Full wwPDB EM Validation Report ⓘ

Mar 19, 2023 – 07:47 am GMT

PDB ID	:	7PQH
EMDB ID	:	EMD-13594
Title	:	Cryo-EM structure of Saccharomyces cerevisiae TOROID (TORC1 Organized in Inhibited Domains).
Authors	:	Felix, J.; Prouteau, M.; Bourgoint, C.; Bonadei, L.; Desfosses, A.; Gabus, C.; Sadian, Y.; Savvides, S.N.; Gutsche, I.; Loewith, R.
Deposited on	:	2021-09-17
Resolution	:	3.87 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

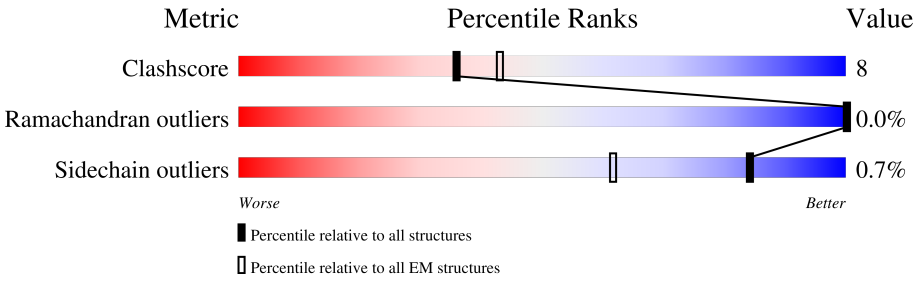
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.87 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1608	10% 60% 15% 25%
1	B	1608	9% 62% 13% 25%
1	G	1608	12% 61% 14% 25%
1	J	1608	10% 61% 14% 25%
2	C	303	26% 72% 27%
2	D	303	28% 75% 24%
2	I	303	78% 77% 22%
2	L	303	72% 78% 21%

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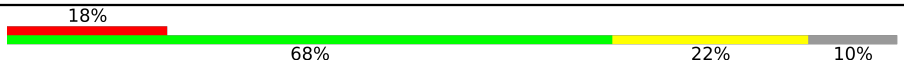
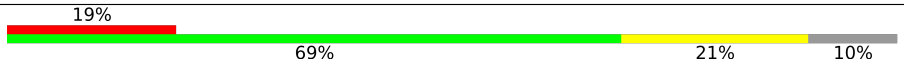
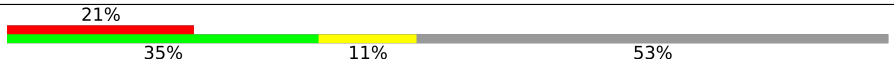
Mol	Chain	Length	Quality of chain
3	E	2474	
3	F	2474	
3	H	2474	
3	K	2474	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 102671 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Target of rapamycin complex 1 subunit KOG1,Target of rapamycin complex 1 subunit Kog1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1209	Total	C	N	O	S	0	0
			9693	6225	1638	1784	46		
1	B	1208	Total	C	N	O	S	0	0
			9686	6223	1636	1781	46		
1	G	1212	Total	C	N	O	S	0	0
			9705	6239	1639	1781	46		
1	J	1213	Total	C	N	O	S	0	0
			9711	6242	1641	1782	46		

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	300	Total	C	N	O	S	0	0
			2366	1465	430	460	11		
2	D	300	Total	C	N	O	S	0	0
			2366	1465	430	460	11		
2	I	300	Total	C	N	O	S	0	0
			2366	1465	430	460	11		
2	L	300	Total	C	N	O	S	0	0
			2366	1465	430	460	11		

- Molecule 3 is a protein called Serine/threonine-protein kinase TOR2.

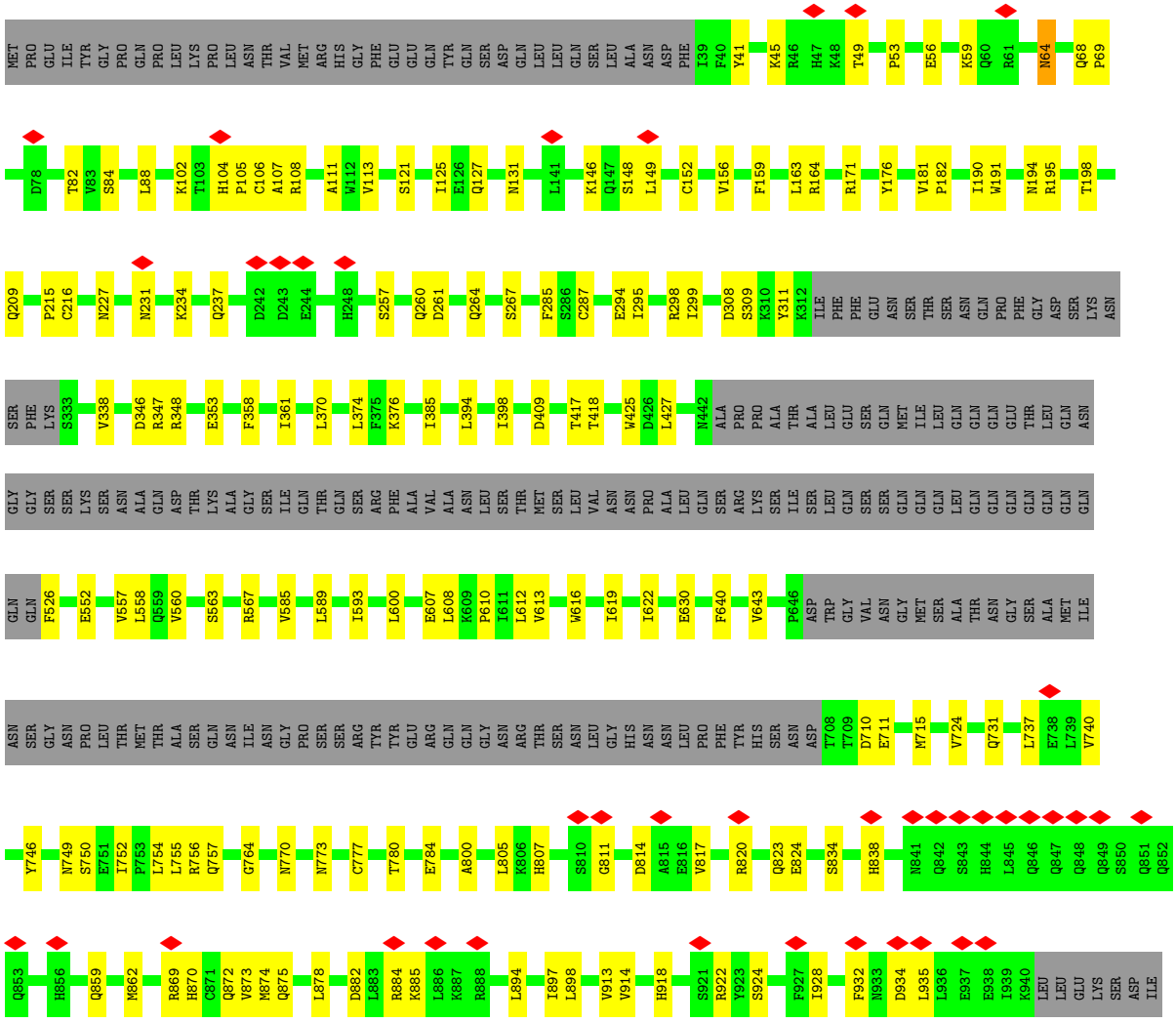
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	2238	Total	C	N	O	S	0	0
			17910	11494	3058	3275	83		
3	F	2238	Total	C	N	O	S	0	0
			17904	11491	3055	3275	83		
3	H	1157	Total	C	N	O	S	0	0
			9299	5981	1588	1684	46		
3	K	1157	Total	C	N	O	S	0	0
			9299	5981	1588	1684	46		

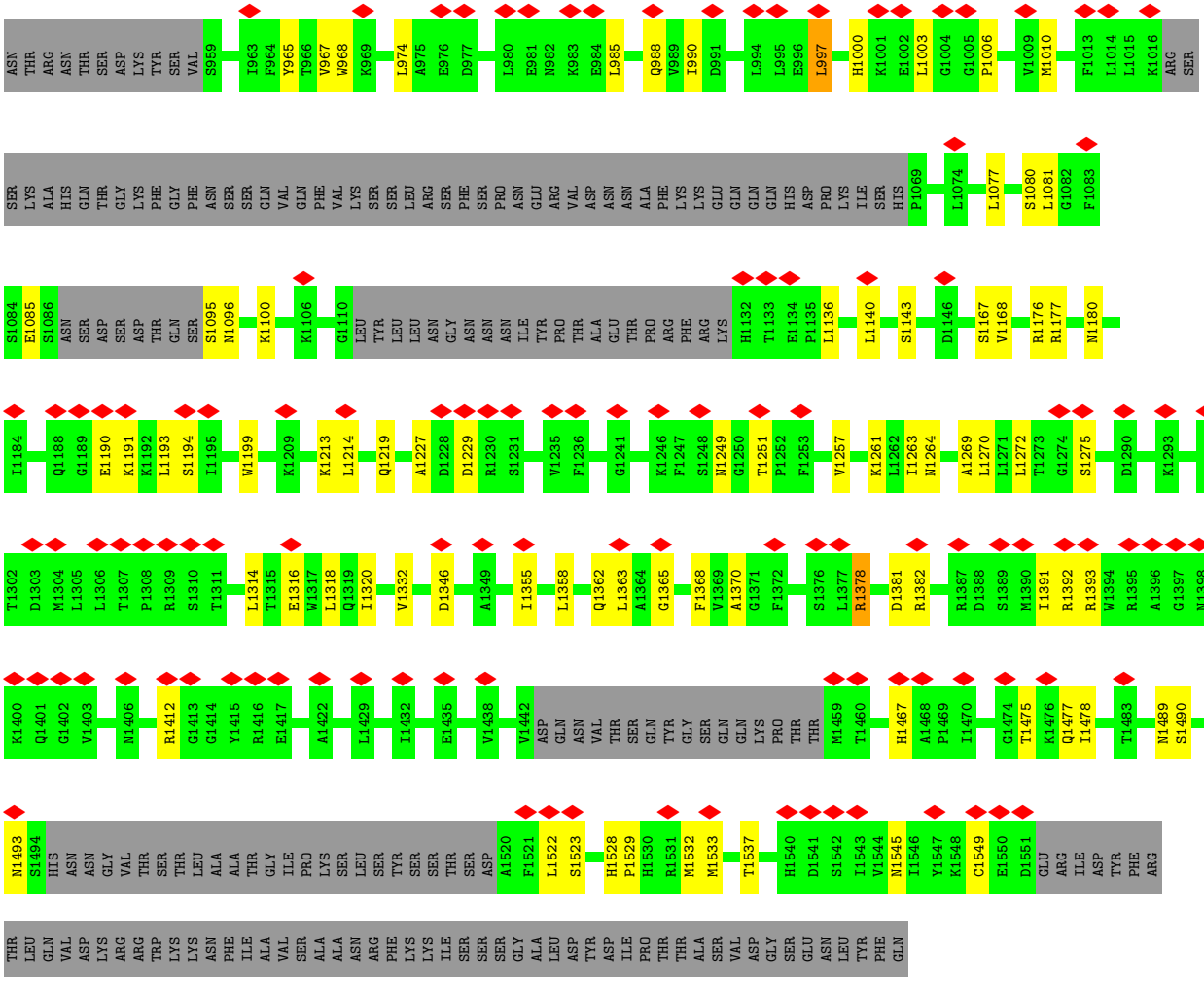
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Target of rapamycin complex 1 subunit KOG1,Target of rapamycin complex 1 subunit Kog1

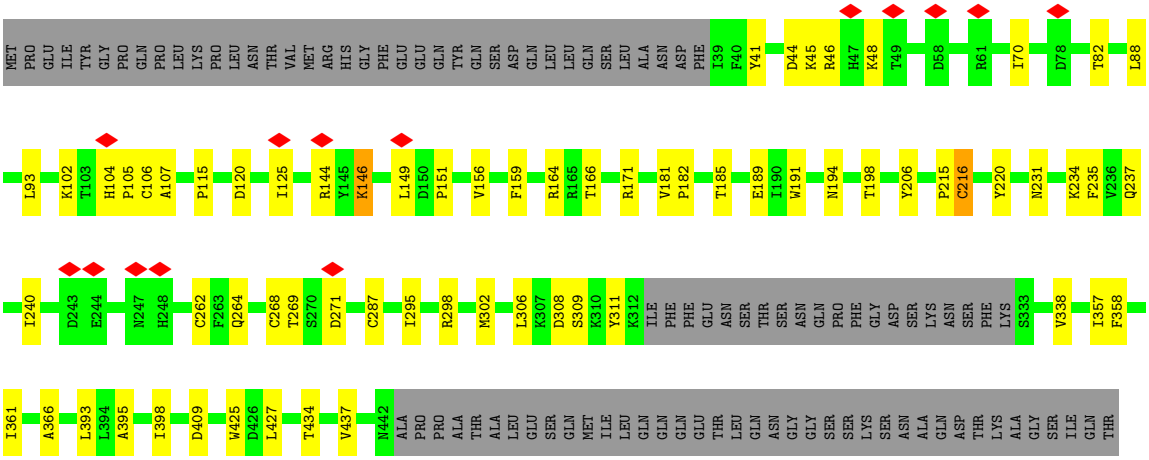
Chain A:

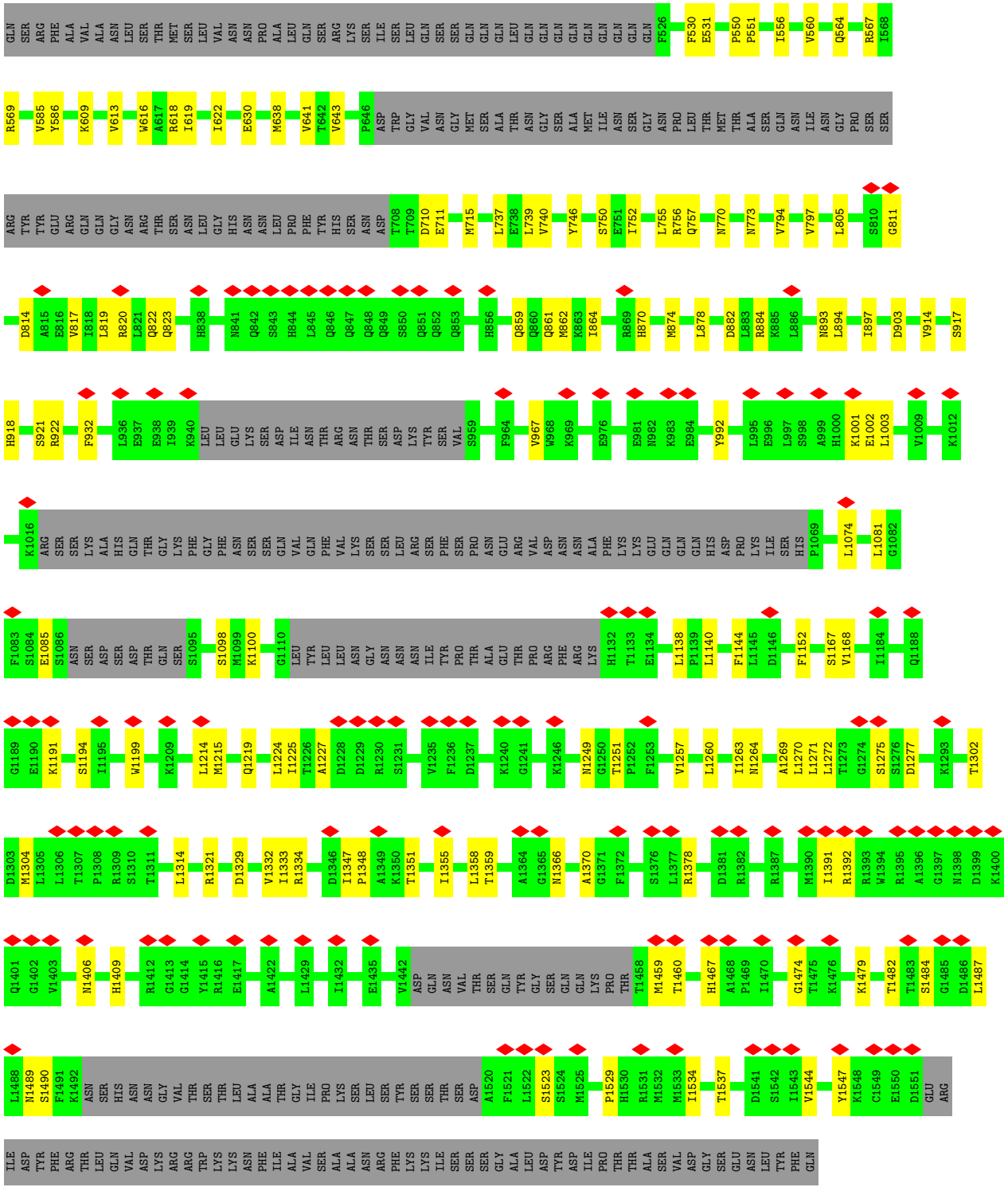




• Molecule 1: Target of rapamycin complex 1 subunit KOG1,Target of rapamycin complex 1 subunit Kog1

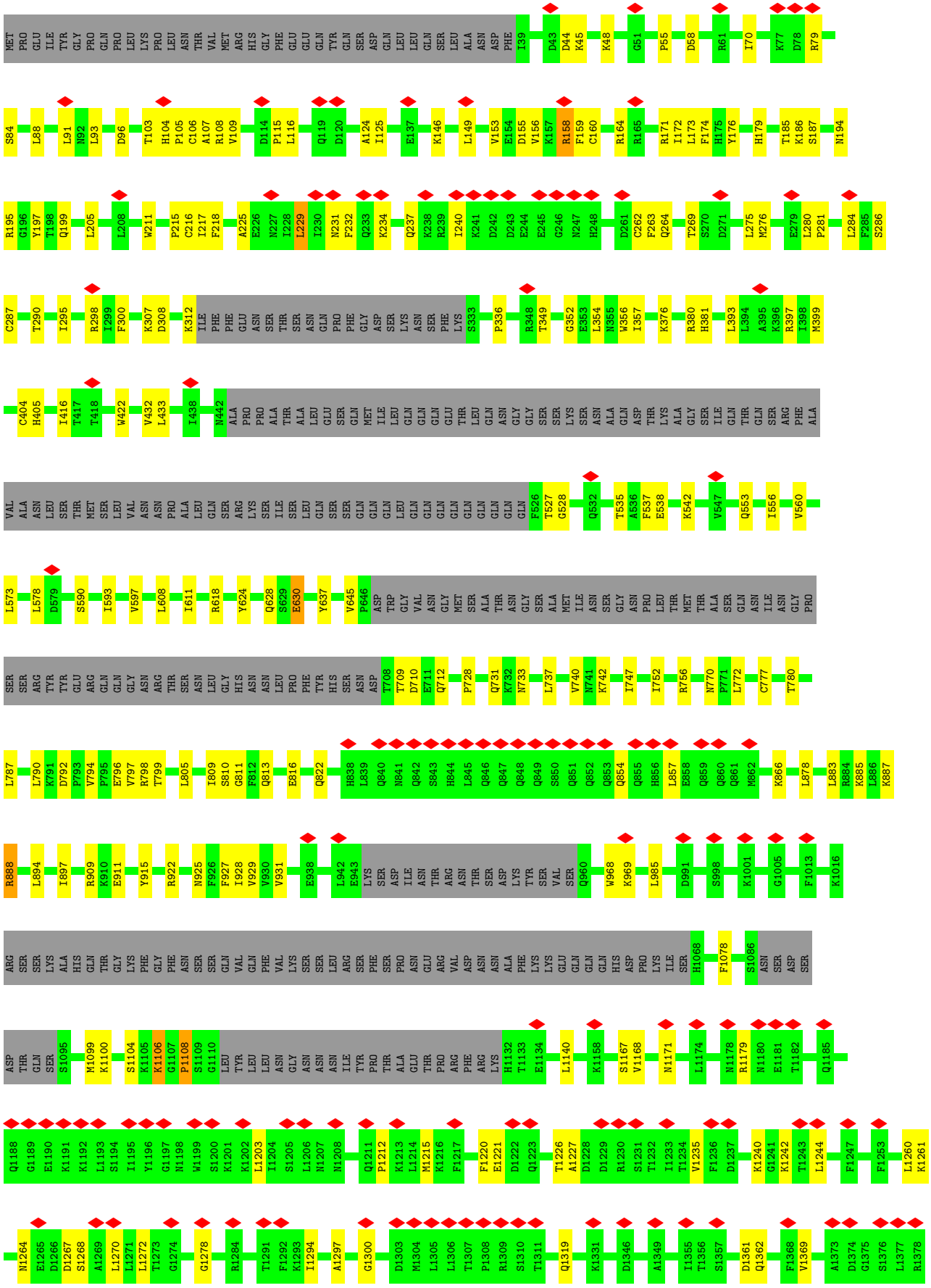
Chain B:

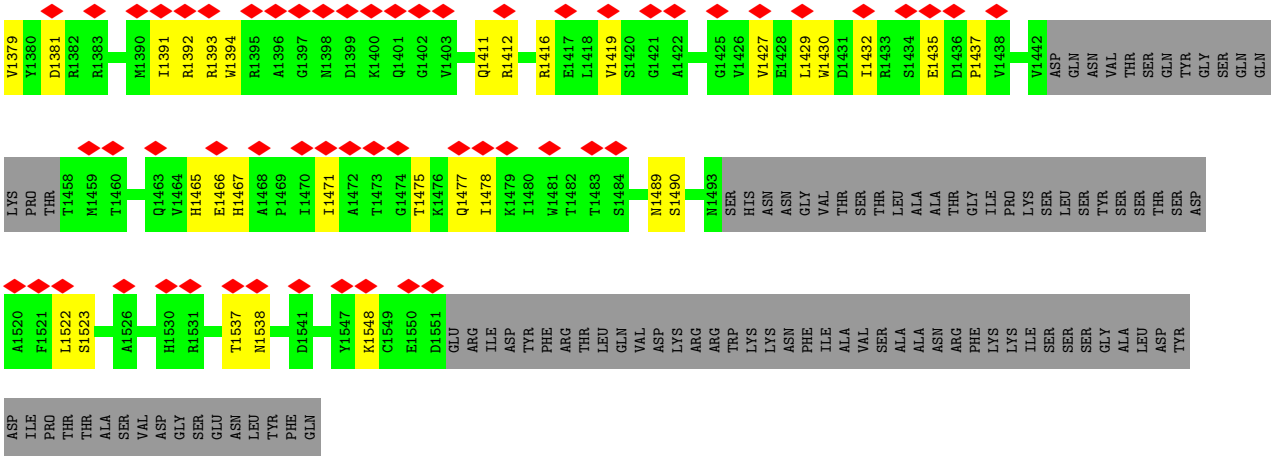




• Molecule 1: Target of rapamycin complex 1 subunit KOG1,Target of rapamycin complex 1 subunit Kog1

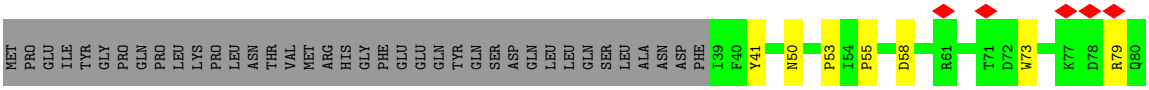
Chain G:

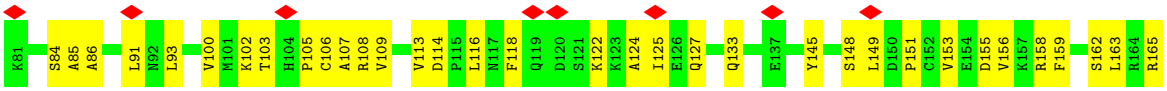


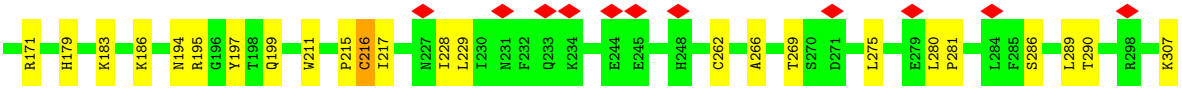


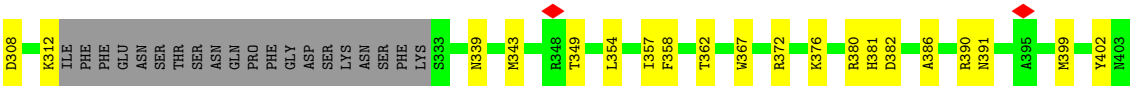
• Molecule 1: Target of rapamycin complex 1 subunit KOG1,Target of rapamycin complex 1 subunit Kog1

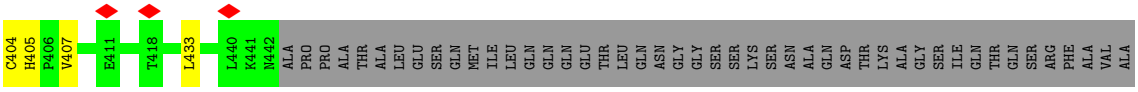
Chain J:

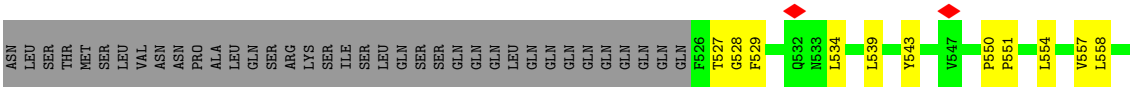


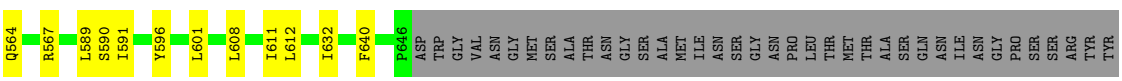


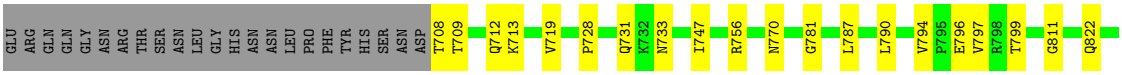


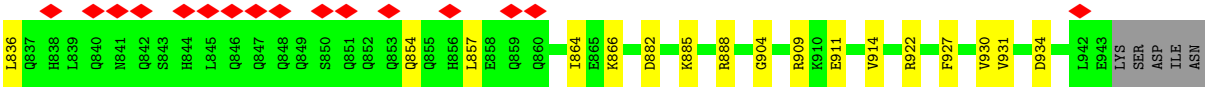


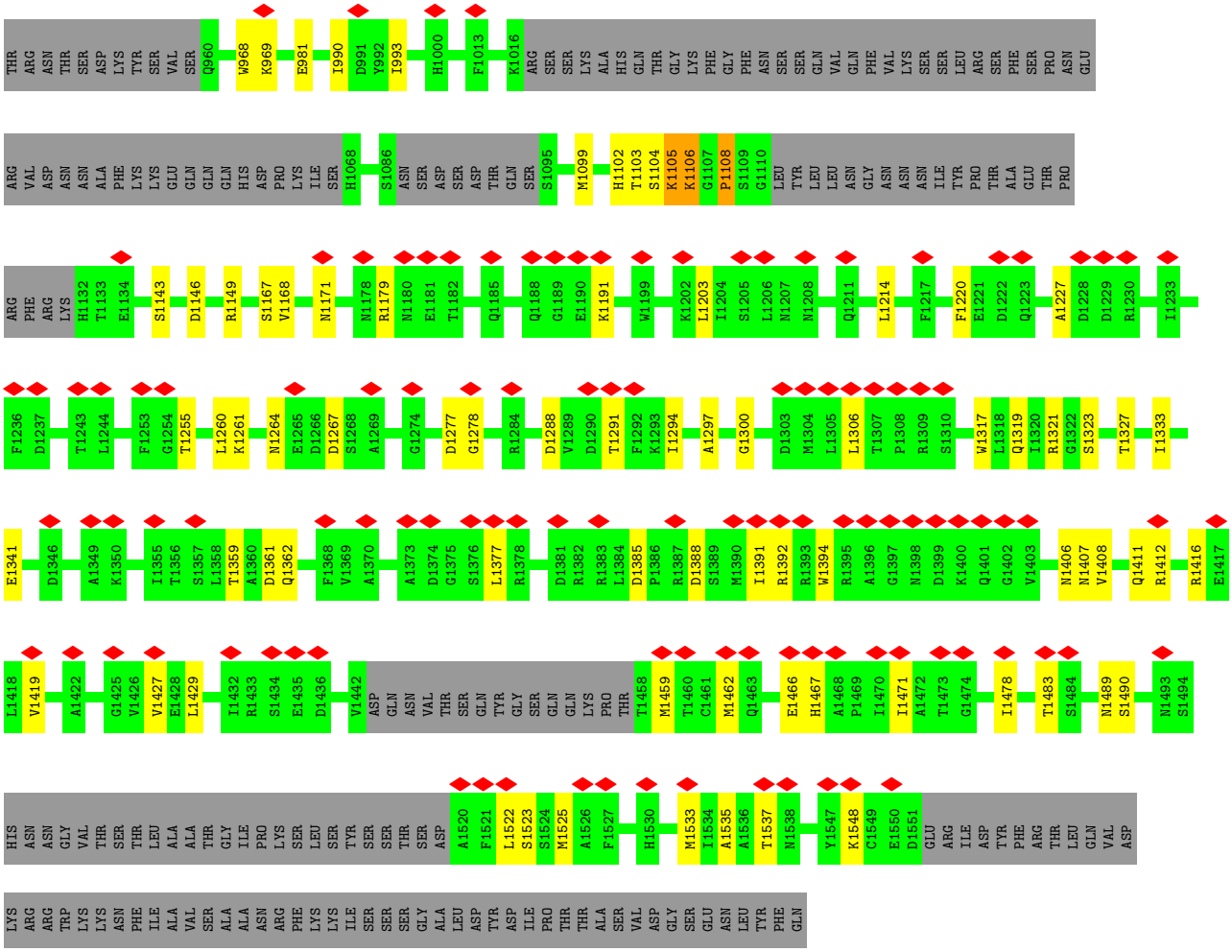






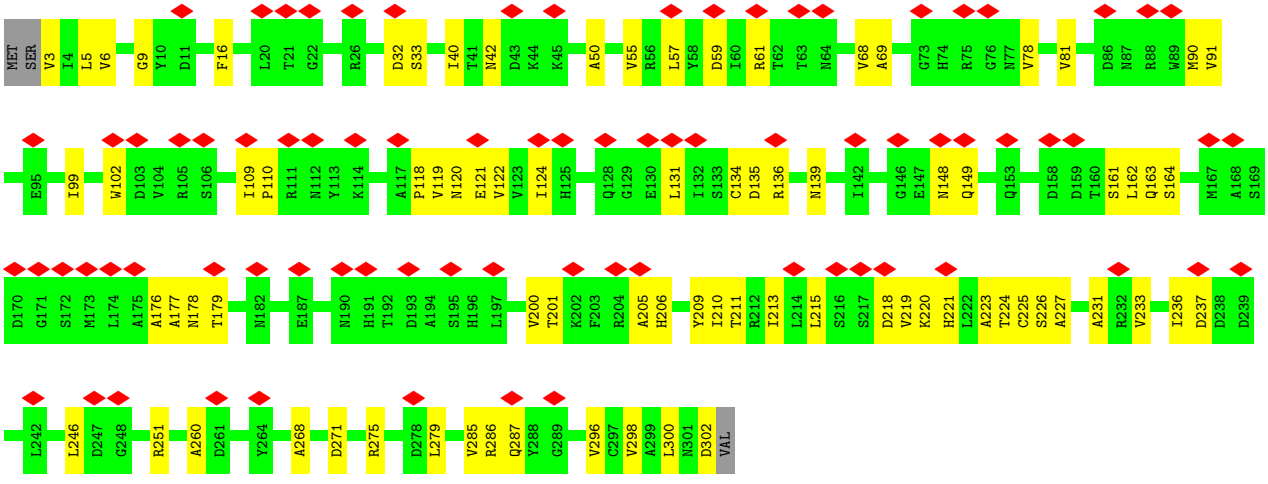






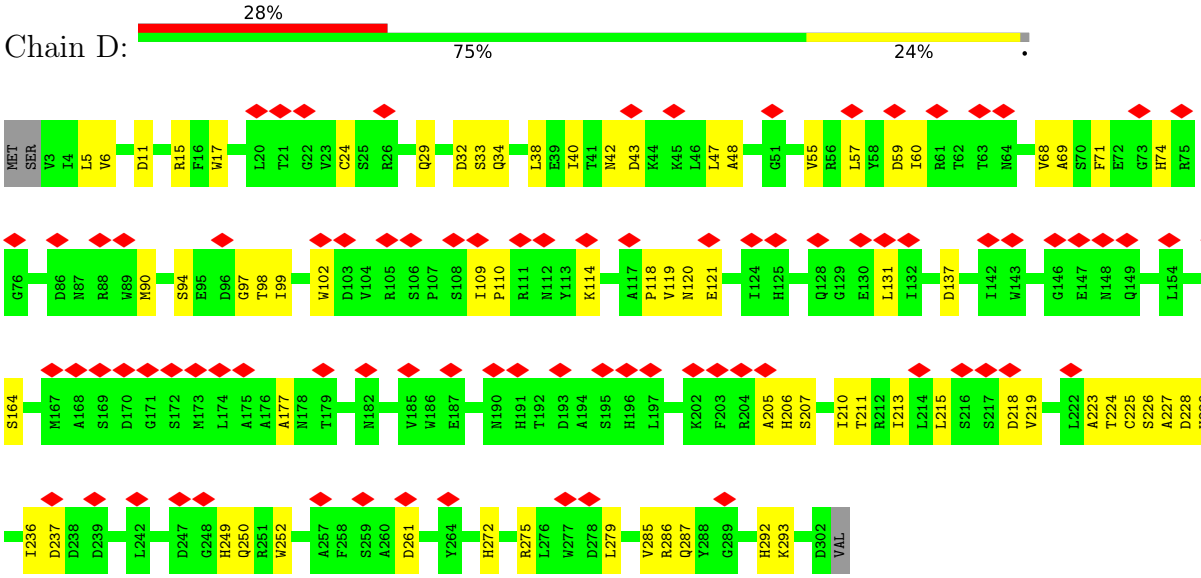
• Molecule 2: Target of rapamycin complex subunit LST8

Chain C:



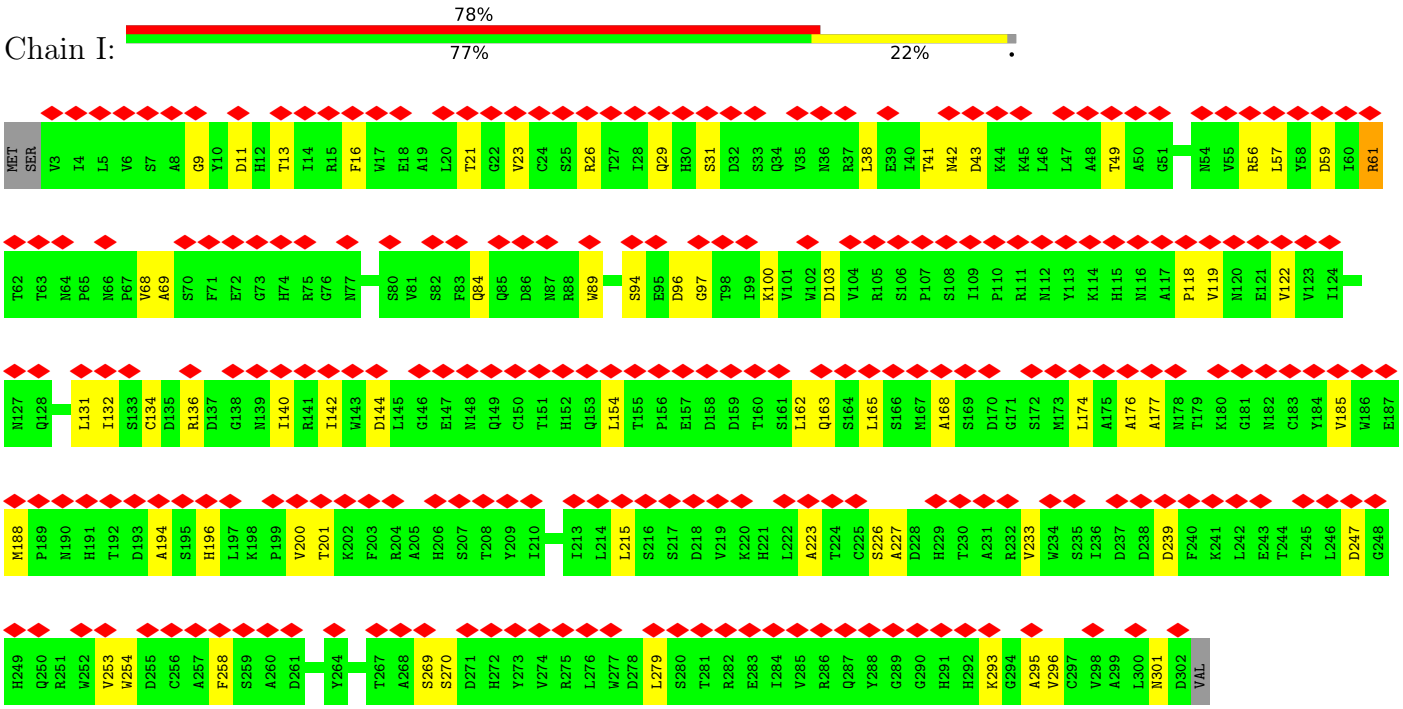
• Molecule 2: Target of rapamycin complex subunit LST8

