Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 12:50 PM EST

PDB ID	:	7U9Q
EMDB ID	:	EMD-26405
Title	:	Structure of PKA phosphorylated human RyR2 in the closed state
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2022-03-11
Resolution	:	3.11 Å(reported)
Based on initial model	:	7U9X

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:

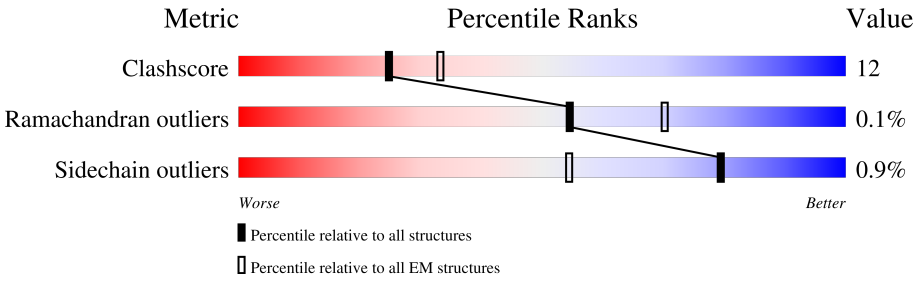
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.11 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	E	108	80% 17%
1	F	108	79% 19%
1	G	108	79% 19%
1	H	108	77% 20%
2	A	4967	13% 62% 22% 15%
2	B	4967	13% 62% 22% 15%
2	C	4967	13% 62% 22% 15%
2	D	4967	13% 62% 22% 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 138608 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

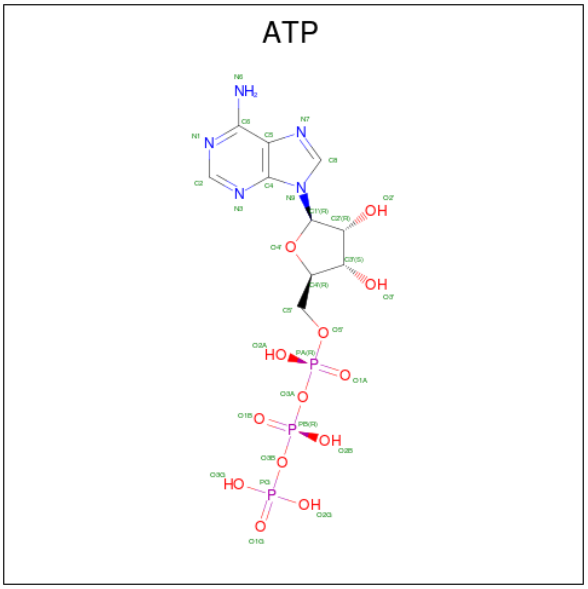
- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	D	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	B	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	C	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



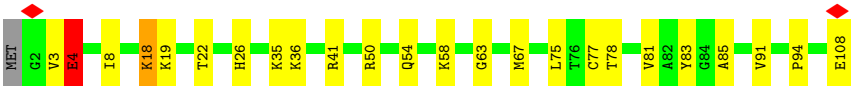
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	C	1	Total	C	N	O	P	0
			62	20	10	26	6	

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.

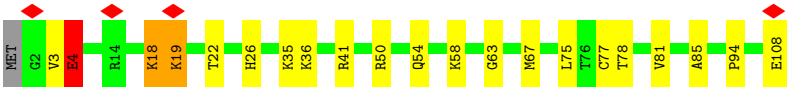
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



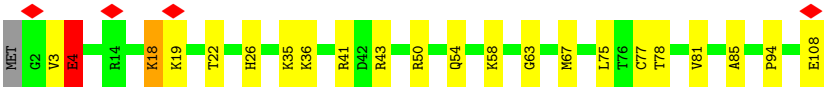
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



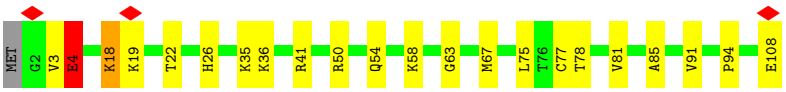
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



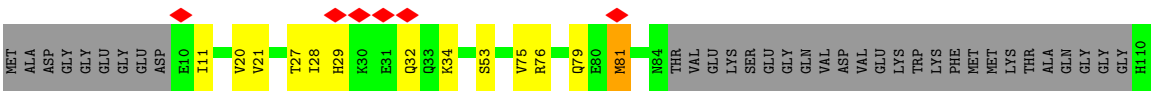
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

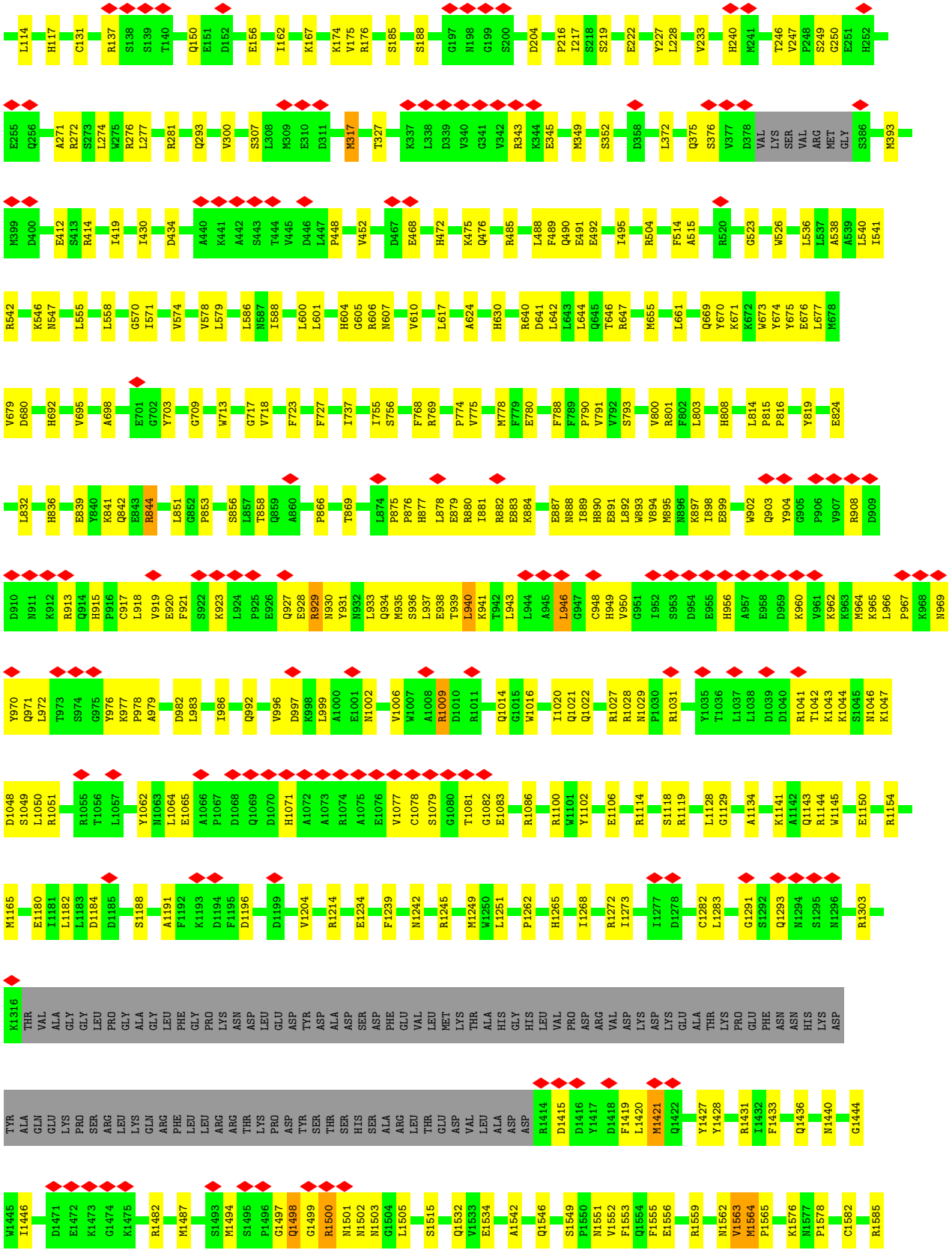
Chain G:

