                     | 0.47              |
| 1:D:215:LYS:HD2   | 1:D:215:LYS:N     | 2.29                     | 0.47              |
| 1:D:320:ASP:OD1   | 2:E:1330:LYS:HE2  | 2.15                     | 0.47              |
| 1:D:77:LEU:HD12   | 1:D:77:LEU:O      | 2.14                     | 0.47              |
| 2:E:1079:ALA:O    | 2:E:1083:THR:HG22 | 2.15                     | 0.47              |
| 2:E:2339:LEU:O    | 2:E:2340:LEU:HD12 | 2.14                     | 0.47              |
| 2:E:969:ILE:HA    | 2:E:981:VAL:O     | 2.15                     | 0.47              |
| 2:B:1471:GLN:O    | 2:B:1473:ARG:HG3  | 2.15                     | 0.47              |
| 2:B:1791:PHE:C    | 2:B:1791:PHE:CD1  | 2.87                     | 0.47              |
| 2:B:1857:VAL:HG13 | 2:B:1894:ILE:HG13 | 1.97                     | 0.47              |
| 2:B:2178:GLU:O    | 2:B:2217:LYS:CG   | 2.62                     | 0.47              |
| 2:E:1019:GLU:HB2  | 2:E:1023:LEU:HD23 | 1.97                     | 0.47              |
| 2:E:1687:HIS:ND1  | 2:E:1688:PRO:CD   | 2.78                     | 0.47              |
| 2:E:2037:TYR:C    | 2:E:2038:HIS:HD2  | 2.17                     | 0.47              |
| 2:E:2177:VAL:HG23 | 2:E:2180:GLN:HB2  | 1.93                     | 0.47              |
| 2:B:1984:PRO:O    | 2:B:1985:GLN:NE2  | 2.48                     | 0.47              |
| 2:B:2208:TYR:CE2  | 2:B:2244:ILE:HD13 | 2.50                     | 0.47              |
| 2:E:1680:SER:OG   | 2:E:1704:GLU:HB2  | 2.15                     | 0.47              |
| 2:B:2007:ARG:CG   | 2:B:2052:GLU:OE2  | 2.62                     | 0.47              |
| 2:E:1067:ASN:ND2  | 2:E:1083:THR:HG21 | 2.11                     | 0.47              |
| 2:B:1721:ASN:HB2  | 2:E:1463:THR:HB   | 1.96                     | 0.47              |
| 2:E:2011:LEU:HD12 | 2:E:2040:TRP:CH2  | 2.49                     | 0.47              |
| 2:E:2210:MET:CE   | 2:E:2252:GLY:CA   | 2.85                     | 0.47              |
| 2:B:1707:HIS:CG   | 2:B:1708:GLU:N    | 2.83                     | 0.46              |
| 2:B:1733:TRP:CD1  | 2:B:1771:THR:O    | 2.68                     | 0.46              |
| 2:B:1840:TYR:OH   | 2:B:2005:PHE:HD2  | 1.98                     | 0.46              |
| 2:B:2184:VAL:CG2  | 2:B:2219:LYS:O    | 2.60                     | 0.46              |
| 1:D:208:VAL:O     | 1:D:213:ILE:HD12  | 2.15                     | 0.46              |
| 2:E:1999:LEU:HD12 | 2:E:2000:SER:O    | 2.15                     | 0.46              |
| 2:E:2056:ARG:O    | 2:E:2060:LEU:N    | 2.42                     | 0.46              |
| 2:E:2260:HIS:HE1  | 2:E:2273:GLU:OE2  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:108:ILE:H     | 1:A:108:ILE:HD12  | 1.80                     | 0.46              |
| 2:B:2032:ILE:HD11 | 2:B:2047:GLN:HE22 | 1.80                     | 0.46              |
| 2:B:2034:ILE:HG23 | 2:B:2040:TRP:O    | 2.15                     | 0.46              |
| 2:B:2210:MET:CE   | 2:B:2253:LEU:CB   | 2.93                     | 0.46              |
| 1:D:75:ASP:OD2    | 1:D:79:LYS:HE2    | 2.11                     | 0.46              |
| 2:E:1687:HIS:CG   | 2:E:1688:PRO:HD2  | 2.50                     | 0.46              |
| 2:E:1760:THR:C    | 2:E:1762:ASP:H    | 2.19                     | 0.46              |
| 2:B:2007:ARG:CD   | 2:B:2052:GLU:OE2  | 2.63                     | 0.46              |
| 2:B:2153:ARG:NH1  | 2:B:2153:ARG:CG   | 2.74                     | 0.46              |
| 2:E:1405:ILE:HB   | 2:E:1437:ILE:HB   | 1.98                     | 0.46              |
| 2:E:1728:ILE:HD13 | 2:E:1728:ILE:N    | 2.26                     | 0.46              |
| 2:E:1834:PHE:HD2  | 2:E:1960:GLU:CG   | 2.28                     | 0.46              |
| 1:A:292:CYS:HA    | 1:A:296:SER:OG    | 2.15                     | 0.46              |
| 2:B:1059:GLU:N    | 2:B:1059:GLU:OE1  | 2.48                     | 0.46              |
| 2:B:1570:TRP:C    | 2:B:1571:GLU:HG3  | 2.36                     | 0.46              |
| 2:B:1679:GLU:HB3  | 2:B:1704:GLU:C    | 2.36                     | 0.46              |
| 1:D:327:ILE:CB    | 1:D:328:TYR:HD1   | 2.13                     | 0.46              |
| 2:E:1370:ARG:CG   | 2:E:1370:ARG:HH11 | 2.28                     | 0.46              |
| 2:E:1730:ASN:N    | 2:E:1730:ASN:OD1  | 2.49                     | 0.46              |
| 2:E:2044:THR:H    | 2:E:2047:GLN:CD   | 2.18                     | 0.46              |
| 2:E:2047:GLN:O    | 2:E:2051:ILE:N    | 2.48                     | 0.46              |
| 2:E:965:LYS:HB3   | 2:E:966:PRO:HD2   | 1.98                     | 0.46              |
| 2:B:1324:GLY:CA   | 2:B:1325:SER:OG   | 2.64                     | 0.46              |
| 2:B:2227:VAL:CG1  | 2:B:2239:SER:CB   | 2.94                     | 0.46              |
| 2:B:2247:LEU:CD1  | 2:B:2248:PRO:CD   | 2.91                     | 0.46              |
| 1:D:354:ARG:HB2   | 1:D:355:PRO:CD    | 2.45                     | 0.46              |
| 2:E:1378:LYS:HE3  | 2:E:1623:PHE:CE2  | 2.50                     | 0.46              |
| 2:E:1733:TRP:CZ2  | 2:E:1767:TYR:CD2  | 3.04                     | 0.46              |
| 2:B:1104:ILE:HG22 | 2:B:1107:LEU:HD13 | 1.97                     | 0.46              |
| 2:B:1465:ARG:HG3  | 2:B:1465:ARG:HH11 | 1.81                     | 0.46              |
| 2:B:2198:ASP:CG   | 2:B:2199:VAL:N    | 2.68                     | 0.46              |
| 2:B:929:LEU:HA    | 2:B:933:GLU:OE1   | 2.16                     | 0.46              |
| 2:E:1679:GLU:HB3  | 2:E:1704:GLU:O    | 2.16                     | 0.46              |
| 2:E:1895:HIS:CD2  | 2:E:1982:THR:C    | 2.89                     | 0.46              |
| 2:E:2159:ASN:HD21 | 2:E:2198:ASP:HA   | 1.81                     | 0.46              |
| 2:B:1286:TRP:CE2  | 2:B:1302:LEU:HD11 | 2.50                     | 0.46              |
| 2:B:2163:TYR:CE1  | 2:B:2164:LEU:CD2  | 2.99                     | 0.46              |
| 2:B:936:GLU:O     | 2:B:940:ILE:HD13  | 2.15                     | 0.46              |
| 2:E:1104:ILE:HG22 | 2:E:1107:LEU:HD13 | 1.97                     | 0.46              |
| 2:E:1565:THR:O    | 2:E:1820:ARG:CZ   | 2.64                     | 0.46              |
| 2:E:2182:VAL:CG1  | 2:E:2338:GLN:HB2  | 2.46                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1137:PRO:HD2  | 2:B:1140:ASN:O    | 2.14                     | 0.46              |
| 2:B:1156:HIS:ND1  | 2:B:1157:PRO:HD2  | 2.31                     | 0.46              |
| 2:B:1991:ILE:HD11 | 2:B:2008:LEU:HD11 | 1.98                     | 0.46              |
| 2:B:2265:GLU:HG3  | 2:B:2294:PHE:CG   | 2.50                     | 0.46              |
| 2:B:2367:ASN:OD1  | 2:B:2370:GLY:CA   | 2.64                     | 0.46              |
| 2:E:1763:ASN:N    | 2:E:1763:ASN:HD22 | 2.13                     | 0.46              |