Chain D:



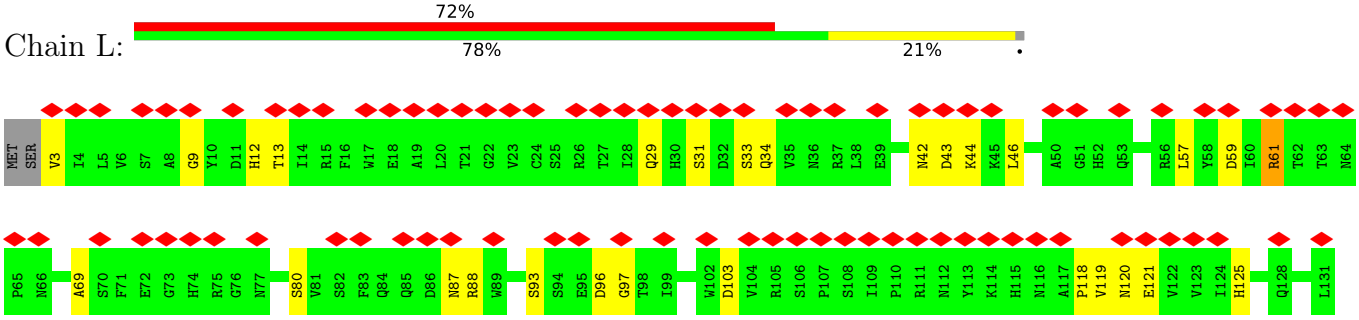
• Molecule 2: Target of rapamycin complex subunit LST8

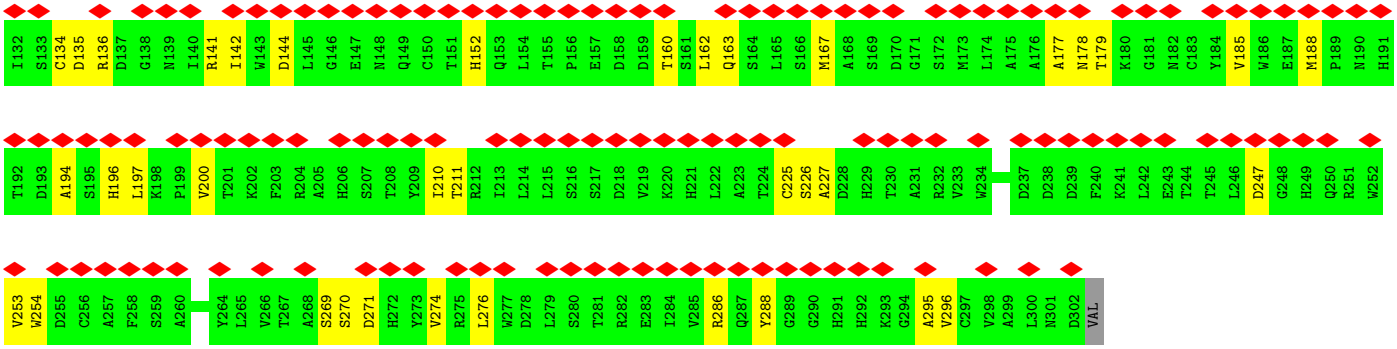
Chain I:



• Molecule 2: Target of rapamycin complex subunit LST8

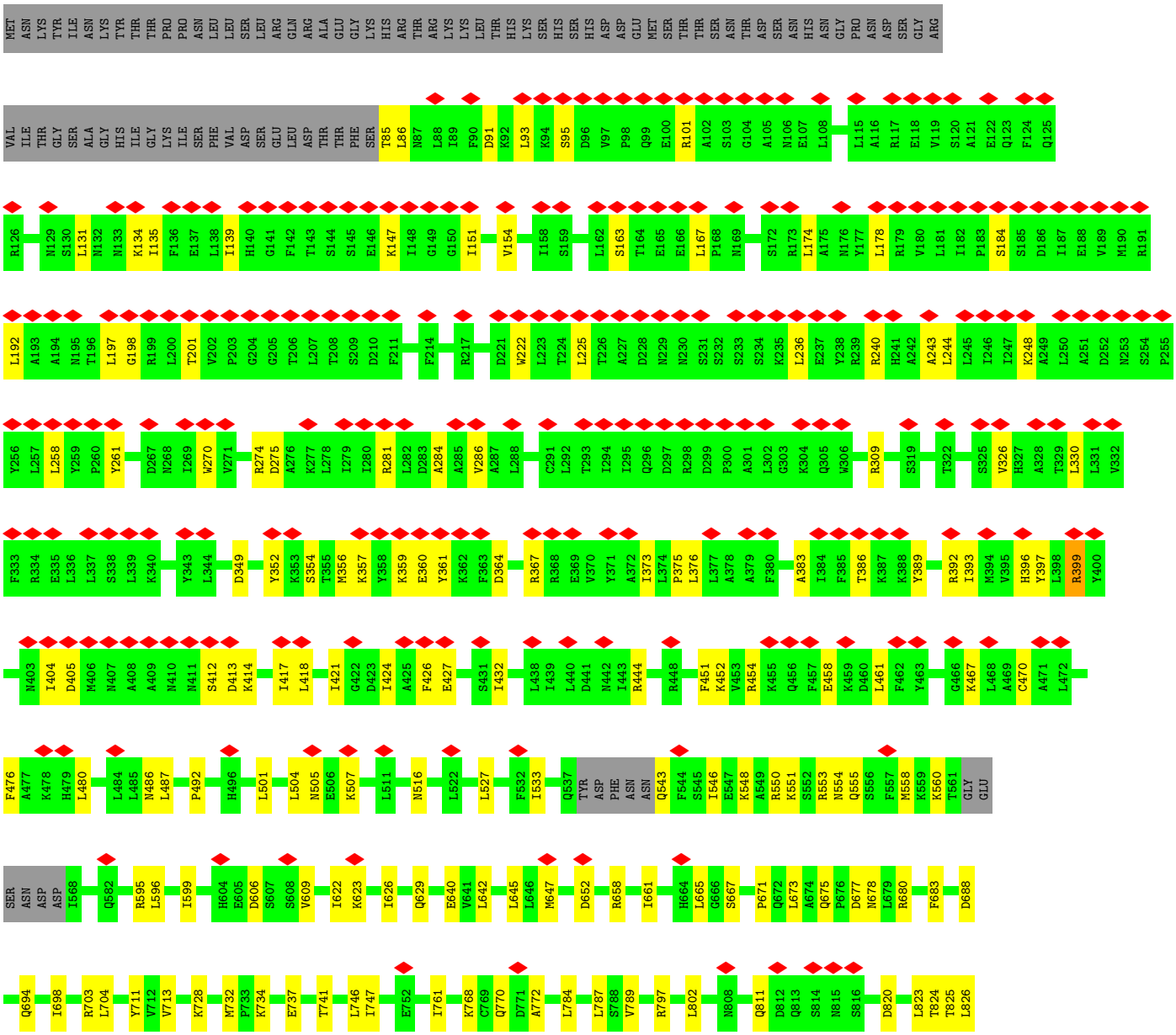
Chain L:

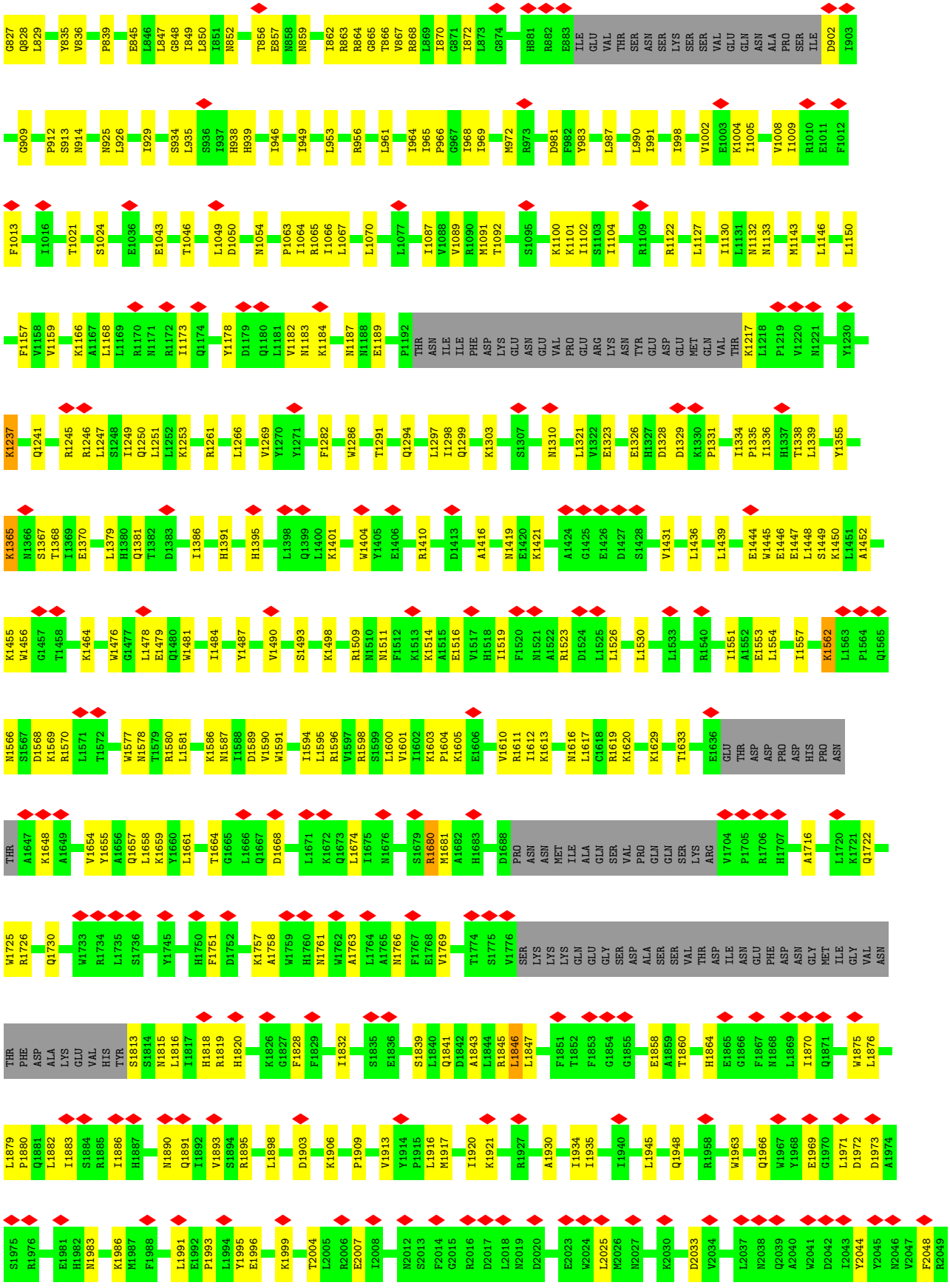




• Molecule 3: Serine/threonine-protein kinase TOR2

Chain E:




G827 Q828 L829 Y835 V836 P839 E845 L846 L847 G848 I849 L850 I851 N852 T856 E857 N858 N859 I862 R863 R864 G865 T866 V867 R868 L869 I870 G871 I872 L873 G874 H881 R882 E883 ILE GLU VAL THR SER ASN SER LYS SER SER VAL GLU GLN ASN ALA PRO SER ILE D902 I903
G909 P912 S913 N914 N925 L926 I929 S934 L935 S936 I937 H938 H939 I946 I949 L953 R956 L961 I964 I965 P966 G967 I968 I969 M972 R973 D981 F982 Y983 L987 L990 I991 I998 V1002 E1003 K1004 I1005 V1008 I1009 R1010 E1011 F1012
F1013 I1016 T1021 S1024 E1036 E1043 T1046 L1049 D1050 N1054 P1063 I1064 R1065 I1066 L1067 L1070 L1077 I1087 V1088 V1089 R1090 M1091 T1092 S1095 K1100 K1101 I1102 S1103 I1104 R1109 R1122 L1127 I1130 L1131 N1132 N1133 M1143 L1146 L1150
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K1237 Q1241 R1245 R1246 L1247 S1248 I1249 Q1250 L1251 L1252 K1253 R1261 L1266 V1269 Y1270 Y1271 F1282 W1286 T1291 Q1294 L1297 I1298 Q1299 K1303 S1307 N1310 L1321 V1322 E1323 E1326 H1327 D1328 D1329 K1330 P1331 I1334 P1335 I1336 H1337 T1338 L1339 Y1355
K1365 N1366 S1367 T1368 I1369 E1370 L1379 H1380 Q1381 T1382 D1383 I1386 H1391 H1395 L1398 Q1399 L1400 K1401 W1404 Y1405 E1406 R1410 D1413 A1416 N1419 E1420 K1421 A1424 G1425 E1426 D1427 S1428 V1431 L1436 L1439 E1444 W1445 E1446 E1447 L1448 S1449 K1450 L1451 A1452
K1455 W1456 G1457 T1458 K1464 W1476 G1477 L1478 E1479 Q1480 W1481 I1484 Y1487 V1490 S1493 K1498 R1509 N1510 N1511 F1512 K1513 K1514 A1515 E1516 V1517 H1518 I1519 F1520 N1521 A1522 R1523 D1524 L1525 L1526 L1530 L1533 R1540 I1551 A1552 E1553 L1554 I1557 K1562 L1563 P1564 Q1565
N1566 S1567 D1568 K1569 R1570 L1571 T1572 W1577 N1578 T1579 R1580 L1581 K1586 N1587 I1588 D1589 V1590 W1591 I1594 L1595 R1596 V1597 R1598 S1599 L1600 V1601 I1602 K1603 P1604 K1605 E1606 V1610 R1611 I1612 K1613 N1616 L1617 C1618 R1619 K1620 K1629 T1633 E1636 GLU THR ASP ASP PRO ASP HIS PRO ASN
THR A1647 K1648 A1649 V1654 Y1655 A1656 Q1657 L1658 K1659 Y1660 L1661 T1664 G1665 L1666 Q1667 D1668 L1671 K1672 Q1673 L1674 I1675 N1676 S1679 R1680 M1681 A1682 H1683 D1688 PRO ASN ASN MET ILE ALA GLN SER VAL PRO GLN GLN SER LYS ARG V1704 P1705 R1706 H1707 A1716 L1720 K1721 Q1722
W1725 R1726 Q1730 W1733 R1734 L1735 S1736 Y1745 H1750 F1751 D1752 K1757 A1758 W1759 H1760 N1761 W1762 A1763 L1764 A1765 N1766 F1767 E1768 V1769 T1774 S1775 V1776 SER LYS LYS LYS GLN GLU GLY SER ASP ALA SER SER VAL THR ASP ILE ASN GLU PHE ASP ASN GLY MET ILE GLY VAL ASN
THR PHE ASP ALA LYS GLU VAL HIS TYR S1813 S1814 N1815 L1816 I1817 H1818 R1819 H1820 K1826 G1827 F1828 F1829 I1832 S1835 E1836 S1839 L1840 Q1841 D1842 A1843 L1844 R1845 L1846 L1847 F1851 T1852 F1853 G1854 G1855 E1858 A1859 T1860 H1864 E1865 G1866 F1867 N1868 L1869 I1870 Q1871 W1875 L1876
L1879 P1880 Q1881 L1882 I1883 S1884 R1885 I1886 H1887 N1890 Q1891 I1892 V1893 S1894 R1895 L1898 D1903 K1906 P1909 V1913 Y1914 P1915 L1916 M1917 I1920 K1921 R1927 A1930 I1934 I1935 I1940 L1945 Q1948 R1958 W1963 Q1966 W1967 Y1968 E1969 G1970 L1971 D1972 D1973 A1974
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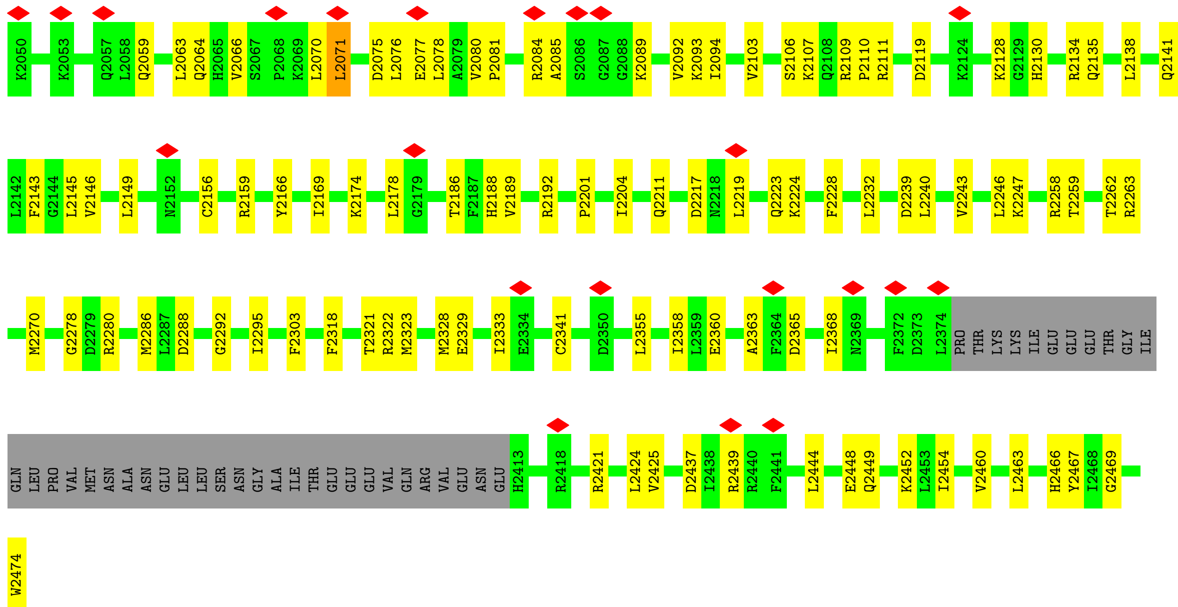
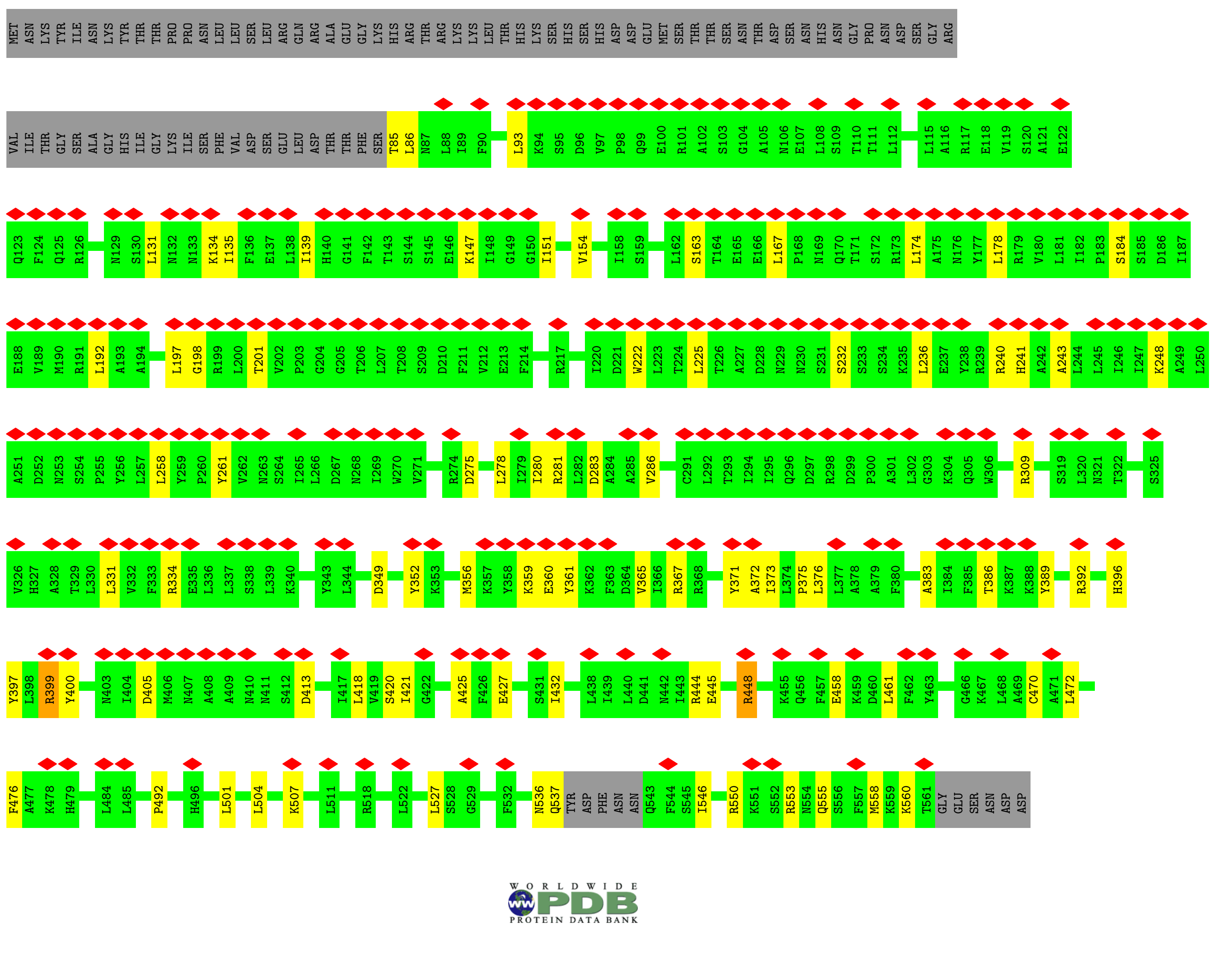
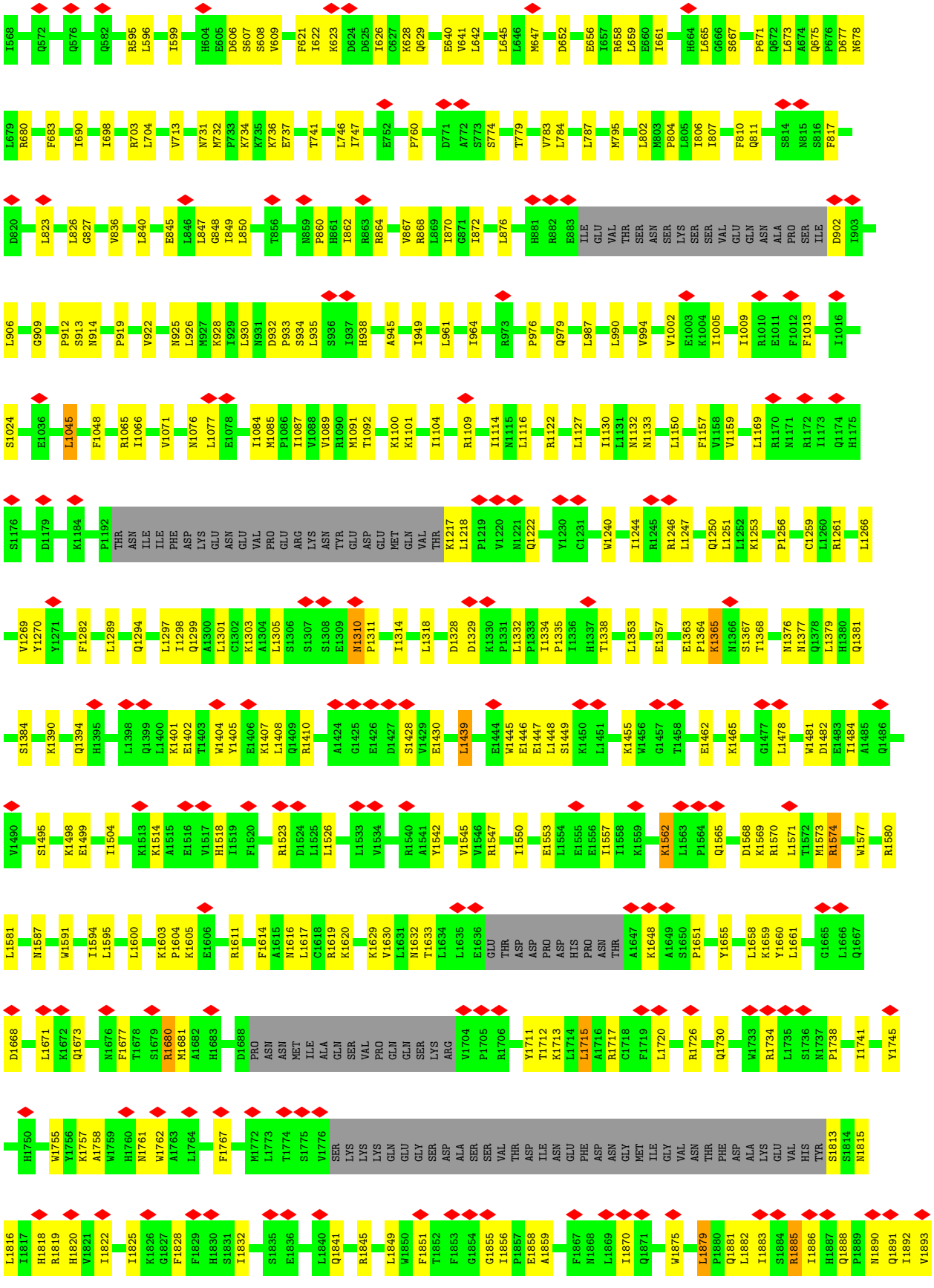
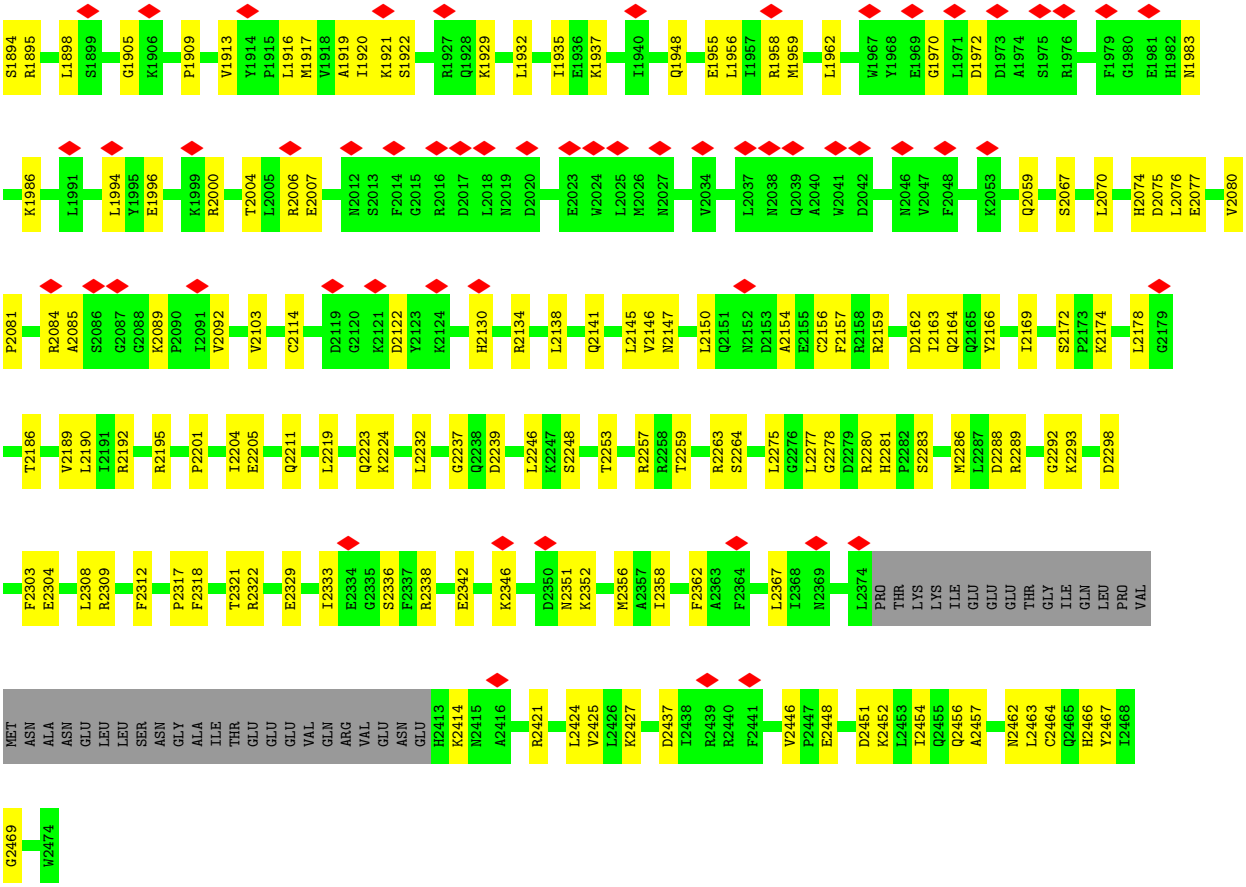


- Molecule 3: Serine/threonine-protein kinase TOR2

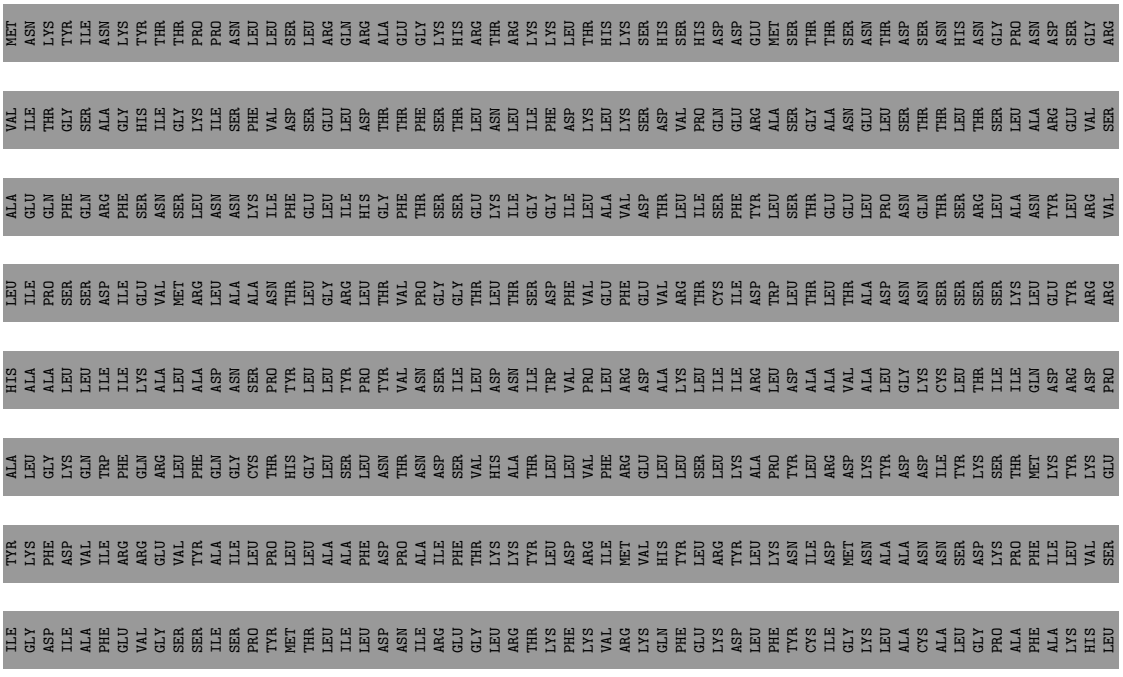


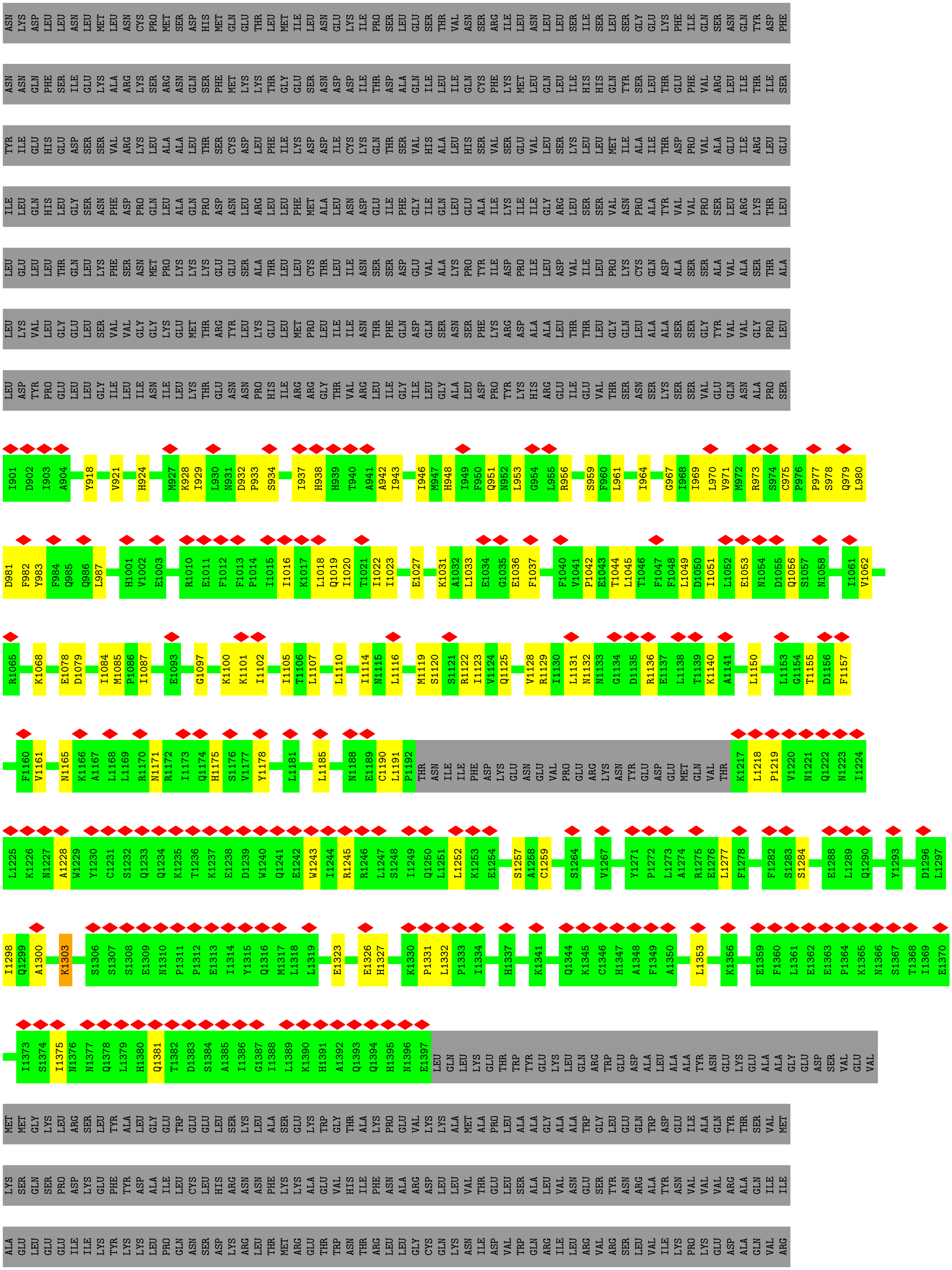


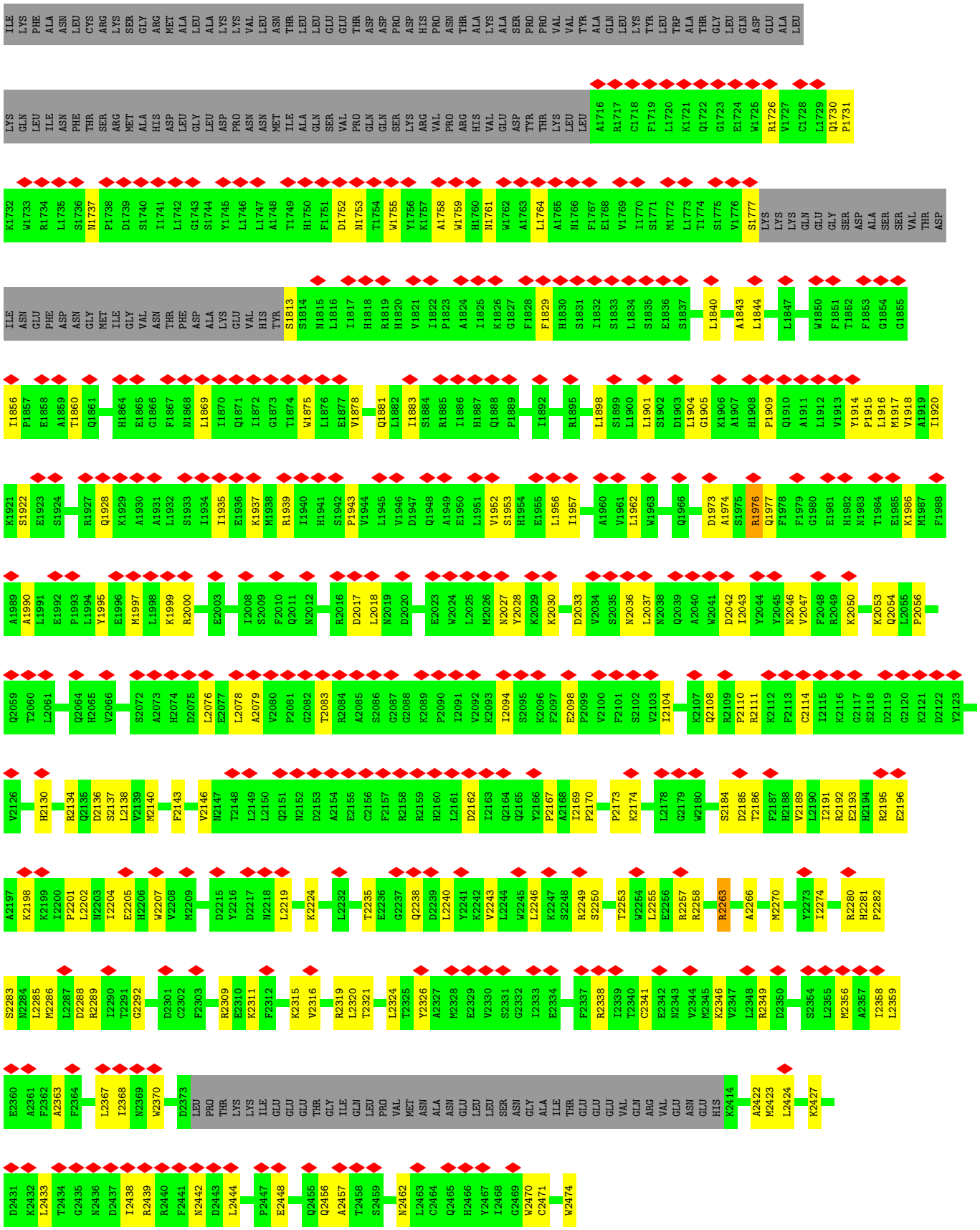


• Molecule 3: Serine/threonine-protein kinase TOR2

Chain H:



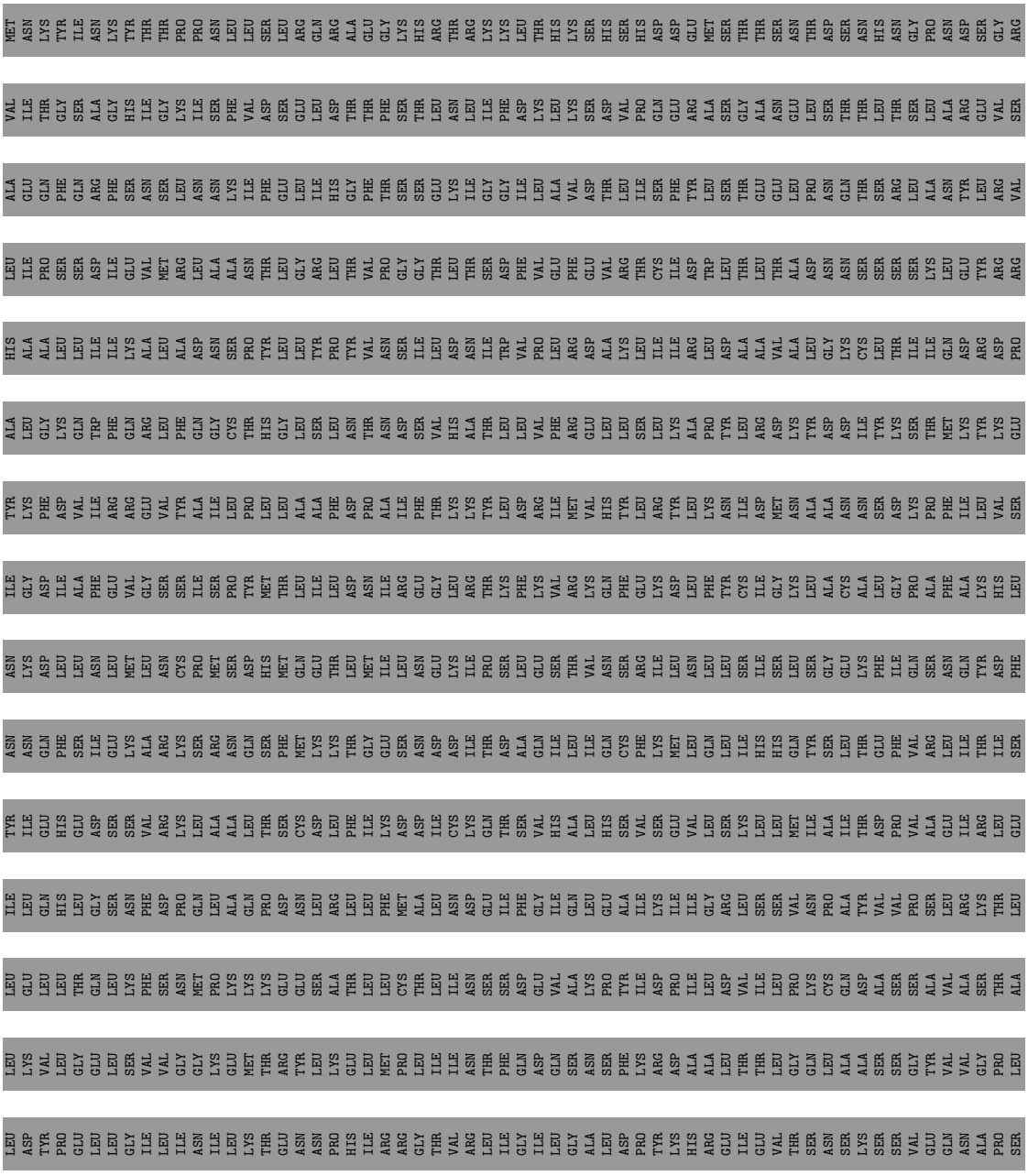

ASN LYS ASP LEU LEU ASN LEU MET LEU ASN CYS PRO MET SER ASP HIS MET GLN GLU THR LEU MET ILE LEU ASN GLU LYS ILE PRO SER LEU GLU SER THR VAL ASN SER ARG ILE LEU ASN LEU LEU SER ILE SER LEU SER GLY GLU LYS PHE ILE GLN SER ASN GLN TYR ASP PHE
ASN ASN GLN PHE SER ILE GLU LYS ALA ARG LYS SER ARG ASN GLN SER PHE MET LYS LYS THR GLY GLU SER ASN ASP ASP ILE THR ASP ALA GLN ILE LEU ILE GLN CYS PHE LYS MET LEU GLN LEU ILE HIS HIS GLN TYR SER LEU THR GLU PHE VAL ARG LEU ILE THR ILE SER
TYR ILE GLU HIS GLU ASP SER SER VAL ARG LYS LEU ALA ALA LEU THR SER CYS ASP LEU PHE ILE LYS ASP ASP ILE CYS LYS GLN THR SER VAL HIS ALA LEU HIS SER VAL SER GLU VAL LEU SER LYS LEU LEU MET ILE ALA ILE THR ASP PRO VAL ALA GLU ILE ARG LEU GLU
ILE LEU GLN HIS LEU GLY SER ASN PHE ASP PRO GLN LEU ALA GLN PRO ASP ASN LEU ARG LEU PHE MET ALA LEU ASN ASP GLU ILE PHE GLY ILE GLN LEU GLU ALA ILE LYS ILE ILE GLY ARG LEU SER SER VAL ASN PRO ALA TYR VAL VAL PRO SER LEU ARG LYS THR LEU
LEU GLU LEU LEU THR GLN LEU LYS PHE SER ASN MET PRO LYS LYS LYS GLU GLU SER ALA THR LEU LEU CYS THR LEU ILE ASN SER SER ASP GLU VAL ALA LYS PRO TYR ILE ASP PRO ILE LEU ASP VAL ILE LEU PRO LYS CYS GLN ASP ALA SER SER ALA VAL ALA SER THR ALA
LEU LYS VAL LEU GLY GLU LEU SER VAL VAL GLY GLY LYS GLU MET THR ARG TYR LEU LYS GLU LEU MET PRO LEU ILE ILE ASN THR PHE GLN ASP GLN SER ASN SER PHE LYS ARG ASP ALA ALA LEU THR THR LEU GLY GLN LEU ALA ALA SER SER GLY TYR VAL VAL GLY PRO LEU
LEU ASP TYR PRO GLU LEU LEU GLY ILE LEU ILE ASN ILE LEU LYS THR GLU ASN ASN PRO HIS ILE ARG ARG GLY THR VAL ARG LEU ILE GLY ILE LEU GLY ALA LEU ASP PRO TYR LYS HIS ARG GLU ILE GLU VAL THR SER ASN SER LYS SER SER VAL GLU GLN ASN ALA PRO SER
I901 D902 I903 A904 Y918 V921 H924 M927 K928 I929 L930 N931 D932 P933 S934 I937 H938 H939 T940 A941 A942 I943 I946 M947 H948 I949 F950 Q951 N952 L953 G954 L955 R956 S959 F960 L961 I964 G967 I968 I969 L970 V971 M972 R973 S974 C975 P976 P977 S978 Q979 L980
D981 F982 Y983 F984 Q985 Q986 L987 H1001 V1002 E1003 R1010 E1011 F1012 F1013 P1014 I1015 I1016 K1017 L1018 Q1019 I1020 T1021 I1022 I1023 E1027 K1031 A1032 L1033 E1034 G1035 E1036 F1037 F1040 V1041 P1042 E1043 T1044 L1045 T1046 F1047 F1048 L1049 D1050 I1051 L1052 E1053 N1054 D1055 Q1056 S1057 N1058 I1061 V1062
R1065 K1068 E1078 D1079 I1084 M1085 P1086 I1087 E1093 G1097 K1100 K1101 I1102 I1105 T1106 L1107 L1110 I1114 N1115 L1116 M1119 S1120 S1121 R1122 I1123 V1124 Q1125 V1128 R1129 I1130 L1131 N1132 N1133 G1134 D1135 R1136 E1137 L1138 T1139 K1140 A1141 L1150 L1153 G1154 T1155 D1156 F1157
F1160 V1161 N1165 K1166 A1167 L1168 L1169 R1170 N1171 R1172 I1173 Q1174 H1175 S1176 V1177 Y1178 L1181 L1185 N1188 E1189 C1190 L1191 P1192 THR ASN ILE ILE PHE ASP LYS GLU ASN GLU VAL PRO GLU ARG LYS ASN TYR GLU ASP GLU MET GLN VAL THR K1217 L1218 P1219 V1220 N1221 Q1222 N1223 I1224
L1225 K1226 N1227 A1228 W1229 Y1230 C1231 S1232 Q1233 Q1234 K1235 T1236 K1237 E1238 D1239 W1240 Q1241 E1242 W1243 I1244 R1245 R1246 L1247 S1248 I1249 Q1250 L1251 L1252 K1253 E1254 S1257 A1258 C1259 S1264 V1267 Y1271 P1272 L1273 A1274 R1275 E1276 L1277 F1278 F1282 S1283 S1284 E1288 L1289 Q1290 Y1293 D1296 L1297
I1298 Q1299 A1300 K1303 S1306 S1307 S1308 E1309 N1310 P1311 P1312 E1313 I1314 Y1315 Q1316 M1317 L1318 L1319 E1323 E1326 H1327 K1330 P1331 L1332 P1333 I1334 H1337 K1341 Q1344 K1345 C1346 H1347 A1348 F1349 A1350 L1353 K1356 E1359 F1360 L1361 E1362 E1363 P1364 K1365 N1366 S1367 T1368 I1369 E1370
I1373 S1374 I1375 N1376 N1377 Q1378 L1379 H1380 Q1381 T1382 D1383 S1384 A1385 I1386 G1387 I1388 L1389 K1390 H1391 A1392 Q1393 Q1394 H1395 N1396 E1397 LEU GLN LEU LYS GLU THR TRP TYR GLU LYS LEU GLN ARG TRP GLU ASP ALA LEU ALA ALA TYR ASN GLU LYS GLU ALA ALA GLY GLU ASP SER VAL GLU VAL
MET MET GLY LYS LEU ARG SER LEU TYR ALA LEU GLY GLU TRP GLU GLU LEU SER LYS LEU ALA SER GLU LYS TRP GLY THR ALA LYS PRO GLU VAL LYS LYS ALA MET ALA PRO LEU ALA ALA GLY ALA ALA TRP GLY LEU GLU GLN TRP ASP GLU ILE ALA GLN TYR THR SER VAL MET
LYS SER GLN SER PRO ASP LYS GLU PHE TYR ASP ALA ILE LEU CYS LEU HIS ARG ASN ASN PHE LYS LYS ALA GLU VAL HIS ILE PHE ASN ALA ARG ASP LEU LEU VAL THR GLU LEU SER ALA LEU VAL ASN GLU SER TYR ASN ARG ALA TYR ASN VAL VAL VAL ARG ALA GLN ILE ILE
ALA GLU LEU GLU GLU ILE ILE LYS TYR LYS LYS LEU PRO GLN ASN SER ASP LYS ARG LEU THR MET ARG GLU THR TRP ASN THR ARG LEU LEU GLY CYS GLN LYS ASN ILE ASP VAL TRP GLN ARG ILE LEU ARG VAL ARG SER LEU VAL ILE LYS PRO LYS GLU ASP ALA GLN VAL ARG

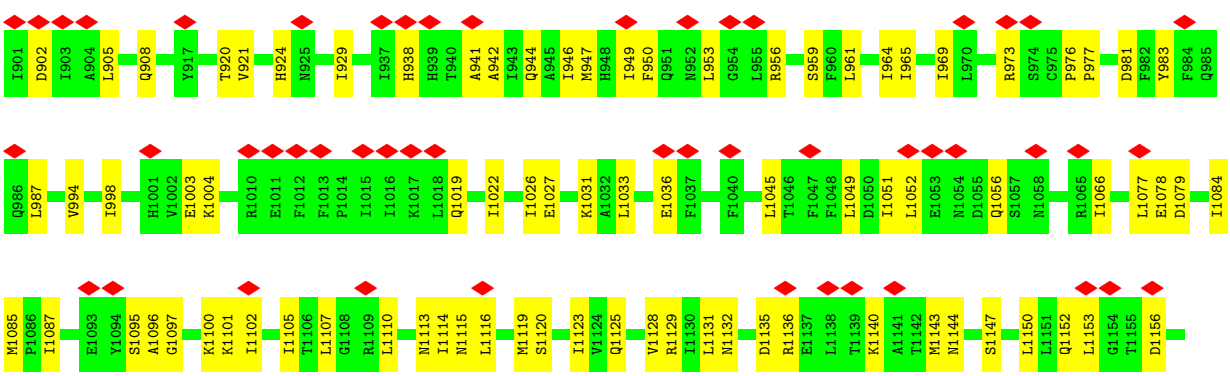


• Molecule 3: Serine/threonine-protein kinase TOR2

Chain K:


20%
35%
11%
53%

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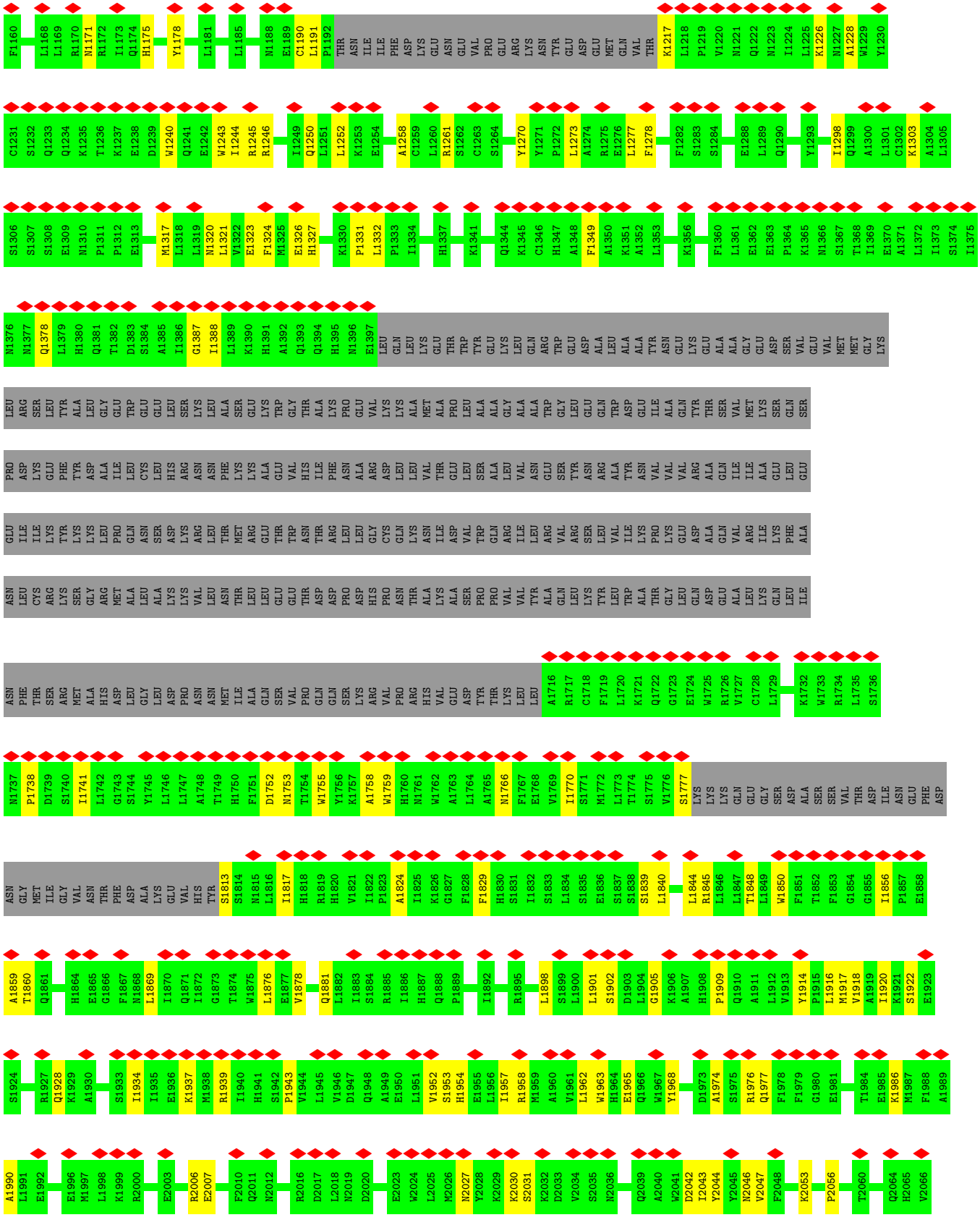
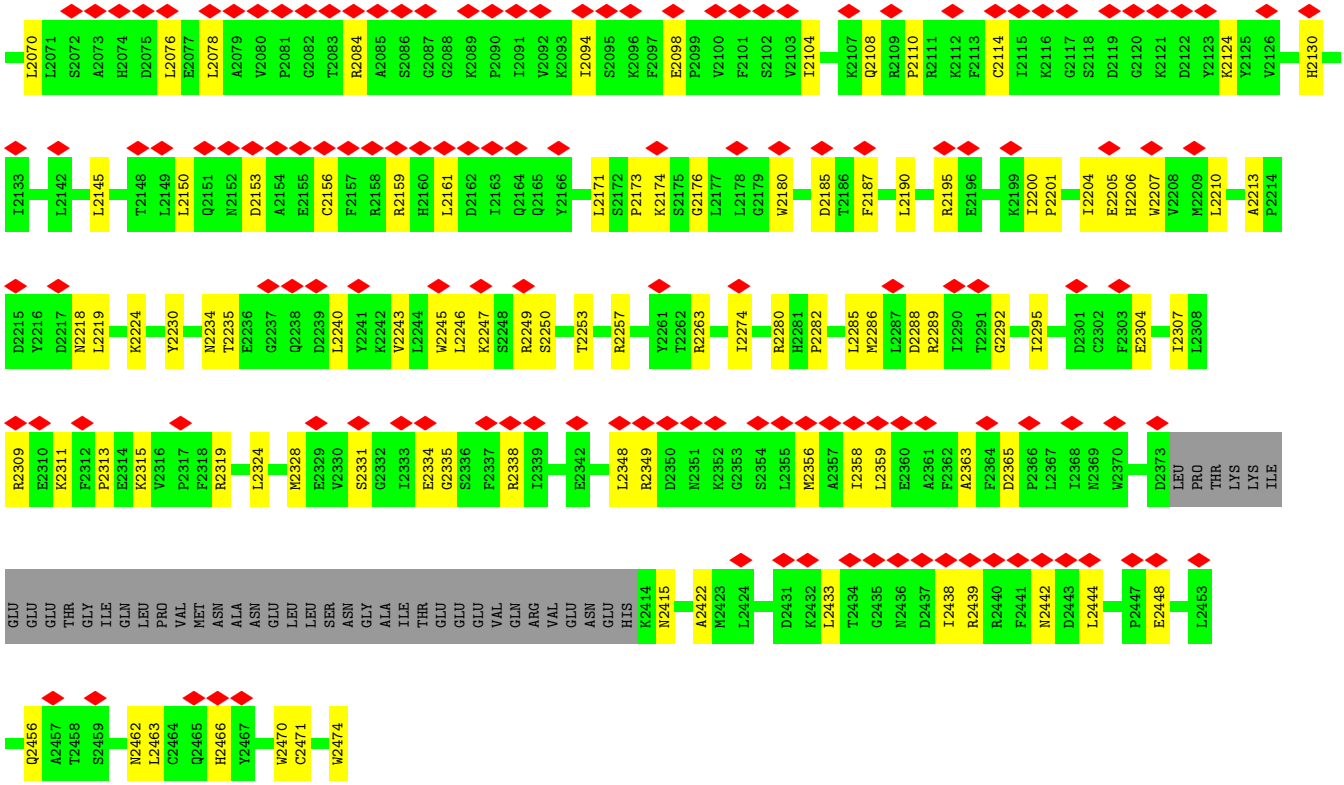
Q986 L987 V994 I998 H1001 V1002 E1003 K1004 R1010 E1011 F1012 F1013 P1014 I1015 I1016 K1017 L1018 Q1019 I1022 I1026 E1027 K1031 A1032 L1033 E1036 F1037 F1040 L1045 T1046 F1047 F1048 L1049 D1050 I1051 L1052 E1053 N1054 D1055 Q1056 S1057 N1058 R1065 I1066 L1077 E1078 D1079 I1084
M1085 P1086 I1087 E1093 Y1094 S1095 A1096 G1097 K1100 K1101 I1102 I1105 T1106 L1107 G1108 R1109 L1110 N1113 I1114 N1115 L1116 M1119 S1120 I1123 V1124 Q1125 V1128 R1129 I1130 L1131 N1132 D1135 R1136 E1137 L1138 T1139 K1140 A1141 T1142 M1143 N1144 S1147 L1150 L1151 Q1152 L1153 G1154 T1155 D1156


F1160 L1168 L1169 R1170 N1171 R1172 I1173 Q1174 H1175 Y1178 L1181 L1185 N1188 E1189 C1190 L1191 P1192 THR ASN ILE ILE PHE ASP LYS GLU ASN GLU VAL PRO GLU ARG LYS ASN TYR GLU ASP GLU MET GLN VAL THR K1217 L1218 P1219 V1220 N1221 Q1222 N1223 I1224 L1225 K1226 N1227 A1228 W1229 Y1230
C1231 S1232 Q1233 Q1234 K1235 T1236 K1237 E1238 D1239 W1240 Q1241 E1242 W1243 I1244 R1245 R1246 I1249 Q1250 L1251 L1252 K1253 E1254 A1258 C1259 L1260 R1261 S1262 C1263 S1264 Y1270 Y1271 P1272 L1273 A1274 R1275 E1276 L1277 F1278 F1282 S1283 S1284 E1288 L1289 Q1290 Y1293 I1298 Q1299 A1300 L1301 C1302 K1303 A1304 L1305
S1306 S1307 S1308 E1309 N1310 P1311 P1312 E1313 M1317 L1318 L1319 N1320 L1321 V1322 E1323 F1324 M1325 E1326 H1327 K1330 P1331 L1332 P1333 I1334 H1337 K1341 Q1344 K1345 C1346 H1347 A1348 F1349 A1350 K1351 A1352 L1353 K1356 F1360 L1361 E1362 E1363 P1364 K1365 N1366 S1367 T1368 I1369 E1370 A1371 L1372 I1373 S1374 I1375
N1376 N1377 Q1378 L1379 H1380 Q1381 T1382 D1383 S1384 A1385 I1386 G1387 I1388 L1389 K1390 H1391 A1392 Q1393 Q1394 H1395 N1396 E1397 LEU GLN LEU LYS GLU THR TRP TYR GLU LYS LEU GLN ARG TRP GLU ASP ALA LEU ALA ALA TYR ASN GLU LYS GLU ALA ALA GLY GLU ASP SER VAL GLU VAL MET MET GLY LYS
LEU ARG SER LEU TYR ALA LEU GLY GLU TRP GLU GLU LEU SER LYS LEU ALA SER GLU LYS TRP GLY THR ALA LYS PRO GLU VAL LYS LYS ALA MET ALA PRO LEU ALA ALA GLY ALA ALA TRP GLY LEU GLU GLN TRP ASP GLU ILE ALA GLN TYR THR SER VAL MET LYS SER GLN SER
PRO ASP LYS GLU PHE TYR ASP ALA ILE LEU CYS LEU HIS ARG ASN ASN PHE LYS LYS ALA GLU VAL HIS ILE PHE ASN ALA ARG ASP LEU LEU VAL THR GLU LEU SER ALA LEU VAL ASN GLU SER TYR ASN ARG ALA TYR ASN VAL VAL VAL ARG ALA GLN ILE ILE ALA GLU LEU GLU
GLU ILE ILE LYS TYR LYS LYS LEU PRO GLN ASN SER ASP LYS ARG LEU THR MET ARG GLU THR TRP ASN THR ARG LEU LEU GLY CYS GLN LYS ASN ILE ASP VAL TRP GLN ARG ILE LEU ARG VAL ARG SER LEU VAL ILE LYS PRO LYS GLU ASP ALA GLN VAL ARG ILE LYS PHE ALA
ASN LEU CYS ARG LYS SER GLY ARG MET ALA LEU ALA LYS LYS VAL LEU ASN THR LEU LEU GLU GLU THR ASP ASP PRO ASP HIS PRO ASN THR ALA LYS ALA SER PRO PRO VAL VAL TYR ALA GLN LEU LYS TYR LEU TRP ALA THR GLY LEU GLN ASP GLU ALA LEU LYS GLN LEU ILE
ASN PHE THR SER ARG MET ALA HIS ASP LEU GLY LEU ASP PRO ASN ASN MET ILE ALA GLN SER VAL PRO GLN GLN SER LYS ARG VAL PRO ARG HIS VAL GLU ASP TYR THR LYS LEU LEU A1716 R1717 C1718 F1719 L1720 K1721 Q1722 G1723 E1724 W1725 R1726 V1727 C1728 L1729 K1732 W1733 R1734 L1735 S1736
N1737 P1738 D1739 S1740 I1741 L1742 G1743 S1744 Y1745 L1746 L1747 A1748 T1749 H1750 F1751 D1752 N1753 T1754 W1755 Y1756 K1757 A1758 W1759 H1760 N1761 W1762 A1763 L1764 A1765 N1766 F1767 E1768 V1769 I1770 S1771 M1772 L1773 T1774 S1775 V1776 S1777 LYS LYS LYS GLN GLU GLY SER ASP ALA SER SER VAL THR ASP ILE ASN GLU PHE ASP
ASN GLY MET ILE GLY VAL ASN THR PHE ASP ALA LYS GLU VAL HIS TYR S1813 S1814 N1815 L1816 I1817 H1818 R1819 H1820 V1821 I1822 P1823 A1824 I1825 K1826 G1827 F1828 F1829 H1830 S1831 I1832 S1833 L1834 S1835 E1836 S1837 S1838 S1839 L1840 L1844 R1845 L1846 L1847 T1848 L1849 W1850 F1851 T1852 F1853 G1854 G1855 I1856 P1857 E1858
A1859 T1860 Q1861 H1864 E1865 G1866 F1867 N1868 L1869 I1870 Q1871 I1872 G1873 T1874 W1875 L1876 E1877 V1878 Q1881 L1882 I1883 S1884 R1885 I1886 H1887 Q1888 P1889 I1892 R1895 L1898 S1899 L1900 L1901 S1902 D1903 L1904 G1905 K1906 A1907 H1908 P1909 Q1910 A1911 L1912 V1913 Y1914 P1915 L1916 M1917 V1918 A1919 I1920 K1921 S1922 E1923
S1924 R1927 Q1928 K1929 A1930 S1933 I1934 I1935 E1936 K1937 M1938 R1939 I1940 H1941 S1942 P1943 V1944 L1945 V1946 D1947 Q1948 A1949 E1950 L1951 V1952 S1953 H1954 E1955 L1956 I1957 R1958 M1959 A1960 V1961 L1962 W1963 H1964 E1965 Q1966 W1967 Y1968 D1973 A1974 S1975 R1976 Q1977 F1978 F1979 G1980 E1981 T1984 E1985 K1986 M1987 F1988 A1989
A1990 L1991 E1992 E1996 M1997 L1998 K1999 R2000 E2003 R2006 E2007 F2010 Q2011 N2012 R2016 D2017 L2018 N2019 D2020 E2023 W2024 L2025 M2026 N2027 Y2028 K2029 K2030 S2031 K2032 D2033 V2034 S2035 N2036 Q2039 A2040 W2041 D2042 I2043 Y2044 Y2045 N2046 V2047 F2048 K2053 P2056 T2060 Q2064 H2065 V2066


L2070 L2071 S2072 A2073 H2074 D2075 L2076 E2077 L2078 A2079 V2080 P2081 G2082 T2083 R2084 A2085 S2086 G2087 G2088 K2089 P2090 I2091 V2092 K2093 I2094 S2095 K2096 F2097 E2098 P2099 V2100 P2101 S2102 V2103 I2104 K2107 Q2108 R2109 P2110 R2111 K2112 F2113 C2114 I2115 K2116 G2117 S2118 D2119 G2120 K2121 D2122 Y2123 K2124 Y2125 V2126 H2130
I2133 L2142 L2145 T2148 L2149 L2150 Q2151 N2152 D2153 A2154 E2155 C2156 F2157 R2158 R2159 H2160 L2161 D2162 I2163 Q2164 Q2165 Y2166 L2171 S2172 P2173 K2174 S2175 G2176 L2177 L2178 G2179 W2180 D2185 T2186 F2187 L2190 R2195 E2196 K2199 I2200 P2201 I2204 E2205 H2206 W2207 V2208 M2209 L2210 A2213 P2214
D2215 Y2216 D2217 N2218 L2219 K2224 Y2230 N2234 T2235 E2236 G2237 Q2238 D2239 L2240 Y2241 K2242 V2243 L2244 W2245 L2246 K2247 S2248 R2249 S2250 T2253 R2257 Y2261 T2262 R2263 I2274 R2280 H2281 P2282 L2285 M2286 L2287 D2288 R2289 I2290 T2291 G2292 I2295 D2301 C2302 F2303 E2304 I2307 L2308
R2309 E2310 K2311 F2312 P2313 E2314 K2315 V2316 P2317 F2318 R2319 L2324 M2328 E2329 V2330 S2331 G2332 I2333 E2334 G2335 S2336 F2337 R2338 I2339 E2342 L2348 R2349 D2350 N2351 K2352 G2353 S2354 L2355 M2356 A2357 I2358 L2359 E2360 A2361 F2362 A2363 F2364 D2365 P2366 L2367 I2368 N2369 W2370 D2373 LEU PRO THR LYS LYS ILE
GLU GLU GLU THR GLY ILE GLN LEU PRO VAL MET ASN ALA ASN GLU LEU LEU SER ASN GLY ALA ILE THR GLU GLU GLU VAL GLN ARG VAL GLU ASN GLU HIS K2414 N2415 A2422 M2423 L2424 D2431 K2432 L2433 T2434 G2435 N2436 D2437 I2438 R2439 R2440 F2441 N2442 D2443 L2444 P2447 E2448 L2453
Q2456 A2457 T2458 S2459 N2462 L2463 C2464 Q2465 H2466 Y2467 W2470 C2471 W2474

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	218872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	37000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.344	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.29	0/9911	0.58	2/13437 (0.0%)
1	B	0.29	0/9904	0.58	1/13427 (0.0%)
1	G	0.28	0/9923	0.56	2/13455 (0.0%)
1	J	0.28	0/9929	0.55	0/13463
2	C	0.26	0/2422	0.60	0/3302
2	D	0.26	0/2422	0.60	2/3302 (0.1%)
2	I	0.25	0/2422	0.59	2/3302 (0.1%)
2	L	0.25	0/2422	0.61	3/3302 (0.1%)
3	E	0.28	0/18271	0.59	2/24746 (0.0%)
3	F	0.27	0/18265	0.59	6/24739 (0.0%)
3	H	0.26	0/9509	0.58	0/12893
3	K	0.26	0/9509	0.56	0/12893
All	All	0.28	0/104909	0.58	20/142261 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	J	0	1
All	All	0	3