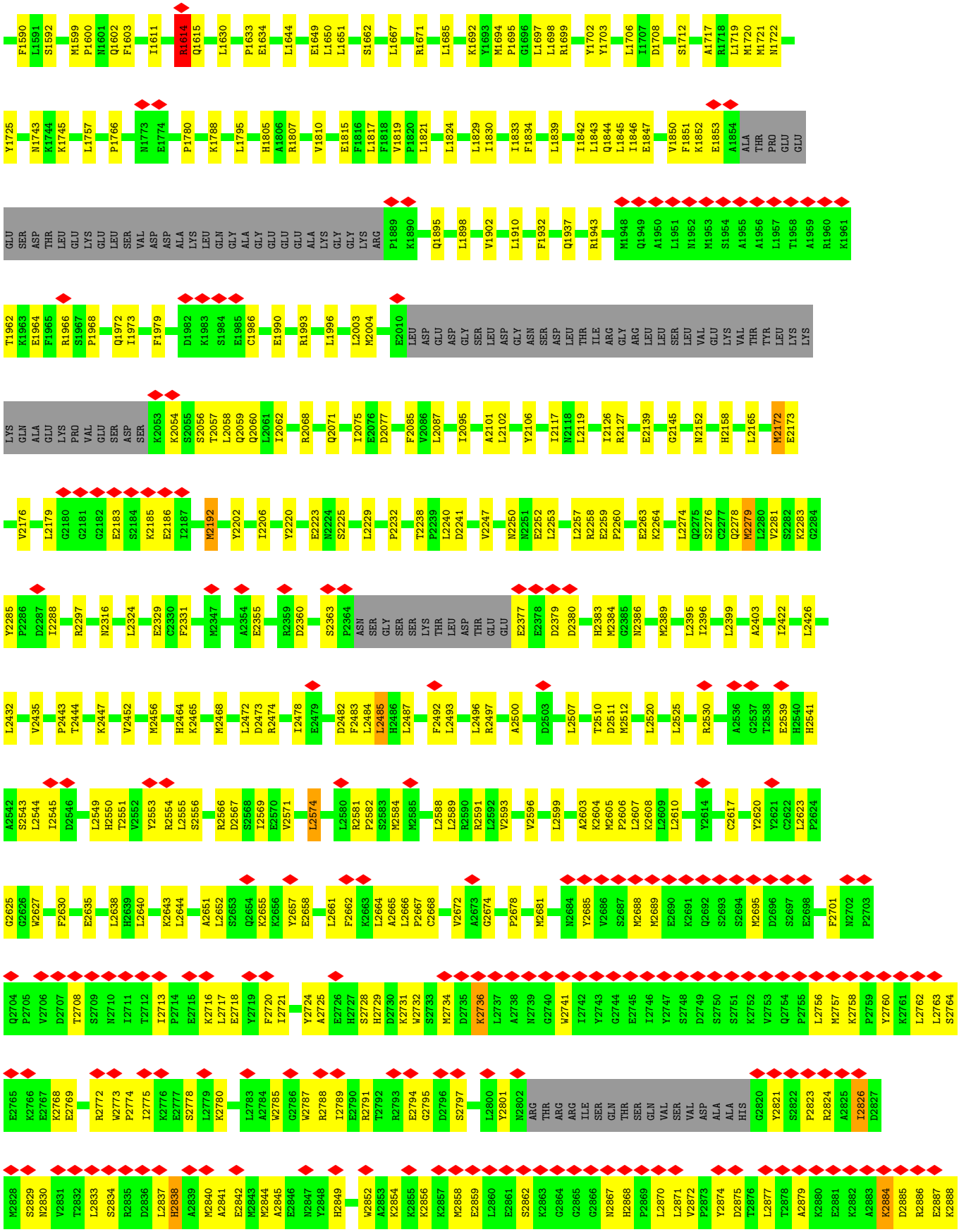


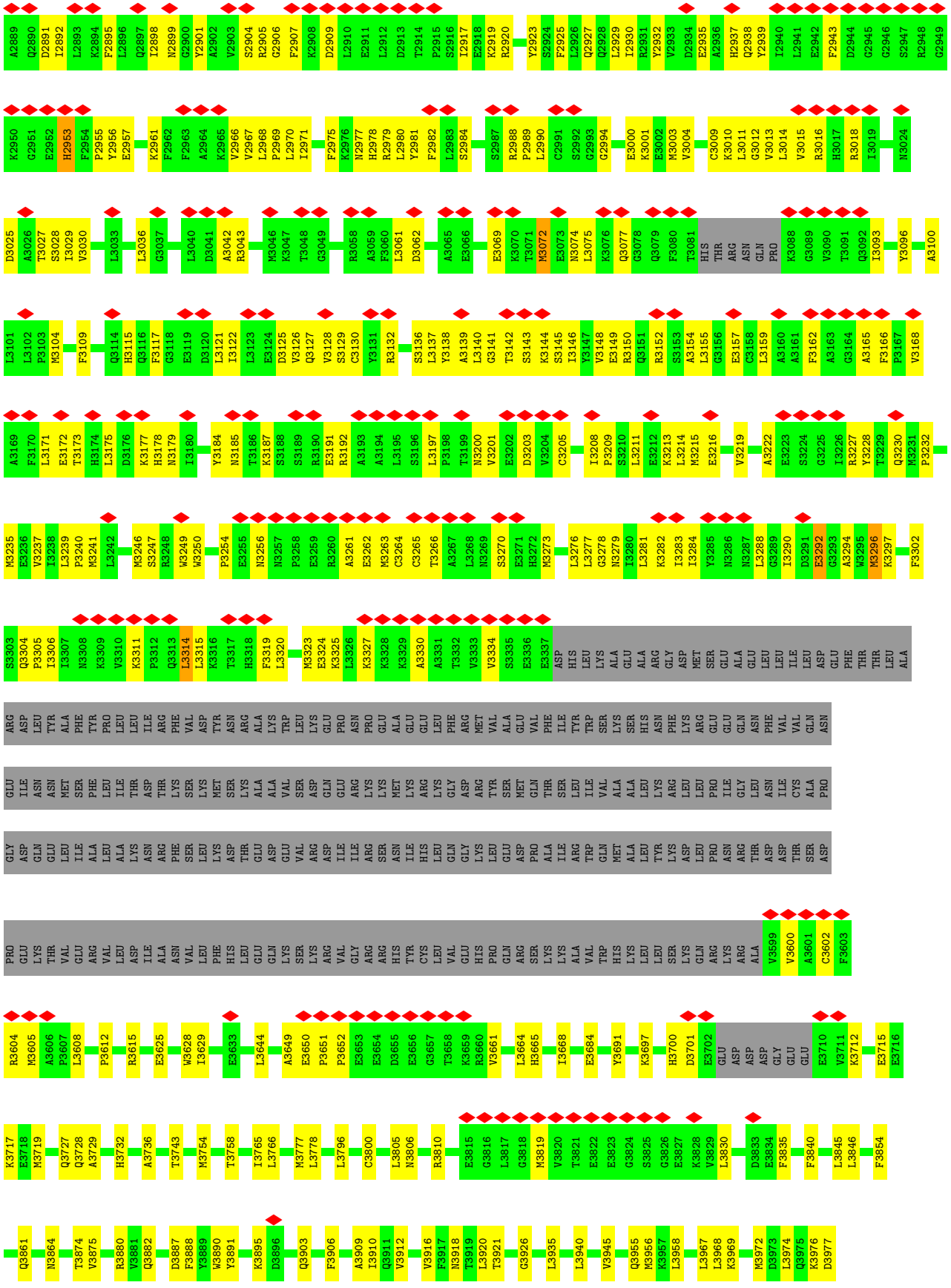