| 2:E:2081:ASP:CG   | 2:E:2082:ILE:HG23 | 2.37                     | 0.46              |
| 2:E:2354:GLY:O    | 2:E:2355:ASN:HB2  | 2.16                     | 0.46              |
| 2:B:1188:ALA:O    | 2:B:1191:PRO:CG   | 2.64                     | 0.46              |
| 2:B:1611:SER:N    | 2:B:1612:PRO:CD   | 2.79                     | 0.46              |
| 2:B:2081:ASP:CG   | 2:B:2082:ILE:HG23 | 2.36                     | 0.46              |
| 2:B:2209:GLY:HA2  | 2:B:2220:GLU:O    | 2.16                     | 0.46              |
| 2:E:1542:TYR:CE2  | 2:E:1546:VAL:HG21 | 2.51                     | 0.46              |
| 2:E:1961:ASN:OD1  | 2:E:2079:ILE:CD1  | 2.63                     | 0.46              |
| 1:A:103:VAL:HG22  | 1:A:104:SER:N     | 2.30                     | 0.46              |
| 1:A:327:ILE:HG21  | 1:A:328:TYR:CE2   | 2.51                     | 0.46              |
| 2:B:2208:TYR:N    | 2:B:2223:THR:O    | 2.40                     | 0.46              |
| 2:B:2282:ALA:HA   | 2:B:2286:ARG:HG2  | 1.98                     | 0.46              |
| 2:E:1425:PHE:CD1  | 2:E:1425:PHE:N    | 2.84                     | 0.46              |
| 2:E:1887:GLY:CA   | 2:E:1992:TYR:CD2  | 2.98                     | 0.46              |
| 2:E:2014:ALA:N    | 2:E:2059:ILE:HD11 | 2.31                     | 0.46              |
| 2:E:2211:SER:HA   | 2:E:2219:LYS:HA   | 1.97                     | 0.46              |
| 2:E:2212:ALA:HB3  | 2:E:2218:VAL:HB   | 1.97                     | 0.46              |
| 2:E:936:GLU:O     | 2:E:940:ILE:HD13  | 2.16                     | 0.46              |
| 2:B:1121:ILE:HD13 | 2:B:1239:THR:CG2  | 2.46                     | 0.45              |
| 2:B:1121:ILE:HD13 | 2:B:1239:THR:HG21 | 1.96                     | 0.45              |
| 2:B:1177:ASP:O    | 2:B:1181:GLU:HB2  | 2.16                     | 0.45              |
| 2:E:1597:GLY:CA   | 2:E:1599:SER:N    | 2.78                     | 0.45              |
| 1:A:280:SER:CB    | 1:A:313:TYR:CE1   | 2.98                     | 0.45              |
| 1:A:86:GLY:O      | 1:A:90:GLU:N      | 2.43                     | 0.45              |
| 2:B:1976:ASP:OD1  | 2:B:1980:LYS:HD2  | 2.16                     | 0.45              |
| 2:B:1996:LEU:HD21 | 2:B:2001:SER:HA   | 1.99                     | 0.45              |
| 2:B:2041:PRO:CG   | 2:B:2043:PHE:CD1  | 2.99                     | 0.45              |
| 2:B:2178:GLU:C    | 2:B:2217:LYS:HZ3  | 2.18                     | 0.45              |
| 2:B:2308:THR:HG23 | 2:B:2333:PHE:C    | 2.19                     | 0.45              |
| 1:D:84:ARG:CG     | 1:D:84:ARG:HH11   | 2.27                     | 0.45              |
| 2:E:2002:TYR:C    | 2:E:2002:TYR:CD1  | 2.89                     | 0.45              |
| 2:B:1727:LEU:C    | 2:B:1728:ILE:HG12 | 2.36                     | 0.45              |
| 2:B:2070:ASN:O    | 2:B:2071:ILE:HG23 | 2.16                     | 0.45              |
| 2:B:2182:VAL:HA   | 2:B:2338:GLN:O    | 2.16                     | 0.45              |
| 2:B:2176:PHE:CA   | 2:B:2338:GLN:NE2  | 2.73                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2339:LEU:HD12 | 2:B:2340:LEU:CA   | 2.41                     | 0.45              |
| 2:E:1459:ALA:O    | 2:E:1463:THR:HG23 | 2.17                     | 0.45              |
| 2:E:1999:LEU:CD1  | 2:E:2004:ALA:HB2  | 2.45                     | 0.45              |
| 2:E:2277:HIS:ND1  | 2:E:2281:PHE:HD2  | 2.07                     | 0.45              |
| 2:E:2264:GLU:C    | 2:E:2294:PHE:CD1  | 2.89                     | 0.45              |
| 2:B:1238:LEU:O    | 2:B:1239:THR:HG22 | 2.16                     | 0.45              |
| 2:B:957:TYR:HD2   | 2:B:991:THR:HG21  | 1.80                     | 0.45              |
| 2:B:1090:ILE:HD11 | 2:B:1104:ILE:HD11 | 1.99                     | 0.45              |
| 2:B:1707:HIS:NE2  | 2:B:1708:GLU:OE1  | 2.50                     | 0.45              |
| 2:B:1843:LEU:HD21 | 2:B:1851:PHE:HE2  | 1.82                     | 0.45              |
| 2:B:2247:LEU:HD23 | 2:B:2374:PHE:HB2  | 1.99                     | 0.45              |
| 1:D:72:ASP:OD2    | 1:D:75:ASP:HB2    | 2.17                     | 0.45              |
| 2:E:2047:GLN:HA   | 2:E:2050:THR:HB   | 1.97                     | 0.45              |
| 2:E:2061:THR:CG2  | 2:E:2062:GLU:N    | 2.79                     | 0.45              |
| 1:A:354:ARG:CB    | 1:A:355:PRO:HD3   | 2.44                     | 0.45              |
| 2:B:1097:HIS:CE1  | 2:B:1098:VAL:O    | 2.70                     | 0.45              |
| 2:B:1844:PHE:CD1  | 2:B:1844:PHE:N    | 2.84                     | 0.45              |
| 2:B:1977:VAL:CG1  | 2:B:1978:VAL:N    | 2.78                     | 0.45              |
| 2:B:2208:TYR:CG   | 2:B:2253:LEU:CD1  | 3.00                     | 0.45              |
| 2:B:2208:TYR:OH   | 2:B:2244:ILE:CG2  | 2.65                     | 0.45              |
| 2:B:2286:ARG:HD3  | 2:B:2312:TYR:CD1  | 2.52                     | 0.45              |
| 2:B:2177:VAL:N    | 2:B:2338:GLN:HE22 | 2.13                     | 0.45              |
| 2:E:1059:GLU:OE1  | 2:E:1059:GLU:N    | 2.49                     | 0.45              |
| 2:E:2070:ASN:O    | 2:E:2071:ILE:HG23 | 2.16                     | 0.45              |
| 2:B:2210:MET:SD   | 2:B:2222:LYS:HD2  | 2.47                     | 0.45              |
| 2:B:2215:HIS:HB3  | 2:B:2218:VAL:CG2  | 2.46                     | 0.45              |
| 2:B:2386:MET:H    | 2:B:2386:MET:HG3  | 1.63                     | 0.45              |
| 2:B:1104:ILE:CG2  | 2:B:1107:LEU:CD1  | 2.95                     | 0.45              |
| 2:B:1472:ASN:HB3  | 2:B:2325:LEU:O    | 2.17                     | 0.45              |
| 2:B:1886:THR:HG1  | 2:B:1888:HIS:CE1  | 2.31                     | 0.45              |
| 2:B:2081:ASP:OD1  | 2:B:2082:ILE:HG23 | 2.16                     | 0.45              |
| 2:B:2208:TYR:CZ   | 2:B:2244:ILE:HG21 | 2.52                     | 0.45              |
| 2:B:2260:HIS:NE2  | 2:B:2273:GLU:OE2  | 2.50                     | 0.45              |
| 2:B:2343:ASP:CB   | 2:B:2344:ARG:NH2  | 2.79                     | 0.45              |
| 1:D:103:VAL:HG22  | 1:D:104:SER:N     | 2.31                     | 0.45              |
| 2:E:1881:THR:O    | 2:E:1889:LEU:HD12 | 2.16                     | 0.45              |
| 2:E:1987:VAL:HB   | 2:E:1989:PHE:HE1  | 1.81                     | 0.45              |
| 2:E:2223:THR:HG21 | 2:E:2350:ILE:HG12 | 1.99                     | 0.45              |
| 2:B:2159:ASN:HD21 | 2:B:2198:ASP:HA   | 1.77                     | 0.45              |
| 2:B:2192:LYS:HA   | 2:B:2195:GLU:HG3  | 1.99                     | 0.45              |
| 1:D:108:ILE:CD1   | 1:D:108:ILE:H     | 2.30                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1763:ASN:N    | 2:E:1763:ASN:ND2  | 2.61                     | 0.45              |
| 2:E:1826:TYR:O    | 2:E:1826:TYR:CG   | 2.70                     | 0.45              |