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	120	ASP	CB-CG-OD1	9.13	126.51	118.30
3	F	1715	LEU	CA-CB-CG	8.74	135.41	115.30
3	E	2071	LEU	CA-CB-CG	6.60	130.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	137	ASP	CB-CG-OD1	6.47	124.13	118.30
2	I	239	ASP	CB-CG-OD1	6.34	124.01	118.30
2	L	96	ASP	CB-CG-OD1	6.29	123.97	118.30
2	L	103	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	997	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	935	LEU	CA-CB-CG	5.89	128.85	115.30
3	E	1846	LEU	CA-CB-CG	5.70	128.41	115.30
3	F	2298	ASP	CB-CG-OD1	5.63	123.37	118.30
1	G	229	LEU	CB-CG-CD1	-5.59	101.50	111.00
3	F	1045	LEU	CB-CG-CD1	-5.55	101.56	111.00
3	F	1879	LEU	CA-CB-CG	5.47	127.89	115.30
2	L	144	ASP	CB-CG-OD1	5.37	123.13	118.30
1	G	96	ASP	CB-CG-OD1	5.37	123.13	118.30
3	F	1439	LEU	CA-CB-CG	5.34	127.58	115.30
2	I	188	MET	CA-CB-CG	5.24	122.20	113.30
2	D	261	ASP	CB-CG-OD1	5.09	122.89	118.30
3	F	906	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	CYS	Peptide
1	B	216	CYS	Peptide
1	J	216	CYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9693	0	9655	137	0
1	B	9686	0	9656	128	0
1	G	9705	0	9676	153	0
1	J	9711	0	9683	149	0
2	C	2366	0	2251	46	0
2	D	2366	0	2251	42	0
2	I	2366	0	2251	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	2366	0	2251	37	0
3	E	17910	0	18236	351	0
3	F	17904	0	18225	331	0
3	H	9299	0	9374	177	0
3	K	9299	0	9374	168	0
All	All	102671	0	102883	1741	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1741) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:632:ILE:HD11	1:J:733:ASN:HD22	1.26	0.97
1:J:1105:LYS:HZ1	1:J:1306:LEU:HD11	1.36	0.90
1:G:630:GLU:N	1:G:630:GLU:OE1	2.08	0.85
3:H:971:VAL:O	3:H:975:CYS:HB3	1.80	0.82
3:E:2286:MET:HB2	3:E:2295:ILE:HB	1.62	0.82
3:E:1680:ARG:NH1	3:E:1681:MET:SD	2.57	0.78
3:F:1619:ARG:HH12	3:F:1659:LYS:HB3	1.49	0.78
3:K:2247:LYS:HB3	3:K:2289:ARG:HH12	1.47	0.78
1:B:585:VAL:HG11	1:B:622:ILE:HG13	1.68	0.76
1:J:1105:LYS:NZ	1:J:1306:LEU:HD11	2.01	0.75
3:K:1777:SER:HG	3:K:1813:SER:N	1.85	0.75
3:E:626:ILE:HA	3:E:629:GLN:HE21	1.51	0.75
1:J:1106:LYS:HD2	1:J:1106:LYS:N	2.03	0.74
1:J:1105:LYS:NZ	1:J:1306:LEU:CD1	2.51	0.73
3:H:1939:ARG:HH21	3:H:1943:PRO:HA	1.54	0.73
3:H:1326:GLU:HG2	3:H:1331:PRO:HB3	1.71	0.72
3:E:824:THR:HG22	3:E:828:GLN:HE22	1.54	0.72
2:L:12:HIS:HE1	2:L:31:SER:HA	1.54	0.71
2:L:57:LEU:HB2	2:L:69:ALA:HB3	1.72	0.71
1:B:1482:THR:HG22	1:B:1484:SER:H	1.53	0.71
3:F:1619:ARG:HE	3:F:1620:LYS:HD2	1.54	0.71
1:B:1081:LEU:O	1:B:1085:GLU:HG2	1.90	0.71
1:A:750:SER:O	1:A:756:ARG:NH2	2.24	0.70
3:H:1777:SER:HG	3:H:1813:SER:N	1.88	0.70
1:B:811:GLY:H	1:B:922:ARG:HH12	1.40	0.70
3:E:2063:LEU:HD22	3:E:2071:LEU:HD12	1.74	0.69
1:J:632:ILE:CD1	1:J:733:ASN:HD22	2.02	0.69
1:B:237:GLN:HA	1:B:240:ILE:HG12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:626:ILE:HA	3:F:629:GLN:HE21	1.58	0.69
3:F:1983:ASN:H	3:F:1986:LYS:HZ1	1.39	0.69
3:H:2134:ARG:HH12	3:H:2138:LEU:HD23	1.57	0.69
2:C:219:VAL:HG12	2:C:236:ILE:HG21	1.76	0.68
1:G:1264:ASN:H	1:G:1319:GLN:HE22	1.42	0.68
1:J:1105:LYS:HE2	1:J:1306:LEU:HD12	1.74	0.68
3:E:533:ILE:HG13	3:E:543:GLN:HE21	1.59	0.68
3:F:1717:ARG:HH21	3:F:1720:LEU:HD13	1.57	0.68
1:A:1176:ARG:O	1:A:1180:ASN:ND2	2.26	0.68
1:J:1214:LEU:HB2	1:J:1227:ALA:HB3	1.76	0.68
3:E:658:ARG:HA	3:E:661:ILE:HG22	1.75	0.68
3:E:961:LEU:HA	3:E:964:ILE:HG22	1.76	0.67
3:E:424:ILE:HG13	3:E:432:ILE:HD11	1.76	0.67
3:K:1120:SER:HA	3:K:1123:ILE:HG12	1.76	0.67
2:I:9:GLY:HA2	2:I:296:VAL:HG22	1.75	0.67
3:F:2134:ARG:HH12	3:F:2367:LEU:HB2	1.59	0.67
3:E:1860:THR:O	3:E:1864:HIS:ND1	2.23	0.67
3:H:1085:MET:HG3	3:H:1119:MET:HG3	1.77	0.67
1:J:41:TYR:O	1:J:1264:ASN:ND2	2.28	0.67
3:E:1447:GLU:HA	3:E:1450:LYS:HG2	1.77	0.66
3:F:546:ILE:HG12	3:F:596:LEU:HD23	1.76	0.66
3:K:1840:LEU:HD13	3:K:1878:VAL:HG22	1.77	0.66
3:K:2053:LYS:O	3:K:2056:PRO:HD2	1.95	0.66
3:E:867:VAL:HA	3:E:870:ILE:HG12	1.76	0.66
2:I:122:VAL:HB	2:I:131:LEU:HD11	1.75	0.66
3:F:658:ARG:HA	3:F:661:ILE:HG22	1.76	0.66
3:E:1587:ASN:HB2	3:E:1590:VAL:HG12	1.77	0.66
3:E:2186:THR:HG22	3:E:2188:HIS:H	1.59	0.66
3:K:1097:GLY:HA2	3:K:1100:LYS:HB2	1.77	0.66
1:J:1105:LYS:HZ1	1:J:1306:LEU:CD1	2.05	0.66
1:G:929:VAL:HG11	1:G:1078:PHE:HB2	1.77	0.66
3:E:1581:LEU:HD13	3:E:1594:ILE:HD11	1.77	0.65
3:H:1228:ALA:O	3:H:1243:TRP:NE1	2.28	0.65
3:H:2047:VAL:HA	3:H:2050:LYS:HG2	1.78	0.65
3:K:2201:PRO:HG2	3:K:2204:ILE:HB	1.78	0.65
1:A:264:GLN:HB2	1:A:409:ASP:HB2	1.79	0.65
3:E:2110:PRO:HB3	3:E:2128:LYS:HG2	1.78	0.65
1:G:1478:ILE:HG12	1:G:1522:LEU:HD11	1.78	0.65
2:C:118:PRO:HG2	2:C:136:ARG:HE	1.61	0.65
3:E:1523:ARG:HH21	3:E:1526:LEU:HD23	1.61	0.65
3:H:1122:ARG:HA	3:H:1125:GLN:HE22	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1336:ILE:HD11	3:E:1355:TYR:HB3	1.78	0.65
3:K:953:LEU:HD13	3:K:956:ARG:HB3	1.77	0.65
3:H:2219:LEU:HD23	3:H:2224:LYS:HG2	1.77	0.65
3:E:2288:ASP:HB3	3:E:2292:GLY:H	1.62	0.65
3:E:2262:THR:HG21	3:E:2329:GLU:HG2	1.79	0.65
1:A:1318:LEU:HD11	1:A:1365:GLY:HA2	1.79	0.64
1:B:819:LEU:HD13	1:B:822:GLN:NE2	2.12	0.64
1:B:822:GLN:O	1:B:822:GLN:HG2	1.94	0.64
1:G:399:MET:HB3	1:G:404:CYS:HB2	1.78	0.64
3:E:1127:LEU:HA	3:E:1130:ILE:HD12	1.79	0.64
3:F:922:VAL:HG11	3:F:1259:CYS:HB3	1.78	0.64
1:J:882:ASP:CG	1:J:885:LYS:HB2	2.18	0.64
1:A:1261:LYS:HE3	1:A:1316:GLU:HA	1.79	0.64
1:B:181:VAL:HG13	1:B:191:TRP:HB2	1.78	0.64
3:K:1974:ALA:HA	3:K:1977:GLN:HE21	1.62	0.64
1:A:898:LEU:HD21	1:A:967:VAL:HG22	1.80	0.64
3:E:824:THR:O	3:E:828:GLN:NE2	2.31	0.64
3:E:826:LEU:HA	3:E:829:LEU:HG	1.79	0.64
1:J:50:ASN:ND2	1:J:981:GLU:OE2	2.31	0.64
3:H:1097:GLY:HA2	3:H:1100:LYS:HB2	1.79	0.64
3:K:956:ARG:NH1	3:K:959:SER:OG	2.29	0.64
1:A:361:ILE:HD13	1:A:425:TRP:HB2	1.80	0.64
2:C:135:ASP:HB3	2:C:139:ASN:H	1.63	0.63
3:E:1009:ILE:O	3:E:1013:PHE:HB2	1.98	0.63
2:L:9:GLY:HA2	2:L:296:VAL:HG12	1.79	0.63
1:B:823:GLN:OE1	1:J:195:ARG:NH1	2.30	0.63
3:F:1439:LEU:HD13	3:F:1447:GLU:HG2	1.79	0.63
2:D:38:LEU:HD12	2:D:47:LEU:HD11	1.79	0.63
3:F:1983:ASN:HB2	3:F:1986:LYS:HG2	1.80	0.63
2:L:163:GLN:N	2:L:177:ALA:O	2.30	0.63
3:E:868:ARG:NH2	3:E:1523:ARG:HD3	2.14	0.63
1:B:1489:ASN:OD1	1:B:1490:SER:N	2.31	0.63
3:F:1246:ARG:O	3:F:1250:GLN:NE2	2.31	0.63
3:F:840:LEU:HG	3:F:876:LEU:HD21	1.81	0.63
2:C:205:ALA:O	2:C:206:HIS:ND1	2.32	0.63
3:E:1983:ASN:HB2	3:E:1986:LYS:HG2	1.80	0.63
3:F:774:SER:HB2	3:F:817:PHE:HB3	1.80	0.63
3:K:1922:SER:O	3:K:1928:GLN:NE2	2.31	0.63
1:B:268:CYS:SG	1:B:269:THR:N	2.72	0.63
1:B:819:LEU:HD13	1:B:822:GLN:HE21	1.63	0.63
1:B:859:GLN:HA	1:B:862:MET:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1452:ALA:HA	3:E:1455:LYS:HE3	1.80	0.63
3:E:1553:GLU:OE2	3:E:1577:TRP:NE1	2.32	0.63
1:G:106:CYS:SG	1:G:107:ALA:N	2.72	0.63
3:H:2288:ASP:HB3	3:H:2292:GLY:H	1.64	0.63
3:H:1918:VAL:HG13	3:H:2173:PRO:HD3	1.79	0.62
3:K:2124:LYS:HG3	3:K:2180:TRP:HB3	1.81	0.62
1:A:164:ARG:HH22	1:A:215:PRO:HD2	1.64	0.62
1:B:914:VAL:HG12	1:B:1140:LEU:HD23	1.81	0.62
3:E:1619:ARG:HH12	3:E:1659:LYS:HB3	1.63	0.62
1:G:747:ILE:HD12	1:G:756:ARG:HG2	1.81	0.62
2:C:59:ASP:HB2	2:C:68:VAL:HG21	1.81	0.62
1:G:298:ARG:NH1	1:G:336:PRO:O	2.32	0.62
3:K:938:HIS:HB3	3:K:942:ALA:HB2	1.81	0.62
3:K:1246:ARG:O	3:K:1250:GLN:NE2	2.32	0.62
1:G:164:ARG:HH12	1:G:215:PRO:HD2	1.64	0.62
3:F:371:TYR:HB3	3:F:420:SER:HB3	1.82	0.62
1:G:1411:GLN:HB2	1:G:1416:ARG:HA	1.79	0.62
2:L:13:THR:HG22	2:L:29:GLN:HA	1.80	0.62
3:E:1439:LEU:HD13	3:E:1447:GLU:HG2	1.81	0.62
1:J:156:VAL:HA	1:J:159:PHE:HB3	1.82	0.62
3:H:2423:MET:SD	3:H:2427:LYS:NZ	2.72	0.62
1:J:539:LEU:O	1:J:543:TYR:HB2	1.99	0.62
3:F:1071:VAL:HB	3:F:1109:ARG:HD2	1.81	0.62
3:F:1996:GLU:O	3:F:2000:ARG:NH1	2.32	0.62
1:B:164:ARG:HH22	1:B:215:PRO:HD2	1.65	0.61
3:F:1818:HIS:ND1	3:F:1858:GLU:OE2	2.33	0.61
3:E:595:ARG:NH2	3:E:640:GLU:OE1	2.34	0.61
3:K:1323:GLU:HA	3:K:1326:GLU:HG2	1.81	0.61
3:K:1918:VAL:HG13	3:K:2173:PRO:HD3	1.81	0.61
1:J:372:ARG:NH1	1:J:590:SER:OG	2.32	0.61
1:J:1264:ASN:H	1:J:1319:GLN:NE2	1.98	0.61
1:J:1406:ASN:ND2	1:J:1459:MET:SD	2.72	0.61
2:C:213:ILE:HG12	2:C:224:THR:HG22	1.81	0.61
1:G:799:THR:HG23	1:G:911:GLU:HG3	1.81	0.61
3:K:953:LEU:HD22	3:K:956:ARG:HE	1.64	0.61
3:E:373:ILE:HA	3:E:376:LEU:HD12	1.82	0.61
3:K:1140:LYS:O	3:K:1144:ASN:ND2	2.33	0.61
3:K:2145:LEU:HD22	3:K:2358:ILE:HG13	1.82	0.61
1:B:814:ASP:HA	1:B:817:VAL:HG12	1.83	0.61
3:F:2424:LEU:HD23	3:F:2427:LYS:HZ3	1.65	0.61
1:G:171:ARG:HH12	1:G:262:CYS:HA	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:163:GLN:N	2:I:177:ALA:O	2.33	0.61
1:B:156:VAL:HA	1:B:159:PHE:HB3	1.83	0.61
3:H:2108:GLN:OE1	3:H:2130:HIS:NE2	2.34	0.61
3:K:1003:GLU:OE1	3:K:1004:LYS:NZ	2.33	0.61
1:G:194:ASN:ND2	1:G:199:GLN:O	2.34	0.61
1:A:181:VAL:HG13	1:A:191:TRP:HB2	1.82	0.61
1:B:1085:GLU:OE1	1:B:1085:GLU:HA	2.01	0.61
3:F:2456:GLN:O	3:F:2462:ASN:ND2	2.33	0.61
1:B:1191:LYS:HE2	1:B:1467:HIS:HB3	1.81	0.61
3:F:1390:LYS:HE2	3:F:1394:GLN:HE22	1.65	0.61
3:K:961:LEU:HA	3:K:964:ILE:HG12	1.80	0.61
1:B:1003:LEU:HD11	1:B:1074:LEU:HD21	1.81	0.60
3:E:2360:GLU:HA	3:E:2363:ALA:HB3	1.83	0.60
3:F:1365:LYS:NZ	3:F:1367:SER:OG	2.26	0.60
3:H:2319:ARG:NH2	3:H:2471:CYS:O	2.34	0.60
1:J:564:GLN:HG2	1:J:567:ARG:HH21	1.65	0.60
3:K:2309:ARG:NH1	3:K:2311:LYS:O	2.34	0.60
3:E:1557:ILE:HD12	3:E:1601:VAL:HG11	1.83	0.60
3:H:1922:SER:O	3:H:1928:GLN:NE2	2.34	0.60
3:H:2349:ARG:NH2	3:H:2433:LEU:O	2.32	0.60
3:K:1131:LEU:O	3:K:1171:ASN:ND2	2.35	0.60
2:L:253:VAL:HA	2:L:269:SER:HB2	1.83	0.60
1:A:1191:LYS:HE2	1:A:1467:HIS:HB3	1.83	0.60
1:B:44:ASP:OD2	1:B:46:ARG:NH1	2.34	0.60
3:F:1365:LYS:HE3	3:F:1368:THR:HG23	1.83	0.60
1:G:1106:LYS:HD2	1:G:1106:LYS:N	2.16	0.60
1:J:794:VAL:HG12	1:J:796:GLU:H	1.67	0.60
1:B:264:GLN:HB2	1:B:409:ASP:HB2	1.84	0.60
3:E:935:LEU:O	3:E:939:HIS:NE2	2.35	0.60
3:E:827:GLY:HA2	3:E:872:ILE:HD13	1.83	0.60
3:K:2153:ASP:HB3	3:K:2156:CYS:HB2	1.84	0.60
2:C:55:VAL:HG21	2:C:81:VAL:HG11	1.84	0.60
3:H:2320:LEU:HA	3:H:2324:LEU:HD12	1.83	0.60
1:J:155:ASP:OD1	1:J:158:ARG:NH2	2.35	0.60
1:A:1213:LYS:NZ	1:A:1229:ASP:OD1	2.31	0.60
3:E:1391:HIS:O	3:E:1395:HIS:HB2	2.01	0.60
3:F:1603:LYS:HD2	3:F:1604:PRO:HD2	1.84	0.60
3:H:1136:ARG:O	3:H:1140:LYS:NZ	2.35	0.60
3:K:2230:TYR:O	3:K:2234:ASN:ND2	2.34	0.60
3:H:953:LEU:HD13	3:H:956:ARG:HB3	1.83	0.59
1:A:552:GLU:OE2	3:E:711:TYR:OH	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ASN:OD1	1:B:234:LYS:NZ	2.34	0.59
2:D:219:VAL:HG12	2:D:236:ILE:HG21	1.83	0.59
3:H:1190:CYS:SG	3:H:1191:LEU:N	2.76	0.59
1:J:799:THR:HG23	1:J:911:GLU:HG3	1.84	0.59
3:K:1147:SER:HA	3:K:1150:LEU:HD12	1.84	0.59
2:L:162:LEU:HA	2:L:178:ASN:HA	1.84	0.59
1:G:710:ASP:HB2	1:G:752:ILE:HD12	1.83	0.59
3:F:275:ASP:O	3:F:281:ARG:NH2	2.35	0.59
1:J:1478:ILE:HG12	1:J:1522:LEU:HD11	1.84	0.59
2:D:11:ASP:HB3	2:D:293:LYS:HB2	1.85	0.59
3:F:1581:LEU:HD13	3:F:1594:ILE:HD11	1.85	0.59
2:C:231:ALA:O	2:C:246:LEU:HB3	2.02	0.59
3:E:458:GLU:HG2	3:E:461:LEU:HD13	1.84	0.59
3:F:919:PRO:HA	3:F:922:VAL:HG12	1.85	0.59
1:J:1105:LYS:CE	1:J:1306:LEU:HD12	2.32	0.59
1:J:1179:ARG:HH12	1:J:1220:PHE:HB3	1.67	0.59
3:F:836:VAL:HG21	3:F:1580:ARG:HE	1.67	0.59
3:F:1816:LEU:O	3:F:1820:HIS:ND1	2.35	0.59
3:F:1958:ARG:HH12	3:F:2004:THR:HB	1.66	0.59
3:H:1150:LEU:HD23	3:H:1157:PHE:HD2	1.68	0.59
2:D:211:THR:HG1	2:D:225:CYS:HG	1.50	0.59
3:E:1876:LEU:HD12	3:E:2084:ARG:HH21	1.68	0.59
3:F:642:LEU:HD21	3:F:673:LEU:HB3	1.84	0.59
2:D:205:ALA:O	2:D:206:HIS:ND1	2.36	0.59
3:E:2333:ILE:HD12	3:E:2454:ILE:HD12	1.85	0.59
3:F:2304:GLU:HG3	3:F:2308:LEU:HD23	1.83	0.59
3:E:836:VAL:HG11	3:E:1580:ARG:HE	1.67	0.59
3:F:2156:CYS:SG	3:F:2159:ARG:NH1	2.76	0.59
3:K:1217:LYS:O	3:K:1261:ARG:NH2	2.36	0.59
3:K:2043:ILE:HA	3:K:2046:ASN:HD22	1.65	0.59
1:A:914:VAL:HG12	1:A:1140:LEU:HD23	1.84	0.58
1:J:194:ASN:HD21	1:J:199:GLN:H	1.50	0.58
3:H:2424:LEU:HA	3:H:2427:LYS:HZ2	1.68	0.58
2:I:118:PRO:HB2	2:I:136:ARG:HH12	1.67	0.58
1:A:1332:VAL:HG11	1:A:1346:ASP:HB3	1.85	0.58
1:B:1332:VAL:HA	1:B:1348:PRO:HA	1.86	0.58
3:E:492:PRO:HD3	3:E:560:LYS:HG2	1.85	0.58
3:E:642:LEU:HD21	3:E:673:LEU:HB3	1.84	0.58
3:F:501:LEU:HD23	3:F:504:LEU:HD21	1.85	0.58
3:K:2108:GLN:OE1	3:K:2130:HIS:NE2	2.37	0.58
1:A:918:HIS:NE2	1:A:1140:LEU:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1365:LYS:HE3	3:E:1368:THR:HG23	1.86	0.58
3:F:2278:GLY:O	3:F:2280:ARG:NH1	2.36	0.58
3:H:2186:THR:HA	3:H:2286:MET:HA	1.86	0.58
1:J:55:PRO:HG2	1:J:58:ASP:HB2	1.84	0.58
1:B:361:ILE:HD13	1:B:425:TRP:HB2	1.86	0.58
3:E:2278:GLY:O	3:E:2280:ARG:NH1	2.36	0.58
3:E:1577:TRP:HB2	3:E:1598:ARG:HH21	1.69	0.58
2:L:194:ALA:HB3	2:L:196:HIS:HD2	1.68	0.58
3:F:823:LEU:HD11	3:F:862:ILE:HG23	1.86	0.58
1:A:353:GLU:HG2	1:A:526:PHE:HB2	1.86	0.58
3:F:1377:ASN:OD1	3:F:1407:LYS:NZ	2.37	0.58
3:E:850:LEU:HD22	3:E:870:ILE:HG22	1.85	0.58
3:H:1101:LYS:HG3	3:H:1102:ILE:HD12	1.86	0.58
3:H:2104:ILE:HB	3:H:2110:PRO:HG2	1.86	0.58
1:J:1411:GLN:HB2	1:J:1416:ARG:HA	1.86	0.58
3:K:1845:ARG:NH1	3:K:1848:THR:OG1	2.37	0.58
1:B:805:LEU:HD22	1:B:897:ILE:HD11	1.86	0.57
3:F:241:HIS:ND1	3:F:283:ASP:OD2	2.32	0.57
3:F:747:ILE:HG12	3:F:787:LEU:HD23	1.85	0.57
3:F:1574:ARG:HA	3:F:1577:TRP:CD1	2.39	0.57
1:B:618:ARG:NH1	1:B:1152:PHE:O	2.37	0.57
3:F:1883:ILE:HA	3:F:1886:ILE:HB	1.86	0.57
3:F:2085:ALA:HB3	3:F:2089:LYS:HB2	1.86	0.57
1:G:1523:SER:HB3	1:G:1537:THR:HG23	1.85	0.57
3:K:2257:ARG:NH2	3:K:2288:ASP:O	2.37	0.57
1:A:616:TRP:HA	1:A:619:ILE:HG22	1.86	0.57
1:A:770:ASN:HB3	1:A:773:ASN:HB2	1.85	0.57
3:E:356:MET:HG2	3:E:360:GLU:HG3	1.86	0.57
3:F:151:ILE:HG21	3:F:192:LEU:HG	1.85	0.57
1:A:41:TYR:O	1:A:1264:ASN:ND2	2.31	0.57
3:E:789:VAL:HB	3:E:828:GLN:HB3	1.87	0.57
1:G:1294:ILE:HD11	1:G:1297:ALA:HB2	1.87	0.57
3:H:1053:GLU:O	3:H:1056:GLN:NE2	2.37	0.57
3:H:1120:SER:HA	3:H:1123:ILE:HG12	1.85	0.57
3:E:823:LEU:HD13	3:E:865:GLY:HA3	1.87	0.57
3:F:1603:LYS:HE3	3:F:1605:LYS:HG2	1.86	0.57
1:A:1214:LEU:HB2	1:A:1227:ALA:HB3	1.86	0.57
1:G:194:ASN:HD21	1:G:199:GLN:H	1.53	0.57
1:G:538:GLU:HB3	1:G:573:LEU:HD11	1.86	0.57
1:J:1264:ASN:H	1:J:1319:GLN:HE22	1.52	0.57
1:J:1427:VAL:HG11	1:J:1471:ILE:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1523:SER:HB3	1:A:1537:THR:HG23	1.85	0.57
2:C:211:THR:OG1	2:C:225:CYS:SG	2.62	0.57
1:B:1351:THR:HB	1:B:1378:ARG:HH12	1.70	0.57
3:E:1237:LYS:O	3:E:1241:GLN:NE2	2.36	0.57
3:E:2134:ARG:NH2	3:E:2365:ASP:OD2	2.38	0.57
3:E:2258:ARG:NH2	3:E:2328:MET:O	2.38	0.57
2:L:9:GLY:HA3	2:L:295:ALA:HA	1.87	0.57
3:F:2138:LEU:HD21	3:F:2362:PHE:CG	2.40	0.56
1:G:537:PHE:HD2	1:G:573:LEU:HD21	1.70	0.56
2:C:215:LEU:HD21	2:C:219:VAL:HG13	1.87	0.56
3:E:236:LEU:HD23	3:E:240:ARG:HG3	1.87	0.56
3:F:811:GLN:HB3	3:F:849:ILE:HG12	1.87	0.56
1:G:55:PRO:HG2	1:G:58:ASP:HB2	1.88	0.56
1:G:1381:ASP:HB2	1:G:1391:ILE:HD11	1.86	0.56
1:J:836:LEU:HB2	1:J:864:ILE:HG21	1.87	0.56
3:K:994:VAL:HG13	3:K:998:ILE:HD11	1.87	0.56
3:K:1753:ASN:O	3:K:1759:TRP:NE1	2.34	0.56
3:K:2104:ILE:HB	3:K:2110:PRO:HG2	1.85	0.56
3:K:2456:GLN:OE1	3:K:2462:ASN:ND2	2.38	0.56
1:B:1263:ILE:HD11	1:B:1272:LEU:HD12	1.87	0.56
2:D:215:LEU:HD21	2:D:219:VAL:HG13	1.88	0.56
3:F:396:HIS:O	3:F:399:ARG:NH1	2.38	0.56
3:F:425:ALA:HA	3:F:432:ILE:HD13	1.87	0.56
3:F:1855:GLY:HA2	3:F:1892:ILE:HD11	1.86	0.56
1:G:925:ASN:HA	1:G:928:ILE:HD12	1.87	0.56
3:H:1878:VAL:O	3:H:1881:GLN:NE2	2.35	0.56
3:H:2050:LYS:O	3:H:2054:GLN:NE2	2.38	0.56
1:J:1294:ILE:HD11	1:J:1297:ALA:HB2	1.88	0.56
3:K:1136:ARG:O	3:K:1140:LYS:NZ	2.38	0.56
3:K:1326:GLU:HB2	3:K:1331:PRO:HB3	1.87	0.56
3:E:151:ILE:HG21	3:E:192:LEU:HG	1.87	0.56
3:E:1603:LYS:HD2	3:E:1604:PRO:HD2	1.87	0.56
1:J:1105:LYS:NZ	1:J:1306:LEU:HD12	2.20	0.56
1:B:306:LEU:HD13	3:F:760:PRO:HB3	1.87	0.56
3:E:93:LEU:HD21	3:E:135:ILE:HG12	1.87	0.56
3:H:1116:LEU:O	3:H:1120:SER:OG	2.23	0.56
2:I:223:ALA:HB3	2:I:258:PHE:HZ	1.70	0.56
3:K:1258:ALA:HA	3:K:1261:ARG:HH11	1.71	0.56
3:K:2319:ARG:NH2	3:K:2471:CYS:O	2.38	0.56
3:K:2439:ARG:HB2	3:K:2442:ASN:HB2	1.87	0.56
2:L:59:ASP:OD1	2:L:61:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1532:MET:HB3	1:A:1549:CYS:HB3	1.87	0.56
1:B:1304:MET:HG3	1:B:1329:ASP:HB2	1.86	0.56
3:F:1890:ASN:HB3	3:F:1893:VAL:HB	1.87	0.56
3:H:2309:ARG:NH1	3:H:2311:LYS:O	2.39	0.56
1:J:194:ASN:ND2	1:J:199:GLN:O	2.39	0.56
3:F:1547:ARG:HA	3:F:1550:ILE:HG12	1.88	0.56
3:F:2338:ARG:NH1	3:F:2451:ASP:OD1	2.39	0.56
3:H:953:LEU:HD22	3:H:956:ARG:HE	1.71	0.56
1:J:1321:ARG:NH1	1:J:1323:SER:OG	2.39	0.56
2:D:275:ARG:NH1	2:D:287:GLN:OE1	2.38	0.56
1:G:287:CYS:HB3	1:G:295:ILE:HG21	1.87	0.56
1:A:1263:ILE:HB	1:A:1270:LEU:HB2	1.86	0.56
1:B:194:ASN:HD21	1:B:198:THR:HG1	1.51	0.56
3:E:1523:ARG:HE	3:E:1526:LEU:HD21	1.71	0.56
3:E:1969:GLU:OE1	3:E:2130:HIS:NE2	2.38	0.56
3:K:1101:LYS:HG3	3:K:1102:ILE:HD12	1.87	0.56
3:K:1905:GLY:HA2	3:K:1909:PRO:HB3	1.87	0.56
3:K:2159:ARG:O	3:K:2263:ARG:NH1	2.38	0.56
3:K:2219:LEU:HD23	3:K:2224:LYS:HG2	1.88	0.56
1:B:882:ASP:OD1	1:B:884:ARG:NH2	2.39	0.56
2:I:59:ASP:HB2	2:I:68:VAL:HG21	1.87	0.56
1:A:710:ASP:HB3	1:A:752:ILE:HD13	1.88	0.55
3:F:976:PRO:HD2	3:F:979:GLN:HE22	1.70	0.55
3:H:2439:ARG:HB2	3:H:2442:ASN:HB2	1.87	0.55
1:B:1523:SER:HB3	1:B:1537:THR:HG23	1.86	0.55
3:E:2004:THR:HG23	3:E:2007:GLU:H	1.71	0.55
3:K:2042:ASP:O	3:K:2046:ASN:ND2	2.39	0.55
3:K:2349:ARG:NH2	3:K:2433:LEU:O	2.39	0.55
3:F:458:GLU:HG2	3:F:461:LEU:HD13	1.87	0.55
3:K:2150:LEU:HD11	3:K:2161:LEU:HB2	1.88	0.55
3:K:2257:ARG:NH1	3:K:2289:ARG:O	2.38	0.55
3:E:147:LYS:NZ	3:E:184:SER:O	2.39	0.55
1:G:1379:VAL:HG12	1:G:1391:ILE:HD12	1.87	0.55
3:H:956:ARG:NH1	3:H:959:SER:OG	2.40	0.55
1:A:64:ASN:O	1:A:64:ASN:ND2	2.30	0.55
1:A:152:CYS:SG	1:A:195:ARG:NH1	2.79	0.55
1:A:814:ASP:HA	1:A:817:VAL:HG12	1.87	0.55
3:F:2004:THR:HG23	3:F:2007:GLU:H	1.72	0.55
3:H:1020:ILE:HD13	3:H:1062:VAL:HG22	1.88	0.55
3:K:1045:LEU:HD21	3:K:1077:LEU:HD11	1.88	0.55
1:B:1214:LEU:HB2	1:B:1227:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1246:ARG:O	3:E:1250:GLN:NE2	2.39	0.55
3:F:2257:ARG:HD2	3:F:2292:GLY:HA3	1.87	0.55
3:E:1479:GLU:OE2	3:E:1596:ARG:NH1	2.40	0.55
1:G:354:LEU:HD11	1:G:432:VAL:HG21	1.88	0.55
3:H:1298:ILE:HD11	3:H:1332:LEU:HD22	1.88	0.55
3:K:2098:GLU:HB2	3:K:2114:CYS:HB3	1.88	0.55
1:B:216:CYS:HB2	1:B:262:CYS:HA	1.89	0.55
3:F:359:LYS:HG3	3:F:361:TYR:H	1.72	0.55
3:F:1299:GLN:O	3:F:1303:LYS:NZ	2.36	0.55
1:G:731:GLN:NE2	1:G:770:ASN:OD1	2.40	0.55
1:J:927:PHE:HA	1:J:930:VAL:HG22	1.87	0.55
3:K:2240:LEU:HA	3:K:2243:VAL:HG12	1.87	0.55
1:A:934:ASP:OD2	1:A:968:TRP:NE1	2.26	0.55
1:A:1177:ARG:HA	1:A:1180:ASN:HD22	1.72	0.55
2:C:200:VAL:HG12	2:C:201:THR:HG23	1.88	0.55
3:E:375:PRO:HB3	3:E:427:GLU:HG3	1.89	0.55
3:E:1299:GLN:O	3:E:1303:LYS:NZ	2.36	0.55
3:E:1386:ILE:HD12	3:E:1410:ARG:HH21	1.71	0.55
3:F:1217:LYS:O	3:F:1261:ARG:NH2	2.40	0.55
3:E:418:LEU:HA	3:E:421:ILE:HG12	1.89	0.55
3:F:1266:LEU:HA	3:F:1269:VAL:HG12	1.88	0.55
3:H:2162:ASP:OD1	3:H:2263:ARG:NH2	2.39	0.55
1:J:84:SER:HB3	1:J:163:LEU:HD22	1.89	0.55
2:L:33:SER:OG	2:L:34:GLN:N	2.40	0.55
1:B:171:ARG:HA	1:B:215:PRO:HB2	1.89	0.54
2:C:163:GLN:N	2:C:177:ALA:O	2.36	0.54
2:C:226:SER:OG	2:C:227:ALA:N	2.40	0.54
1:G:44:ASP:O	1:G:48:LYS:NZ	2.40	0.54
3:H:1128:VAL:HA	3:H:1131:LEU:HB2	1.89	0.54
2:C:121:GLU:HG3	2:C:164:SER:HA	1.88	0.54
1:A:784:GLU:HG2	2:I:13:THR:HG21	1.89	0.54
1:B:41:TYR:O	1:B:1264:ASN:ND2	2.38	0.54
1:B:1257:VAL:HA	1:B:1275:SER:HA	1.90	0.54
2:D:59:ASP:OD1	2:D:60:ILE:N	2.40	0.54
3:F:2333:ILE:HD12	3:F:2454:ILE:HD12	1.88	0.54
3:K:921:VAL:HA	3:K:924:HIS:CE1	2.41	0.54
1:A:823:GLN:HE22	1:G:195:ARG:HH12	1.56	0.54
3:E:359:LYS:HG3	3:E:361:TYR:H	1.72	0.54
1:G:186:LYS:O	1:G:231:ASN:ND2	2.40	0.54
3:H:1019:GLN:HA	3:H:1022:ILE:HD12	1.90	0.54
2:I:59:ASP:OD1	2:I:61:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:904:GLY:HA3	1:J:1341:GLU:HB3	1.90	0.54
1:A:805:LEU:HD12	1:A:897:ILE:HD11	1.89	0.54
1:B:616:TRP:HA	1:B:619:ILE:HG22	1.88	0.54
3:F:925:ASN:OD1	3:F:926:LEU:N	2.40	0.54
3:H:2186:THR:HG23	3:H:2189:VAL:H	1.73	0.54
1:B:1302:THR:HG23	1:B:1334:ARG:HH12	1.73	0.54
2:C:90:MET:HB2	2:C:102:TRP:HB2	1.90	0.54
2:C:275:ARG:NH1	2:C:287:GLN:OE1	2.41	0.54
1:A:257:SER:O	1:A:260:GLN:NE2	2.41	0.54
3:F:236:LEU:HD23	3:F:240:ARG:HG3	1.90	0.54
3:F:595:ARG:NH2	3:F:640:GLU:OE1	2.41	0.54
1:J:275:LEU:HD23	1:J:280:LEU:HD22	1.90	0.54
1:J:1525:MET:HA	1:J:1535:ALA:O	2.08	0.54
2:L:135:ASP:OD1	2:L:136:ARG:N	2.38	0.54
1:B:1391:ILE:HG22	1:B:1392:ARG:HG3	1.89	0.54
3:E:1616:ASN:OD1	3:E:1617:LEU:N	2.41	0.54
3:F:2145:LEU:HD21	3:F:2358:ILE:HG12	1.88	0.54
1:G:171:ARG:NH1	1:G:216:CYS:O	2.40	0.54
2:L:87:ASN:OD1	2:L:88:ARG:NH2	2.40	0.54
2:L:120:ASN:ND2	2:L:163:GLN:O	2.41	0.54
3:F:527:LEU:O	3:F:553:ARG:NH2	2.41	0.54
2:L:211:THR:OG1	2:L:225:CYS:SG	2.58	0.54
1:A:156:VAL:HA	1:A:159:PHE:HB3	1.90	0.54
1:B:805:LEU:HD23	1:B:893:ASN:HB3	1.90	0.54
3:E:1476:TRP:HE1	3:E:1600:LEU:HD13	1.73	0.54
2:I:9:GLY:HA3	2:I:295:ALA:HA	1.90	0.54
3:F:1856:ILE:HG22	3:F:1859:ALA:H	1.73	0.53
1:G:70:ILE:HD11	1:G:590:SER:HB3	1.89	0.53
2:I:165:LEU:HD12	2:I:174:LEU:HD11	1.91	0.53
3:E:820:ASP:OD1	3:E:820:ASP:N	2.42	0.53
1:G:108:ARG:HD2	1:G:116:LEU:HB2	1.89	0.53
1:J:79:ARG:NH1	1:J:381:HIS:O	2.41	0.53
3:E:354:SER:HB3	3:E:357:LYS:HZ1	1.72	0.53
3:E:966:PRO:HA	3:E:969:ILE:HG12	1.89	0.53
3:E:1655:TYR:HA	3:E:1658:LEU:HB2	1.91	0.53
3:K:1019:GLN:HA	3:K:1022:ILE:HD12	1.91	0.53
3:E:2219:LEU:HB2	3:E:2224:LYS:HG3	1.91	0.53
3:F:1024:SER:OG	3:F:1065:ARG:NH2	2.41	0.53
3:H:1730:GLN:NE2	3:H:1731:PRO:O	2.40	0.53
2:I:38:LEU:HA	2:I:49:THR:HA	1.90	0.53
1:J:125:ILE:HG21	1:J:149:LEU:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1876:LEU:O	3:K:2084:ARG:NH2	2.42	0.53
3:K:2365:ASP:N	3:K:2365:ASP:OD1	2.39	0.53
1:A:746:TYR:HB3	1:A:755:LEU:HD21	1.89	0.53
1:B:144:ARG:HH21	1:B:166:THR:HG21	1.72	0.53
3:E:1291:THR:HA	3:E:1294:GLN:HG2	1.91	0.53
3:E:2146:VAL:HG12	3:E:2355:LEU:HD11	1.91	0.53
1:J:854:GLN:HA	1:J:857:LEU:HD12	1.90	0.53
2:C:3:VAL:HG12	2:C:302:ASP:HA	1.90	0.53
3:F:1428:SER:OG	3:F:1430:GLU:OE1	2.27	0.53
3:H:2043:ILE:HA	3:H:2046:ASN:HD22	1.73	0.53
3:H:2240:LEU:HA	3:H:2243:VAL:HG12	1.90	0.53
2:I:162:LEU:HD11	2:I:176:ALA:HB1	1.90	0.53
3:K:920:THR:O	3:K:924:HIS:ND1	2.42	0.53
3:K:1049:LEU:HD12	3:K:1087:ILE:HD11	1.88	0.53
2:L:254:TRP:HE1	2:L:270:SER:HB3	1.74	0.53
1:A:1391:ILE:HG22	1:A:1392:ARG:HG3	1.91	0.53
2:D:121:GLU:HG3	2:D:164:SER:HA	1.90	0.53
3:E:1050:ASP:O	3:E:1054:ASN:HB2	2.08	0.53
3:E:1569:LYS:HE2	3:E:1570:ARG:HH22	1.73	0.53
3:E:1766:ASN:HA	3:E:1769:VAL:HG12	1.90	0.53
3:F:622:ILE:HG13	3:F:623:LYS:H	1.74	0.53
3:F:698:ILE:HD11	3:F:746:LEU:HD13	1.90	0.53
3:F:1132:ASN:OD1	3:F:1133:ASN:N	2.42	0.53
3:F:2463:LEU:O	3:F:2466:HIS:ND1	2.41	0.53
3:K:1085:MET:HG3	3:K:1119:MET:HG3	1.91	0.53
1:B:1537:THR:HB	1:B:1544:VAL:HG13	1.89	0.53
3:E:1365:LYS:NZ	3:E:1367:SER:OG	2.27	0.53
3:F:93:LEU:HD21	3:F:135:ILE:HG12	1.90	0.53
3:F:1301:LEU:HD21	3:F:1318:LEU:HD12	1.91	0.53
3:F:1402:GLU:HG3	3:F:1405:TYR:HD2	1.74	0.53
1:G:787:LEU:HA	1:G:790:LEU:HD12	1.91	0.53
1:G:854:GLN:HA	1:G:857:LEU:HD12	1.91	0.53
3:K:1175:HIS:HB3	3:K:1178:TYR:HB3	1.91	0.53
1:B:710:ASP:HB3	1:B:752:ILE:HD13	1.91	0.53
2:D:59:ASP:HB2	2:D:68:VAL:HG21	1.90	0.53
2:D:177:ALA:HB2	2:D:213:ILE:HD12	1.89	0.53
3:E:673:LEU:HD12	3:E:704:LEU:HD21	1.91	0.53
3:E:2085:ALA:HB3	3:E:2089:LYS:HB2	1.90	0.53
3:F:827:GLY:HA2	3:F:872:ILE:HD11	1.91	0.53
3:F:2329:GLU:HG3	3:F:2336:SER:HB3	1.91	0.53
1:G:217:ILE:HA	1:G:263:PHE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1175:HIS:HB3	3:H:1178:TYR:HB3	1.89	0.53
3:H:1777:SER:OG	3:H:1813:SER:N	2.41	0.53
3:H:2130:HIS:N	3:H:2174:LYS:O	2.41	0.53
2:D:97:GLY:HA2	2:D:118:PRO:HA	1.91	0.53
2:D:120:ASN:ND2	2:D:163:GLN:O	2.42	0.53
3:E:533:ILE:CG1	3:E:543:GLN:HE21	2.19	0.53
3:E:1401:LYS:HB2	3:E:1404:TRP:CE2	2.44	0.53
3:E:1726:ARG:HD3	3:E:1730:GLN:HE22	1.74	0.53
3:E:2109:ARG:O	3:E:2111:ARG:NH1	2.42	0.53
3:H:1042:PRO:HA	3:H:1045:LEU:HD12	1.90	0.53
1:J:376:LYS:HD3	1:J:380:ARG:HG3	1.91	0.53
1:A:567:ARG:HH22	1:A:600:LEU:HG	1.74	0.52
1:A:1362:GLN:HG3	1:A:1412:ARG:HG2	1.91	0.52
1:B:220:TYR:OH	1:B:264:GLN:OE1	2.27	0.52
2:C:6:VAL:HG21	2:C:40:ILE:HD11	1.91	0.52
3:F:198:GLY:O	3:F:201:THR:OG1	2.26	0.52
1:G:811:GLY:O	1:G:922:ARG:NH1	2.42	0.52
3:H:2193:GLU:HA	3:H:2196:GLU:HG3	1.91	0.52
2:I:226:SER:OG	2:I:227:ALA:N	2.42	0.52
3:K:1125:GLN:HA	3:K:1128:VAL:HG22	1.91	0.52
1:A:640:PHE:HA	1:A:643:VAL:HG12	1.91	0.52
3:E:761:ILE:HD13	3:E:787:LEU:HD21	1.91	0.52
3:E:1654:VAL:HA	3:E:1657:GLN:HE22	1.74	0.52
3:E:2063:LEU:HD21	3:E:2070:LEU:HB2	1.90	0.52
2:I:94:SER:OG	2:I:96:ASP:OD1	2.26	0.52
1:A:894:LEU:HD21	1:A:967:VAL:HG21	1.90	0.52
2:C:220:LYS:O	2:C:221:HIS:ND1	2.42	0.52
3:E:91:ASP:O	3:E:95:SER:HB2	2.10	0.52
3:E:198:GLY:O	3:E:201:THR:OG1	2.26	0.52
1:G:794:VAL:HG12	1:G:796:GLU:H	1.74	0.52
1:J:354:LEU:HA	1:J:357:ILE:HG22	1.91	0.52
3:K:1755:TRP:CE3	3:K:1758:ALA:HB2	2.44	0.52
3:E:969:ILE:CG2	3:E:1004:LYS:HZ2	2.23	0.52
3:E:2211:GLN:HE21	1:J:888:ARG:HH12	1.57	0.52
3:F:1002:VAL:HA	3:F:1005:ILE:HG22	1.91	0.52
3:F:2080:VAL:HG12	3:F:2092:VAL:HG11	1.91	0.52
2:I:168:ALA:HA	2:I:215:LEU:HD11	1.91	0.52
1:J:308:ASP:OD1	1:J:308:ASP:N	2.41	0.52
2:C:268:ALA:HB2	2:C:298:VAL:HB	1.92	0.52
3:E:1132:ASN:OD1	3:E:1133:ASN:N	2.43	0.52
3:E:1217:LYS:O	3:E:1261:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1816:LEU:O	3:E:1820:HIS:ND1	2.42	0.52
3:E:1948:GLN:HE22	3:E:2077:GLU:HG2	1.74	0.52
3:F:397:TYR:HA	3:F:400:TYR:HD2	1.75	0.52
3:H:1986:LYS:NZ	3:H:1990:ALA:HB2	2.25	0.52
1:J:747:ILE:HD12	1:J:756:ARG:HG2	1.90	0.52
1:J:968:TRP:HE1	1:J:990:ILE:HD11	1.75	0.52
3:K:941:ALA:HA	3:K:944:GLN:HG2	1.91	0.52
3:K:1190:CYS:SG	3:K:1191:LEU:N	2.82	0.52
1:A:1478:ILE:HG12	1:A:1522:LEU:HD11	1.92	0.52
3:E:1449:SER:HB3	3:E:1478:LEU:HD22	1.92	0.52
3:F:1955:GLU:OE1	3:F:2067:SER:OG	2.24	0.52
3:K:1829:PHE:HB3	3:K:1869:LEU:HD23	1.92	0.52
3:K:2076:LEU:HB3	3:K:2094:ILE:HB	1.92	0.52
2:L:118:PRO:HB2	2:L:136:ARG:HH12	1.73	0.52
3:E:2189:VAL:HA	3:E:2192:ARG:HG2	1.90	0.52
3:F:375:PRO:HB3	3:F:427:GLU:HG3	1.90	0.52
3:F:667:SER:OG	3:F:703:ARG:NH1	2.42	0.52
3:H:1019:GLN:HG2	3:H:1051:ILE:HD11	1.92	0.52
3:H:2363:ALA:HB1	3:H:2422:ALA:HB1	1.92	0.52
1:G:1523:SER:N	1:G:1537:THR:O	2.40	0.52
3:H:1049:LEU:HD12	3:H:1087:ILE:HD11	1.91	0.52
1:J:1106:LYS:N	1:J:1106:LYS:CD	2.72	0.52
3:E:622:ILE:HG13	3:E:623:LYS:H	1.74	0.52
3:E:1249:ILE:O	3:E:1253:LYS:NZ	2.35	0.52
3:F:864:ARG:O	3:F:868:ARG:NH1	2.42	0.52
1:G:91:LEU:HD21	1:G:179:HIS:HB2	1.91	0.52
1:G:156:VAL:HA	1:G:159:PHE:HB3	1.92	0.52
1:G:185:THR:HG22	1:G:187:SER:H	1.74	0.52
3:H:1898:LEU:HD23	3:H:1901:LEU:HD21	1.92	0.52
3:H:2444:LEU:HD22	3:H:2448:GLU:HG2	1.92	0.52
3:K:2130:HIS:N	3:K:2174:LYS:O	2.42	0.52
3:E:2145:LEU:HD21	3:E:2358:ILE:HG21	1.92	0.52
3:F:356:MET:HG2	3:F:360:GLU:HG3	1.91	0.52
3:F:1009:ILE:O	3:F:1013:PHE:HB2	2.09	0.52
1:G:624:TYR:O	1:G:628:GLN:HB3	2.10	0.52
3:H:981:ASP:OD1	3:H:982:PHE:N	2.42	0.52
1:J:1523:SER:N	1:J:1537:THR:O	2.39	0.52
1:A:824:GLU:OE1	1:A:824:GLU:N	2.35	0.51
3:E:396:HIS:O	3:E:399:ARG:NH1	2.43	0.51
3:F:1087:ILE:O	3:F:1091:MET:HG3	2.10	0.51
3:F:1614:PHE:CE2	3:F:1630:VAL:HG21	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1757:LYS:O	3:F:1761:ASN:ND2	2.43	0.51
1:G:237:GLN:HA	1:G:240:ILE:HG12	1.92	0.51
1:G:792:ASP:OD1	1:G:798:ARG:NH1	2.43	0.51
3:K:944:GLN:HA	3:K:947:MET:HE2	1.91	0.51
3:K:2444:LEU:HD22	3:K:2448:GLU:HG2	1.91	0.51
1:B:1263:ILE:HB	1:B:1270:LEU:HB2	1.91	0.51