• Molecule 2: Ryanodine receptor 2

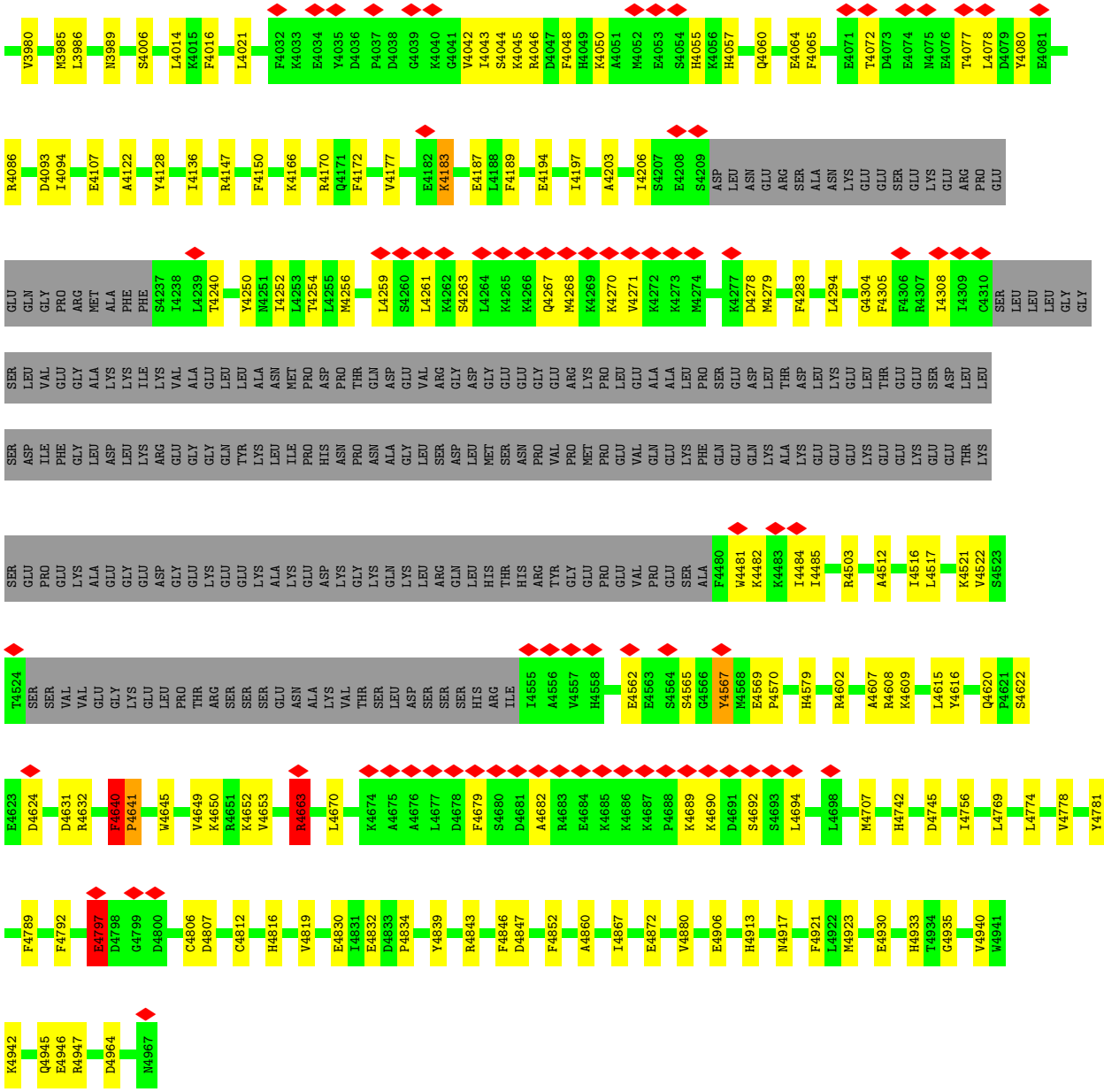
Chain A:




L114 H117 C131 R137 S138 S139 T140 Q150 E151 D152 E156 I162 K167 K174 V175 R176 S185 S188 G197 N198 G199 S200 D204 P216 I217 S218 S219 E222 Y227 L228 V233 H240 M241 T246 V247 P248 S249 G250 E251 H252
E255 Q256 A271 R272 S273 L274 W275 R276 L277 R281 Q293 V300 S307 L308 M309 E310 D311 M317 T327 K337 L338 D339 V340 G341 V342 R343 K344 E345 M349 S352 D358 L372 Q375 S376 V377 D378 VAL LYS SER VAL ARG MET GLY S386 M393
M399 D400 E412 S413 R414 I419 I430 D434 A440 K441 A442 S443 T444 V445 D446 L447 P448 V452 D467 E468 H472 K475 Q476 R485 L488 F489 Q490 E491 E492 I495 R504 F514 A515 R520 G523 W526 L536 L537 A538 A539 L540 I541
R542 K546 N547 L555 L558 G570 I571 V574 V578 L579 L586 N587 I588 L600 L601 H604 G605 R606 N607 V610 L617 A624 H630 R640 D641 L642 L643 L644 Q645 T646 R647 M655 L661 Q669 Y670 K671 K672 W673 Y674 Y675 E676 L677 M678
V679 D680 H692 V695 A698 E701 G702 Y703 G709 W713 G717 V718 F723 F727 I737 I755 S756 F768 R769 P774 V775 M778 F779 E780 F788 F789 P790 V791 V792 S793 V800 R801 F802 L803 H808 L814 P815 P816 Y819 E824
L832 H836 E839 Y840 K841 Q842 E843 R844 L851 G852 P853 S856 L857 T858 Q859 A860 P866 T869 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 K884 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 W902 Q903 Y904 G905 P906 V907 R908 D909
D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956 A957 E958 D959 K960 V961 K962 K963 M964 K965 L966 P967 K968 N969
Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 D982 L983 I986 Q992 V996 D997 K998 L999 A1000 E1001 N1002 V1006 W1007 A1008 R1009 D1010 R1011 Q1014 G1015 W1016 I1020 Q1021 Q1022 R1027 R1028 N1029 P1030 R1031 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047
D1048 S1049 L1050 R1051 R1055 T1056 L1057 Y1062 N1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1086 R1100 W1101 Y1102 E1106 R1114 S1118 R1119 L1128 G1129 A1134 K1141 A1142 Q1143 R1144 W1145 E1150 R1154
M1165 E1180 I1181 L1182 L1183 D1184 D1185 S1188 A1191 F1192 K1193 D1194 F1195 D1196 D1199 V1204 R1214 E1234 F1239 N1242 R1245 M1249 W1250 L1251 P1262 H1265 I1268 R1272 I1273 I1277 D1278 C1282 L1283 G1291 S1292 Q1293 N1294 S1295 N1296 R1303
K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP
TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418 F1419 L1420 M1421 Q1422 Y1427 Y1428 R1431 I1432 F1433 Q1436 N1440 G1444
W1445 I1446 D1471 E1472 K1473 G1474 K1475 R1482 M1487 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 S1515 Q1532 V1533 E1534 A1542 Q1546 S1549 P1550 N1551 V1552 F1553 Q1554 F1555 E1556 R1559 N1562 V1563 M1564 P1565 K1576 N1577 P1578 C1582 R1585