| 2:E:1837:SER:O    | 2:E:1840:TYR:HB2  | 2.17                     | 0.45              |
| 2:E:2183:TYR:CE1  | 2:E:2289:ILE:HD13 | 2.52                     | 0.45              |
| 1:A:263:LYS:HD2   | 1:A:263:LYS:HA    | 1.60                     | 0.45              |
| 2:B:2185:LEU:HA   | 2:B:2186:PRO:HD3  | 1.57                     | 0.45              |
| 2:B:2192:LYS:C    | 2:B:2195:GLU:HB2  | 2.35                     | 0.45              |
| 2:B:2278:SER:HG   | 2:B:2316:GLU:HG3  | 1.80                     | 0.45              |
| 2:E:1156:HIS:ND1  | 2:E:1157:PRO:HD2  | 2.32                     | 0.45              |
| 2:E:2081:ASP:OD1  | 2:E:2082:ILE:HG23 | 2.17                     | 0.45              |
| 1:A:343:ASN:HD22  | 1:A:343:ASN:HA    | 1.64                     | 0.44              |
| 2:B:2264:GLU:HG2  | 2:B:2265:GLU:O    | 2.16                     | 0.44              |
| 2:E:1195:PHE:CD1  | 2:E:1217:ARG:HD2  | 2.52                     | 0.44              |
| 2:E:1684:GLU:CD   | 2:E:1702:THR:OG1  | 2.52                     | 0.44              |
| 2:E:1996:LEU:CD2  | 2:E:2001:SER:HA   | 2.47                     | 0.44              |
| 2:E:2037:TYR:CE1  | 2:E:2038:HIS:CD2  | 3.01                     | 0.44              |
| 2:E:2089:LYS:HA   | 2:E:2090:ALA:HA   | 1.66                     | 0.44              |
| 1:A:224:LEU:C     | 1:A:224:LEU:HD23  | 2.37                     | 0.44              |
| 2:B:2240:ASN:O    | 2:B:2241:ILE:C    | 2.56                     | 0.44              |
| 2:B:2354:GLY:O    | 2:B:2355:ASN:HB2  | 2.17                     | 0.44              |
| 2:E:1093:LYS:HD3  | 2:E:1094:ASP:HA   | 2.00                     | 0.44              |
| 2:E:1370:ARG:CG   | 2:E:1370:ARG:NH1  | 2.79                     | 0.44              |
| 2:E:1710:GLU:HA   | 2:E:1727:LEU:O    | 2.17                     | 0.44              |
| 2:E:2039:LEU:CA   | 2:E:2040:TRP:CD1  | 3.00                     | 0.44              |
| 2:B:1999:LEU:HD21 | 2:B:2003:THR:CB   | 2.48                     | 0.44              |
| 2:B:2210:MET:HE1  | 2:B:2253:LEU:N    | 2.31                     | 0.44              |
| 2:B:2305:TYR:HB3  | 2:B:2334:SER:CB   | 2.47                     | 0.44              |
| 2:E:958:LEU:HA    | 2:E:1081:TYR:CD2  | 2.52                     | 0.44              |
| 2:B:2277:HIS:CE1  | 2:B:2288:CYS:O    | 2.70                     | 0.44              |
| 2:E:1347:ARG:HD3  | 2:E:1445:THR:O    | 2.17                     | 0.44              |
| 2:E:1825:ILE:HG22 | 2:E:1825:ILE:O    | 2.16                     | 0.44              |
| 2:E:2003:THR:O    | 2:E:2007:ARG:N    | 2.50                     | 0.44              |
| 2:E:2227:VAL:HG12 | 2:E:2239:SER:OG   | 2.14                     | 0.44              |
| 2:B:2043:PHE:CZ   | 2:B:2051:ILE:CD1  | 2.78                     | 0.44              |
| 2:B:2178:GLU:O    | 2:B:2217:LYS:HG2  | 2.17                     | 0.44              |
| 2:B:2277:HIS:ND1  | 2:B:2307:LEU:HD23 | 2.32                     | 0.44              |
| 2:B:2284:LYS:CE   | 2:B:2285:LYS:HA   | 2.47                     | 0.44              |
| 2:E:1347:ARG:NH1  | 2:E:1445:THR:O    | 2.38                     | 0.44              |
| 2:E:1763:ASN:CA   | 2:E:1766:MET:HE1  | 2.46                     | 0.44              |
| 2:E:2190:LEU:O    | 2:E:2190:LEU:HG   | 2.17                     | 0.44              |
| 2:B:2048:TRP:CE3  | 2:B:2048:TRP:HA   | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2232:HIS:HB2  | 2:B:2235:SER:O    | 2.17                     | 0.44              |
| 2:B:2262:GLN:HG2  | 2:B:2293:ILE:O    | 2.18                     | 0.44              |
| 1:D:263:LYS:HD2   | 1:D:263:LYS:HA    | 1.80                     | 0.44              |
| 2:E:1362:LYS:O    | 2:E:1366:ARG:HG3  | 2.17                     | 0.44              |
| 2:E:1431:HIS:C    | 2:E:1433:ASP:N    | 2.71                     | 0.44              |
| 2:E:1558:GLU:HG3  | 2:E:1558:GLU:O    | 2.18                     | 0.44              |
| 2:E:2046:GLU:O    | 2:E:2049:ILE:HG23 | 2.04                     | 0.44              |
| 2:E:2174:ASP:CG   | 2:E:2175:ASP:H    | 2.14                     | 0.44              |
| 2:E:2248:PRO:C    | 2:E:2249:ASP:OD1  | 2.56                     | 0.44              |
| 2:E:2357:TRP:H    | 2:E:2387:HIS:HE1  | 1.64                     | 0.44              |
| 2:B:1343:PHE:HB3  | 2:B:1444:ILE:CD1  | 2.48                     | 0.44              |
| 2:B:2163:TYR:CE1  | 2:B:2164:LEU:HD23 | 2.53                     | 0.44              |
| 2:B:2183:TYR:CD1  | 2:B:2219:LYS:CD   | 2.90                     | 0.44              |
| 2:E:2191:LYS:HE2  | 2:E:2195:GLU:OE2  | 2.17                     | 0.44              |
| 2:E:2202:GLN:HE22 | 2:E:2235:SER:N    | 2.10                     | 0.44              |
| 1:A:109:ASP:O     | 1:A:109:ASP:OD1   | 2.35                     | 0.44              |
| 2:B:1887:GLY:HA2  | 2:B:1992:TYR:CD2  | 2.44                     | 0.44              |
| 2:B:2301:SER:C    | 2:B:2302:LEU:HD12 | 2.39                     | 0.44              |
| 2:B:965:LYS:HB3   | 2:B:966:PRO:HD2   | 1.98                     | 0.44              |
| 2:E:1104:ILE:CG2  | 2:E:1107:LEU:CD1  | 2.96                     | 0.44              |
| 2:E:2043:PHE:HD2  | 2:E:2051:ILE:CG1  | 2.21                     | 0.44              |
| 1:A:48:HIS:CG     | 1:A:53:SER:HG     | 2.32                     | 0.44              |
| 2:B:2067:TYR:CD1  | 2:B:2067:TYR:N    | 2.86                     | 0.44              |
| 2:E:1090:ILE:HD11 | 2:E:1104:ILE:HD11 | 1.99                     | 0.44              |
| 2:E:1431:HIS:O    | 2:E:1433:ASP:N    | 2.51                     | 0.44              |
| 2:B:1784:TYR:CD1  | 2:B:1806:MET:HG3  | 2.53                     | 0.43              |
| 2:B:2011:LEU:HB3  | 2:B:2040:TRP:CZ3  | 2.53                     | 0.43              |
| 2:B:2040:TRP:CD1  | 2:B:2040:TRP:N    | 2.86                     | 0.43              |
| 2:B:2044:THR:CG2  | 2:B:2047:GLN:CD   | 2.80                     | 0.43              |
| 2:E:1093:LYS:HD3  | 2:E:1093:LYS:HA   | 1.79                     | 0.43              |
| 2:E:1059:GLU:OE2  | 2:E:1105:ARG:NH2  | 2.51                     | 0.43              |
| 2:E:1624:LEU:HD21 | 2:E:1633:PHE:HB3  | 2.00                     | 0.43              |
| 2:E:1992:TYR:O    | 2:E:1993:ASP:HB2  | 2.18                     | 0.43              |
| 2:E:2029:ASP:OD2  | 2:E:2032:ILE:CD1  | 2.65                     | 0.43              |
| 2:E:908:ASP:OD1   | 2:E:994:TYR:OH    | 2.25                     | 0.43              |
| 2:B:1305:SER:O    | 2:B:1309:ILE:HG13 | 2.18                     | 0.43              |
| 2:B:1354:GLU:N    | 2:B:1355:PRO:CD   | 2.81                     | 0.43              |
| 2:B:2024:MET:SD   | 2:B:2157:ILE:HG21 | 2.58                     | 0.43              |
| 2:E:2066:LYS:CB   | 2:E:2067:TYR:CD1  | 2.97                     | 0.43              |