1:B:1314:LEU:HD13	1:B:1355:ILE:HG22	1.91	0.51
3:E:86:LEU:HD23	3:E:131:LEU:HD13	1.92	0.51
3:E:688:ASP:H	3:E:694:GLN:HE21	1.58	0.51
3:E:2217:ASP:N	3:E:2217:ASP:OD1	2.43	0.51
1:G:813:GLN:HB3	1:G:816:GLU:HB3	1.92	0.51
1:J:811:GLY:O	1:J:922:ARG:NH1	2.44	0.51
1:J:1419:VAL:HG22	1:J:1429:LEU:HG	1.92	0.51
1:A:1006:PRO:O	1:A:1010:MET:HG2	2.11	0.51
2:D:99:ILE:HD11	2:D:119:VAL:HB	1.93	0.51
3:E:864:ARG:HA	3:E:867:VAL:HG12	1.91	0.51
3:E:1184:LYS:NZ	3:E:1189:GLU:OE2	2.44	0.51
3:E:1763:ALA:HB1	3:E:1828:PHE:HE1	1.76	0.51
3:E:2463:LEU:O	3:E:2466:HIS:ND1	2.43	0.51
3:F:278:LEU:HD11	3:F:365:VAL:HG13	1.92	0.51
3:H:1327:HIS:HD2	3:H:2246:LEU:HA	1.75	0.51
3:H:2201:PRO:HG2	3:H:2204:ILE:HB	1.91	0.51
2:L:226:SER:OG	2:L:227:ALA:N	2.44	0.51
2:L:276:LEU:HB3	2:L:286:ARG:HB2	1.91	0.51
1:B:1219:GLN:HA	1:B:1529:PRO:HG2	1.93	0.51
2:C:50:ALA:HB1	2:C:78:VAL:HG13	1.92	0.51
3:F:147:LYS:NZ	3:F:184:SER:O	2.42	0.51
3:F:2424:LEU:HA	3:F:2427:LYS:HZ3	1.74	0.51
1:G:1278:GLY:O	1:G:1300:GLY:N	2.40	0.51
1:G:1369:VAL:HG22	1:G:1379:VAL:HG22	1.91	0.51
2:I:200:VAL:HG12	2:I:201:THR:HG23	1.91	0.51
2:I:253:VAL:HA	2:I:269:SER:HB2	1.91	0.51
1:J:1317:TRP:HE1	1:J:1319:GLN:NE2	2.09	0.51
1:A:227:ASN:O	1:A:231:ASN:ND2	2.43	0.51
2:D:57:LEU:HB2	2:D:69:ALA:HB3	1.92	0.51
3:E:258:LEU:HD12	3:E:261:TYR:HB2	1.91	0.51
3:F:652:ASP:O	3:F:658:ARG:NH2	2.43	0.51
3:F:961:LEU:HA	3:F:964:ILE:HG22	1.93	0.51
3:F:2085:ALA:H	3:F:2089:LYS:HZ3	1.59	0.51
3:H:1257:SER:HG	3:H:1259:CYS:HG	1.57	0.51
3:H:2098:GLU:HB2	3:H:2114:CYS:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:2253:THR:O	3:H:2257:ARG:HG2	2.10	0.51
1:A:870:HIS:O	1:A:874:MET:HG2	2.11	0.51
1:B:1460:THR:OG1	1:B:1474:GLY:O	2.29	0.51
3:E:698:ILE:HD11	3:E:746:LEU:HD13	1.92	0.51
3:F:373:ILE:HA	3:F:376:LEU:HD12	1.93	0.51
3:F:806:ILE:HD12	3:F:826:LEU:HG	1.91	0.51
3:F:1948:GLN:HB2	3:F:2076:LEU:HD13	1.93	0.51
3:F:278:LEU:HD23	3:F:281:ARG:HH11	1.76	0.51
3:H:1755:TRP:CE3	3:H:1758:ALA:HB2	2.45	0.51
3:H:1829:PHE:HB3	3:H:1869:LEU:HD22	1.93	0.51
3:H:1905:GLY:HA2	3:H:1909:PRO:HB3	1.93	0.51
3:K:1898:LEU:HD23	3:K:1901:LEU:HD21	1.91	0.51
3:E:606:ASP:HB3	3:E:609:VAL:H	1.76	0.51
3:E:1519:ILE:O	3:E:1523:ARG:NH1	2.44	0.51
3:E:1916:LEU:HB3	3:E:1935:ILE:HD11	1.93	0.51
3:F:470:CYS:HA	3:F:507:LYS:HG2	1.92	0.51
1:G:307:LYS:NZ	1:G:312:LYS:O	2.38	0.51
3:H:1997:MET:HA	3:H:2000:ARG:HB2	1.93	0.51
1:A:1320:ILE:HD12	1:A:1363:LEU:HA	1.92	0.51
1:B:530:PHE:HD1	1:B:560:VAL:HG22	1.75	0.51
3:E:275:ASP:O	3:E:281:ARG:NH2	2.38	0.51
3:E:913:SER:OG	3:E:914:ASN:N	2.44	0.51
3:F:1851:PHE:HE2	3:F:1885:ARG:HE	1.58	0.51
3:F:2084:ARG:HA	3:F:2089:LYS:HZ3	1.76	0.51
1:G:772:LEU:HB2	1:G:878:LEU:HD13	1.92	0.51
3:H:1381:GLN:HG3	3:H:2258:ARG:HH22	1.76	0.51
1:J:93:LEU:HD12	1:J:124:ALA:HA	1.93	0.51
3:K:1324:PHE:HA	3:K:1327:HIS:CE1	2.45	0.51
3:E:671:PRO:O	3:E:675:GLN:NE2	2.43	0.51
3:E:2033:ASP:OD1	3:E:2033:ASP:N	2.43	0.51
1:G:164:ARG:HH22	1:G:215:PRO:HD2	1.76	0.51
1:G:1475:THR:OG1	1:G:1477:GLN:O	2.29	0.51
3:H:1125:GLN:HA	3:H:1128:VAL:HG22	1.92	0.51
3:H:1353:LEU:HB2	3:H:1375:ILE:HG21	1.93	0.51
1:J:1267:ASP:OD1	1:J:1267:ASP:N	2.43	0.51
2:C:91:VAL:HG21	2:C:124:ILE:HD11	1.93	0.50
2:C:161:SER:O	2:C:178:ASN:ND2	2.44	0.50
1:G:1264:ASN:HD22	1:G:1270:LEU:HD12	1.76	0.50
2:I:254:TRP:HE1	2:I:270:SER:HB3	1.76	0.50
2:C:120:ASN:ND2	2:C:163:GLN:O	2.44	0.50
3:F:784:LEU:HD11	3:F:802:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:969:ILE:HG22	3:H:973:ARG:HH22	1.74	0.50
1:A:1167:SER:OG	1:A:1168:VAL:N	2.44	0.50
3:F:961:LEU:HD11	3:F:994:VAL:HG11	1.94	0.50
2:I:194:ALA:HB3	2:I:196:HIS:HD2	1.77	0.50
3:K:1140:LYS:HA	3:K:1143:MET:HE2	1.92	0.50
1:B:870:HIS:O	1:B:874:MET:HG2	2.11	0.50
3:E:451:PHE:H	3:E:454:ARG:HB2	1.77	0.50
3:E:926:LEU:HA	3:E:929:ILE:HG12	1.92	0.50
3:E:2232:LEU:HD13	3:E:2322:ARG:HH21	1.76	0.50
3:E:2084:ARG:HA	3:E:2089:LYS:HZ3	1.76	0.50
3:E:2186:THR:HB	3:E:2189:VAL:HG22	1.93	0.50
3:F:2162:ASP:OD1	3:F:2163:ILE:N	2.44	0.50
1:J:608:LEU:HD13	1:J:611:ILE:HD11	1.94	0.50
1:A:106:CYS:SG	1:A:107:ALA:N	2.84	0.50
1:A:308:ASP:OD1	1:A:309:SER:N	2.44	0.50
1:B:874:MET:O	1:B:878:LEU:HG	2.12	0.50
3:E:349:ASP:N	3:E:349:ASP:OD1	2.43	0.50
3:E:555:GLN:HA	3:E:558:MET:HG3	1.94	0.50
3:F:2342:GLU:HB2	3:F:2446:VAL:HG12	1.94	0.50
1:G:909:ARG:NH1	1:G:1297:ALA:O	2.45	0.50
3:K:2282:PRO:HA	3:K:2285:LEU:HB2	1.93	0.50
1:A:859:GLN:HA	1:A:862:MET:SD	2.52	0.50
1:B:1321:ARG:NH1	1:B:1366:ASN:OD1	2.45	0.50
3:E:383:ALA:HB1	3:E:386:THR:HB	1.94	0.50
3:E:1605:LYS:NZ	3:E:1633:THR:O	2.45	0.50
3:E:1891:GLN:O	3:E:1895:ARG:NH1	2.45	0.50
3:E:2085:ALA:H	3:E:2089:LYS:HZ3	1.59	0.50
3:F:1481:TRP:HA	3:F:1484:ILE:HD12	1.94	0.50
3:H:2047:VAL:HG12	3:H:2050:LYS:HE2	1.94	0.50
3:K:1323:GLU:OE2	3:K:2245:TRP:NE1	2.44	0.50
3:E:1519:ILE:O	3:E:1523:ARG:HG2	2.10	0.50
3:F:1449:SER:HB3	3:F:1478:LEU:HD22	1.93	0.50
3:F:1712:THR:O	3:F:1715:LEU:HB3	2.12	0.50
1:G:173:LEU:HA	1:G:217:ILE:HG23	1.94	0.50
3:H:1995:TYR:HE1	3:H:2018:LEU:HB3	1.76	0.50
2:I:57:LEU:HB2	2:I:69:ALA:HB3	1.94	0.50
1:J:194:ASN:OD1	1:J:197:TYR:N	2.44	0.50
3:E:154:VAL:HG13	3:E:174:LEU:HD13	1.94	0.50
3:E:680:ARG:HA	3:E:683:PHE:CE1	2.47	0.50
3:E:1237:LYS:HB2	3:E:1241:GLN:HE22	1.77	0.50
3:E:1328:ASP:OD1	3:E:1329:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1883:ILE:HA	3:E:1886:ILE:HB	1.93	0.50
3:F:154:VAL:HG13	3:F:174:LEU:HD13	1.93	0.50
1:G:792:ASP:OD2	1:G:797:VAL:HG23	2.12	0.50
3:K:2185:ASP:N	3:K:2185:ASP:OD1	2.45	0.50
2:L:46:LEU:HD13	2:L:57:LEU:HD13	1.94	0.50
2:L:97:GLY:HA2	2:L:119:VAL:HG22	1.94	0.50
3:E:1444:GLU:HA	3:E:1629:LYS:HE3	1.93	0.49
3:F:934:SER:O	3:F:938:HIS:ND1	2.45	0.49
3:F:1570:ARG:O	3:F:1574:ARG:NH1	2.34	0.49
3:H:1952:VAL:O	3:H:1956:LEU:HD23	2.12	0.49
3:H:2192:ARG:HA	3:H:2202:LEU:HD11	1.93	0.49
1:J:794:VAL:HB	1:J:797:VAL:HG22	1.94	0.49
3:K:961:LEU:O	3:K:965:ILE:HG12	2.12	0.49
3:E:1841:GLN:OE1	3:E:1841:GLN:N	2.44	0.49
3:F:932:ASP:HA	3:F:935:LEU:HB2	1.94	0.49
3:K:905:LEU:O	3:K:908:GLN:NE2	2.45	0.49
3:K:2250:SER:H	3:K:2253:THR:HB	1.78	0.49
3:E:546:ILE:HD13	3:E:599:ILE:HD12	1.92	0.49
3:E:2421:ARG:HD3	3:E:2424:LEU:HD12	1.94	0.49
3:F:645:LEU:HD22	3:F:665:LEU:HD21	1.95	0.49
3:F:1726:ARG:HH21	3:F:1730:GLN:HE22	1.60	0.49
1:G:79:ARG:NH1	1:G:381:HIS:O	2.45	0.49
1:G:156:VAL:HG23	1:G:211:TRP:HZ3	1.77	0.49
1:A:111:ALA:O	1:A:131:ASN:ND2	2.46	0.49
1:A:113:VAL:HG21	1:A:127:GLN:HG2	1.94	0.49
1:A:882:ASP:OD1	1:A:885:LYS:N	2.37	0.49
3:E:486:ASN:OD1	3:E:487:LEU:N	2.45	0.49
3:E:550:ARG:HA	3:E:553:ARG:HG2	1.94	0.49
3:E:784:LEU:HD21	3:E:802:LEU:HD11	1.93	0.49
3:E:1334:ILE:HD11	3:E:1339:LEU:HD12	1.94	0.49
3:E:1523:ARG:NH2	3:E:1551:ILE:HG12	2.27	0.49
3:F:492:PRO:HD3	3:F:560:LYS:HG2	1.94	0.49
3:H:2033:ASP:OD2	3:H:2036:ASN:ND2	2.40	0.49
3:H:2205:GLU:HB3	3:H:2235:THR:HG21	1.93	0.49
3:K:2205:GLU:HB3	3:K:2235:THR:HG21	1.93	0.49
3:E:845:GLU:O	3:E:848:GLY:N	2.46	0.49
3:E:1903:ASP:HA	3:E:1906:LYS:HD3	1.95	0.49
3:F:1651:PRO:HD2	3:F:1711:TYR:HE1	1.78	0.49
1:G:792:ASP:O	1:G:798:ARG:NH1	2.42	0.49
3:H:932:ASP:OD1	3:H:933:PRO:HD3	2.12	0.49
3:H:978:SER:OG	3:H:979:GLN:OE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1844:LEU:HD21	3:H:2358:ILE:HD13	1.94	0.49
1:J:399:MET:HB3	1:J:404:CYS:HB2	1.93	0.49
3:E:1183:ASN:O	3:E:1187:ASN:ND2	2.45	0.49
3:F:987:LEU:HD12	3:F:990:LEU:HD12	1.94	0.49
1:G:84:SER:HB3	1:G:172:ILE:HG12	1.93	0.49
1:G:269:THR:HB	1:G:405:HIS:HB2	1.95	0.49
1:J:100:VAL:HG23	1:J:102:LYS:HZ1	1.77	0.49
1:J:343:MET:H	1:J:349:THR:HG21	1.77	0.49
1:J:708:THR:OG1	1:J:713:LYS:NZ	2.40	0.49
1:A:171:ARG:HA	1:A:215:PRO:HB2	1.95	0.49
1:B:917:SER:OG	1:B:1138:LEU:O	2.28	0.49
1:B:932:PHE:HB3	1:B:1074:LEU:HD13	1.92	0.49
2:C:210:ILE:HD11	2:C:224:THR:HB	1.93	0.49
3:F:909:GLY:HA2	3:F:912:PRO:HD2	1.95	0.49
1:G:931:VAL:HA	1:G:968:TRP:HZ3	1.76	0.49
3:H:1033:LEU:HB3	3:H:1036:GLU:HB2	1.94	0.49
1:A:267:SER:HG	1:A:285:PHE:HD2	1.60	0.49
1:A:299:ILE:HD13	1:A:398:ILE:HG23	1.94	0.49
2:C:233:VAL:HG11	2:C:279:LEU:HD21	1.94	0.49
1:G:1203:LEU:HD11	1:G:1548:LYS:HB2	1.95	0.49
1:G:1267:ASP:OD1	1:G:1268:SER:N	2.45	0.49
1:B:287:CYS:HB3	1:B:295:ILE:HG21	1.94	0.49
2:C:162:LEU:HD11	2:C:176:ALA:HB1	1.95	0.49
3:E:85:THR:OG1	3:E:86:LEU:N	2.45	0.49
1:G:107:ALA:HB2	1:G:276:MET:HA	1.95	0.49
3:H:1027:GLU:HB2	3:H:1031:LYS:NZ	2.28	0.49
3:H:2027:ASN:HA	3:H:2030:LYS:HG2	1.95	0.49
1:J:1191:LYS:HE2	1:J:1467:HIS:HB3	1.93	0.49
2:L:135:ASP:OD2	2:L:141:ARG:NH2	2.46	0.49
1:A:194:ASN:HD21	1:A:198:THR:HG1	1.59	0.49
3:E:1993:PRO:HA	3:E:1996:GLU:HG2	1.94	0.49
3:F:847:LEU:HA	3:F:850:LEU:HG	1.94	0.49
3:F:2201:PRO:HB2	3:F:2204:ILE:HB	1.95	0.49
1:G:88:LEU:HD23	1:G:176:TYR:HD1	1.77	0.49
1:G:1261:LYS:HB2	1:G:1272:LEU:HD23	1.95	0.49
1:A:764:GLY:O	1:A:807:HIS:ND1	2.35	0.48
1:A:1095:SER:OG	1:A:1096:ASN:N	2.44	0.48
1:B:1263:ILE:O	1:B:1269:ALA:HA	2.13	0.48
1:B:1359:THR:HG21	1:B:1409:HIS:HA	1.95	0.48
3:E:1024:SER:OG	3:E:1065:ARG:NH2	2.45	0.48
3:E:1445:TRP:HA	3:E:1448:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1332:LEU:HB3	3:F:1334:ILE:HG23	1.95	0.48
1:J:156:VAL:HG13	1:J:211:TRP:HZ3	1.78	0.48
3:K:2304:GLU:HB3	3:K:2307:ILE:HD13	1.95	0.48
3:E:548:LYS:HA	3:E:551:LYS:HE2	1.95	0.48
3:E:1909:PRO:O	3:E:1913:VAL:HG13	2.13	0.48
3:H:1914:TYR:HA	3:H:1917:MET:SD	2.52	0.48
3:K:1349:PHE:HB3	3:K:1378:GLN:HE22	1.78	0.48
3:K:1770:ILE:HG12	3:K:1817:ILE:HG22	1.95	0.48
1:B:182:PRO:HG2	1:B:191:TRP:CD1	2.48	0.48
1:B:308:ASP:OD1	1:B:309:SER:N	2.44	0.48
1:B:1167:SER:OG	1:B:1168:VAL:N	2.46	0.48
3:H:929:ILE:HG21	3:H:942:ALA:HB1	1.95	0.48
3:K:1878:VAL:O	3:K:1881:GLN:NE2	2.39	0.48
1:B:185:THR:OG1	1:B:189:GLU:OE1	2.31	0.48
2:C:122:VAL:HG13	2:C:131:LEU:HD11	1.94	0.48
3:E:1266:LEU:HA	3:E:1269:VAL:HG12	1.95	0.48
3:E:1603:LYS:HE3	3:E:1605:LYS:HG2	1.95	0.48
3:E:2075:ASP:HA	3:E:2093:LYS:HZ1	1.79	0.48
3:F:1244:ILE:HD11	3:F:1314:ILE:HD11	1.94	0.48
1:G:1167:SER:O	1:G:1171:ASN:ND2	2.46	0.48
1:J:931:VAL:HA	1:J:968:TRP:CZ3	2.48	0.48
3:H:2136:ASP:OD1	3:H:2137:SER:N	2.46	0.48
3:H:2169:ILE:HD12	3:H:2170:PRO:HD2	1.96	0.48
3:K:2356:MET:HA	3:K:2359:LEU:HG	1.94	0.48
1:B:82:THR:HG22	1:B:171:ARG:HB3	1.96	0.48
3:F:546:ILE:HD13	3:F:599:ILE:HD12	1.95	0.48
3:F:671:PRO:O	3:F:675:GLN:NE2	2.46	0.48
3:F:864:ARG:O	3:F:867:VAL:HG22	2.13	0.48
3:F:1401:LYS:HB2	3:F:1404:TRP:CE2	2.48	0.48
1:G:160:CYS:HB2	1:G:211:TRP:HB3	1.94	0.48
1:G:1430:TRP:CD1	1:G:1437:PRO:HA	2.48	0.48
1:B:1225:ILE:HD13	1:B:1271:LEU:HD13	1.95	0.48
2:C:260:ALA:N	2:C:302:ASP:OD2	2.46	0.48
3:E:154:VAL:HG22	3:E:174:LEU:HD22	1.93	0.48
3:E:225:LEU:HB2	3:E:240:ARG:HH22	1.78	0.48
3:F:1616:ASN:OD1	3:F:1617:LEU:N	2.47	0.48
3:F:1671:LEU:HD22	3:F:1726:ARG:HH22	1.78	0.48
1:J:1146:ASP:HA	1:J:1149:ARG:HG2	1.96	0.48
1:J:1261:LYS:HZ2	1:J:1317:TRP:H	1.62	0.48
3:K:1027:GLU:HB2	3:K:1031:LYS:NZ	2.29	0.48
3:K:1116:LEU:O	3:K:1120:SER:OG	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:991:ILE:HD12	3:E:998:ILE:HD13	1.96	0.48
3:E:1841:GLN:O	3:E:1845:ARG:HG2	2.13	0.48
3:E:2228:PHE:HD2	3:E:2460:VAL:HG13	1.79	0.48
1:G:275:LEU:HD23	1:G:280:LEU:HD22	1.95	0.48
1:G:931:VAL:HA	1:G:968:TRP:CZ3	2.49	0.48
3:K:1317:MET:HA	3:K:1320:ASN:HD22	1.78	0.48
3:K:2307:ILE:HA	3:K:2313:PRO:HB3	1.96	0.48
3:E:2064:GLN:HE21	3:E:2071:LEU:HD11	1.78	0.48
3:E:2243:VAL:O	3:E:2247:LYS:HG2	2.13	0.48
3:F:86:LEU:HD23	3:F:131:LEU:HD13	1.95	0.48
1:G:153:VAL:HA	1:G:156:VAL:HG22	1.96	0.48
1:G:194:ASN:OD1	1:G:197:TYR:N	2.47	0.48
3:H:1122:ARG:HA	3:H:1125:GLN:NE2	2.29	0.48
1:J:106:CYS:SG	1:J:107:ALA:N	2.87	0.48
1:J:113:VAL:HG11	1:J:127:GLN:HE22	1.78	0.48
1:A:1219:GLN:HA	1:A:1529:PRO:HG2	1.96	0.48
1:B:1199:TRP:H	1:B:1489:ASN:ND2	2.12	0.48
3:E:1087:ILE:O	3:E:1091:MET:HG3	2.14	0.48
3:E:1436:LEU:HD21	3:E:1455:LYS:HZ2	1.79	0.48
3:F:795:MET:N	3:F:795:MET:SD	2.87	0.48
3:F:2189:VAL:HA	3:F:2192:ARG:HG2	1.96	0.48
3:H:2309:ARG:HD2	3:H:2311:LYS:HG3	1.96	0.48
3:H:2456:GLN:O	3:H:2462:ASN:ND2	2.42	0.48
1:J:1391:ILE:HG22	1:J:1392:ARG:HG3	1.96	0.48
3:K:1051:ILE:O	3:K:1056:GLN:NE2	2.47	0.48
3:K:2363:ALA:HB1	3:K:2422:ALA:HB1	1.94	0.48
1:A:607:GLU:HG2	1:A:608:LEU:HD12	1.95	0.47
2:D:32:ASP:OD1	2:D:33:SER:N	2.47	0.47
3:E:677:ASP:OD1	3:E:678:ASN:N	2.47	0.47
3:E:925:ASN:OD1	3:E:926:LEU:N	2.47	0.47
3:F:1668:ASP:N	3:F:1668:ASP:OD1	2.46	0.47
1:G:308:ASP:OD1	1:G:308:ASP:N	2.46	0.47
1:G:354:LEU:HA	1:G:357:ILE:HG22	1.95	0.47
1:J:228:ILE:HG13	1:J:229:LEU:HD22	1.96	0.47
1:J:357:ILE:HD11	1:J:529:PHE:HB3	1.96	0.47
3:K:981:ASP:OD1	3:K:981:ASP:N	2.46	0.47
3:K:1914:TYR:HA	3:K:1917:MET:SD	2.54	0.47
1:A:287:CYS:HB3	1:A:295:ILE:HG21	1.96	0.47
2:C:285:VAL:O	2:C:286:ARG:NE	2.38	0.47
3:E:1948:GLN:HB2	3:E:2076:LEU:HD13	1.96	0.47
3:E:2174:LYS:HA	3:E:2174:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:349:THR:HG23	1:G:352:GLY:H	1.79	0.47
1:J:1359:THR:OG1	1:J:1408:VAL:O	2.31	0.47
3:E:405:ASP:N	3:E:405:ASP:OD1	2.47	0.47
3:E:1063:PRO:HA	3:E:1066:ILE:HG22	1.96	0.47
3:E:2080:VAL:HG12	3:E:2092:VAL:HG11	1.95	0.47
3:F:1673:GLN:HB3	3:F:1677:PHE:CE2	2.48	0.47
1:G:109:VAL:HG13	1:G:281:PRO:HA	1.96	0.47
1:G:985:LEU:HD11	1:G:1140:LEU:HD22	1.95	0.47
1:J:1167:SER:O	1:J:1171:ASN:ND2	2.48	0.47
3:K:1228:ALA:O	3:K:1243:TRP:NE1	2.46	0.47
3:E:505:ASN:ND2	3:E:516:ASN:OD1	2.47	0.47
3:E:909:GLY:HA2	3:E:912:PRO:HD2	1.96	0.47
3:E:1064:ILE:HG12	3:E:1102:ILE:HG13	1.96	0.47
3:H:1129:ARG:HA	3:H:1132:ASN:HD21	1.78	0.47
1:J:1288:ASP:OD2	1:J:1291:THR:OG1	2.32	0.47
3:K:1752:ASP:HB3	3:K:1755:TRP:HB2	1.96	0.47
3:K:1953:SER:O	3:K:1957:ILE:HD12	2.15	0.47
3:K:2210:LEU:HA	3:K:2213:ALA:HB3	1.96	0.47
1:B:106:CYS:SG	1:B:107:ALA:N	2.87	0.47
3:E:1595:LEU:HD21	3:E:1611:ARG:CZ	2.45	0.47
3:E:2259:THR:O	3:E:2263:ARG:HG3	2.14	0.47
3:F:248:LYS:HE3	3:F:286:VAL:HB	1.95	0.47
1:G:1419:VAL:HG22	1:G:1429:LEU:HG	1.97	0.47
3:H:1323:GLU:HA	3:H:1326:GLU:HB2	1.95	0.47
1:A:125:ILE:HG13	1:A:149:LEU:HA	1.97	0.47
1:B:609:LYS:O	1:B:613:VAL:HG23	2.15	0.47
1:B:921:SER:HB2	1:B:1138:LEU:HB3	1.96	0.47
3:E:2119:ASP:N	3:E:2119:ASP:OD1	2.47	0.47
3:F:1962:LEU:HD12	3:F:2006:ARG:HG2	1.96	0.47
1:G:728:PRO:HA	1:G:731:GLN:HG2	1.96	0.47
3:H:2274:ILE:HG23	3:H:2433:LEU:HD11	1.95	0.47
1:A:608:LEU:HB3	1:A:612:LEU:HD23	1.97	0.47
2:D:163:GLN:N	2:D:177:ALA:O	2.46	0.47
3:E:1416:ALA:HA	3:E:1419:ASN:HD22	1.80	0.47
3:E:1587:ASN:O	3:E:1591:TRP:HB2	2.15	0.47
3:E:2081:PRO:HB3	3:E:2169:ILE:HD11	1.95	0.47
3:E:2138:LEU:HD21	3:E:2368:ILE:HD12	1.97	0.47
3:F:383:ALA:HB1	3:F:386:THR:HB	1.97	0.47
3:F:1581:LEU:HD11	3:F:1591:TRP:CE2	2.50	0.47
3:F:1841:GLN:OE1	3:F:1841:GLN:N	2.43	0.47
3:F:2248:SER:OG	3:F:2253:THR:OG1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2275:LEU:HD22	3:F:2277:LEU:HB2	1.96	0.47
3:F:2437:ASP:OD1	3:F:2437:ASP:N	2.47	0.47
1:G:556:ILE:O	1:G:560:VAL:HG23	2.15	0.47
1:G:709:THR:N	1:G:712:GLN:OE1	2.48	0.47
1:J:286:SER:O	1:J:290:THR:HG22	2.14	0.47
1:J:382:ASP:N	1:J:382:ASP:OD1	2.48	0.47
3:K:1079:ASP:OD1	3:K:1079:ASP:N	2.47	0.47
3:K:1153:LEU:HG	3:K:1156:ASP:HB2	1.97	0.47
3:K:1839:SER:O	3:K:1839:SER:OG	2.27	0.47
1:A:1194:SER:HB2	1:A:1199:TRP:HZ2	1.79	0.47
1:A:1358:LEU:HD13	1:A:1370:ALA:HB2	1.95	0.47
2:D:109:ILE:HD12	2:D:110:PRO:HD2	1.97	0.47
3:E:397:TYR:CD1	3:E:417:ILE:HD11	2.50	0.47
3:E:667:SER:OG	3:E:703:ARG:NH1	2.47	0.47
3:E:2130:HIS:N	3:E:2174:LYS:O	2.48	0.47
3:F:225:LEU:HB2	3:F:240:ARG:HH22	1.80	0.47
3:F:1553:GLU:O	3:F:1557:ILE:HG12	2.15	0.47
3:F:1870:ILE:HG21	3:F:1875:TRP:HE1	1.80	0.47
1:G:608:LEU:HD13	1:G:611:ILE:HD11	1.97	0.47
3:H:2134:ARG:HH21	3:H:2367:LEU:HB3	1.80	0.47
3:H:2280:ARG:N	3:H:2470:TRP:HE1	2.13	0.47
1:J:882:ASP:OD2	1:J:885:LYS:HB2	2.15	0.47
3:K:1252:LEU:HD21	3:K:1277:LEU:HD21	1.97	0.47
3:K:2006:ARG:HD3	3:K:2006:ARG:HA	1.63	0.47
1:A:182:PRO:HG2	1:A:191:TRP:CD1	2.50	0.47
1:A:294:GLU:O	1:A:298:ARG:HG3	2.14	0.47
2:D:272:HIS:ND1	2:D:292:HIS:O	2.47	0.47
3:E:902:ASP:N	3:E:902:ASP:OD1	2.47	0.47
3:F:2224:LYS:HB3	3:F:2464:CYS:SG	2.55	0.47
1:G:737:LEU:HA	1:G:740:VAL:HG22	1.95	0.47
1:G:1522:LEU:HA	1:G:1538:ASN:HA	1.96	0.47
2:I:84:GLN:HE22	2:I:89:TRP:HD1	1.63	0.47
2:D:237:ASP:OD1	2:D:237:ASP:N	2.46	0.47
3:E:1616:ASN:O	3:E:1620:LYS:HG2	2.15	0.47
3:E:1879:LEU:HG	3:E:1880:PRO:HD3	1.96	0.47
3:F:677:ASP:OD1	3:F:678:ASN:N	2.48	0.47
3:H:961:LEU:HA	3:H:964:ILE:HG12	1.96	0.47
3:H:2195:ARG:HH22	3:H:2204:ILE:HG21	1.80	0.47
1:J:109:VAL:HG13	1:J:281:PRO:HA	1.97	0.47
1:J:787:LEU:HA	1:J:790:LEU:HD12	1.96	0.47
1:A:884:ARG:HD2	3:H:2207:TRP:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:2138:LEU:O	3:E:2141:GLN:HG3	2.15	0.46
3:H:2280:ARG:O	3:H:2470:TRP:NE1	2.48	0.46
1:J:171:ARG:HD3	1:J:217:ILE:HG12	1.97	0.46
1:J:1203:LEU:HD11	1:J:1548:LYS:HB2	1.96	0.46
1:B:641:VAL:HG23	1:B:739:LEU:HD13	1.98	0.46
3:E:546:ILE:HG12	3:E:596:LEU:HD23	1.97	0.46
3:E:1972:ASP:OD1	3:E:1973:ASP:N	2.48	0.46
3:F:1655:TYR:HA	3:F:1658:LEU:HB2	1.96	0.46
3:F:2211:GLN:OE1	1:G:888:ARG:NE	2.49	0.46
1:G:218:PHE:HB2	1:G:264:GLN:HB3	1.97	0.46
3:H:1037:PHE:HZ	3:H:1044:THR:HG21	1.81	0.46
2:I:16:PHE:HD2	2:I:26:ARG:HB3	1.80	0.46
1:J:269:THR:HB	1:J:405:HIS:HB2	1.96	0.46
3:E:1818:HIS:ND1	3:E:1858:GLU:OE2	2.47	0.46
3:E:2093:LYS:NZ	3:E:2094:ILE:O	2.48	0.46
3:E:2239:ASP:OD1	3:E:2240:LEU:N	2.48	0.46
3:F:1879:LEU:HA	3:F:1882:LEU:HB2	1.96	0.46
3:F:1970:GLY:HA3	3:F:1994:LEU:HD11	1.98	0.46
1:G:1392:ARG:HD3	1:G:1435:GLU:HG2	1.97	0.46
3:K:1965:GLU:HA	3:K:1968:TYR:HB3	1.98	0.46
1:A:1378:ARG:HD2	1:A:1393:ARG:HG3	1.97	0.46
3:E:1551:ILE:HD12	3:E:1554:LEU:HD21	1.97	0.46
3:F:258:LEU:HD12	3:F:261:TYR:HB2	1.98	0.46
3:F:1218:LEU:HD12	3:F:1256:PRO:HD3	1.96	0.46
3:F:1376:ASN:ND2	3:F:1384:SER:OG	2.34	0.46
3:F:1542:TYR:HA	3:F:1545:VAL:HG12	1.96	0.46
3:H:1914:TYR:OH	3:H:2079:ALA:O	2.34	0.46
3:H:2266:ALA:O	3:H:2270:MET:HG2	2.15	0.46
2:I:144:ASP:N	2:I:144:ASP:OD1	2.48	0.46
1:J:527:THR:OG1	1:J:528:GLY:N	2.49	0.46
3:K:2319:ARG:NH2	3:K:2474:TRP:O	2.49	0.46
1:B:750:SER:O	1:B:756:ARG:NE	2.48	0.46
2:C:135:ASP:OD1	2:C:136:ARG:N	2.48	0.46
3:E:404:ILE:HD11	3:E:412:SER:H	1.80	0.46
3:E:2444:LEU:HB3	3:E:2449:GLN:HB2	1.97	0.46
3:F:1282:PHE:HZ	3:F:1297:LEU:HD21	1.79	0.46
3:F:1629:LYS:HE2	3:F:1629:LYS:HB2	1.71	0.46
3:F:1948:GLN:HE22	3:F:2077:GLU:HG2	1.81	0.46
1:G:1264:ASN:N	1:G:1319:GLN:HE22	2.09	0.46
2:I:97:GLY:HA2	2:I:119:VAL:HG22	1.97	0.46
1:J:216:CYS:N	1:J:262:CYS:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:289:LEU:HA	1:J:391:ASN:HB3	1.98	0.46
1:A:874:MET:O	1:A:878:LEU:HG	2.16	0.46
2:D:90:MET:HB2	2:D:102:TRP:HB2	1.96	0.46
3:E:2201:PRO:HB2	3:E:2204:ILE:HB	1.98	0.46
3:F:1455:LYS:HA	3:F:1455:LYS:HD2	1.61	0.46
3:F:1605:LYS:NZ	3:F:1633:THR:O	2.48	0.46
3:F:1909:PRO:O	3:F:1913:VAL:HG13	2.15	0.46
3:F:2219:LEU:HB2	3:F:2224:LYS:HG3	1.98	0.46
1:A:234:LYS:HA	1:A:237:GLN:HG3	1.98	0.46
3:E:1722:GLN:HA	3:E:1725:TRP:HB2	1.97	0.46
3:F:349:ASP:OD1	3:F:349:ASP:N	2.49	0.46
3:F:913:SER:OG	3:F:914:ASN:N	2.47	0.46
1:G:927:PHE:O	1:G:931:VAL:HG23	2.16	0.46
3:H:921:VAL:HA	3:H:924:HIS:CE1	2.50	0.46
2:I:132:ILE:HG12	2:I:142:ILE:HG12	1.97	0.46
1:J:1278:GLY:O	1:J:1300:GLY:N	2.39	0.46
3:K:1240:TRP:O	3:K:1244:ILE:HG12	2.16	0.46
1:A:872:GLN:HA	1:A:875:GLN:HB2	1.97	0.46
3:E:867:VAL:HG13	3:E:868:ARG:NH2	2.31	0.46
3:E:2166:TYR:HE2	3:E:2178:LEU:HD12	1.81	0.46
3:F:810:PHE:HE1	3:F:823:LEU:HD23	1.81	0.46
3:F:1305:LEU:HD21	3:F:1318:LEU:HB2	1.97	0.46
1:J:731:GLN:NE2	1:J:770:ASN:OD1	2.48	0.46
1:J:1407:ASN:HB2	1:J:1462:MET:HB3	1.98	0.46
3:K:2044:TYR:HA	3:K:2047:VAL:HG22	1.96	0.46
3:K:2315:LYS:NZ	3:K:2456:GLN:OE1	2.48	0.46
2:L:142:ILE:HB	2:L:152:HIS:HB2	1.97	0.46
1:A:610:PRO:HA	1:A:613:VAL:HG12	1.98	0.46
1:A:1000:HIS:HB3	1:A:1003:LEU:HB3	1.97	0.46
1:B:125:ILE:HG13	1:B:149:LEU:HA	1.98	0.46
1:B:609:LYS:HD3	1:B:643:VAL:HG23	1.97	0.46
3:E:857:GLU:OE1	3:E:859:ASN:N	2.38	0.46
3:E:1335:PRO:HG2	3:E:1338:THR:HG22	1.98	0.46
2:I:134:CYS:HB3	2:I:165:LEU:HD22	1.98	0.46
1:J:73:TRP:CE3	1:J:589:LEU:HB3	2.51	0.46
3:K:1755:TRP:HE3	3:K:1758:ALA:HB2	1.79	0.46
3:K:2076:LEU:HG	3:K:2078:LEU:HG	1.97	0.46
2:D:55:VAL:HG13	2:D:71:PHE:HD2	1.81	0.46
3:E:1002:VAL:HA	3:E:1005:ILE:HG22	1.97	0.46
3:E:1578:ASN:ND2	3:E:1610:VAL:HG11	2.30	0.46
3:E:1972:ASP:HB3	3:E:2048:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:902:ASP:OD1	3:F:902:ASP:N	2.49	0.46
3:F:1089:VAL:HG11	3:F:1122:ARG:HG2	1.96	0.46
3:F:1127:LEU:HD23	3:F:1130:ILE:HD12	1.97	0.46
3:F:2424:LEU:HD23	3:F:2427:LYS:NZ	2.30	0.46
1:G:1235:VAL:O	1:G:1244:LEU:N	2.46	0.46
3:H:2076:LEU:HB3	3:H:2094:ILE:HB	1.98	0.46
1:J:358:PHE:O	1:J:362:THR:HG22	2.15	0.46
3:E:622:ILE:HG13	3:E:623:LYS:N	2.31	0.45
3:F:1294:GLN:O	3:F:1298:ILE:HD12	2.16	0.45
3:K:1095:SER:OG	3:K:1096:ALA:N	2.48	0.45
1:B:357:ILE:HG23	1:B:425:TRP:HZ3	1.81	0.45
3:E:1589:ASP:OD1	3:E:1589:ASP:N	2.48	0.45
3:E:2318:PHE:HZ	3:E:2454:ILE:HG22	1.81	0.45
1:G:286:SER:O	1:G:290:THR:HG22	2.16	0.45
1:G:1179:ARG:HH22	1:G:1220:PHE:HB3	1.81	0.45
1:G:1215:MET:HG2	1:G:1226:THR:HG22	1.98	0.45
1:A:1257:VAL:HA	1:A:1275:SER:HA	1.98	0.45
1:B:564:GLN:HB2	1:B:567:ARG:HH12	1.80	0.45
2:C:237:ASP:OD1	2:C:237:ASP:N	2.48	0.45
3:E:647:MET:HG2	3:F:1159:VAL:HG23	1.97	0.45
3:E:934:SER:O	3:E:938:HIS:ND1	2.50	0.45
3:E:1493:SER:O	3:E:1498:LYS:NZ	2.45	0.45
3:E:1568:ASP:OD1	3:E:1569:LYS:N	2.49	0.45
3:F:154:VAL:HG22	3:F:174:LEU:HD22	1.97	0.45
3:F:1632:ASN:OD1	3:F:1633:THR:N	2.50	0.45
3:F:2154:ALA:HA	3:F:2157:PHE:HB2	1.98	0.45
1:G:125:ILE:HG21	1:G:149:LEU:HA	1.98	0.45
3:H:1976:ARG:NH1	3:H:1977:GLN:HB3	2.31	0.45
1:J:171:ARG:HG3	1:J:215:PRO:HB2	1.97	0.45
1:J:367:TRP:CE2	1:J:591:ILE:HD11	2.51	0.45
1:J:554:LEU:HA	1:J:557:VAL:HG12	1.99	0.45
1:J:601:LEU:HD23	1:J:612:LEU:HD21	1.98	0.45
3:E:1995:TYR:O	3:E:1999:LYS:NZ	2.50	0.45
3:F:550:ARG:HA	3:F:553:ARG:HG2	1.98	0.45
3:F:1247:LEU:O	3:F:1251:LEU:HG	2.17	0.45
3:F:1328:ASP:OD1	3:F:1329:ASP:N	2.49	0.45
3:F:1767:PHE:HD1	3:F:1849:LEU:HD21	1.81	0.45
1:G:103:THR:OG1	1:G:105:PRO:O	2.27	0.45
1:G:216:CYS:HB2	1:G:262:CYS:HB2	1.55	0.45
1:G:578:LEU:O	1:G:618:ARG:NH1	2.49	0.45
3:H:2338:ARG:O	3:H:2341:CYS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:TYR:HD2	1:A:1100:LYS:HE2	1.82	0.45
1:B:556:ILE:O	1:B:560:VAL:HG23	2.17	0.45
1:B:921:SER:HA	1:B:1138:LEU:HD23	1.98	0.45
1:B:992:TYR:CD2	1:B:1138:LEU:HD22	2.51	0.45
1:B:1479:LYS:HZ3	1:B:1487:LEU:HD13	1.82	0.45
2:D:6:VAL:HG21	2:D:40:ILE:HD11	1.98	0.45
2:D:42:ASN:OD1	2:D:43:ASP:N	2.50	0.45
3:E:330:LEU:HB3	3:E:373:ILE:HD13	1.99	0.45
3:E:1282:PHE:HZ	3:E:1297:LEU:HD21	1.82	0.45
3:E:1991:LEU:HD13	3:E:2025:LEU:HD21	1.97	0.45
3:E:2156:CYS:HA	3:E:2159:ARG:HH21	1.81	0.45
3:F:673:LEU:HD12	3:F:704:LEU:HD21	1.97	0.45
1:J:103:THR:OG1	1:J:105:PRO:O	2.27	0.45
3:K:1078:GLU:HB3	3:K:1114:ILE:HG22	1.97	0.45
3:K:2334:GLU:HA	3:K:2338:ARG:HG3	1.99	0.45
1:A:1077:LEU:O	1:A:1080:SER:OG	2.34	0.45
3:E:770:GLN:HG2	3:E:772:ALA:H	1.81	0.45
3:E:1758:ALA:HA	3:E:1761:ASN:HD21	1.81	0.45
3:E:1813:SER:OG	3:E:1815:ASN:OD1	2.35	0.45
3:E:2059:GLN:HA	3:E:2103:VAL:HG22	1.97	0.45
3:E:2448:GLU:O	3:E:2452:LYS:HG2	2.16	0.45
3:F:240:ARG:HB2	3:F:280:ILE:HD13	1.99	0.45
3:F:367:ARG:NH1	3:F:413:ASP:OD2	2.49	0.45
3:F:606:ASP:OD1	3:F:608:SER:N	2.46	0.45
3:F:1045:LEU:HD11	3:F:1084:ILE:HG13	1.99	0.45
3:F:1916:LEU:HB3	3:F:1935:ILE:HD11	1.97	0.45
3:F:2303:PHE:HB3	3:F:2425:VAL:HG21	1.98	0.45
1:G:205:LEU:HD23	1:G:232:PHE:HD1	1.82	0.45
3:H:1840:LEU:HD13	3:H:1878:VAL:HG22	1.98	0.45
3:H:1875:TRP:HB2	3:H:1904:LEU:HD21	1.97	0.45
1:A:88:LEU:HD23	1:A:176:TYR:HD1	1.82	0.45
1:A:811:GLY:H	1:A:922:ARG:HH12	1.65	0.45
1:B:1333:ILE:N	1:B:1347:ILE:O	2.44	0.45
2:C:57:LEU:HB2	2:C:69:ALA:HB3	1.98	0.45
2:D:210:ILE:HD11	2:D:224:THR:HB	1.97	0.45
2:D:211:THR:OG1	2:D:225:CYS:SG	2.63	0.45
2:D:218:ASP:OD1	2:D:218:ASP:N	2.46	0.45
3:E:732:MET:SD	3:E:734:LYS:HB3	2.57	0.45
3:E:987:LEU:HD12	3:E:990:LEU:HD12	1.98	0.45
3:E:2437:ASP:N	3:E:2437:ASP:OD1	2.50	0.45
3:E:2467:TYR:HD2	3:E:2469:GLY:H	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:85:THR:OG1	3:F:86:LEU:N	2.47	0.45
3:F:178:LEU:HD13	3:F:197:LEU:HG	1.99	0.45
3:F:925:ASN:HA	3:F:928:LYS:NZ	2.32	0.45
3:F:2081:PRO:HB3	3:F:2169:ILE:HD11	1.97	0.45
1:G:1361:ASP:N	1:G:1361:ASP:OD1	2.45	0.45
1:G:1412:ARG:N	1:G:1466:GLU:O	2.50	0.45
1:A:557:VAL:HA	1:A:560:VAL:HG12	1.98	0.45
1:A:558:LEU:HG	1:A:593:ILE:HD13	1.98	0.45
3:E:527:LEU:O	3:E:553:ARG:NH2	2.50	0.45
3:E:747:ILE:HG12	3:E:787:LEU:HD23	1.99	0.45
3:E:823:LEU:HD11	3:E:862:ILE:HG23	1.98	0.45
3:E:825:THR:HG23	3:E:826:LEU:HD12	1.98	0.45
3:E:1446:GLU:O	3:E:1449:SER:OG	2.27	0.45
3:E:1913:VAL:HA	3:E:1916:LEU:HD12	1.98	0.45
3:E:1963:TRP:HA	3:E:1966:GLN:OE1	2.17	0.45
3:F:945:ALA:O	3:F:949:ILE:HG12	2.16	0.45
1:J:1429:LEU:HD21	1:J:1483:THR:HB	1.99	0.45
3:K:1135:ASP:OD1	3:K:1135:ASP:N	2.49	0.45
1:A:988:GLN:HB3	1:A:1136:LEU:HD21	1.98	0.45
1:B:1249:ASN:HB3	1:B:1251:THR:HG23	1.98	0.45
2:C:42:ASN:OD1	2:C:42:ASN:N	2.50	0.45
3:E:501:LEU:HD23	3:E:504:LEU:HD21	1.99	0.45
3:E:768:LYS:HA	3:E:768:LYS:HD2	1.84	0.45
3:E:867:VAL:HG23	3:E:870:ILE:HD11	1.99	0.45
3:E:1370:GLU:HG2	3:E:1404:TRP:HE1	1.82	0.45
3:E:2143:PHE:HA	3:E:2146:VAL:HG22	1.99	0.45
3:F:418:LEU:HA	3:F:421:ILE:HG12	1.97	0.45
3:F:1660:TYR:HD2	3:F:1661:LEU:HD22	1.81	0.45
3:F:1713:LYS:HZ1	3:F:1717:ARG:HG2	1.82	0.45
1:G:433:LEU:HD23	1:G:433:LEU:HA	1.80	0.45
3:H:918:TYR:HE2	3:H:1284:SER:HB3	1.82	0.45
3:H:967:GLY:O	3:H:971:VAL:HG23	2.17	0.45
3:H:1102:ILE:HA	3:H:1105:ILE:HG12	1.99	0.45
3:H:2017:ASP:OD2	3:H:2050:LYS:NZ	2.43	0.45
3:H:2083:THR:HB	3:H:2167:PRO:HG3	1.98	0.45
2:I:185:VAL:HG13	2:I:200:VAL:HB	1.99	0.45
1:J:386:ALA:O	1:J:390:ARG:HB2	2.17	0.45
3:K:1844:LEU:O	3:K:1848:THR:HG23	2.17	0.45
3:K:2195:ARG:HE	3:K:2200:ILE:HG13	1.81	0.45
1:B:794:VAL:HG23	1:B:797:VAL:HG22	1.98	0.45
2:C:9:GLY:HA2	2:C:296:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:847:LEU:HA	3:E:850:LEU:HG	1.97	0.45
1:G:155:ASP:HA	1:G:158:ARG:NH1	2.32	0.45
1:G:174:PHE:HB3	1:G:218:PHE:CD1	2.52	0.45
1:J:86:ALA:HB1	1:J:159:PHE:CZ	2.52	0.45
1:J:433:LEU:HD23	1:J:433:LEU:HA	1.80	0.45
3:K:1766:ASN:HB2	3:K:1824:ALA:HB2	1.99	0.45
3:K:1939:ARG:HE	3:K:1943:PRO:HB3	1.82	0.45
3:K:2027:ASN:HA	3:K:2030:LYS:HG2	1.98	0.45
2:L:3:VAL:N	2:L:44:LYS:HZ1	2.14	0.45
2:L:160:THR:OG1	2:L:178:ASN:ND2	2.46	0.45
1:A:376:LYS:HB3	1:A:376:LYS:HE2	1.73	0.44
1:A:834:SER:O	1:A:838:HIS:ND1	2.50	0.44
2:C:109:ILE:HD12	2:C:110:PRO:HD2	1.99	0.44
2:D:99:ILE:HG21	2:D:131:LEU:HD21	1.99	0.44
3:E:383:ALA:HB3	3:E:389:TYR:H	1.82	0.44
3:E:811:GLN:HB3	3:E:849:ILE:HG12	1.99	0.44
3:E:1168:LEU:HD22	3:E:1173:ILE:HB	1.99	0.44
3:E:1178:TYR:O	3:E:1182:VAL:HG23	2.18	0.44
3:E:1247:LEU:HA	3:E:1250:GLN:HE22	1.82	0.44
3:E:1481:TRP:HA	3:E:1484:ILE:HD12	1.99	0.44
3:F:622:ILE:HG13	3:F:623:LYS:N	2.31	0.44
3:F:1353:LEU:O	3:F:1357:GLU:HG2	2.16	0.44
3:F:1972:ASP:OD1	3:F:1972:ASP:N	2.49	0.44
3:H:2134:ARG:NH2	3:H:2367:LEU:HB3	2.31	0.44
1:J:927:PHE:HB3	1:J:993:ILE:HD11	1.98	0.44
2:D:5:LEU:HG	2:D:17:TRP:HB2	1.98	0.44
2:D:226:SER:OG	2:D:227:ALA:N	2.50	0.44
3:E:1945:LEU:HD12	3:E:1948:GLN:HE21	1.82	0.44
3:F:1405:TYR:HB3	3:F:1410:ARG:HB2	1.98	0.44
1:G:376:LYS:HD3	1:G:380:ARG:HG3	1.98	0.44
1:A:1249:ASN:HB3	1:A:1251:THR:HG23	1.98	0.44
1:A:1314:LEU:HD13	1:A:1355:ILE:HG22	1.99	0.44
1:B:427:LEU:HD11	3:F:713:VAL:HG12	1.98	0.44
1:B:1406:ASN:ND2	1:B:1459:MET:O	2.49	0.44
2:D:229:HIS:NE2	2:D:250:GLN:O	2.46	0.44
3:E:309:ARG:HA	3:E:309:ARG:HD3	1.73	0.44