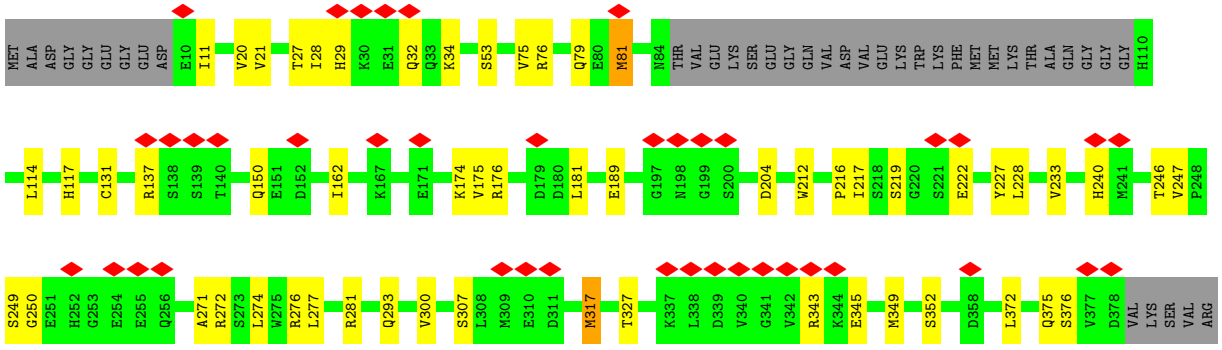


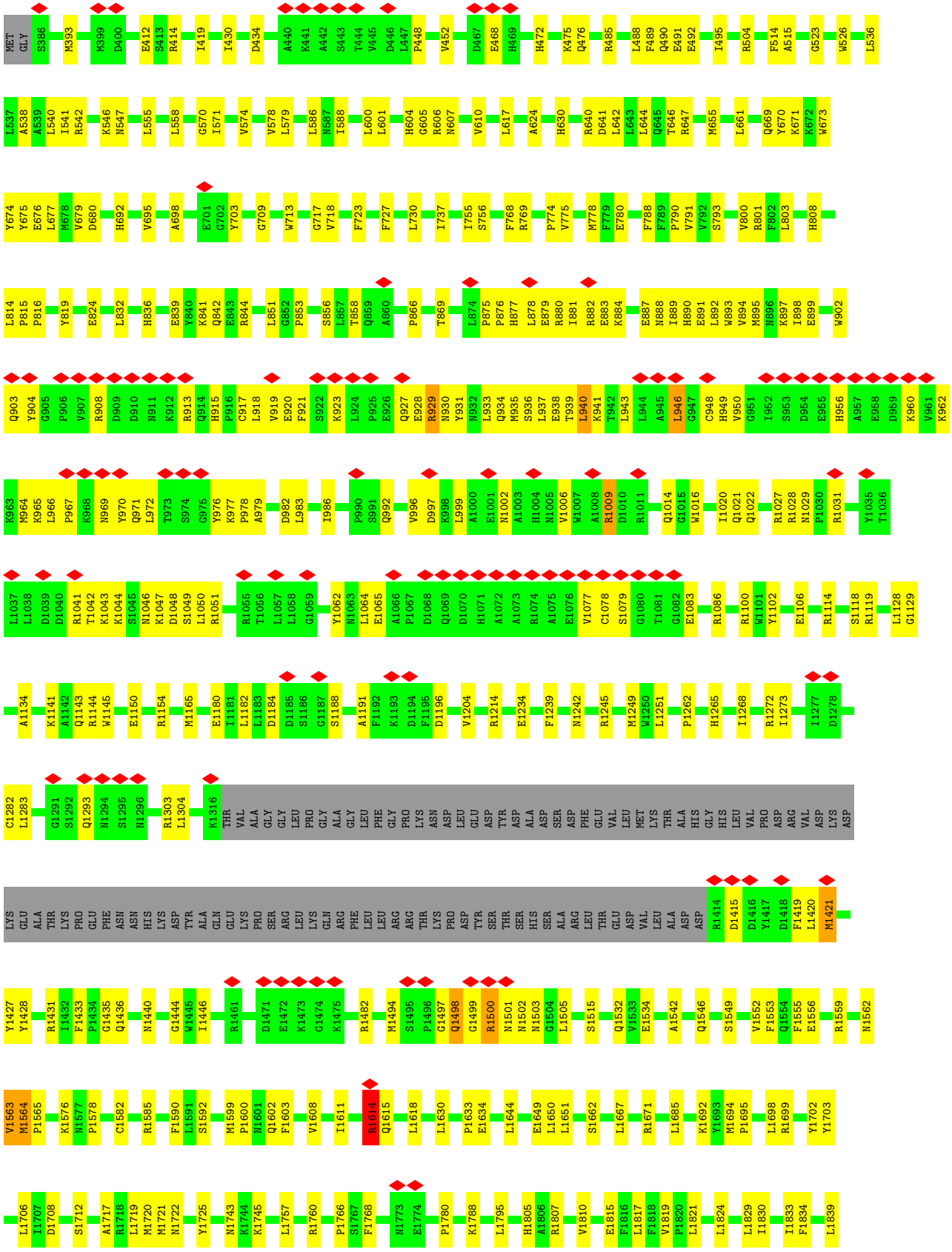


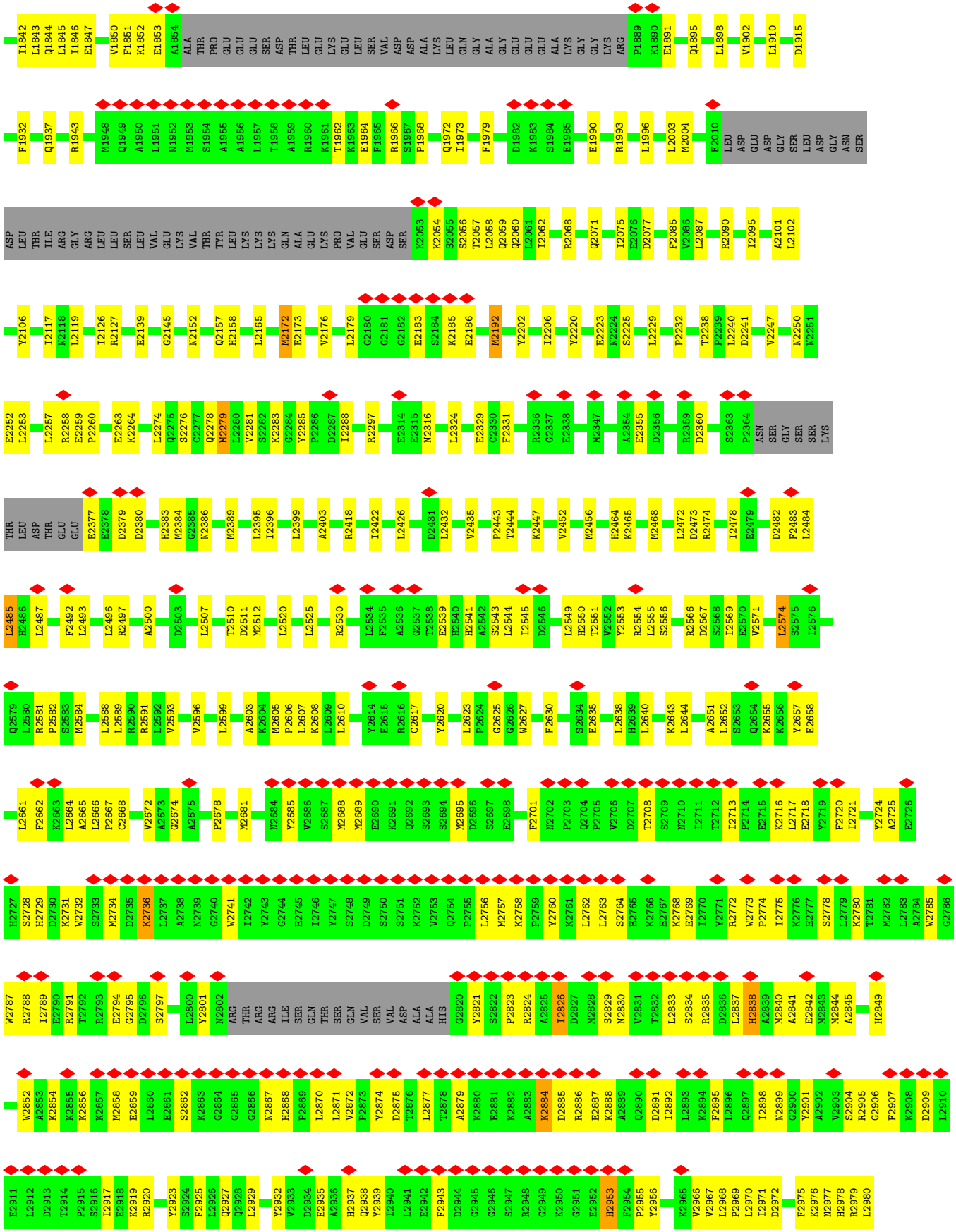