| 2:E:2242:PRO:CB   | 2:E:2374:PHE:CE2  | 3.01                     | 0.43              |
| 2:B:1842:GLU:O    | 2:B:1844:PHE:N    | 2.51                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1894:ILE:HD13 | 2:B:1894:ILE:HA   | 1.86                     | 0.43              |
| 2:B:2045:ASP:O    | 2:B:2048:TRP:HB2  | 2.18                     | 0.43              |
| 2:B:2179:GLU:HA   | 2:B:2217:LYS:HE2  | 2.01                     | 0.43              |
| 2:B:953:ARG:CG    | 2:B:953:ARG:HH11  | 2.31                     | 0.43              |
| 1:D:20:TYR:CE2    | 1:D:106:PRO:HG2   | 2.53                     | 0.43              |
| 2:E:1292:ARG:NH1  | 2:E:1293:THR:HG22 | 2.33                     | 0.43              |
| 2:E:2083:ILE:CG2  | 2:E:2084:LEU:H    | 2.32                     | 0.43              |
| 2:E:2223:THR:HG21 | 2:E:2350:ILE:CG1  | 2.48                     | 0.43              |
| 2:B:2054:GLN:HE21 | 2:B:2054:GLN:HB3  | 1.64                     | 0.43              |
| 2:B:2017:THR:HG21 | 2:B:2062:GLU:HG3  | 1.99                     | 0.43              |
| 2:B:2020:GLU:HG3  | 2:B:2164:LEU:HD12 | 2.00                     | 0.43              |
| 2:B:2342:SER:OG   | 2:B:2344:ARG:N    | 2.37                     | 0.43              |
| 2:B:2358:ASN:CB   | 2:B:2387:HIS:HD1  | 2.18                     | 0.43              |
| 1:D:25:LYS:O      | 1:D:28:GLN:CB     | 2.66                     | 0.43              |
| 2:E:930:ASN:ND2   | 2:E:933:GLU:HB2   | 2.32                     | 0.43              |
| 2:B:1906:SER:O    | 2:B:1909:ALA:HB3  | 2.19                     | 0.43              |
| 2:B:2087:ASN:CB   | 2:B:2089:LYS:HG3  | 2.46                     | 0.43              |
| 2:B:2166:LEU:O    | 2:B:2167:LYS:C    | 2.56                     | 0.43              |
| 2:E:1354:GLU:N    | 2:E:1355:PRO:CD   | 2.81                     | 0.43              |
| 2:E:1788:GLY:O    | 2:E:1790:TRP:CD1  | 2.71                     | 0.43              |
| 2:E:2181:ASN:O    | 2:E:2338:GLN:HG3  | 2.18                     | 0.43              |
| 2:B:1853:ASP:OD1  | 2:B:1854:ASP:N    | 2.51                     | 0.43              |
| 2:B:2270:ALA:HB1  | 2:B:2324:VAL:HA   | 2.00                     | 0.43              |
| 1:D:35:ASP:O      | 1:D:107:LYS:NZ    | 2.34                     | 0.43              |
| 2:E:1784:TYR:CD1  | 2:E:1806:MET:HG3  | 2.53                     | 0.43              |
| 2:E:2063:TYR:O    | 2:E:2067:TYR:CD1  | 2.71                     | 0.43              |
| 2:E:2154:LYS:O    | 2:E:2157:ILE:HB   | 2.18                     | 0.43              |
| 2:E:953:ARG:HG3   | 2:E:953:ARG:HH11  | 1.83                     | 0.43              |
| 2:B:1542:TYR:CE2  | 2:B:1546:VAL:HG21 | 2.53                     | 0.43              |
| 2:B:1864:LYS:NZ   | 2:B:1865:THR:O    | 2.44                     | 0.43              |
| 2:B:2281:PHE:HB3  | 2:B:2286:ARG:O    | 2.19                     | 0.43              |
| 2:E:2253:LEU:HA   | 2:E:2253:LEU:HD23 | 1.90                     | 0.43              |
| 2:E:2384:ASN:HB3  | 2:E:2387:HIS:HD2  | 1.83                     | 0.43              |
| 2:B:1187:LEU:O    | 2:B:1191:PRO:CG   | 2.66                     | 0.43              |
| 2:B:2085:GLY:HA3  | 2:B:2086:GLN:HA   | 1.79                     | 0.43              |
| 2:B:2153:ARG:HH11 | 2:B:2153:ARG:HG3  | 1.82                     | 0.43              |
| 2:B:2178:GLU:HB3  | 2:B:2217:LYS:HZ2  | 1.84                     | 0.43              |
| 2:B:2231:GLY:O    | 2:B:2232:HIS:CD2  | 2.71                     | 0.43              |
| 2:B:2329:PHE:C    | 2:B:2330:GLU:HG2  | 2.39                     | 0.43              |
| 2:B:2357:TRP:CZ3  | 2:B:2382:PHE:CE1  | 3.04                     | 0.43              |
| 1:D:9:ALA:N       | 1:D:10:PRO:HD3    | 2.34                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2185:LEU:HG   | 2:B:2186:PRO:HD2  | 2.00                     | 0.43              |
| 2:E:1091:ASN:HB3  | 2:E:1093:LYS:HE2  | 2.00                     | 0.43              |
| 2:E:2318:ASN:HB3  | 2:E:2321:ILE:HD11 | 2.01                     | 0.43              |
| 2:B:1704:GLU:CG   | 2:B:1705:SER:N    | 2.81                     | 0.43              |
| 2:B:1707:HIS:CE1  | 2:B:1708:GLU:CD   | 2.92                     | 0.43              |
| 1:D:327:ILE:HG21  | 1:D:328:TYR:HE1   | 1.84                     | 0.43              |
| 2:E:1835:LEU:HB3  | 2:E:1959:THR:HB   | 2.00                     | 0.42              |
| 2:E:2065:ARG:HH11 | 2:E:2065:ARG:HB3  | 1.81                     | 0.42              |
| 2:E:2302:LEU:CD1  | 2:E:2302:LEU:N    | 2.82                     | 0.42              |
| 2:B:1051:GLU:HG3  | 2:B:1169:TYR:CE2  | 2.54                     | 0.42              |
| 2:B:1383:PHE:CE2  | 2:B:1387:VAL:HG21 | 2.54                     | 0.42              |
| 2:B:1961:ASN:HA   | 2:B:2079:ILE:CD1  | 2.49                     | 0.42              |
| 2:B:2076:GLN:OE1  | 2:B:2076:GLN:HA   | 2.19                     | 0.42              |
| 2:B:2230:LEU:CB   | 2:B:2237:GLN:HG3  | 2.47                     | 0.42              |
| 2:B:1721:ASN:HB3  | 2:E:1463:THR:HB   | 2.00                     | 0.42              |
| 2:E:2086:GLN:O    | 2:E:2088:ILE:HG12 | 2.20                     | 0.42              |
| 2:E:2155:SER:HB3  | 2:E:2383:TYR:CE2  | 2.53                     | 0.42              |
| 2:B:1847:ASP:O    | 2:B:1849:LYS:HD2  | 2.19                     | 0.42              |
| 2:B:1917:VAL:O    | 2:B:1921:VAL:HG23 | 2.19                     | 0.42              |
| 2:B:2189:LEU:HD21 | 2:B:2347:GLY:HA3  | 2.01                     | 0.42              |
| 2:E:958:LEU:HD23  | 2:E:1081:TYR:CD2  | 2.55                     | 0.42              |
| 2:E:1596:THR:O    | 2:E:1598:LEU:HB3  | 2.19                     | 0.42              |
| 2:E:1763:ASN:HD22 | 2:E:1764:VAL:N    | 2.17                     | 0.42              |
| 2:E:2061:THR:HG22 | 2:E:2062:GLU:N    | 2.34                     | 0.42              |
| 2:B:1321:MET:HA   | 2:B:1321:MET:CE   | 2.49                     | 0.42              |
| 2:B:2064:GLY:O    | 2:B:2068:ASN:HA   | 2.19                     | 0.42              |
| 2:B:2373:ASN:O    | 2:B:2374:PHE:CG   | 2.72                     | 0.42              |
| 2:E:1567:PHE:CE2  | 2:E:1820:ARG:NH1  | 2.84                     | 0.42              |
| 2:E:1837:SER:O    | 2:E:1840:TYR:CB   | 2.68                     | 0.42              |
| 2:E:2087:ASN:O    | 2:E:2088:ILE:HG12 | 2.19                     | 0.42              |
| 2:B:1097:HIS:ND1  | 2:B:1097:HIS:C    | 2.73                     | 0.42              |
| 2:B:2063:TYR:CE1  | 2:B:2081:ASP:O    | 2.73                     | 0.42              |
| 2:E:1435:LYS:HD3  | 2:E:1549:ALA:O    | 2.19                     | 0.42              |
| 2:E:2075:THR:HG22 | 2:E:2076:GLN:N    | 2.34                     | 0.42              |
| 2:E:2086:GLN:HG2  | 2:E:2086:GLN:O    | 2.19                     | 0.42              |