3:E:737:GLU:O	3:E:741:THR:HG22	2.18	0.44
3:E:863:ARG:O	3:E:866:THR:OG1	2.30	0.44
3:E:1101:LYS:HA	3:E:1104:ILE:HG12	1.97	0.44
3:F:472:LEU:HD23	3:F:472:LEU:HA	1.87	0.44
3:F:1591:TRP:CD1	3:F:1614:PHE:HD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:527:THR:OG1	1:G:528:GLY:N	2.49	0.44
1:J:153:VAL:HA	1:J:156:VAL:HG12	2.00	0.44
1:J:1489:ASN:OD1	1:J:1490:SER:N	2.49	0.44
1:A:84:SER:HB3	1:A:163:LEU:HD22	1.99	0.44
1:B:395:ALA:HA	1:B:398:ILE:HG22	1.99	0.44
1:B:1479:LYS:NZ	1:B:1487:LEU:HD13	2.32	0.44
3:E:1049:LEU:HD21	3:E:1087:ILE:HG13	1.99	0.44
3:F:281:ARG:HB3	3:F:331:LEU:HD13	1.98	0.44
3:F:1587:ASN:O	3:F:1591:TRP:HB2	2.17	0.44
3:F:1891:GLN:HG2	3:F:1892:ILE:H	1.82	0.44
1:G:356:TRP:HZ2	1:G:560:VAL:HA	1.83	0.44
1:G:1489:ASN:OD1	1:G:1490:SER:N	2.50	0.44
3:H:1752:ASP:HB3	3:H:1755:TRP:HB2	2.00	0.44
3:H:2053:LYS:O	3:H:2056:PRO:HD2	2.17	0.44
1:J:148:SER:HB2	1:J:151:PRO:HG3	2.00	0.44
1:J:911:GLU:HA	1:J:914:VAL:HG12	1.99	0.44
3:K:1115:ASN:OD1	3:K:1152:GLN:NE2	2.50	0.44
3:E:367:ARG:NH1	3:E:413:ASP:OD2	2.50	0.44
3:F:606:ASP:OD1	3:F:607:SER:N	2.51	0.44
1:G:1429:LEU:HD11	1:G:1471:ILE:HD11	2.00	0.44
3:H:2250:SER:H	3:H:2253:THR:HB	1.83	0.44
3:H:2315:LYS:O	3:H:2456:GLN:NE2	2.43	0.44
1:J:367:TRP:CD2	1:J:591:ILE:HD11	2.52	0.44
1:J:934:ASP:HB3	1:J:968:TRP:HZ3	1.82	0.44
1:A:45:LYS:O	1:A:49:THR:OG1	2.23	0.44
1:A:171:ARG:NH1	1:A:261:ASP:OD1	2.39	0.44
3:E:1323:GLU:OE1	3:E:1355:TYR:OH	2.32	0.44
3:H:1726:ARG:NE	3:H:1730:GLN:OE1	2.42	0.44
1:A:711:GLU:O	1:A:715:MET:HG2	2.17	0.44
1:A:777:CYS:HA	1:A:780:THR:HG22	1.99	0.44
1:B:311:TYR:HE1	1:B:338:VAL:HG22	1.83	0.44
1:B:903:ASP:OD1	1:B:903:ASP:N	2.46	0.44
3:E:2135:GLN:HA	3:E:2138:LEU:HG	1.99	0.44
3:F:222:TRP:HE3	3:F:243:ALA:HB2	1.83	0.44
3:F:309:ARG:HD3	3:F:309:ARG:HA	1.71	0.44
3:F:732:MET:SD	3:F:734:LYS:HB3	2.58	0.44
3:F:1439:LEU:HD12	3:F:1448:LEU:HD23	2.00	0.44
3:F:1570:ARG:NH2	3:F:1573:MET:HG3	2.33	0.44
3:F:1738:PRO:HA	3:F:1741:ILE:HG12	2.00	0.44
3:F:2186:THR:HG22	3:F:2286:MET:HE2	1.99	0.44
1:G:645:VAL:HG22	1:G:742:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:794:VAL:HB	1:G:797:VAL:HG22	1.99	0.44
3:H:924:HIS:O	3:H:928:LYS:NZ	2.40	0.44
3:H:1157:PHE:O	3:H:1161:VAL:HG23	2.17	0.44
3:H:1953:SER:O	3:H:1957:ILE:HD12	2.18	0.44
1:J:133:GLN:HE21	1:J:145:TYR:HD2	1.66	0.44
1:J:728:PRO:HA	1:J:731:GLN:HG2	1.98	0.44
3:K:1952:VAL:HG23	3:K:2070:LEU:HD22	1.99	0.44
1:A:348:ARG:HH12	1:A:563:SER:HB2	1.83	0.44
1:A:924:SER:O	1:A:928:ILE:HG12	2.18	0.44
3:E:946:ILE:HA	3:E:949:ILE:HG12	1.99	0.44
3:F:334:ARG:HH22	3:F:372:ALA:HB3	1.83	0.44
3:F:555:GLN:HA	3:F:558:MET:HG3	2.00	0.44
3:F:731:ASN:HA	3:F:736:LYS:HE3	2.00	0.44
3:F:1363:GLU:HA	3:F:1364:PRO:HD3	1.91	0.44
3:F:1379:LEU:HB3	3:F:1381:GLN:OE1	2.18	0.44
3:H:977:PRO:HA	3:H:980:LEU:HG	2.00	0.44
2:I:42:ASN:OD1	2:I:43:ASP:N	2.51	0.44
3:K:950:PHE:HD1	3:K:953:LEU:HD21	1.82	0.44
3:K:2280:ARG:H	3:K:2470:TRP:HE1	1.66	0.44
1:A:934:ASP:OD1	1:A:965:TYR:OH	2.32	0.44
1:B:884:ARG:HD2	3:K:2207:TRP:CD2	2.53	0.44
2:C:32:ASP:OD1	2:C:33:SER:N	2.51	0.44
3:E:244:LEU:HD22	3:E:284:ALA:HA	1.99	0.44
3:F:536:ASN:OD1	3:F:537:GLN:N	2.51	0.44
3:F:659:LEU:HD21	3:F:690:ILE:HG13	2.00	0.44
3:F:737:GLU:O	3:F:741:THR:HG22	2.18	0.44
3:K:1298:ILE:HD11	3:K:1332:LEU:HD22	1.99	0.44
1:A:56:GLU:HA	1:A:59:LYS:HB2	2.00	0.43
1:B:613:VAL:HG21	1:B:643:VAL:HG21	2.00	0.43
3:F:139:ILE:HG22	3:F:147:LYS:HA	1.98	0.43
3:F:1495:SER:O	3:F:1498:LYS:HG2	2.17	0.43
3:F:1822:ILE:HA	3:F:1825:ILE:HG12	2.00	0.43
3:F:1895:ARG:HA	3:F:1898:LEU:HG	1.99	0.43
3:H:1761:ASN:HA	3:H:1764:LEU:HG	2.00	0.43
1:A:171:ARG:HD2	1:A:385:ILE:HD11	2.00	0.43
1:A:869:ARG:O	1:A:873:VAL:HG23	2.18	0.43
2:D:29:GLN:OE1	1:J:781:GLY:O	2.36	0.43
3:F:163:SER:HB2	3:F:167:LEU:HG	2.00	0.43
3:F:1523:ARG:HA	3:F:1526:LEU:HG	1.99	0.43
3:F:1929:LYS:HD3	3:F:1932:LEU:HD21	2.00	0.43
3:H:1020:ILE:HD12	3:H:1023:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1161:VAL:O	3:H:1165:ASN:ND2	2.51	0.43
1:J:1103:THR:HB	1:J:1105:LYS:HE3	2.00	0.43
1:J:1361:ASP:N	1:J:1361:ASP:OD1	2.48	0.43
3:K:1963:TRP:NE1	3:K:2007:GLU:HG3	2.34	0.43
3:E:1004:LYS:NZ	3:E:1008:VAL:HG21	2.33	0.43
3:F:383:ALA:HB3	3:F:389:TYR:HB2	2.00	0.43
3:F:606:ASP:HB3	3:F:609:VAL:H	1.83	0.43
3:F:1101:LYS:HA	3:F:1104:ILE:HG12	2.00	0.43
3:F:1250:GLN:HA	3:F:1253:LYS:HE2	1.99	0.43
3:F:1446:GLU:O	3:F:1449:SER:OG	2.26	0.43
3:F:1571:LEU:HA	3:F:1574:ARG:NH1	2.34	0.43
3:F:1595:LEU:HD21	3:F:1611:ARG:CZ	2.48	0.43
3:F:2237:GLY:N	3:F:2322:ARG:HH21	2.16	0.43
1:G:1430:TRP:HE1	1:G:1437:PRO:HB3	1.83	0.43
3:H:2249:ARG:H	3:H:2253:THR:HG21	1.83	0.43
1:J:909:ARG:NH1	1:J:1297:ALA:O	2.51	0.43
3:K:2286:MET:HB3	3:K:2295:ILE:HB	2.00	0.43
1:B:358:PHE:HB2	1:B:425:TRP:CH2	2.53	0.43
1:B:638:MET:HA	1:B:641:VAL:HG12	1.99	0.43
1:B:757:GLN:HE22	1:B:1144:PHE:HE2	1.65	0.43
2:D:223:ALA:HA	2:D:233:VAL:HA	2.00	0.43
3:E:389:TYR:O	3:E:393:ILE:HG12	2.18	0.43
3:F:1445:TRP:HA	3:F:1448:LEU:HD12	2.00	0.43
3:F:1620:LYS:HE3	3:F:1620:LYS:HA	2.00	0.43
3:F:1888:GLN:HG2	3:F:1894:SER:HA	1.99	0.43
3:F:2114:CYS:SG	3:F:2122:ASP:HB3	2.59	0.43
3:H:1078:GLU:HB3	3:H:1114:ILE:HG22	2.00	0.43
3:H:1084:ILE:HD12	3:H:1087:ILE:HD12	1.99	0.43
3:H:1878:VAL:HG12	3:H:1881:GLN:NE2	2.34	0.43
2:I:140:ILE:HB	2:I:154:LEU:HB2	2.00	0.43
3:K:2288:ASP:HB3	3:K:2292:GLY:H	1.83	0.43
1:A:68:GLN:HA	1:A:69:PRO:HD3	1.93	0.43
1:B:861:GLN:HA	1:B:864:ILE:HD12	2.00	0.43
1:B:1358:LEU:HD13	1:B:1370:ALA:HB2	2.01	0.43
2:D:285:VAL:O	2:D:286:ARG:NE	2.44	0.43
3:F:656:GLU:HA	3:F:659:LEU:HD23	1.99	0.43
3:F:1335:PRO:HB2	3:F:1338:THR:HG22	1.99	0.43
3:F:1482:ASP:OD1	3:F:1482:ASP:N	2.47	0.43
3:F:2174:LYS:HE3	3:F:2174:LYS:HA	2.00	0.43
3:F:2467:TYR:HD2	3:F:2469:GLY:H	1.65	0.43
1:G:93:LEU:HD12	1:G:124:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1255:THR:HG21	1:J:1277:ASP:HB3	2.01	0.43
3:E:470:CYS:HA	3:E:507:LYS:HG2	1.99	0.43
3:E:953:LEU:O	3:E:956:ARG:NH2	2.52	0.43
3:E:1043:GLU:O	3:E:1046:THR:OG1	2.31	0.43
3:F:1568:ASP:OD1	3:F:1569:LYS:N	2.52	0.43
3:F:2421:ARG:HA	3:F:2424:LEU:HD12	2.01	0.43
1:G:216:CYS:N	1:G:262:CYS:HB2	2.34	0.43
1:G:225:ALA:O	1:G:229:LEU:HD23	2.19	0.43
1:G:809:ILE:HD11	1:G:915:TYR:HE1	1.82	0.43
3:H:948:HIS:O	3:H:951:GLN:HG3	2.19	0.43
3:H:2076:LEU:HD21	3:H:2078:LEU:HD12	1.99	0.43
3:H:2281:HIS:ND1	3:H:2283:SER:HB2	2.34	0.43
2:I:247:ASP:OD1	2:I:247:ASP:N	2.52	0.43
3:K:1954:HIS:O	3:K:1958:ARG:HG2	2.18	0.43
3:K:1962:LEU:O	3:K:1965:GLU:HG2	2.19	0.43
1:A:757:GLN:NE2	1:A:800:ALA:HB2	2.33	0.43
1:B:206:TYR:HB2	1:B:235:PHE:CE2	2.54	0.43
1:B:434:THR:HA	1:B:437:VAL:HG12	2.01	0.43
1:B:894:LEU:HD21	1:B:967:VAL:HG21	2.01	0.43
3:E:645:LEU:HD22	3:E:665:LEU:HD21	2.01	0.43
3:E:1843:ALA:HA	3:E:1846:LEU:HG	2.01	0.43
3:H:938:HIS:HB3	3:H:942:ALA:HB2	2.01	0.43
1:J:108:ARG:NE	1:J:114:ASP:OD1	2.51	0.43
3:K:2171:LEU:H	3:K:2176:GLY:HA2	1.84	0.43
2:L:188:MET:HB2	2:L:197:LEU:HD23	2.00	0.43
1:A:932:PHE:HE1	1:A:997:LEU:HB2	1.84	0.43
1:B:1138:LEU:HD12	1:B:1138:LEU:HA	1.85	0.43
2:C:99:ILE:HD11	2:C:119:VAL:HB	2.01	0.43
3:E:452:LYS:HD3	3:E:452:LYS:HA	1.77	0.43
3:E:1067:LEU:HD23	3:E:1070:LEU:HD12	1.99	0.43
3:E:1159:VAL:HG23	3:F:647:MET:HG2	2.01	0.43
3:E:1648:LYS:HD2	3:E:1648:LYS:HA	1.88	0.43
3:F:225:LEU:HD13	3:F:232:SER:HB2	2.01	0.43
3:H:2191:ILE:O	3:H:2195:ARG:HG2	2.19	0.43
3:H:2319:ARG:NH2	3:H:2474:TRP:OXT	2.51	0.43
1:J:339:ASN:N	1:J:339:ASN:OD1	2.52	0.43
1:J:534:LEU:HA	1:J:534:LEU:HD23	1.86	0.43
1:J:1106:LYS:HD2	1:J:1106:LYS:H	1.76	0.43
3:K:976:PRO:HA	3:K:977:PRO:HD3	1.89	0.43
1:B:146:LYS:NZ	1:B:159:PHE:HA	2.34	0.43
1:B:366:ALA:HB2	1:B:393:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:248:LYS:HE3	3:E:286:VAL:HB	2.00	0.43
3:E:1456:TRP:CD1	3:E:1464:LYS:HE2	2.54	0.43
3:F:1499:GLU:HG3	3:F:1518:HIS:CD2	2.54	0.43
3:F:2232:LEU:HD13	3:F:2322:ARG:HD2	2.00	0.43
3:F:2246:LEU:HD23	3:F:2246:LEU:HA	1.88	0.43
3:F:2259:THR:O	3:F:2263:ARG:HG3	2.19	0.43
1:J:564:GLN:OE1	1:J:567:ARG:NE	2.52	0.43
3:K:1084:ILE:HD12	3:K:1087:ILE:HD12	2.01	0.43
3:K:2463:LEU:HA	3:K:2466:HIS:CE1	2.54	0.43
2:L:42:ASN:OD1	2:L:43:ASP:N	2.51	0.43
2:L:247:ASP:OD1	2:L:247:ASP:N	2.50	0.43
1:B:1001:LYS:HG3	1:B:1002:GLU:HG3	2.01	0.43
2:C:223:ALA:HA	2:C:233:VAL:HA	2.00	0.43
3:E:139:ILE:HG22	3:E:147:LYS:HA	2.01	0.43
3:E:835:TYR:CE2	3:E:839:PRO:HG3	2.54	0.43
3:E:852:ASN:O	3:E:856:THR:OG1	2.34	0.43
3:E:1100:LYS:HE3	3:E:1100:LYS:HB2	1.92	0.43
3:E:1516:GLU:HA	3:E:1519:ILE:HG22	2.00	0.43
3:F:1240:TRP:CD1	3:F:1311:PRO:HG3	2.54	0.43
3:F:1266:LEU:O	3:F:1270:TYR:HB3	2.19	0.43
3:F:1755:TRP:HD1	3:F:1758:ALA:HB2	1.83	0.43
3:F:2166:TYR:HE2	3:F:2178:LEU:HD12	1.84	0.43
1:G:630:GLU:O	1:G:630:GLU:HG2	2.19	0.43
2:I:21:THR:HG23	2:I:23:VAL:H	1.84	0.43
1:J:85:ALA:HB3	1:J:145:TYR:CD1	2.54	0.43
1:J:558:LEU:HD11	1:J:596:TYR:HD2	1.83	0.43
1:J:1412:ARG:N	1:J:1466:GLU:O	2.52	0.43
3:K:1107:LEU:HD23	3:K:1110:LEU:HD21	2.00	0.43
3:K:1327:HIS:HD2	3:K:2246:LEU:HA	1.84	0.43
2:L:210:ILE:HA	2:L:226:SER:HA	2.01	0.43
1:A:585:VAL:HG11	1:A:622:ILE:HD13	2.01	0.42
1:A:589:LEU:HD11	1:A:619:ILE:HD11	2.01	0.42
1:A:1368:PHE:HE1	1:A:1382:ARG:HG3	1.84	0.42
1:B:271:ASP:OD1	1:B:271:ASP:N	2.44	0.42
2:D:15:ARG:HB2	2:D:24:CYS:SG	2.59	0.42
3:E:326:VAL:HG11	3:E:357:LYS:HZ1	1.83	0.42
3:F:930:LEU:HA	3:F:935:LEU:HD11	2.01	0.42
3:F:2317:PRO:HG2	3:F:2457:ALA:HB2	2.01	0.42
1:G:229:LEU:HD11	1:G:264:GLN:OE1	2.19	0.42
1:G:630:GLU:OE1	1:G:630:GLU:CA	2.66	0.42
1:G:1465:HIS:CD2	1:G:1467:HIS:H	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:SER:HB2	1:A:159:PHE:CE2	2.54	0.42
1:B:1227:ALA:HB2	1:B:1260:LEU:HD11	2.00	0.42
3:E:1100:LYS:O	3:E:1104:ILE:HG23	2.20	0.42
3:E:1948:GLN:HG3	3:E:2078:LEU:HD11	2.00	0.42
3:E:2186:THR:HG22	3:E:2188:HIS:N	2.32	0.42
3:F:352:TYR:HE2	3:F:392:ARG:HE	1.65	0.42
3:F:1246:ARG:HE	3:F:1246:ARG:HB2	1.65	0.42
3:F:2281:HIS:CE1	3:F:2283:SER:HB3	2.54	0.42
1:G:229:LEU:HA	1:G:229:LEU:HD13	1.81	0.42
3:H:1131:LEU:O	3:H:1171:ASN:ND2	2.52	0.42
3:H:1155:THR:HG22	3:H:1185:LEU:HG	2.00	0.42
2:I:196:HIS:O	2:I:196:HIS:ND1	2.52	0.42
1:J:108:ARG:HD3	1:J:116:LEU:HD23	1.99	0.42
3:K:929:ILE:HG21	3:K:942:ALA:HB1	2.01	0.42
3:K:1856:ILE:HG22	3:K:1859:ALA:H	1.84	0.42
1:A:311:TYR:HE1	1:A:338:VAL:HG22	1.83	0.42
1:B:88:LEU:HD11	1:B:151:PRO:HG3	2.01	0.42
3:E:476:PHE:CZ	3:E:480:LEU:HB2	2.54	0.42
3:E:1150:LEU:HD13	3:E:1157:PHE:CD2	2.54	0.42
3:E:2270:MET:SD	3:E:2341:CYS:HB2	2.59	0.42
3:F:131:LEU:HA	3:F:134:LYS:HG2	2.01	0.42
3:F:1717:ARG:NH2	3:F:1720:LEU:HD13	2.29	0.42
3:F:2195:ARG:NH2	3:F:2205:GLU:OE2	2.47	0.42
3:H:2282:PRO:HA	3:H:2285:LEU:HB2	2.01	0.42
3:H:2321:THR:HG22	3:H:2324:LEU:HG	2.01	0.42
3:K:1850:TRP:HH2	3:K:1860:THR:HG22	1.84	0.42
1:A:370:LEU:HD22	1:A:374:LEU:HD23	2.01	0.42
1:A:805:LEU:HD23	1:A:805:LEU:HA	1.84	0.42
1:A:1489:ASN:OD1	1:A:1490:SER:N	2.52	0.42
1:B:45:LYS:HA	1:B:48:LYS:HG2	2.02	0.42
1:B:530:PHE:CD1	1:B:560:VAL:HG22	2.54	0.42
1:B:1194:SER:HB2	1:B:1199:TRP:HZ2	1.85	0.42
2:D:38:LEU:HA	2:D:48:ALA:O	2.20	0.42
2:D:227:ALA:HB1	2:D:252:TRP:CE2	2.53	0.42
3:E:222:TRP:HE3	3:E:243:ALA:HB2	1.85	0.42
3:E:1004:LYS:HZ3	3:E:1008:VAL:HG21	1.84	0.42
3:E:1143:MET:HA	3:E:1146:LEU:HG	2.00	0.42
3:E:1846:LEU:HD12	3:E:1847:LEU:HD22	2.01	0.42
3:E:1916:LEU:O	3:E:1920:ILE:HG12	2.20	0.42
3:E:1917:MET:O	3:E:1921:LYS:HG2	2.19	0.42
3:F:472:LEU:HB3	3:F:476:PHE:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1100:LYS:HE3	3:F:1100:LYS:HB2	1.90	0.42
1:G:397:ARG:HD2	1:G:422:TRP:CD2	2.54	0.42
1:G:790:LEU:HD11	1:G:805:LEU:HD11	2.01	0.42
1:J:85:ALA:HB3	1:J:145:TYR:HD1	1.84	0.42
1:J:266:ALA:HB3	1:J:407:VAL:H	1.83	0.42
3:K:2150:LEU:HD12	3:K:2156:CYS:HB3	2.00	0.42
3:K:2438:ILE:HG22	3:K:2439:ARG:HG2	2.01	0.42
1:A:1493:ASN:OD1	1:A:1545:ASN:ND2	2.46	0.42
1:B:70:ILE:HG12	1:B:586:TYR:HB3	2.02	0.42
2:D:233:VAL:HG11	2:D:279:LEU:HD21	2.01	0.42
3:E:1326:GLU:HA	3:E:1331:PRO:HG3	2.01	0.42
3:F:1085:MET:HE2	3:F:1116:LEU:HD21	2.00	0.42
3:F:1841:GLN:O	3:F:1845:ARG:HG2	2.19	0.42
3:F:2146:VAL:O	3:F:2150:LEU:HG	2.19	0.42
1:G:1362:GLN:HG3	1:G:1412:ARG:HG2	2.01	0.42
3:H:2184:SER:HA	3:H:2289:ARG:H	1.84	0.42
2:I:41:THR:O	2:I:301:ASN:ND2	2.53	0.42
1:J:53:PRO:HD3	1:J:1143:SER:HB3	2.01	0.42
3:K:2274:ILE:HG21	3:K:2348:LEU:HD13	2.01	0.42
1:A:358:PHE:HB2	1:A:425:TRP:CH2	2.54	0.42
1:A:417:THR:HG23	1:A:418:THR:HG23	2.02	0.42
3:E:364:ASP:OD1	3:E:364:ASP:N	2.51	0.42
3:E:1294:GLN:O	3:E:1298:ILE:HG12	2.19	0.42
3:F:867:VAL:HA	3:F:870:ILE:HG12	2.01	0.42
3:F:1713:LYS:HA	3:F:1713:LYS:HD2	1.81	0.42
3:F:2074:HIS:ND1	3:F:2075:ASP:OD2	2.46	0.42
3:H:934:SER:HA	3:H:937:ILE:HG12	2.02	0.42
3:H:1068:LYS:HA	3:H:1068:LYS:HD2	1.77	0.42
3:H:1252:LEU:HD21	3:H:1277:LEU:HD21	2.01	0.42
3:H:2198:LYS:HA	3:H:2198:LYS:HD2	1.84	0.42
1:J:367:TRP:HZ2	1:J:372:ARG:HH22	1.68	0.42
3:K:965:ILE:O	3:K:969:ILE:HG12	2.19	0.42
3:K:1102:ILE:HA	3:K:1105:ILE:HG12	2.01	0.42
3:K:1387:GLY:HA3	3:K:2335:GLY:HA2	2.00	0.42
1:A:990:ILE:HD12	1:A:990:ILE:HA	1.93	0.42
1:B:298:ARG:O	1:B:302:MET:HG2	2.20	0.42
2:D:74:HIS:ND1	2:D:94:SER:OG	2.41	0.42
3:E:1668:ASP:OD1	3:E:1668:ASP:N	2.52	0.42
3:F:1377:ASN:HD21	3:F:1408:LEU:HD21	1.84	0.42
3:F:1648:LYS:HD2	3:F:1648:LYS:HA	1.85	0.42
3:F:2138:LEU:O	3:F:2141:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:ARG:NH1	1:G:215:PRO:HD2	2.32	0.42
1:G:792:ASP:OD1	1:G:798:ARG:HG3	2.19	0.42
1:G:1427:VAL:HG11	1:G:1471:ILE:HG21	2.01	0.42
3:H:1300:ALA:O	3:H:1303:LYS:HG3	2.19	0.42
3:H:2238:GLN:HG2	3:H:2326:TYR:HB3	2.01	0.42
1:J:275:LEU:HD11	1:J:402:TYR:HB3	2.01	0.42
1:J:1523:SER:HB3	1:J:1537:THR:HG23	2.02	0.42
1:A:1263:ILE:HD11	1:A:1272:LEU:HD12	2.01	0.42
3:E:131:LEU:HA	3:E:134:LYS:HG2	2.01	0.42
3:E:397:TYR:CE1	3:E:417:ILE:HD11	2.55	0.42
3:E:554:ASN:OD1	3:E:555:GLN:N	2.53	0.42
3:E:1379:LEU:HB3	3:E:1381:GLN:OE1	2.20	0.42
3:E:1716:ALA:HB2	3:E:1751:PHE:HB3	2.02	0.42
3:E:2321:THR:HG1	3:E:2474:TRP:C	2.22	0.42
3:F:1813:SER:OG	3:F:1815:ASN:OD1	2.29	0.42
3:F:2130:HIS:N	3:F:2174:LYS:O	2.53	0.42
1:G:894:LEU:HA	1:G:897:ILE:HG22	2.01	0.42
1:G:1212:PRO:HG2	1:G:1537:THR:HG21	2.02	0.42
3:K:969:ILE:HG22	3:K:973:ARG:HH12	1.85	0.42
3:K:1052:LEU:HD11	3:K:1066:ILE:HG21	2.02	0.42
3:K:2206:HIS:ND1	3:K:2210:LEU:HD23	2.35	0.42
2:L:185:VAL:HG23	2:L:200:VAL:HB	2.02	0.42
1:A:913:VAL:HG12	1:A:974:LEU:HD13	2.01	0.42
1:B:531:GLU:OE1	1:B:569:ARG:NH1	2.52	0.42
1:B:550:PRO:HA	1:B:551:PRO:HD3	1.89	0.42
1:B:711:GLU:O	1:B:715:MET:HG2	2.19	0.42
1:B:770:ASN:HB3	1:B:773:ASN:HB2	2.02	0.42
3:E:414:LYS:HA	3:E:417:ILE:HG22	2.00	0.42
3:E:652:ASP:O	3:E:658:ARG:NH2	2.35	0.42
3:E:1661:LEU:O	3:E:1664:THR:OG1	2.34	0.42
3:E:1879:LEU:HA	3:E:1882:LEU:HB2	2.01	0.42
3:F:860:PRO:HB2	3:F:864:ARG:HH22	1.85	0.42
3:F:1169:LEU:HD23	3:F:1169:LEU:HA	1.92	0.42
3:F:1881:GLN:O	3:F:1885:ARG:HD3	2.20	0.42
1:G:104:HIS:HB2	1:G:105:PRO:HD3	2.02	0.42
1:G:234:LYS:HA	1:G:234:LYS:HD2	1.77	0.42
1:G:885:LYS:HE2	1:G:885:LYS:HB2	1.65	0.42
1:G:1179:ARG:NH2	1:G:1221:GLU:OE2	2.46	0.42
2:I:103:ASP:N	2:I:103:ASP:OD1	2.53	0.42
1:J:709:THR:N	1:J:712:GLN:OE1	2.52	0.42
1:J:1377:LEU:HB2	1:J:1394:TRP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1226:LYS:HA	3:K:1226:LYS:HD3	1.81	0.42
1:A:346:ASP:OD1	1:A:347:ARG:N	2.51	0.42
1:B:1225:ILE:HG22	1:B:1260:LEU:HD13	2.00	0.42
1:B:1534:ILE:HG23	1:B:1547:TYR:HB2	2.02	0.42
3:E:270:TRP:HH2	3:E:309:ARG:HB3	1.84	0.42
3:E:1619:ARG:HH22	3:E:1659:LYS:HD3	1.84	0.42
3:E:1930:ALA:O	3:E:1934:ILE:HG12	2.20	0.42
3:F:1916:LEU:O	3:F:1920:ILE:HG12	2.19	0.42
3:F:2309:ARG:NH2	3:F:2312:PHE:O	2.52	0.42
1:G:108:ARG:HG2	1:G:115:PRO:HD2	2.02	0.42
3:H:1843:ALA:HB3	3:H:1878:VAL:HG11	2.02	0.42
1:J:1385:ASP:OD1	1:J:1388:ASP:N	2.50	0.42
3:K:1027:GLU:HB2	3:K:1031:LYS:HZ3	1.83	0.42
2:L:269:SER:OG	2:L:270:SER:N	2.53	0.42
1:A:190:ILE:HG22	1:A:191:TRP:H	1.84	0.41
1:A:394:LEU:HD21	1:A:398:ILE:HD12	2.02	0.41
1:A:985:LEU:HD12	1:A:985:LEU:HA	1.85	0.41
1:A:1081:LEU:O	1:A:1085:GLU:HG2	2.19	0.41
1:B:918:HIS:NE2	1:B:1140:LEU:O	2.39	0.41
3:E:1237:LYS:H	3:E:1310:ASN:HD22	1.68	0.41
3:E:1586:LYS:HE2	3:E:1586:LYS:HB2	1.82	0.41
3:F:445:GLU:O	3:F:448:ARG:NE	2.50	0.41
3:F:1745:TYR:HB3	3:F:1762:TRP:HB2	2.02	0.41
1:G:1240:LYS:NZ	1:G:1242:LYS:HB3	2.35	0.41
1:J:162:SER:HA	1:J:165:ARG:HG2	2.02	0.41
1:J:1327:THR:HB	1:J:1333:ILE:HG12	2.01	0.41
1:A:1190:GLU:HA	1:A:1193:LEU:HD23	2.01	0.41
3:E:968:ILE:O	3:E:972:MET:HG2	2.20	0.41
3:E:1487:TYR:HA	3:E:1490:VAL:HG22	2.02	0.41
3:E:1612:ILE:HG13	3:E:1613:LYS:HD2	2.02	0.41
3:E:2246:LEU:HA	3:E:2246:LEU:HD23	1.86	0.41
3:F:1504:ILE:HG23	3:F:1600:LEU:HD11	2.02	0.41
3:F:1913:VAL:HA	3:F:1916:LEU:HD12	2.02	0.41
3:F:1917:MET:O	3:F:1921:LYS:HG2	2.20	0.41
3:F:2318:PHE:HZ	3:F:2454:ILE:HG22	1.85	0.41
1:G:593:ILE:HG13	1:G:597:VAL:HG13	2.02	0.41
3:H:1327:HIS:CD2	3:H:2246:LEU:HA	2.53	0.41
1:J:118:PHE:HE2	1:J:122:LYS:HB2	1.84	0.41
1:J:640:PHE:CZ	1:J:719:VAL:HG11	2.55	0.41
1:J:969:LYS:HA	1:J:969:LYS:HD3	1.86	0.41
1:J:1168:VAL:HA	1:J:1171:ASN:HD21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1107:LEU:HA	3:K:1110:LEU:HG	2.00	0.41
3:K:2027:ASN:O	3:K:2031:SER:OG	2.30	0.41
1:A:82:THR:HG22	1:A:171:ARG:HB3	2.01	0.41
1:A:231:ASN:HA	1:A:234:LYS:HZ2	1.85	0.41
3:E:352:TYR:HE2	3:E:392:ARG:HE	1.68	0.41
3:E:550:ARG:HD2	3:E:553:ARG:HD2	2.01	0.41
3:E:965:ILE:O	3:E:969:ILE:HG23	2.20	0.41
3:E:1674:LEU:HD11	3:E:1726:ARG:NH1	2.35	0.41
3:E:2219:LEU:HB3	3:E:2223:GLN:HB2	2.03	0.41
3:F:845:GLU:O	3:F:848:GLY:N	2.53	0.41
3:F:1828:PHE:O	3:F:1832:ILE:HD12	2.20	0.41
3:H:1027:GLU:HB2	3:H:1031:LYS:HZ3	1.85	0.41
3:H:2134:ARG:NH1	3:H:2138:LEU:HD23	2.29	0.41
3:H:2185:ASP:OD1	3:H:2185:ASP:N	2.53	0.41
3:H:2356:MET:HA	3:H:2359:LEU:HG	2.02	0.41
3:K:946:ILE:HA	3:K:949:ILE:HG12	2.03	0.41
3:K:1270:TYR:HD2	3:K:1273:LEU:HD22	1.85	0.41
1:A:53:PRO:HG3	1:A:1143:SER:HB2	2.01	0.41
1:A:121:SER:O	1:A:121:SER:OG	2.33	0.41
2:D:249:HIS:NE2	2:D:275:ARG:HD2	2.35	0.41
3:E:981:ASP:OD1	3:E:1021:THR:OG1	2.34	0.41
3:E:1509:ARG:NH1	3:E:1511:ASN:HB3	2.34	0.41
3:E:1757:LYS:O	3:E:1761:ASN:ND2	2.53	0.41
3:F:1289:LEU:HD12	3:F:1294:GLN:HG2	2.02	0.41
3:F:2321:THR:OG1	3:F:2322:ARG:N	2.53	0.41
1:G:777:CYS:HA	1:G:780:THR:HG22	2.02	0.41
3:H:943:ILE:HA	3:H:946:ILE:HD13	2.02	0.41
3:H:1218:LEU:HD12	3:H:1219:PRO:HD2	2.03	0.41
3:K:902:ASP:OD1	3:K:2249:ARG:NH2	2.53	0.41
1:A:752:ILE:HG22	1:A:754:LEU:H	1.85	0.41
1:A:1528:HIS:HB2	1:A:1533:MET:HB2	2.02	0.41
1:B:746:TYR:HB3	1:B:755:LEU:HD21	2.03	0.41
3:E:364:ASP:HA	3:E:367:ARG:HE	1.85	0.41
3:E:1089:VAL:HG11	3:E:1122:ARG:HG2	2.03	0.41
3:E:1526:LEU:HD13	3:E:1530:LEU:HD11	2.02	0.41
3:E:1895:ARG:HA	3:E:1898:LEU:HG	2.03	0.41
3:F:1048:PHE:HA	3:F:1066:ILE:HD11	2.01	0.41
1:G:393:LEU:HD22	1:G:416:ILE:HD12	2.01	0.41
3:H:1916:LEU:O	3:H:1920:ILE:HG12	2.21	0.41
3:H:1935:ILE:O	3:H:1939:ARG:HG2	2.19	0.41
1:J:122:LYS:HA	1:J:122:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1388:ILE:HG13	3:K:2331:SER:HB3	2.02	0.41
3:K:1902:SER:HA	3:K:1937:LYS:HE3	2.02	0.41
3:K:2324:LEU:O	3:K:2328:MET:HG2	2.21	0.41
3:K:2415:ASN:OD1	3:K:2415:ASN:N	2.53	0.41
1:A:630:GLU:N	1:A:630:GLU:OE1	2.54	0.41
2:C:148:ASN:O	2:C:149:GLN:NE2	2.54	0.41
3:E:1870:ILE:HD13	3:E:1875:TRP:HE1	1.85	0.41
3:E:2004:THR:OG1	3:E:2066:VAL:O	2.36	0.41
3:F:804:PRO:HA	3:F:807:ILE:HG12	2.02	0.41
3:F:1562:LYS:HZ2	3:F:1565:GLN:HG2	1.86	0.41
3:F:1816:LEU:C	3:F:1820:HIS:HD1	2.24	0.41
3:F:1921:LYS:HD2	3:F:2172:SER:HA	2.03	0.41
3:F:2264:SER:HB3	3:F:2293:LYS:HB2	2.02	0.41
1:G:637:TYR:OH	1:G:733:ASN:O	2.30	0.41
3:H:1016:ILE:HD11	3:H:1018:LEU:HD22	2.02	0.41
3:H:1856:ILE:O	3:H:1860:THR:HG23	2.20	0.41
1:J:969:LYS:HD2	1:J:1102:HIS:CE1	2.56	0.41
1:J:1533:MET:HG3	1:J:1548:LYS:HB2	2.03	0.41
3:K:1110:LEU:HA	3:K:1113:ASN:HB2	2.03	0.41
3:K:1278:PHE:CE2	3:K:1321:LEU:HD22	2.55	0.41
1:A:737:LEU:HA	1:A:740:VAL:HG22	2.01	0.41
2:C:5:LEU:HD21	2:C:300:LEU:HD12	2.03	0.41
3:E:1832:ILE:HG13	3:E:1839:SER:HB2	2.03	0.41
1:G:1168:VAL:HA	1:G:1171:ASN:HD21	1.86	0.41
1:G:1394:TRP:HH2	1:G:1432:ILE:HA	1.85	0.41
3:H:2143:PHE:HA	3:H:2146:VAL:HG12	2.01	0.41
1:J:550:PRO:HA	1:J:551:PRO:HD2	1.80	0.41
1:J:1362:GLN:HG3	1:J:1412:ARG:HG2	2.03	0.41
2:C:6:VAL:HG12	2:C:16:PHE:CD1	2.56	0.41
3:E:178:LEU:HD13	3:E:197:LEU:HG	2.02	0.41
3:E:1247:LEU:O	3:E:1251:LEU:HG	2.20	0.41
3:E:1421:LYS:HZ3	3:E:1431:VAL:HG11	1.86	0.41
3:F:1562:LYS:HG2	3:F:1569:LYS:NZ	2.36	0.41
3:F:1919:ALA:O	3:F:1922:SER:OG	2.26	0.41
1:G:810:SER:OG	1:G:811:GLY:N	2.54	0.41
3:H:983:TYR:O	3:H:987:LEU:HG	2.21	0.41
3:H:1107:LEU:HD23	3:H:1110:LEU:HD21	2.03	0.41
2:I:29:GLN:OE1	2:I:31:SER:OG	2.38	0.41
3:K:1022:ILE:O	3:K:1026:ILE:HG12	2.20	0.41
3:K:1033:LEU:HG	3:K:1036:GLU:HB2	2.01	0.41
3:K:1934:ILE:HA	3:K:1937:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:121:GLU:HB2	2:L:134:CYS:SG	2.61	0.41
2:L:178:ASN:OD1	2:L:179:THR:N	2.54	0.41
1:B:93:LEU:HD23	1:B:115:PRO:HB3	2.02	0.41
2:C:218:ASP:OD1	2:C:218:ASP:N	2.45	0.41
2:C:251:ARG:HG2	2:C:271:ASP:HA	2.03	0.41
3:E:197:LEU:O	3:E:201:THR:HG23	2.21	0.41
3:E:426:PHE:HB2	3:E:467:LYS:HD3	2.03	0.41
3:E:1282:PHE:CE2	3:E:1321:LEU:HD21	2.55	0.41
3:E:1890:ASN:HB3	3:E:1893:VAL:HB	2.03	0.41
3:E:2303:PHE:HB3	3:E:2425:VAL:HG21	2.03	0.41
3:F:405:ASP:N	3:F:405:ASP:OD1	2.53	0.41
3:F:860:PRO:HB2	3:F:864:ARG:NH2	2.35	0.41
3:F:932:ASP:OD1	3:F:933:PRO:HD3	2.21	0.41
3:F:1150:LEU:HD13	3:F:1157:PHE:CD2	2.55	0.41
3:F:1680:ARG:NH1	3:F:1681:MET:HB3	2.36	0.41
3:F:2190:LEU:HD23	3:F:2190:LEU:HA	1.97	0.41
3:F:2219:LEU:HB3	3:F:2223:GLN:HB2	2.03	0.41
3:F:2239:ASP:OD1	3:F:2239:ASP:N	2.53	0.41
3:F:2346:LYS:HE3	3:F:2346:LYS:HB3	1.92	0.41
1:G:1227:ALA:HB2	1:G:1260:LEU:HD11	2.03	0.41
3:H:1753:ASN:O	3:H:1759:TRP:NE1	2.48	0.41
3:H:1883:ILE:HG12	3:H:1915:PRO:HB2	2.02	0.41
3:H:2028:TYR:CZ	3:H:2037:LEU:HD22	2.56	0.41
3:H:2438:ILE:HG22	3:H:2439:ARG:HG2	2.03	0.41
2:I:11:ASP:OD1	2:I:293:LYS:N	2.50	0.41
2:I:233:VAL:HG11	2:I:279:LEU:HD21	2.02	0.41
3:K:1110:LEU:HD13	3:K:1114:ILE:HD11	2.03	0.41
3:K:1129:ARG:HA	3:K:1132:ASN:HD21	1.86	0.41
3:K:1986:LYS:HZ3	3:K:1990:ALA:HB2	1.86	0.41
1:A:104:HIS:HB2	1:A:105:PRO:HD3	2.03	0.41
1:A:724:VAL:HG13	1:A:731:GLN:HG2	2.03	0.41
1:A:823:GLN:NE2	1:G:195:ARG:HH12	2.19	0.41
1:B:1098:SER:O	1:B:1100:LYS:N	2.52	0.41
1:B:1215:MET:HE1	1:B:1224:LEU:HD21	2.03	0.41
3:E:972:MET:HE1	3:E:983:TYR:CD2	2.56	0.41
3:E:1089:VAL:O	3:E:1092:THR:HG22	2.20	0.41
3:E:1562:LYS:O	3:E:1566:ASN:ND2	2.39	0.41
3:F:779:THR:O	3:F:783:VAL:HG23	2.21	0.41
3:F:1407:LYS:HG3	3:F:1408:LEU:HG	2.03	0.41
3:F:1956:LEU:HA	3:F:1959:MET:HE1	2.03	0.41
3:F:2352:LYS:HD3	3:F:2356:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:792:ASP:OD1	1:G:792:ASP:N	2.54	0.41
3:H:932:ASP:OD1	3:H:932:ASP:N	2.54	0.41
3:H:2042:ASP:O	3:H:2046:ASN:ND2	2.54	0.41
3:H:2255:LEU:O	3:H:2258:ARG:HG3	2.21	0.41
3:H:2368:ILE:O	3:H:2370:TRP:N	2.52	0.41
1:J:1214:LEU:HD13	1:J:1260:LEU:HG	2.03	0.41
1:A:1475:THR:OG1	1:A:1477:GLN:O	2.39	0.40
1:B:737:LEU:HA	1:B:740:VAL:HG22	2.03	0.40
2:C:121:GLU:HB2	2:C:134:CYS:SG	2.61	0.40
3:E:1241:GLN:O	3:E:1245:ARG:HG2	2.21	0.40
3:F:1077:LEU:HB2	3:F:1114:ILE:HG13	2.03	0.40
3:F:1310:ASN:C	3:F:1310:ASN:HD22	2.24	0.40
3:F:1462:GLU:HA	3:F:1465:LYS:HG2	2.03	0.40
3:F:1905:GLY:HA3	3:F:1937:LYS:NZ	2.36	0.40
3:F:2059:GLN:HA	3:F:2103:VAL:HG22	2.04	0.40
1:J:91:LEU:HD21	1:J:179:HIS:HB2	2.03	0.40
1:A:194:ASN:ND2	1:A:198:THR:OG1	2.41	0.40
1:A:427:LEU:HD11	3:E:713:VAL:HG12	2.02	0.40
1:A:1263:ILE:O	1:A:1269:ALA:HA	2.20	0.40
1:B:1214:LEU:HD13	1:B:1260:LEU:HG	2.02	0.40
2:D:98:THR:HG22	2:D:114:LYS:HG3	2.03	0.40
3:E:101:ARG:H	3:E:101:ARG:HG2	1.74	0.40
3:E:163:SER:HB2	3:E:167:LEU:HG	2.03	0.40
3:E:1250:GLN:HA	3:E:1253:LYS:HE2	2.03	0.40
3:E:1613:LYS:HD2	3:E:1613:LYS:H	1.85	0.40
3:E:2106:SER:O	3:E:2107:LYS:CB	2.69	0.40
3:F:621:PHE:HE2	3:F:641:VAL:HG11	1.86	0.40
3:F:1247:LEU:HA	3:F:1250:GLN:HE22	1.86	0.40
3:F:1734:ARG:HB2	3:F:1738:PRO:HD3	2.02	0.40
3:F:2164:GLN:HG2	3:F:2293:LYS:NZ	2.37	0.40
3:F:2288:ASP:OD1	3:F:2289:ARG:N	2.54	0.40
1:G:284:LEU:HA	1:G:287:CYS:HB2	2.03	0.40
1:G:1393:ARG:HD2	1:G:1393:ARG:HA	1.86	0.40
3:H:1995:TYR:O	3:H:1999:LYS:NZ	2.54	0.40
1:J:100:VAL:HG13	1:J:183:LYS:NZ	2.36	0.40
3:K:983:TYR:O	3:K:987:LEU:HG	2.20	0.40
2:L:274:VAL:HG23	2:L:288:TYR:HD2	1.86	0.40
1:B:1215:MET:HE3	1:B:1224:LEU:HD11	2.03	0.40
1:B:1277:ASP:OD1	1:B:1277:ASP:N	2.49	0.40
3:E:417:ILE:HA	3:E:417:ILE:HD12	1.92	0.40
3:E:1971:LEU:HD11	3:E:2044:TYR:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1089:VAL:O	3:F:1092:THR:HG22	2.22	0.40
3:F:1959:MET:HE3	3:F:2070:LEU:HD21	2.03	0.40
3:F:2448:GLU:O	3:F:2452:LYS:HG2	2.22	0.40
1:G:537:PHE:CD1	1:G:553:GLN:HB2	2.56	0.40
3:H:1973:ASP:OD1	3:H:1974:ALA:N	2.54	0.40
3:H:2316:VAL:HG23	3:H:2457:ALA:HA	2.02	0.40
1:J:591:ILE:HD13	1:J:591:ILE:HA	1.91	0.40
1:B:104:HIS:HB2	1:B:105:PRO:HD3	2.04	0.40
1:B:630:GLU:N	1:B:630:GLU:OE1	2.53	0.40
2:C:179:THR:HB	2:C:209:TYR:HD1	1.86	0.40
3:F:359:LYS:HE3	3:F:361:TYR:HB3	2.03	0.40
3:H:970:LEU:HD13	3:H:973:ARG:HH21	1.86	0.40
3:H:1730:GLN:HE22	3:H:1737:ASN:HB2	1.84	0.40
1:J:307:LYS:NZ	1:J:312:LYS:O	2.48	0.40
3:K:1738:PRO:HA	3:K:1741:ILE:HG12	2.02	0.40
3:K:2187:PHE:HA	3:K:2190:LEU:HD12	2.04	0.40
2:L:125:HIS:HA	2:L:167:MET:HE1	2.02	0.40
1:A:1381:ASP:HB2	1:A:1391:ILE:HD11	2.02	0.40
2:D:207:SER:OG	2:D:228:ASP:OD2	2.35	0.40
3:E:1286:TRP:CZ3	3:E:1294:GLN:HB2	2.57	0.40
3:E:2149:LEU:HD22	3:E:2355:LEU:HD21	2.04	0.40
3:F:680:ARG:HA	3:F:683:PHE:CE1	2.57	0.40
1:G:300:PHE:CE2	1:G:433:LEU:HD12	2.57	0.40
1:G:535:THR:HA	1:G:538:GLU:HG2	2.03	0.40
1:G:883:LEU:O	1:G:887:LYS:HG2	2.22	0.40
1:G:969:LYS:NZ	1:G:1100:LYS:O	2.49	0.40
3:H:1079:ASP:OD1	3:H:1079:ASP:N	2.52	0.40
3:H:1962:LEU:HB2	3:H:2111:ARG:HH21	1.86	0.40
3:H:2140:MET:HA	3:H:2143:PHE:HD2	1.86	0.40
3:K:1916:LEU:O	3:K:1920:ILE:HG12	2.21	0.40
2:L:80:SER:OG	2:L:93:SER:OG	2.35	0.40
2:L:271:ASP:OD1	2:L:271:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1189/1608 (74%)	1121 (94%)	68 (6%)	0	100	100
1	B	1188/1608 (74%)	1128 (95%)	60 (5%)	0	100	100
1	G	1192/1608 (74%)	1131 (95%)	59 (5%)	2 (0%)	47	79
1	J	1193/1608 (74%)	1126 (94%)	65 (5%)	2 (0%)	47	79
2	C	298/303 (98%)	267 (90%)	31 (10%)	0	100	100
2	D	298/303 (98%)	267 (90%)	31 (10%)	0	100	100
2	I	298/303 (98%)	266 (89%)	32 (11%)	0	100	100
2	L	298/303 (98%)	268 (90%)	30 (10%)	0	100	100
3	E	2220/2474 (90%)	2072 (93%)	148 (7%)	0	100	100
3	F	2220/2474 (90%)	2069 (93%)	151 (7%)	0	100	100
3	H	1147/2474 (46%)	1097 (96%)	50 (4%)	0	100	100
3	K	1147/2474 (46%)	1091 (95%)	56 (5%)	0	100	100
All	All	12688/17540 (72%)	11903 (94%)	781 (6%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	1099	MET
1	G	1099	MET
1	J	1108	PRO
1	G	1108	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1080/1458 (74%)	1072 (99%)	8 (1%)	84	90
1	B	1079/1458 (74%)	1076 (100%)	3 (0%)	92	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	1079/1458 (74%)	1068 (99%)	11 (1%)	76	86
1	J	1080/1458 (74%)	1073 (99%)	7 (1%)	86	91
2	C	263/267 (98%)	262 (100%)	1 (0%)	91	94
2	D	263/267 (98%)	262 (100%)	1 (0%)	91	94
2	I	263/267 (98%)	260 (99%)	3 (1%)	73	84
2	L	263/267 (98%)	262 (100%)	1 (0%)	91	94
3	E	1991/2219 (90%)	1977 (99%)	14 (1%)	84	90
3	F	1990/2219 (90%)	1973 (99%)	17 (1%)	78	87
3	H	1037/2219 (47%)	1031 (99%)	6 (1%)	86	91
3	K	1037/2219 (47%)	1033 (100%)	4 (0%)	91	94
All	All	11425/15776 (72%)	11349 (99%)	76 (1%)	84	90