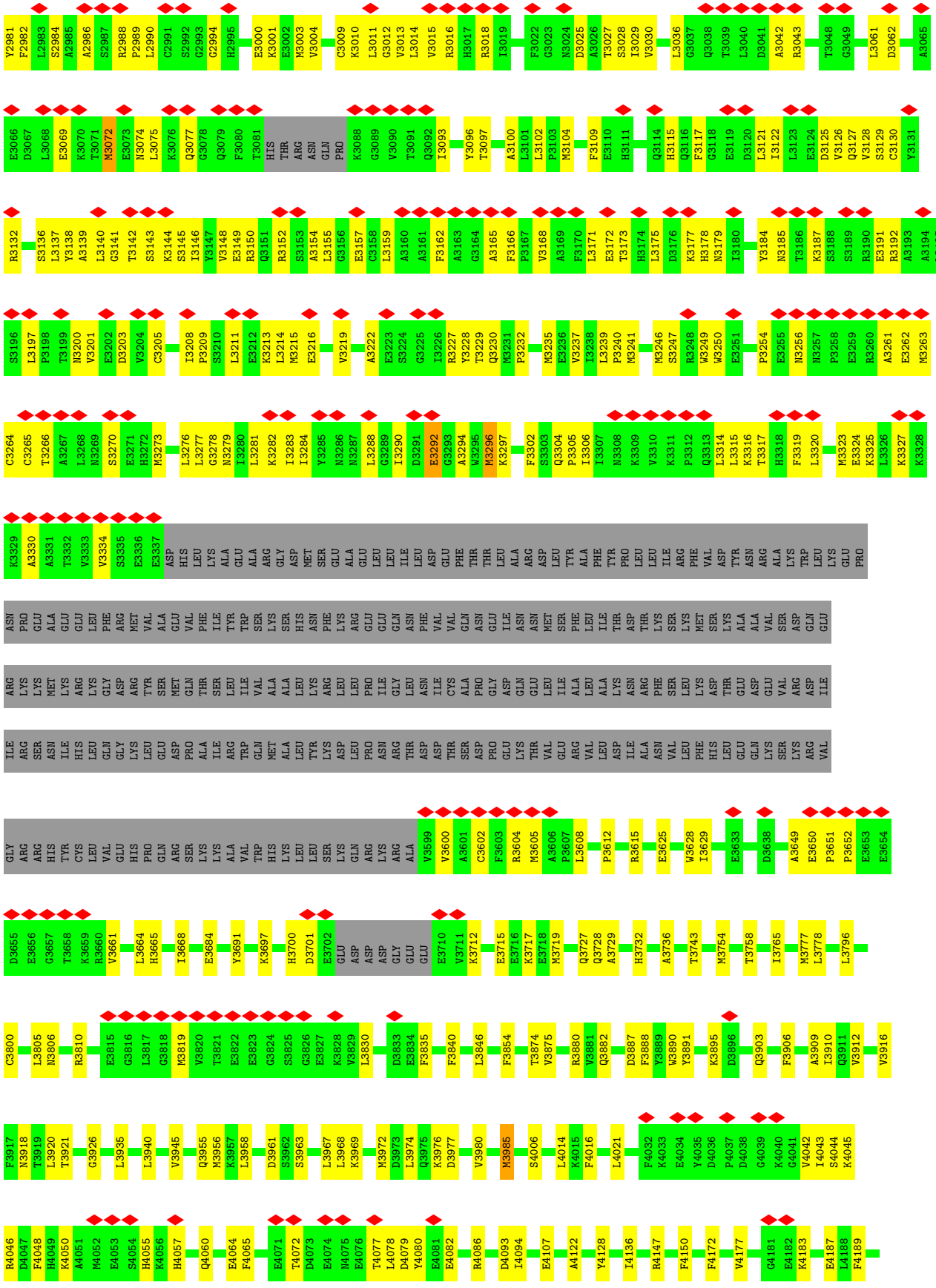
• Molecule 2: Ryanodine receptor 2

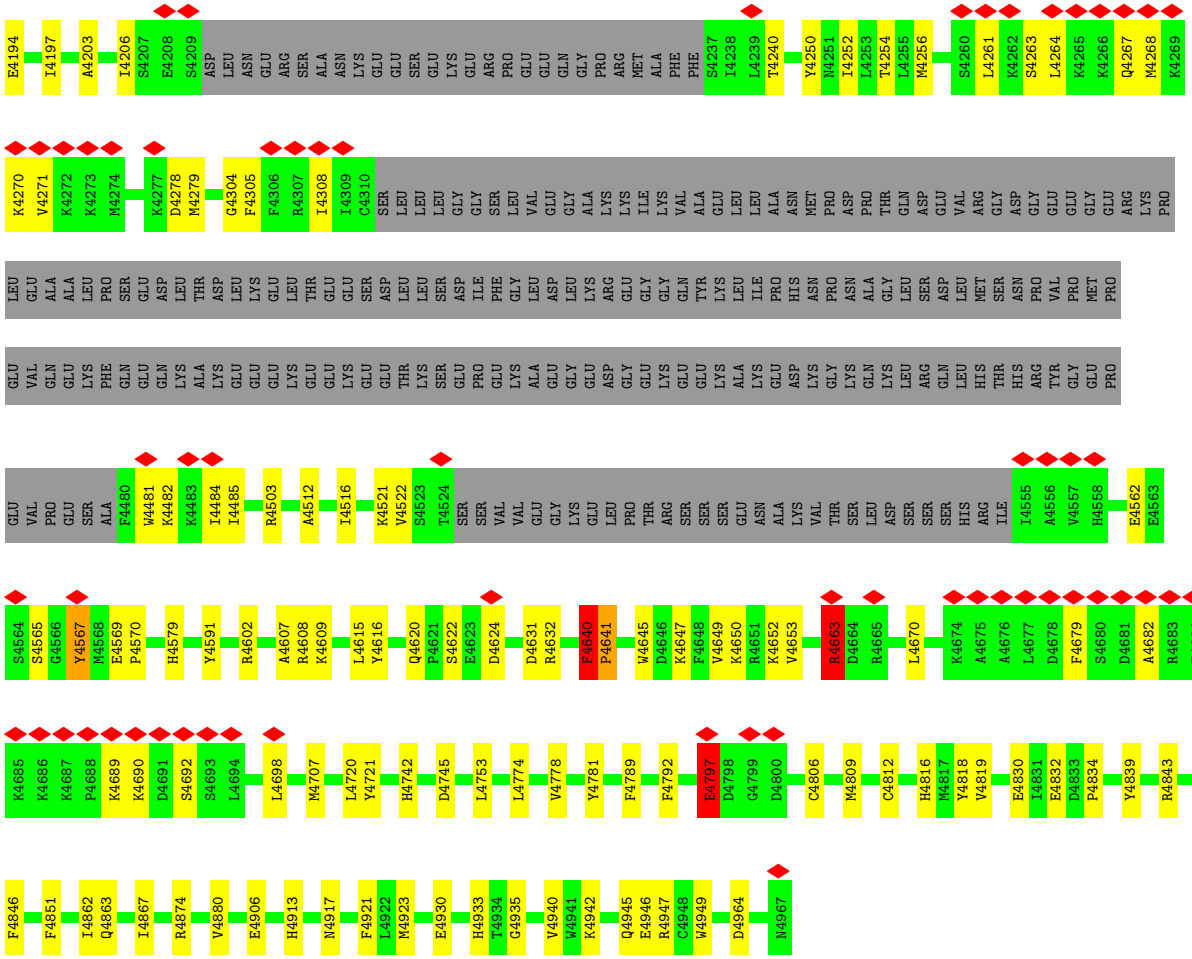
Chain D:




MET GLY S386 M393 M399 D400 E412 S413 R414 I419 I430 D434 A440 K441 A442 S443 T444 V445 D446 L447 P448 V452 D467 E468 H469 H472 K475 Q476 R485 L488 F489 Q490 E491 E492 I495 R504 F514 A515 G523 W526 L536
L537 A538 A539 L540 I541 R542 K546 N547 L555 L558 G570 I571 V574 V578 L579 L586 N587 I588 L600 L601 H604 G605 R606 N607 V610 L617 A624 H630 R640 D641 L642 L643 L644 Q645 T646 R647 M655 L661 Q669 Y670 K671 K672 W673
Y674 Y675 E676 L677 M678 V679 D680 H692 V695 A698 E701 G702 Y703 G709 W713 G717 V718 F723 F727 L730 I737 I755 S756 F768 R769 P774 V775 M778 F779 E780 F788 F789 P790 V791 V792 S793 V800 R801 F802 L803 H808
L814 P815 P816 Y819 E824 L832 H836 E839 Y840 K841 Q842 E843 R844 L851 G852 P853 S856 L857 T858 Q859 A860 P866 T869 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 K884 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 W902
Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956 A957 E958 D959 K960 V961 K962
K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 D982 L983 I986 P990 S991 Q992 V996 D997 K998 L999 A1000 E1001 N1002 A1003 H1004 N1005 V1006 W1007 A1008 R1009 D1010 R1011 Q1014 G1015 W1016 I1020 Q1021 Q1022 R1027 R1028 N1029 P1030 R1031 Y1035 T1036
L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 R1055 T1056 L1057 L1058 G1059 Y1062 N1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1086 R1100 W1101 Y1102 E1106 R1114 S1118 R1119 L1128 G1129
A1134 K1141 A1142 Q1143 R1144 W1145 E1150 R1154 M1165 E1180 I1181 L1182 L1183 D1184 D1185 S1186 G1187 S1188 A1191 F1192 K1193 D1194 F1195 D1196 V1204 R1214 E1234 F1239 N1242 R1245 M1249 W1250 L1251 P1262 H1265 I1268 R1272 I1273 I1277 D1278
C1282 L1283 G1291 S1292 Q1293 N1294 S1295 N1296 R1303 L1304 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP
LYS GLU ALA THR LYS PRO GLU PHE ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP R1414 D1415 D1416 Y1417 D1418 F1419 L1420 M1421
Y1427 Y1428 R1431 I1432 F1433 P1434 G1435 Q1436 N1440 G1444 W1445 I1446 R1461 D1471 E1472 K1473 G1474 K1475 R1482 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 S1515 Q1532 V1533 E1534 A1542 Q1546 S1549 V1552 F1553 Q1554 F1555 E1556 R1559 N1562
V1563 M1564 P1565 K1576 M1577 P1578 C1582 R1585 F1590 L1591 S1592 M1599 P1600 N1601 Q1602 F1603 V1608 I1611 R1614 Q1615 L1618 L1630 P1633 E1634 L1644 E1649 L1650 L1651 S1662 L1667 R1671 L1685 K1692 Y1693 M1694 P1695 L1698 R1699 Y1702 Y1703
L1706 I1707 D1708 S1712 A1717 R1718 L1719 M1720 M1721 N1722 Y1725 N1743 K1744 K1745 L1757 R1760 P1766 S1767 F1768 N1773 E1774 P1780 K1788 L1795 H1805 A1806 R1807 V1810 E1815 F1816 L1817 F1818 V1819 P1820 L1821 L1824 L1829 I1830 I1833 F1834 L1839