| 2:B:1894:ILE:HG22 | 2:B:1894:ILE:O    | 2.18                     | 0.42              |
| 2:B:1848:ILE:HD11 | 2:B:1928:GLU:O    | 2.14                     | 0.42              |
| 2:B:957:TYR:O     | 2:B:961:GLN:N     | 2.48                     | 0.42              |
| 2:E:1234:VAL:HG11 | 2:E:1239:THR:CG2  | 2.49                     | 0.42              |
| 2:E:1596:THR:O    | 2:E:1598:LEU:CB   | 2.67                     | 0.42              |
| 2:E:1604:ARG:HH22 | 2:E:1822:GLY:C    | 2.23                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1674:ASP:OD1  | 2:E:1674:ASP:N    | 2.52                     | 0.42              |
| 2:E:1717:LEU:HB2  | 2:E:1786:ALA:HB3  | 2.02                     | 0.42              |
| 2:E:1964:PRO:HG3  | 2:E:2013:ARG:CZ   | 2.49                     | 0.42              |
| 2:E:2020:GLU:HG3  | 2:E:2164:LEU:HD12 | 2.02                     | 0.42              |
| 2:E:2259:ILE:HD11 | 2:E:2293:ILE:HD11 | 2.01                     | 0.42              |
| 2:B:1015:PRO:HD2  | 2:B:1165:LEU:CD2  | 2.36                     | 0.42              |
| 2:B:1661:ILE:HG12 | 2:B:1805:ILE:CD1  | 2.50                     | 0.42              |
| 2:B:2035:LYS:O    | 2:B:2037:TYR:N    | 2.53                     | 0.42              |
| 1:D:23:ASN:ND2    | 1:D:23:ASN:N      | 2.68                     | 0.42              |
| 2:B:1800:ASN:OD1  | 2:B:1803:ARG:NH1  | 2.53                     | 0.42              |
| 2:B:1854:ASP:CA   | 2:B:1857:VAL:HG23 | 2.49                     | 0.42              |
| 2:B:1944:LEU:O    | 2:B:1948:MET:HG2  | 2.20                     | 0.42              |
| 2:B:2208:TYR:HB3  | 2:B:2253:LEU:CG   | 2.45                     | 0.42              |
| 2:B:2232:HIS:HE1  | 2:B:2237:GLN:HE21 | 1.68                     | 0.42              |
| 1:D:3:THR:HG22    | 1:D:5:PRO:HD3     | 2.01                     | 0.42              |
| 2:B:2063:TYR:HE1  | 2:B:2081:ASP:O    | 2.02                     | 0.42              |
| 2:B:969:ILE:HG22  | 2:B:982:TYR:CD2   | 2.55                     | 0.42              |
| 2:E:1484:TRP:CH2  | 2:E:1495:PHE:HB2  | 2.55                     | 0.42              |
| 2:E:2388:ARG:HD3  | 2:E:2389:PRO:HD2  | 2.02                     | 0.42              |
| 1:A:214:PHE:CD1   | 1:A:220:TYR:HA    | 2.55                     | 0.42              |
| 2:B:1904:ARG:HD3  | 2:B:1907:GLN:OE1  | 2.20                     | 0.42              |
| 2:B:2229:GLN:NE2  | 2:B:2357:TRP:CE3  | 2.88                     | 0.42              |
| 1:D:282:ILE:HD13  | 2:E:1604:ARG:HD2  | 2.02                     | 0.42              |
| 2:E:2021:SER:O    | 2:E:2024:MET:HB3  | 2.20                     | 0.42              |
| 2:B:1893:ILE:CG2  | 2:B:1978:VAL:HG13 | 2.50                     | 0.41              |
| 2:B:2010:LEU:HA   | 2:B:2010:LEU:HD12 | 1.82                     | 0.41              |
| 2:B:2230:LEU:HA   | 2:B:2230:LEU:HD12 | 1.84                     | 0.41              |
| 1:D:48:HIS:HE1    | 1:D:56:TYR:OH     | 2.03                     | 0.41              |
| 2:E:1370:ARG:HG2  | 2:E:1370:ARG:NH1  | 2.36                     | 0.41              |
| 2:E:1611:SER:N    | 2:E:1612:PRO:CD   | 2.83                     | 0.41              |
| 2:E:1712:SER:OG   | 2:E:1713:LYS:N    | 2.51                     | 0.41              |
| 2:E:2078:GLU:O    | 2:E:2079:ILE:HD13 | 2.20                     | 0.41              |
| 2:B:1717:LEU:HB2  | 2:B:1786:ALA:HB3  | 2.02                     | 0.41              |
| 2:B:2082:ILE:O    | 2:B:2083:ILE:CG1  | 2.69                     | 0.41              |
| 2:B:2309:ASP:O    | 2:B:2312:TYR:N    | 2.53                     | 0.41              |
| 2:E:1849:LYS:C    | 2:E:1850:LEU:HD23 | 2.40                     | 0.41              |
| 2:B:1674:ASP:OD1  | 2:B:1674:ASP:N    | 2.53                     | 0.41              |
| 2:B:1843:LEU:HD11 | 2:B:1884:PRO:HG3  | 1.94                     | 0.41              |
| 2:B:1853:ASP:CG   | 2:B:1855:THR:OG1  | 2.57                     | 0.41              |
| 2:B:1990:ASN:OD1  | 2:B:1992:TYR:N    | 2.52                     | 0.41              |
| 2:B:2183:TYR:CD1  | 2:B:2219:LYS:CB   | 3.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2309:ASP:N    | 2:B:2310:GLU:OE1  | 2.54                     | 0.41              |
| 2:B:2351:ILE:HG21 | 2:B:2379:PRO:HA   | 2.02                     | 0.41              |
| 2:E:2070:ASN:O    | 2:E:2071:ILE:CG2  | 2.69                     | 0.41              |
| 2:E:2386:MET:C    | 2:E:2388:ARG:N    | 2.74                     | 0.41              |
| 2:B:2258:TRP:N    | 2:B:2258:TRP:CD1  | 2.82                     | 0.41              |
| 2:B:2278:SER:OG   | 2:B:2312:TYR:O    | 2.38                     | 0.41              |
| 2:B:2318:ASN:ND2  | 2:B:2318:ASN:N    | 2.68                     | 0.41              |
| 1:D:84:ARG:NH1    | 1:D:84:ARG:CG     | 2.84                     | 0.41              |
| 1:D:328:TYR:CD2   | 2:E:1543:ARG:NH1  | 2.89                     | 0.41              |
| 2:E:2304:ALA:HB3  | 2:E:2339:LEU:HD23 | 1.98                     | 0.41              |
| 2:E:965:LYS:HE3   | 2:E:985:ASP:CG    | 2.41                     | 0.41              |
| 2:E:995:LEU:O     | 2:E:999:LEU:HG    | 2.21                     | 0.41              |
| 1:A:282:ILE:HD13  | 2:B:1604:ARG:HD2  | 2.03                     | 0.41              |
| 2:E:1705:SER:HB3  | 2:E:1709:TRP:CE3  | 2.55                     | 0.41              |
| 2:E:1762:ASP:CG   | 2:E:1763:ASN:H    | 2.23                     | 0.41              |
| 2:E:2084:LEU:C    | 2:E:2084:LEU:HD22 | 2.37                     | 0.41              |
| 2:E:2182:VAL:HG12 | 2:E:2338:GLN:HB3  | 2.02                     | 0.41              |
| 2:E:2280:LEU:HB2  | 2:E:2281:PHE:CD2  | 2.56                     | 0.41              |
| 2:E:986:PRO:O     | 2:E:990:ILE:HD12  | 2.20                     | 0.41              |
| 1:A:16:GLY:HA3    | 1:A:45:HIS:CE1    | 2.54                     | 0.41              |
| 2:B:1673:LEU:HA   | 2:B:1678:ILE:HB   | 2.03                     | 0.41              |
| 2:B:1686:VAL:HG12 | 2:B:1687:HIS:N    | 2.36                     | 0.41              |
| 2:B:1963:LEU:HD23 | 2:B:1963:LEU:HA   | 1.95                     | 0.41              |
| 2:B:1435:LYS:NZ   | 2:E:1351:VAL:HG13 | 2.36                     | 0.41              |
| 2:E:1624:LEU:CD2  | 2:E:1625:VAL:N    | 2.83                     | 0.41              |
| 2:E:1996:LEU:HD21 | 2:E:2001:SER:HA   | 2.02                     | 0.41              |
| 2:B:1137:PRO:O    | 2:B:1140:ASN:C    | 2.59                     | 0.41              |
| 2:B:1889:LEU:HD23 | 2:B:1891:LEU:HB2  | 2.03                     | 0.41              |
| 2:B:2307:LEU:HD12 | 2:B:2308:THR:O    | 2.21                     | 0.41              |
| 2:B:2386:MET:CE   | 2:B:2387:HIS:CD2  | 3.03                     | 0.41              |