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

Mol	Chain	Res	Type
1	A	64	ASN
1	A	102	LYS
1	A	108	ARG
1	A	146	LYS
1	A	209	GLN
1	A	749	ASN
1	A	820	ARG
1	A	1378	ARG
1	B	102	LYS
1	B	146	LYS
1	B	820	ARG
2	C	61	ARG
2	D	34	GLN
3	E	274	ARG
3	E	399	ARG
3	E	444	ARG
3	E	728	LYS
3	E	797	ARG
3	E	1166	LYS
3	E	1237	LYS
3	E	1365	LYS
3	E	1514	LYS
3	E	1562	LYS

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Mol	Chain	Res	Type
3	E	1680	ARG
3	E	1819	ARG
3	E	2323	MET
3	E	2439	ARG
3	F	399	ARG
3	F	444	ARG
3	F	448	ARG
3	F	628	LYS
3	F	1076	ASN
3	F	1222	GLN
3	F	1310	ASN
3	F	1365	LYS
3	F	1514	LYS
3	F	1562	LYS
3	F	1574	ARG
3	F	1680	ARG
3	F	1819	ARG
3	F	1885	ARG
3	F	2147	ASN
3	F	2351	ASN
3	F	2414	LYS
1	G	45	LYS
1	G	146	LYS
1	G	158	ARG
1	G	542	LYS
1	G	630	GLU
1	G	822	GLN
1	G	866	LYS
1	G	888	ARG
1	G	1104	SER
1	G	1106	LYS
1	G	1108	PRO
3	H	1245	ARG
3	H	1303	LYS
3	H	1937	LYS
3	H	1976	ARG
3	H	2263	ARG
3	H	2346	LYS
2	I	56	ARG
2	I	61	ARG
2	I	100	LYS
1	J	186	LYS

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Mol	Chain	Res	Type
1	J	822	GLN
1	J	866	LYS
1	J	1104	SER
1	J	1105	LYS
1	J	1106	LYS
1	J	1108	PRO
3	K	1245	ARG
3	K	1303	LYS
3	K	1976	ARG
3	K	2218	ASN
2	L	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	749	ASN
1	A	822	GLN
1	A	823	GLN
1	A	1180	ASN
1	B	1406	ASN
2	D	29	GLN
3	E	543	GLN
3	E	629	GLN
3	E	828	GLN
3	E	1241	GLN
3	E	1294	GLN
3	E	1761	ASN
3	E	1948	GLN
3	E	2211	GLN
3	F	629	GLN
3	F	1394	GLN
3	F	1761	ASN
3	F	1948	GLN
3	F	2462	ASN
1	G	131	ASN
1	G	1171	ASN
1	G	1319	GLN
3	H	908	GLN
3	H	1171	ASN
1	J	733	ASN
1	J	822	GLN

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Mol	Chain	Res	Type
1	J	823	GLN
1	J	1102	HIS
1	J	1171	ASN
1	J	1319	GLN
3	K	1056	GLN
3	K	1250	GLN
3	K	1320	ASN
3	K	1378	GLN
3	K	1977	GLN
2	L	12	HIS
2	L	29	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

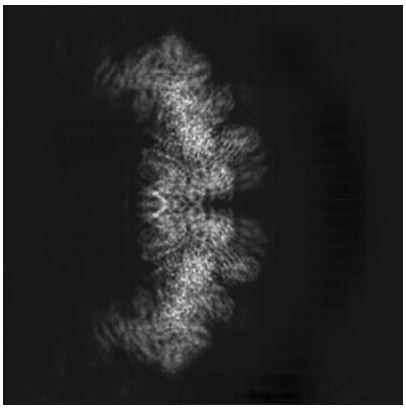
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13594. These allow visual inspection of the internal detail of the map and identification of artifacts.