| 2:E:1763:ASN:O    | 2:E:1766:MET:HE3  | 2.18                     | 0.41              |
| 2:E:2014:ALA:CA   | 2:E:2059:ILE:CD1  | 2.72                     | 0.41              |
| 2:E:2157:ILE:HD12 | 2:E:2157:ILE:HA   | 1.74                     | 0.41              |
| 2:E:2189:LEU:HD21 | 2:E:2347:GLY:C    | 2.41                     | 0.41              |
| 1:A:89:PHE:C      | 1:A:89:PHE:CD1    | 2.94                     | 0.41              |
| 2:B:1405:ILE:HB   | 2:B:1437:ILE:HB   | 2.02                     | 0.41              |
| 2:B:2017:THR:HG23 | 2:B:2062:GLU:HG3  | 2.03                     | 0.41              |
| 2:E:1279:VAL:HG12 | 2:E:1280:SER:N    | 2.36                     | 0.41              |
| 2:E:1826:TYR:CA   | 2:E:1827:GLN:HB2  | 2.50                     | 0.41              |
| 2:E:1865:THR:OG1  | 2:E:1869:ASN:HB2  | 2.20                     | 0.41              |
| 2:E:2030:PRO:CG   | 2:E:2153:ARG:NE   | 2.77                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:2267:LYS:C    | 2:E:2305:TYR:OH   | 2.58                     | 0.41              |
| 1:A:7:THR:HG21    | 1:A:70:GLN:OE1    | 2.21                     | 0.41              |
| 2:B:1080:ASP:O    | 2:B:1084:ALA:HB2  | 2.21                     | 0.41              |
| 2:B:1150:LYS:HD2  | 2:B:1292:ARG:HH22 | 1.84                     | 0.41              |
| 2:E:2028:SER:C    | 2:E:2030:PRO:HD3  | 2.37                     | 0.41              |
| 2:B:2157:ILE:C    | 2:B:2160:THR:OG1  | 2.44                     | 0.41              |
| 2:B:2386:MET:HE1  | 2:B:2387:HIS:CD2  | 2.56                     | 0.41              |
| 2:E:1826:TYR:CA   | 2:E:1827:GLN:CB   | 2.99                     | 0.41              |
| 2:E:2067:TYR:CD1  | 2:E:2067:TYR:N    | 2.89                     | 0.41              |
| 2:B:2247:LEU:HD23 | 2:B:2374:PHE:CB   | 2.51                     | 0.40              |
| 2:B:995:LEU:O     | 2:B:999:LEU:HG    | 2.21                     | 0.40              |
| 1:D:16:GLY:HA3    | 1:D:45:HIS:CE1    | 2.56                     | 0.40              |
| 2:E:1466:GLN:O    | 2:E:1469:ILE:CA   | 2.69                     | 0.40              |
| 2:E:1766:MET:C    | 2:E:1767:TYR:CD1  | 2.94                     | 0.40              |
| 2:E:2057:ASP:O    | 2:E:2061:THR:HB   | 2.22                     | 0.40              |
| 2:E:2230:LEU:HD23 | 2:E:2237:GLN:NE2  | 2.36                     | 0.40              |
| 2:B:2070:ASN:O    | 2:B:2071:ILE:CG2  | 2.69                     | 0.40              |
| 2:B:2082:ILE:O    | 2:B:2083:ILE:HG13 | 2.21                     | 0.40              |
| 2:B:2089:LYS:HA   | 2:B:2090:ALA:HA   | 1.74                     | 0.40              |
| 2:B:2191:LYS:O    | 2:B:2195:GLU:CG   | 2.44                     | 0.40              |
| 2:B:2184:VAL:O    | 2:B:2221:ILE:CG1  | 2.69                     | 0.40              |
| 2:E:1168:ILE:O    | 2:E:1168:ILE:HG13 | 2.21                     | 0.40              |
| 2:E:1889:LEU:HA   | 2:E:1889:LEU:HD12 | 1.86                     | 0.40              |
| 2:E:1995:TRP:HZ3  | 2:E:2007:ARG:HG2  | 1.58                     | 0.40              |
| 2:E:946:ASN:HB3   | 2:E:949:ASP:OD2   | 2.21                     | 0.40              |
| 2:B:1107:LEU:HD23 | 2:B:1109:PHE:CZ   | 2.56                     | 0.40              |
| 2:B:1153:GLU:O    | 2:B:1159:ARG:HD3  | 2.21                     | 0.40              |
| 2:B:1168:ILE:HG13 | 2:B:1168:ILE:O    | 2.21                     | 0.40              |
| 2:B:1324:GLY:HA2  | 2:B:1325:SER:HB3  | 2.03                     | 0.40              |
| 2:B:2207:ILE:CG1  | 2:B:2257:GLY:O    | 2.70                     | 0.40              |
| 1:D:107:LYS:HA    | 1:D:108:ILE:HA    | 1.87                     | 0.40              |
| 2:E:1477:PHE:C    | 2:E:1477:PHE:CD1  | 2.94                     | 0.40              |
| 2:E:1624:LEU:HD21 | 2:E:1633:PHE:CD1  | 2.57                     | 0.40              |
| 2:E:1894:ILE:O    | 2:E:1894:ILE:HG22 | 2.21                     | 0.40              |
| 2:E:2029:ASP:OD2  | 2:E:2032:ILE:HD11 | 2.21                     | 0.40              |
| 2:E:930:ASN:ND2   | 2:E:933:GLU:CD    | 2.74                     | 0.40              |
| 2:E:969:ILE:HG22  | 2:E:982:TYR:CD2   | 2.57                     | 0.40              |
| 2:B:1187:LEU:HA   | 2:B:1187:LEU:HD23 | 1.85                     | 0.40              |
| 2:B:2153:ARG:NH1  | 2:B:2153:ARG:HG2  | 2.36                     | 0.40              |
| 1:D:141:ASP:OD1   | 1:D:141:ASP:C     | 2.60                     | 0.40              |
| 2:E:1383:PHE:CE2  | 2:E:1387:VAL:HG21 | 2.55                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1727:LEU:C    | 2:E:1728:ILE:CD1  | 2.71                     | 0.40              |
| 2:E:2203:VAL:HG22 | 2:E:2357:TRP:CZ3  | 2.57                     | 0.40              |
| 2:B:1762:ASP:OD1  | 2:B:1764:VAL:HG22 | 2.22                     | 0.40              |
| 2:B:1893:ILE:HG23 | 2:B:1978:VAL:HG13 | 2.02                     | 0.40              |
| 2:B:2060:LEU:O    | 2:B:2063:TYR:CA   | 2.70                     | 0.40              |
| 2:B:2162:LEU:HD23 | 2:B:2165:ARG:HE   | 1.86                     | 0.40              |
| 2:B:2224:VAL:CA   | 2:B:2349:PHE:CE1  | 3.04                     | 0.40              |
| 2:E:2177:VAL:O    | 2:E:2177:VAL:HG23 | 2.21                     | 0.40              |

All (1) 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) |
|------------------|-------------------------|--------------------------|-------------------|
| 2:B:1685:THR:OG1 | 2:E:2309:ASP:OD2[4_545] | 1.96                     | 0.24              |

## 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     | 319/355 (90%)   | 310 (97%)  | 9 (3%)  | 0        | 100         | 100 |
| 1   | D     | 307/355 (86%)   | 298 (97%)  | 8 (3%)  | 1 (0%)   | 41          | 73  |
| 2   | B     | 1384/1531 (90%) | 1345 (97%) | 38 (3%) | 1 (0%)   | 51          | 83  |
| 2   | E     | 1406/1531 (92%) | 1360 (97%) | 42 (3%) | 4 (0%)   | 41          | 73  |
| All | All   | 3416/3772 (91%) | 3313 (97%) | 97 (3%) | 6 (0%)   | 47          | 79  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 2088 | ILE  |
| 2   | E     | 2286 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 2088 | ILE  |
| 1   | D     | 29   | PRO  |
| 2   | E     | 1726 | GLY  |
| 2   | E     | 2215 | HIS  |

### 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     | 293/326 (90%)   | 284 (97%)  | 9 (3%)    | 40          | 70 |
| 1   | D     | 289/326 (89%)   | 269 (93%)  | 20 (7%)   | 15          | 45 |
| 2   | B     | 1256/1373 (92%) | 1108 (88%) | 148 (12%) | 5           | 21 |
| 2   | E     | 1278/1373 (93%) | 1151 (90%) | 127 (10%) | 8           | 29 |
| All | All   | 3116/3398 (92%) | 2812 (90%) | 304 (10%) | 8           | 29 |

All (304) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 93  | VAL  |
| 1   | A     | 95  | ASN  |
| 1   | A     | 107 | LYS  |
| 1   | A     | 110 | GLU  |
| 1   | A     | 132 | LYS  |
| 1   | A     | 215 | LYS  |
| 1   | A     | 263 | LYS  |
| 1   | A     | 299 | LYS  |
| 1   | A     | 343 | ASN  |
| 2   | B     | 883 | SER  |
| 2   | B     | 885 | VAL  |
| 2   | B     | 908 | ASP  |
| 2   | B     | 929 | LEU  |
| 2   | B     | 952 | ASN  |
| 2   | B     | 953 | ARG  |
| 2   | B     | 956 | LYS  |
| 2   | B     | 960 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 969  | ILE  |
| 2   | B     | 987  | LEU  |
| 2   | B     | 1018 | SER  |
| 2   | B     | 1019 | GLU  |
| 2   | B     | 1042 | SER  |
| 2   | B     | 1074 | VAL  |
| 2   | B     | 1096 | SER  |
| 2   | B     | 1097 | HIS  |
| 2   | B     | 1105 | ARG  |
| 2   | B     | 1139 | ASN  |
| 2   | B     | 1165 | LEU  |
| 2   | B     | 1177 | ASP  |
| 2   | B     | 1213 | MET  |
| 2   | B     | 1218 | GLN  |
| 2   | B     | 1237 | SER  |
| 2   | B     | 1239 | THR  |
| 2   | B     | 1273 | GLN  |
| 2   | B     | 1282 | ASP  |
| 2   | B     | 1305 | SER  |
| 2   | B     | 1321 | MET  |
| 2   | B     | 1348 | GLU  |
| 2   | B     | 1377 | SER  |
| 2   | B     | 1406 | LEU  |
| 2   | B     | 1430 | THR  |
| 2   | B     | 1465 | ARG  |
| 2   | B     | 1466 | GLN  |
| 2   | B     | 1467 | GLU  |
| 2   | B     | 1478 | GLU  |
| 2   | B     | 1510 | ILE  |
| 2   | B     | 1512 | ARG  |
| 2   | B     | 1521 | ARG  |
| 2   | B     | 1569 | SER  |
| 2   | B     | 1571 | GLU  |
| 2   | B     | 1573 | LEU  |
| 2   | B     | 1594 | GLN  |
| 2   | B     | 1595 | ARG  |
| 2   | B     | 1598 | LEU  |
| 2   | B     | 1679 | GLU  |
| 2   | B     | 1691 | SER  |
| 2   | B     | 1703 | MET  |
| 2   | B     | 1706 | VAL  |
| 2   | B     | 1710 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1713 | LYS  |
| 2   | B     | 1727 | LEU  |
| 2   | B     | 1739 | ARG  |
| 2   | B     | 1742 | ASP  |
| 2   | B     | 1750 | ARG  |
| 2   | B     | 1802 | MET  |
| 2   | B     | 1804 | THR  |
| 2   | B     | 1805 | ILE  |
| 2   | B     | 1817 | GLU  |
| 2   | B     | 1821 | LYS  |
| 2   | B     | 1842 | GLU  |
| 2   | B     | 1845 | ASN  |
| 2   | B     | 1848 | ILE  |
| 2   | B     | 1849 | LYS  |
| 2   | B     | 1858 | TYR  |
| 2   | B     | 1859 | ARG  |
| 2   | B     | 1864 | LYS  |
| 2   | B     | 1867 | GLU  |
| 2   | B     | 1869 | ASN  |
| 2   | B     | 1882 | LEU  |
| 2   | B     | 1896 | THR  |
| 2   | B     | 1897 | SER  |
| 2   | B     | 1904 | ARG  |
| 2   | B     | 1926 | LYS  |
| 2   | B     | 1927 | GLU  |
| 2   | B     | 1932 | GLN  |
| 2   | B     | 1962 | ARG  |
| 2   | B     | 1972 | ASP  |
| 2   | B     | 1979 | MET  |
| 2   | B     | 1980 | LYS  |
| 2   | B     | 1988 | LEU  |
| 2   | B     | 1997 | ASP  |
| 2   | B     | 2001 | SER  |
| 2   | B     | 2002 | TYR  |
| 2   | B     | 2006 | SER  |
| 2   | B     | 2016 | LYS  |
| 2   | B     | 2018 | ASN  |
| 2   | B     | 2026 | LEU  |
| 2   | B     | 2032 | ILE  |
| 2   | B     | 2038 | HIS  |
| 2   | B     | 2039 | LEU  |
| 2   | B     | 2044 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 2045 | ASP  |
| 2   | B     | 2047 | GLN  |
| 2   | B     | 2048 | TRP  |
| 2   | B     | 2050 | THR  |
| 2   | B     | 2053 | SER  |
| 2   | B     | 2054 | GLN  |
| 2   | B     | 2057 | ASP  |
| 2   | B     | 2153 | ARG  |
| 2   | B     | 2155 | SER  |
| 2   | B     | 2160 | THR  |
| 2   | B     | 2163 | TYR  |
| 2   | B     | 2165 | ARG  |
| 2   | B     | 2187 | LYS  |
| 2   | B     | 2199 | VAL  |
| 2   | B     | 2202 | GLN  |
| 2   | B     | 2210 | MET  |
| 2   | B     | 2222 | LYS  |
| 2   | B     | 2237 | GLN  |
| 2   | B     | 2238 | ILE  |
| 2   | B     | 2239 | SER  |
| 2   | B     | 2243 | ASP  |
| 2   | B     | 2246 | ASP  |
| 2   | B     | 2247 | LEU  |
| 2   | B     | 2250 | THR  |
| 2   | B     | 2253 | LEU  |
| 2   | B     | 2254 | GLU  |
| 2   | B     | 2256 | LEU  |
| 2   | B     | 2258 | TRP  |
| 2   | B     | 2265 | GLU  |
| 2   | B     | 2268 | PHE  |
| 2   | B     | 2277 | HIS  |
| 2   | B     | 2280 | LEU  |
| 2   | B     | 2283 | ASP  |
| 2   | B     | 2284 | LYS  |
| 2   | B     | 2286 | ARG  |
| 2   | B     | 2295 | SER  |
| 2   | B     | 2301 | SER  |
| 2   | B     | 2303 | SER  |
| 2   | B     | 2306 | ASN  |
| 2   | B     | 2307 | LEU  |
| 2   | B     | 2309 | ASP  |
| 2   | B     | 2318 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 2332 | THR  |
| 2   | B     | 2334 | SER  |
| 2   | B     | 2336 | HIS  |
| 2   | B     | 2339 | LEU  |
| 2   | B     | 2341 | LEU  |
| 2   | B     | 2343 | ASP  |
| 2   | B     | 2344 | ARG  |
| 2   | B     | 2345 | ILE  |
| 2   | B     | 2349 | PHE  |
| 2   | B     | 2362 | MET  |
| 2   | B     | 2367 | ASN  |
| 2   | B     | 2382 | PHE  |
| 2   | B     | 2384 | ASN  |
| 2   | B     | 2386 | MET  |
| 1   | D     | 21   | SER  |
| 1   | D     | 23   | ASN  |
| 1   | D     | 24   | VAL  |
| 1   | D     | 27   | ASN  |
| 1   | D     | 83   | GLU  |
| 1   | D     | 84   | ARG  |
| 1   | D     | 85   | ASP  |
| 1   | D     | 101  | MET  |
| 1   | D     | 102  | MET  |
| 1   | D     | 104  | SER  |
| 1   | D     | 108  | ILE  |
| 1   | D     | 109  | ASP  |
| 1   | D     | 113  | THR  |
| 1   | D     | 215  | LYS  |
| 1   | D     | 216  | ASN  |
| 1   | D     | 299  | LYS  |
| 1   | D     | 300  | ASN  |
| 1   | D     | 326  | LEU  |
| 1   | D     | 327  | ILE  |
| 1   | D     | 355  | PRO  |
| 2   | E     | 885  | VAL  |
| 2   | E     | 908  | ASP  |
| 2   | E     | 909  | THR  |
| 2   | E     | 930  | ASN  |
| 2   | E     | 942  | GLU  |
| 2   | E     | 945  | ASP  |
| 2   | E     | 953  | ARG  |
| 2   | E     | 956  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 969  | ILE  |
| 2   | E     | 987  | LEU  |
| 2   | E     | 1093 | LYS  |
| 2   | E     | 1095 | MET  |
| 2   | E     | 1096 | SER  |
| 2   | E     | 1165 | LEU  |
| 2   | E     | 1166 | ASP  |
| 2   | E     | 1189 | GLU  |
| 2   | E     | 1213 | MET  |
| 2   | E     | 1272 | ARG  |
| 2   | E     | 1273 | GLN  |
| 2   | E     | 1275 | MET  |
| 2   | E     | 1281 | ASN  |
| 2   | E     | 1282 | ASP  |
| 2   | E     | 1292 | ARG  |
| 2   | E     | 1321 | MET  |
| 2   | E     | 1348 | GLU  |
| 2   | E     | 1370 | ARG  |
| 2   | E     | 1377 | SER  |
| 2   | E     | 1382 | ARG  |
| 2   | E     | 1426 | ARG  |
| 2   | E     | 1432 | GLU  |
| 2   | E     | 1465 | ARG  |
| 2   | E     | 1477 | PHE  |
| 2   | E     | 1510 | ILE  |
| 2   | E     | 1512 | ARG  |
| 2   | E     | 1530 | SER  |
| 2   | E     | 1568 | ASN  |
| 2   | E     | 1574 | PHE  |
| 2   | E     | 1596 | THR  |
| 2   | E     | 1598 | LEU  |
| 2   | E     | 1600 | GLN  |
| 2   | E     | 1624 | LEU  |
| 2   | E     | 1679 | GLU  |
| 2   | E     | 1691 | SER  |
| 2   | E     | 1693 | LYS  |
| 2   | E     | 1694 | MET  |
| 2   | E     | 1702 | THR  |
| 2   | E     | 1704 | GLU  |
| 2   | E     | 1707 | HIS  |
| 2   | E     | 1710 | GLU  |
| 2   | E     | 1713 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 1715 | SER  |
| 2   | E     | 1722 | ASP  |
| 2   | E     | 1723 | SER  |
| 2   | E     | 1727 | LEU  |