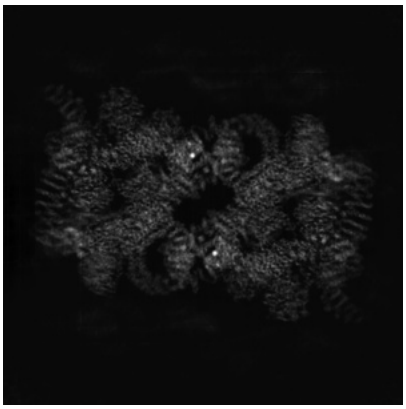
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

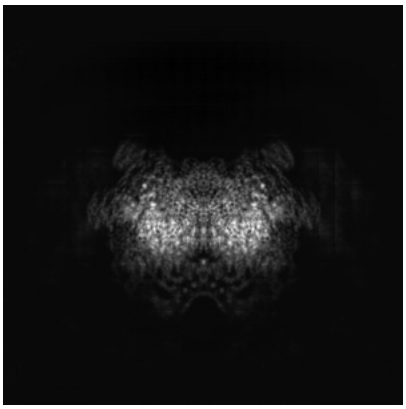
6.1.1 Primary map



X

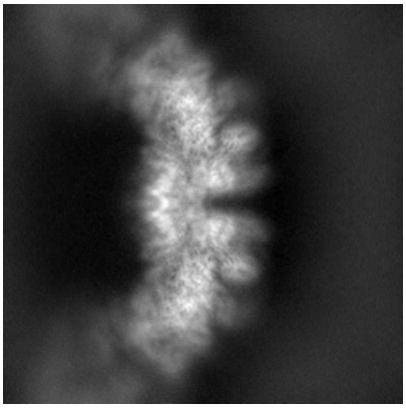


Y

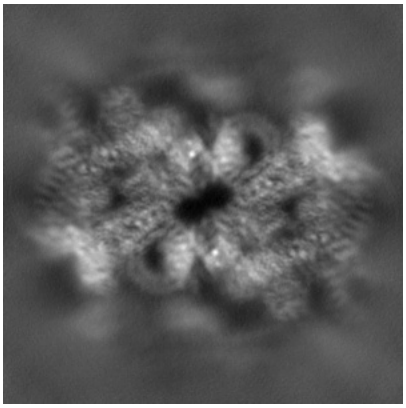


Z

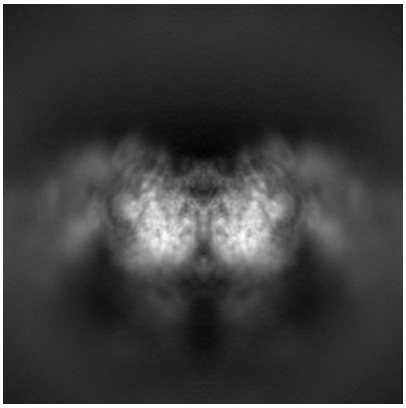
6.1.2 Raw map



X



Y



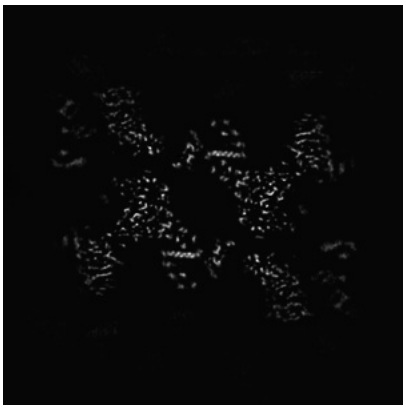
Z

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

6.2 Central slices (i)

6.2.1 Primary map

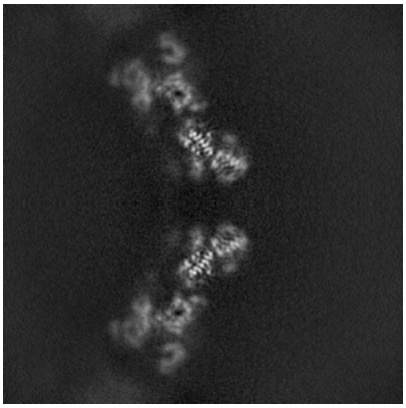
X Index: 150



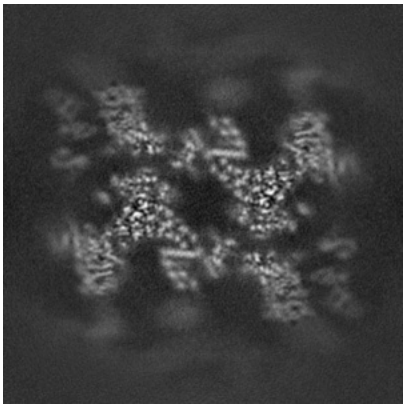
Y Index: 150

Z Index: 150

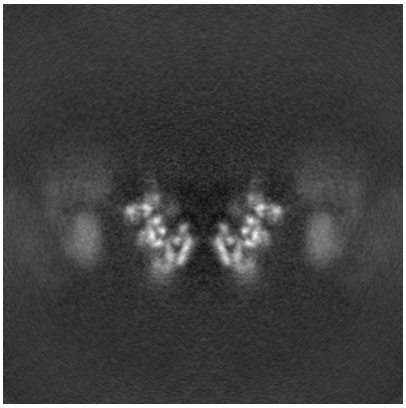
6.2.2 Raw map



X Index: 150



Y Index: 150



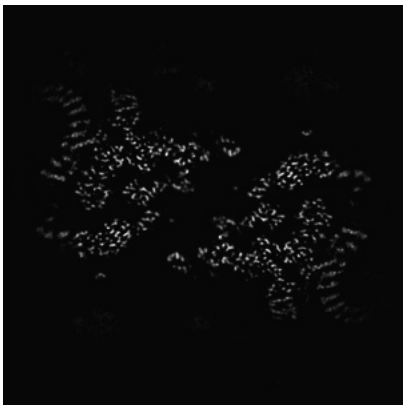
Z Index: 150

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

6.3 Largest variance slices (i)

6.3.1 Primary map

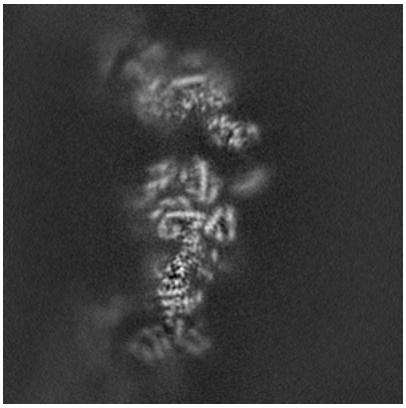
X Index: 187



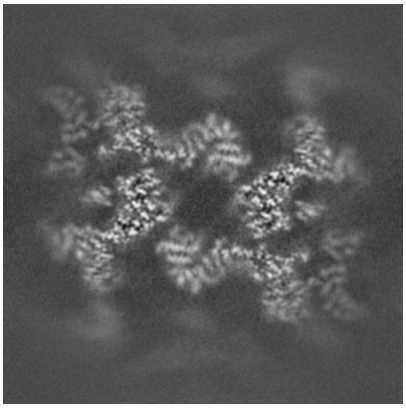
Y Index: 136

Z Index: 195

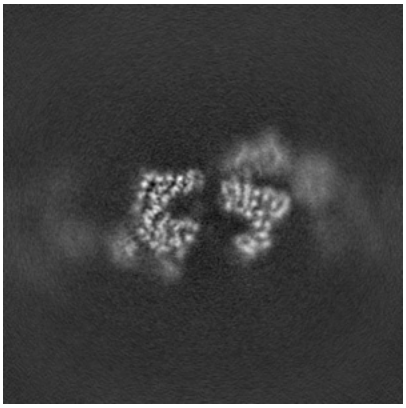
6.3.2 Raw map



X Index: 187



Y Index: 143



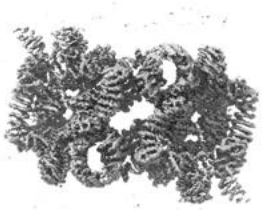
Z Index: 166

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



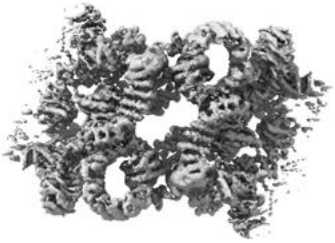
Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X



Y

Z

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

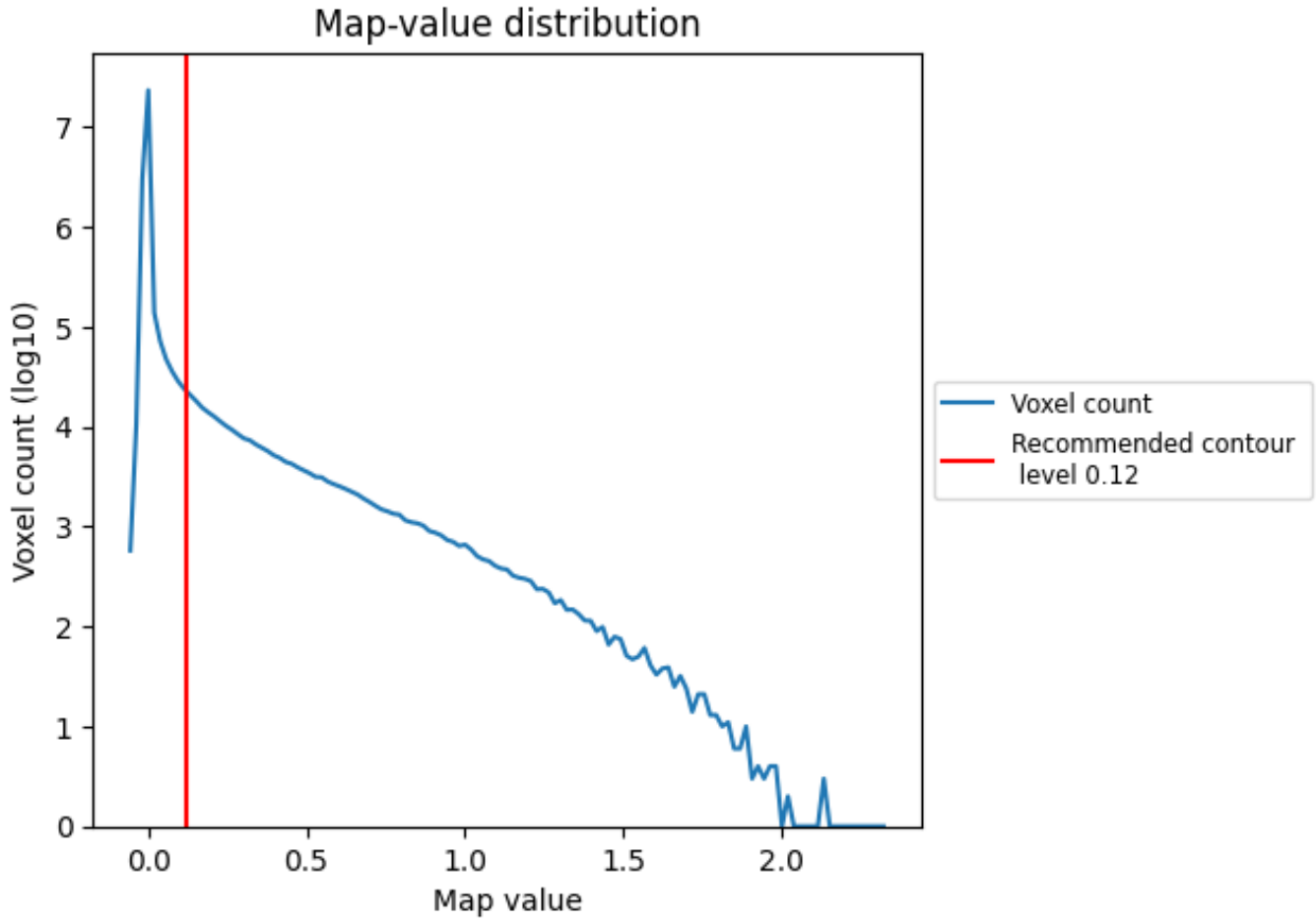
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

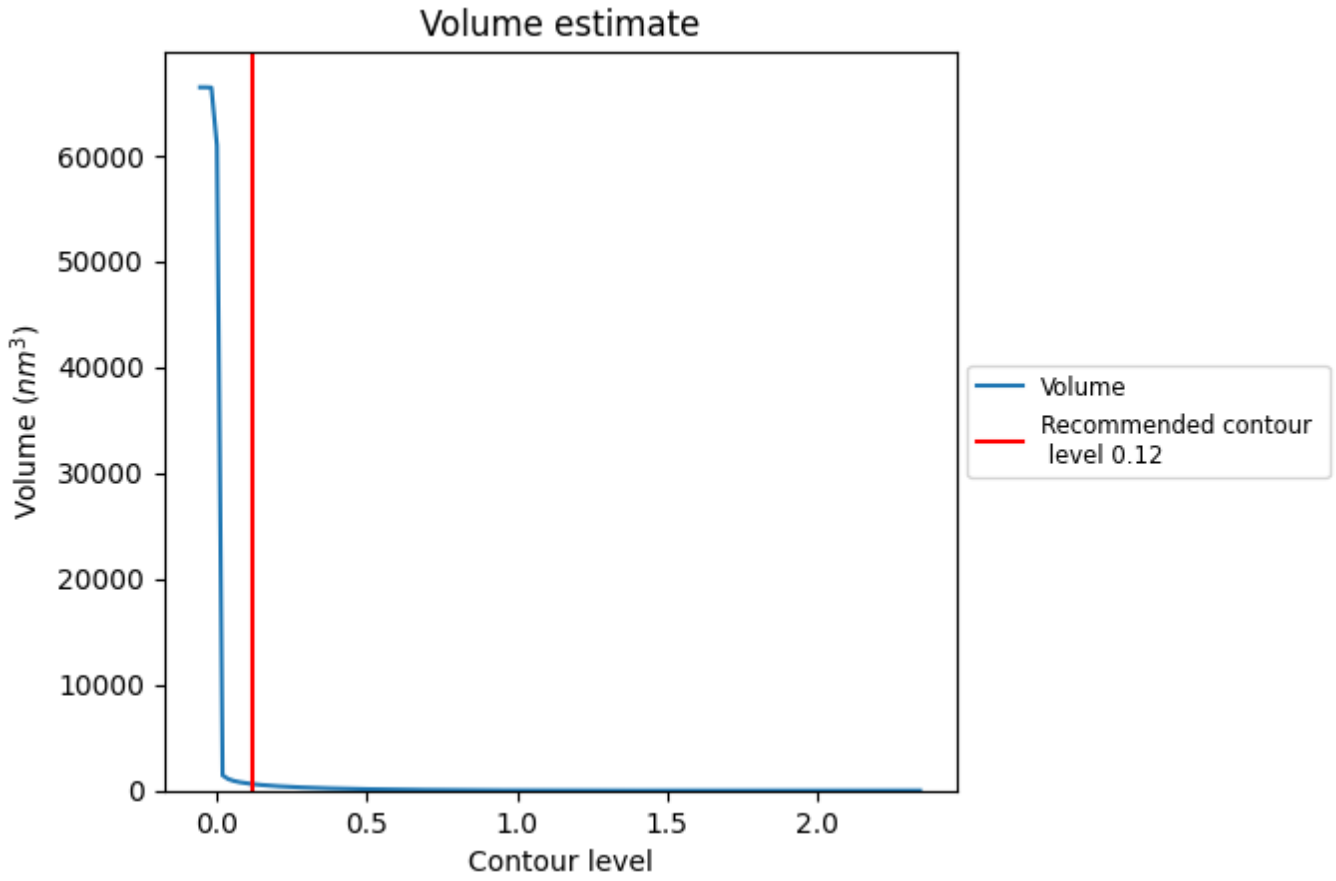
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

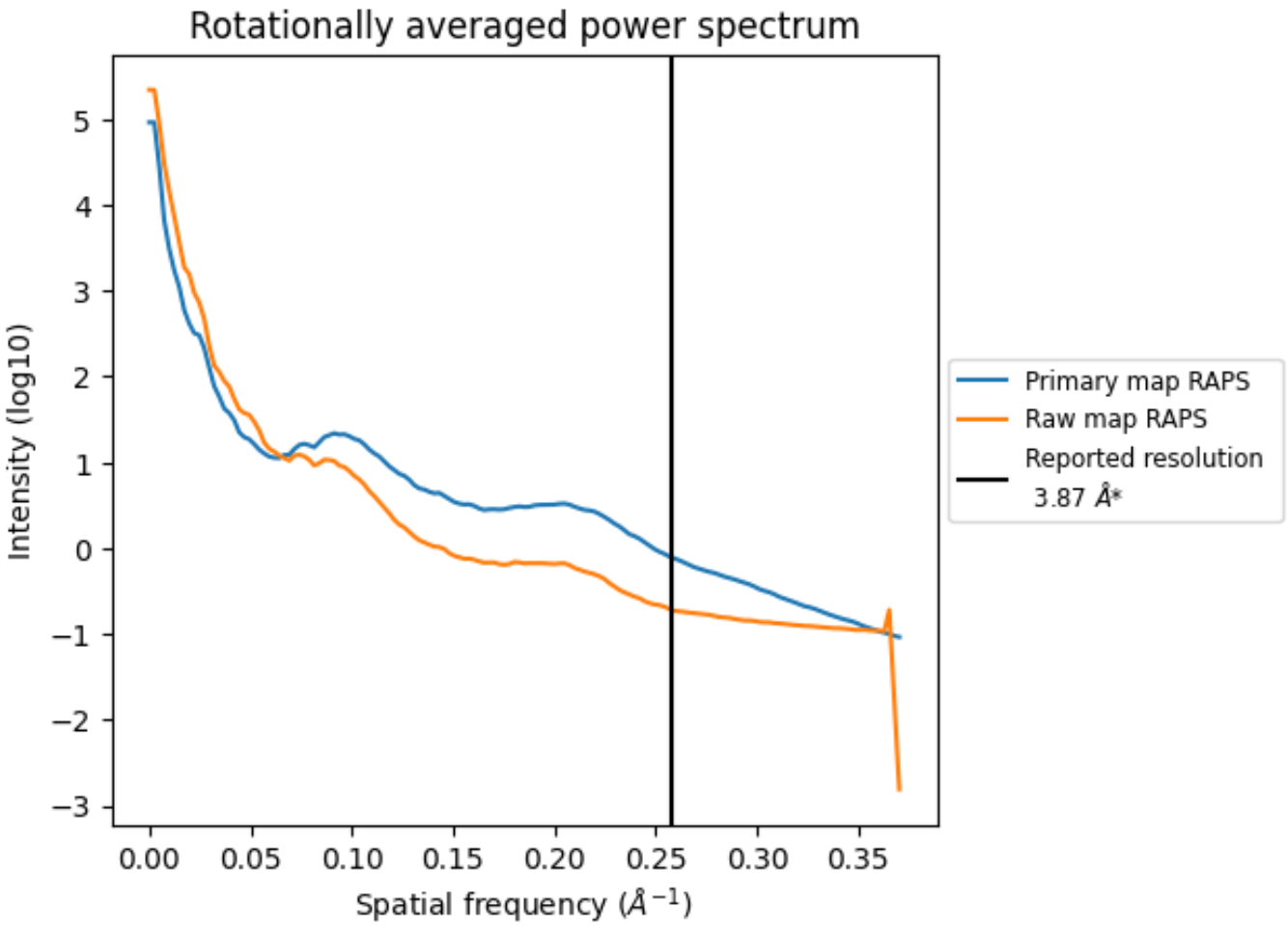
7.2 Volume estimate



The volume at the recommended contour level is 609 nm^3; this corresponds to an approximate mass of 550 kDa.

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

7.3 Rotationally averaged power spectrum (i)

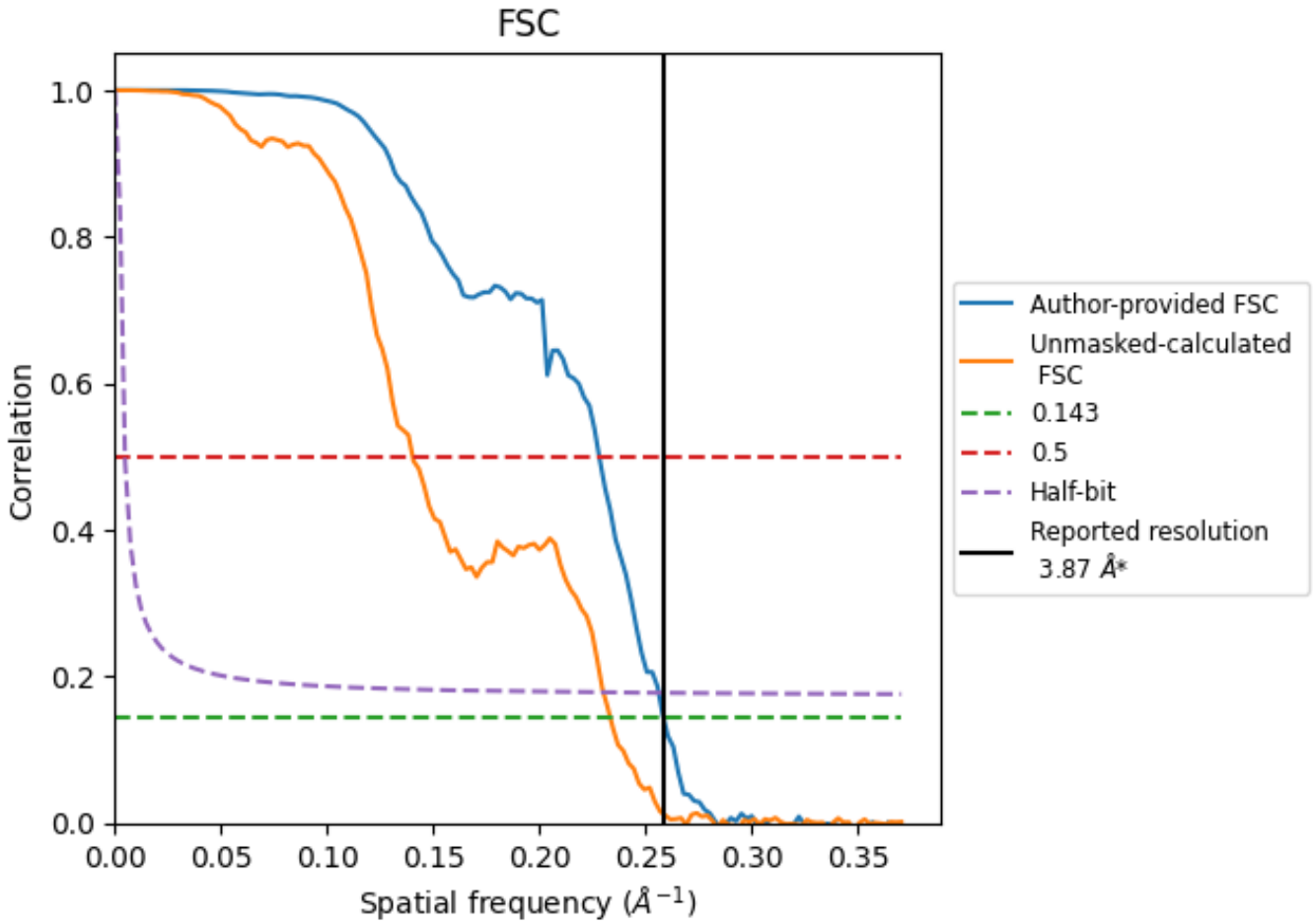


*Reported resolution corresponds to spatial frequency of 0.258 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.258 Å^{-1}

8.2 Resolution estimates (i)

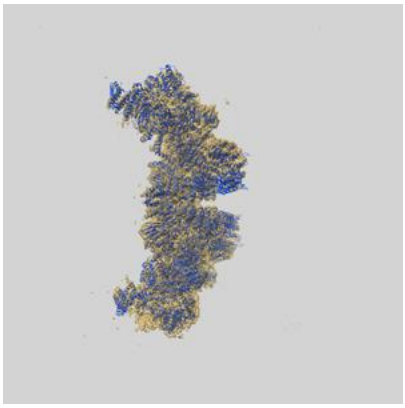
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.87	-	-
Author-provided FSC curve	3.87	4.38	3.90
Unmasked-calculated*	4.28	7.13	4.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.28 differs from the reported value 3.87 by more than 10 %

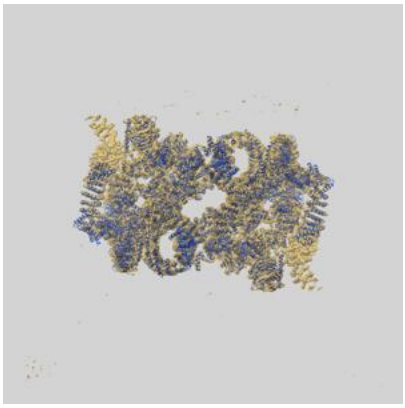
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13594 and PDB model 7PQH. Per-residue inclusion information can be found in section 3 on page 5.

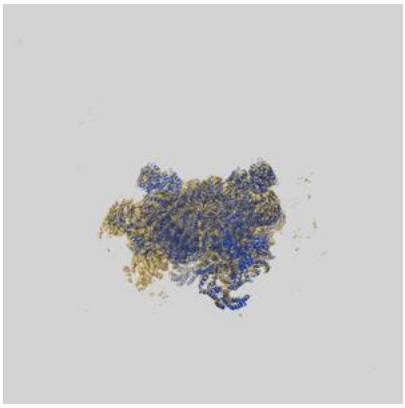
9.1 Map-model overlay



X



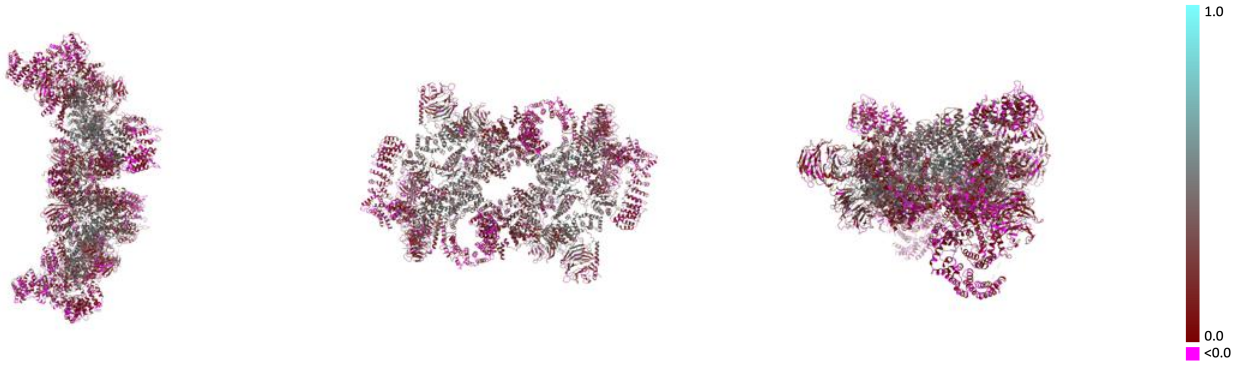
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

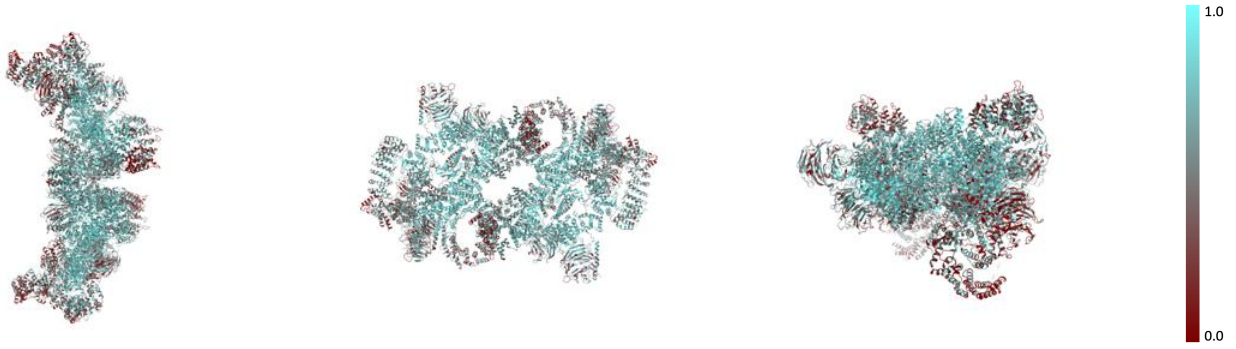
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

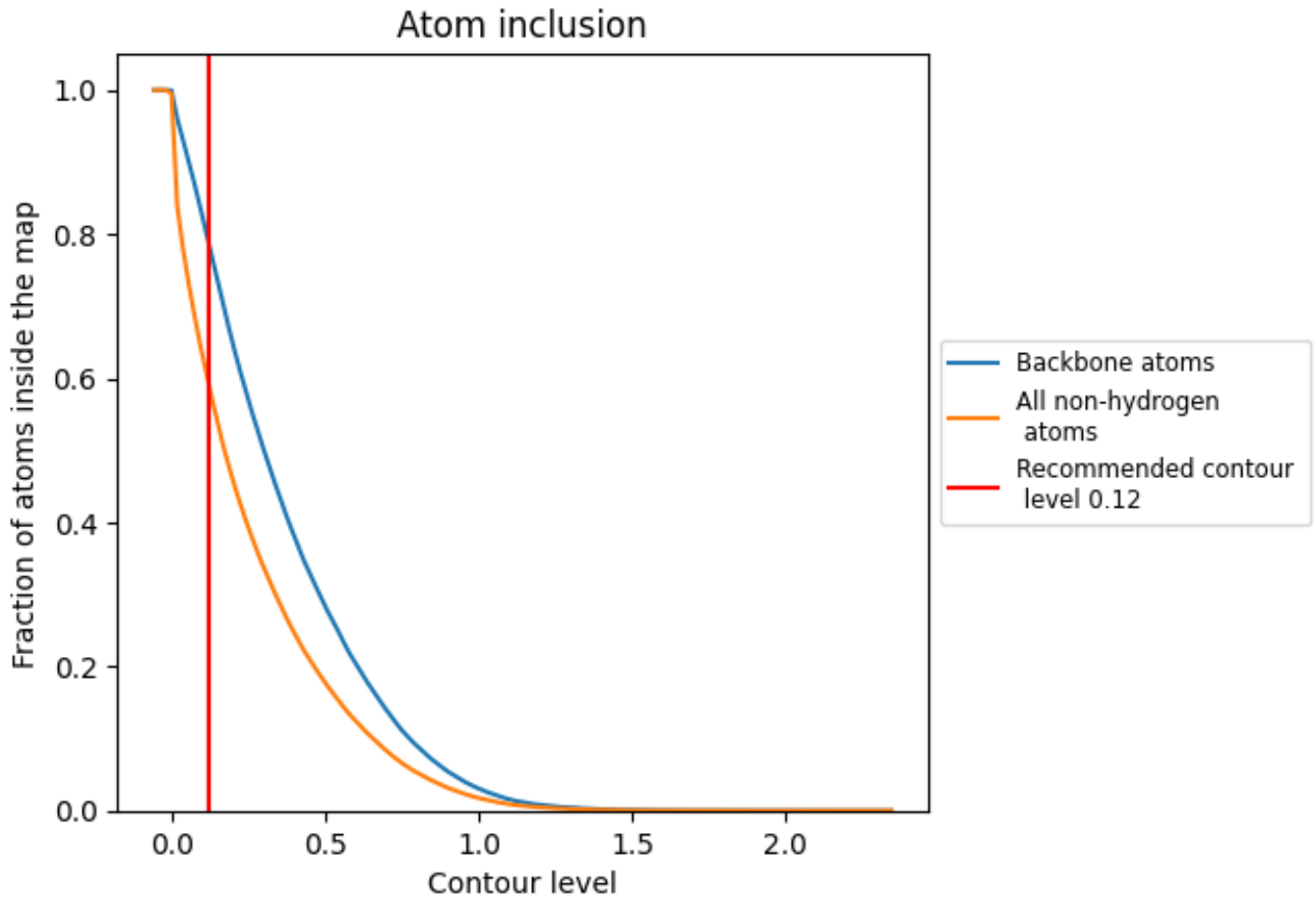
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5920	0.2410
A	0.7000	0.3320
B	0.7191	0.3360
C	0.5663	0.2680
D	0.5482	0.2640
E	0.6176	0.2290
F	0.6111	0.2270
G	0.6837	0.3160
H	0.4175	0.1110
I	0.2017	0.1100
J	0.6972	0.3160
K	0.4346	0.1150
L	0.2449	0.1250