| 2   | E     | 1729 | THR  |
| 2   | E     | 1730 | ASN  |
| 2   | E     | 1732 | MET  |
| 2   | E     | 1761 | THR  |
| 2   | E     | 1763 | ASN  |
| 2   | E     | 1765 | SER  |
| 2   | E     | 1767 | TYR  |
| 2   | E     | 1769 | SER  |
| 2   | E     | 1817 | GLU  |
| 2   | E     | 1821 | LYS  |
| 2   | E     | 1842 | GLU  |
| 2   | E     | 1859 | ARG  |
| 2   | E     | 1862 | VAL  |
| 2   | E     | 1882 | LEU  |
| 2   | E     | 1897 | SER  |
| 2   | E     | 1927 | GLU  |
| 2   | E     | 1962 | ARG  |
| 2   | E     | 1972 | ASP  |
| 2   | E     | 1985 | GLN  |
| 2   | E     | 2001 | SER  |
| 2   | E     | 2002 | TYR  |
| 2   | E     | 2007 | ARG  |
| 2   | E     | 2018 | ASN  |
| 2   | E     | 2020 | GLU  |
| 2   | E     | 2021 | SER  |
| 2   | E     | 2033 | THR  |
| 2   | E     | 2034 | ILE  |
| 2   | E     | 2035 | LYS  |
| 2   | E     | 2047 | GLN  |
| 2   | E     | 2048 | TRP  |
| 2   | E     | 2059 | ILE  |
| 2   | E     | 2061 | THR  |
| 2   | E     | 2065 | ARG  |
| 2   | E     | 2077 | THR  |
| 2   | E     | 2080 | LYS  |
| 2   | E     | 2084 | LEU  |
| 2   | E     | 2086 | GLN  |
| 2   | E     | 2087 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 2095 | ARG  |
| 2   | E     | 2163 | TYR  |
| 2   | E     | 2172 | SER  |
| 2   | E     | 2178 | GLU  |
| 2   | E     | 2179 | GLU  |
| 2   | E     | 2182 | VAL  |
| 2   | E     | 2183 | TYR  |
| 2   | E     | 2189 | LEU  |
| 2   | E     | 2197 | SER  |
| 2   | E     | 2201 | ILE  |
| 2   | E     | 2214 | ASP  |
| 2   | E     | 2215 | HIS  |
| 2   | E     | 2222 | LYS  |
| 2   | E     | 2249 | ASP  |
| 2   | E     | 2264 | GLU  |
| 2   | E     | 2266 | LEU  |
| 2   | E     | 2267 | LYS  |
| 2   | E     | 2277 | HIS  |
| 2   | E     | 2296 | THR  |
| 2   | E     | 2326 | SER  |
| 2   | E     | 2327 | GLU  |
| 2   | E     | 2332 | THR  |
| 2   | E     | 2339 | LEU  |
| 2   | E     | 2340 | LEU  |
| 2   | E     | 2360 | THR  |
| 2   | E     | 2362 | MET  |
| 2   | E     | 2367 | ASN  |
| 2   | E     | 2368 | GLN  |
| 2   | E     | 2371 | ASP  |
| 2   | E     | 2375 | LYS  |
| 2   | E     | 2380 | LEU  |
| 2   | E     | 2384 | ASN  |
| 2   | E     | 2388 | ARG  |
| 2   | E     | 2393 | LEU  |
| 2   | E     | 2396 | SER  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 136  | GLN  |
| 1   | A     | 343  | ASN  |
| 2   | B     | 1030 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1087 | ASN  |
| 2   | B     | 1139 | ASN  |
| 2   | B     | 1470 | GLN  |
| 2   | B     | 1471 | GLN  |
| 2   | B     | 1863 | HIS  |
| 2   | B     | 1869 | ASN  |
| 2   | B     | 1895 | HIS  |
| 2   | B     | 1985 | GLN  |
| 2   | B     | 2038 | HIS  |
| 2   | B     | 2054 | GLN  |
| 2   | B     | 2087 | ASN  |
| 2   | B     | 2202 | GLN  |
| 2   | B     | 2237 | GLN  |
| 2   | B     | 2318 | ASN  |
| 2   | B     | 2338 | GLN  |
| 2   | B     | 2368 | GLN  |
| 2   | B     | 2373 | ASN  |
| 2   | B     | 2384 | ASN  |
| 2   | B     | 2387 | HIS  |
| 1   | D     | 48   | HIS  |
| 1   | D     | 219  | ASN  |
| 1   | D     | 244  | HIS  |
| 2   | E     | 930  | ASN  |
| 2   | E     | 1087 | ASN  |
| 2   | E     | 1091 | ASN  |
| 2   | E     | 1097 | HIS  |
| 2   | E     | 1140 | ASN  |
| 2   | E     | 1218 | GLN  |
| 2   | E     | 1281 | ASN  |
| 2   | E     | 1470 | GLN  |
| 2   | E     | 1540 | ASN  |
| 2   | E     | 1600 | GLN  |
| 2   | E     | 1655 | GLN  |
| 2   | E     | 1763 | ASN  |
| 2   | E     | 1863 | HIS  |
| 2   | E     | 1985 | GLN  |
| 2   | E     | 2018 | ASN  |
| 2   | E     | 2054 | GLN  |
| 2   | E     | 2087 | ASN  |
| 2   | E     | 2159 | ASN  |
| 2   | E     | 2202 | GLN  |
| 2   | E     | 2232 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 2237 | GLN  |
| 2   | E     | 2260 | HIS  |
| 2   | E     | 2358 | ASN  |
| 2   | E     | 2373 | ASN  |
| 2   | E     | 2384 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|---------------|-----------------------|--------|
| 1   | A     | 327/355 (92%)   | -0.32  | 4 (1%) 79 61  | 40, 75, 133, 168      | 1 (0%) |
| 1   | D     | 317/355 (89%)   | -0.37  | 0 100 100     | 38, 73, 131, 170      | 0      |
| 2   | B     | 1398/1531 (91%) | -0.10  | 35 (2%) 57 34 | 38, 103, 176, 253     | 0      |
| 2   | E     | 1420/1531 (92%) | -0.15  | 26 (1%) 68 47 | 37, 90, 160, 245      | 0      |
| All | All   | 3462/3772 (91%) | -0.17  | 65 (1%) 66 46 | 37, 92, 165, 253      | 1 (0%) |

All (65) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | E     | 2096 | GLN  | 15.9 |
| 2   | E     | 2093 | VAL  | 6.8  |
| 2   | E     | 2323 | ASN  | 6.5  |
| 2   | B     | 2385 | GLU  | 5.8  |
| 2   | E     | 2321 | ILE  | 5.4  |
| 2   | B     | 2174 | ASP  | 5.3  |
| 2   | B     | 2268 | PHE  | 5.2  |
| 2   | E     | 2326 | SER  | 5.1  |
| 2   | B     | 2059 | ILE  | 5.1  |
| 2   | E     | 2325 | LEU  | 5.0  |
| 2   | B     | 2361 | PHE  | 4.7  |
| 2   | E     | 2322 | MET  | 4.5  |
| 2   | B     | 2221 | ILE  | 3.9  |
| 2   | B     | 2251 | GLU  | 3.7  |
| 2   | B     | 2322 | MET  | 3.6  |
| 2   | E     | 2059 | ILE  | 3.6  |
| 2   | E     | 2095 | ARG  | 3.5  |
| 2   | B     | 1433 | ASP  | 3.5  |
| 2   | B     | 2060 | LEU  | 3.5  |
| 2   | E     | 2361 | PHE  | 3.5  |
| 1   | A     | 329  | GLY  | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 1324 | GLY  | 3.4  |
| 2   | E     | 2081 | ASP  | 3.2  |
| 2   | E     | 1680 | SER  | 3.1  |
| 2   | E     | 2082 | ILE  | 3.1  |
| 2   | B     | 2320 | ASP  | 3.1  |
| 2   | E     | 2057 | ASP  | 3.1  |
| 2   | E     | 2324 | VAL  | 3.0  |
| 2   | B     | 2052 | GLU  | 2.9  |
| 2   | B     | 2072 | SER  | 2.9  |
| 2   | E     | 2214 | ASP  | 2.9  |
| 2   | E     | 2094 | LYS  | 2.8  |
| 2   | B     | 1292 | ARG  | 2.8  |
| 2   | E     | 2072 | SER  | 2.8  |
| 2   | E     | 2071 | ILE  | 2.7  |
| 2   | E     | 2385 | GLU  | 2.7  |
| 2   | B     | 1899 | TRP  | 2.7  |
| 2   | B     | 2275 | ALA  | 2.6  |
| 2   | E     | 2092 | SER  | 2.6  |
| 2   | B     | 2262 | GLN  | 2.5  |
| 2   | B     | 2384 | ASN  | 2.5  |
| 2   | B     | 1238 | LEU  | 2.4  |
| 2   | B     | 2288 | CYS  | 2.4  |
| 2   | B     | 2179 | GLU  | 2.4  |
| 2   | B     | 2091 | PRO  | 2.4  |
| 1   | A     | 110  | GLU  | 2.3  |
| 2   | E     | 1323 | SER  | 2.3  |
| 2   | E     | 2382 | PHE  | 2.3  |
| 2   | B     | 2087 | ASN  | 2.3  |
| 2   | E     | 1681 | VAL  | 2.3  |
| 2   | E     | 2320 | ASP  | 2.2  |
| 2   | B     | 1894 | ILE  | 2.2  |
| 2   | B     | 2289 | ILE  | 2.2  |
| 1   | A     | 40   | HIS  | 2.2  |
| 2   | B     | 2183 | TYR  | 2.2  |
| 2   | B     | 2264 | GLU  | 2.2  |
| 2   | B     | 1674 | ASP  | 2.2  |
| 1   | A     | 169  | GLU  | 2.2  |
| 2   | B     | 2286 | ARG  | 2.1  |
| 2   | B     | 2214 | ASP  | 2.1  |
| 2   | B     | 2311 | GLY  | 2.1  |
| 2   | B     | 2333 | PHE  | 2.0  |
| 2   | B     | 2317 | GLU  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | E     | 2060 | LEU  | 2.0  |
| 2   | B     | 2210 | MET  | 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.