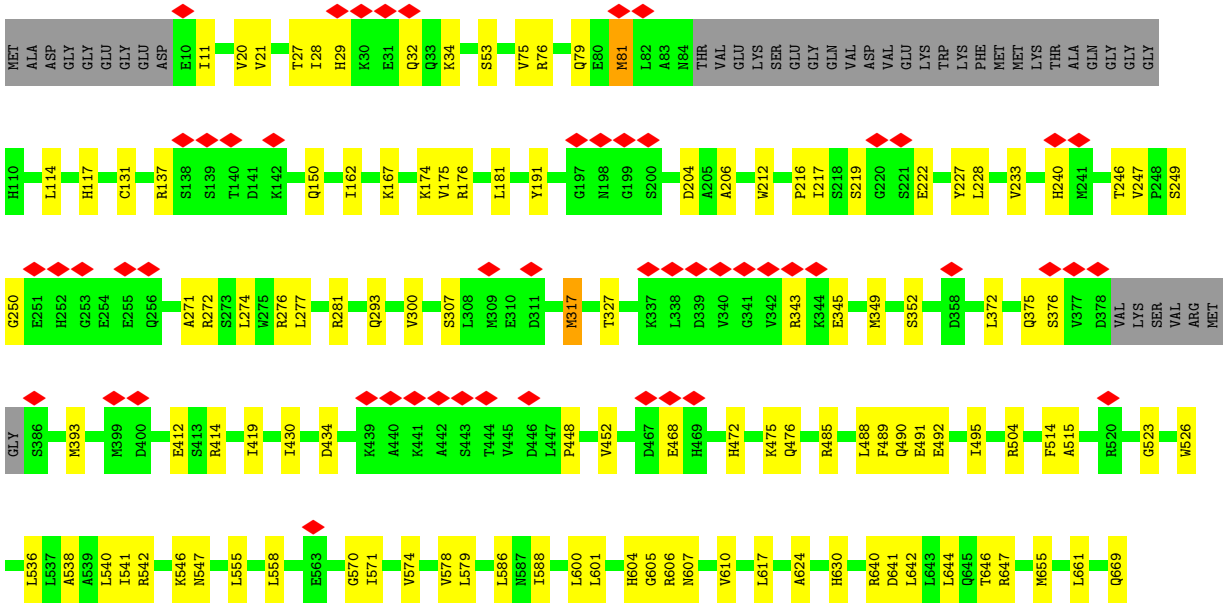


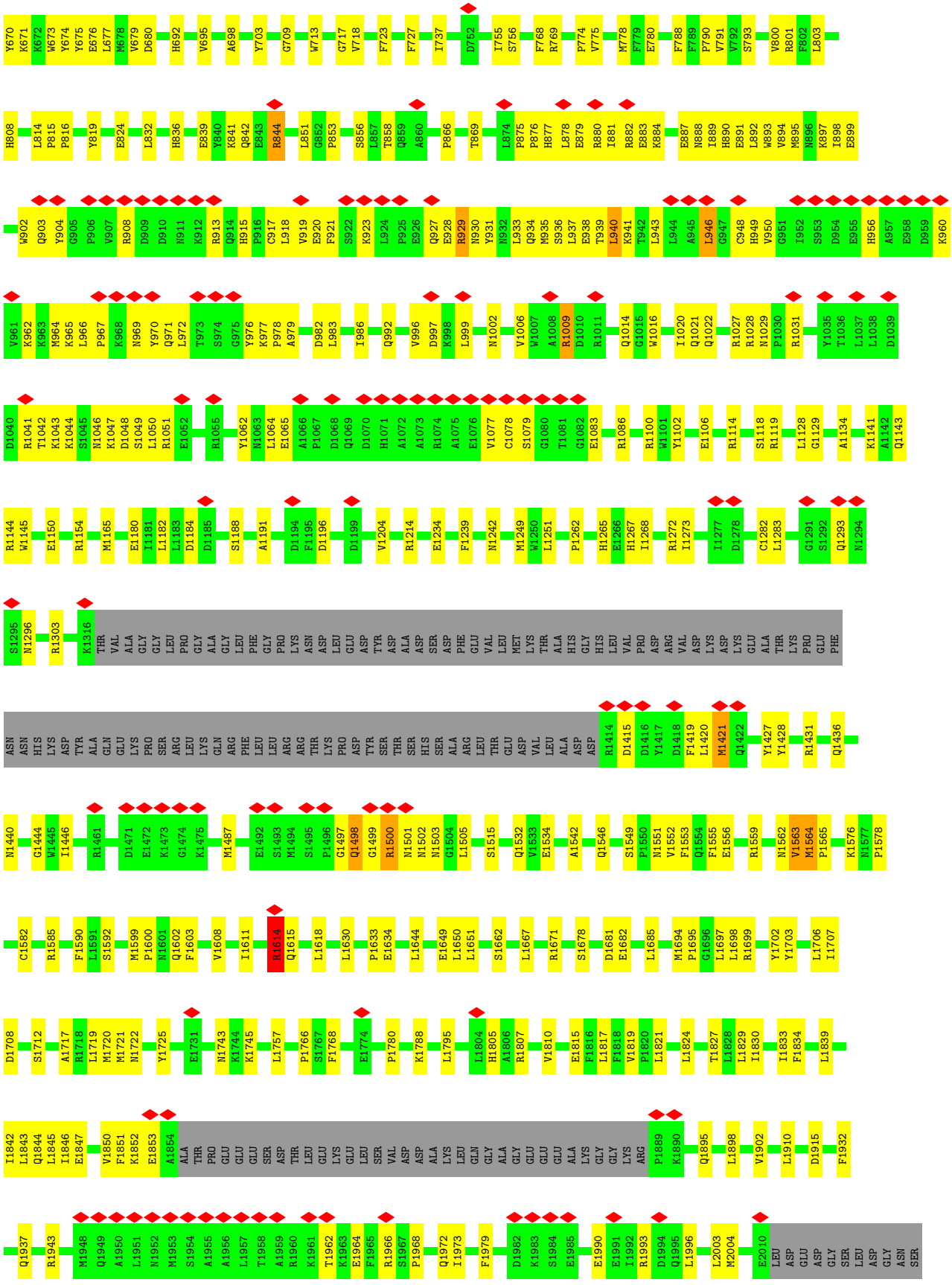


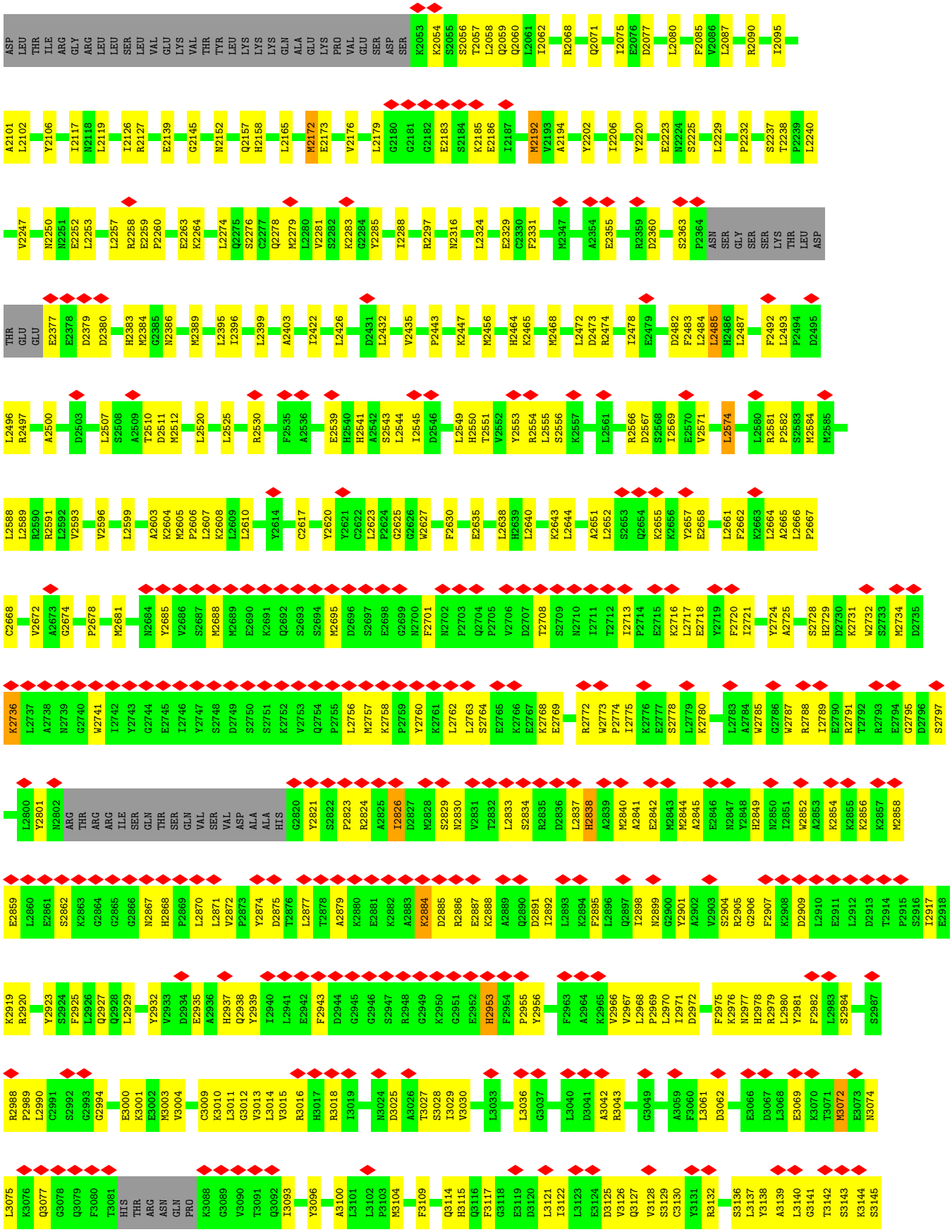


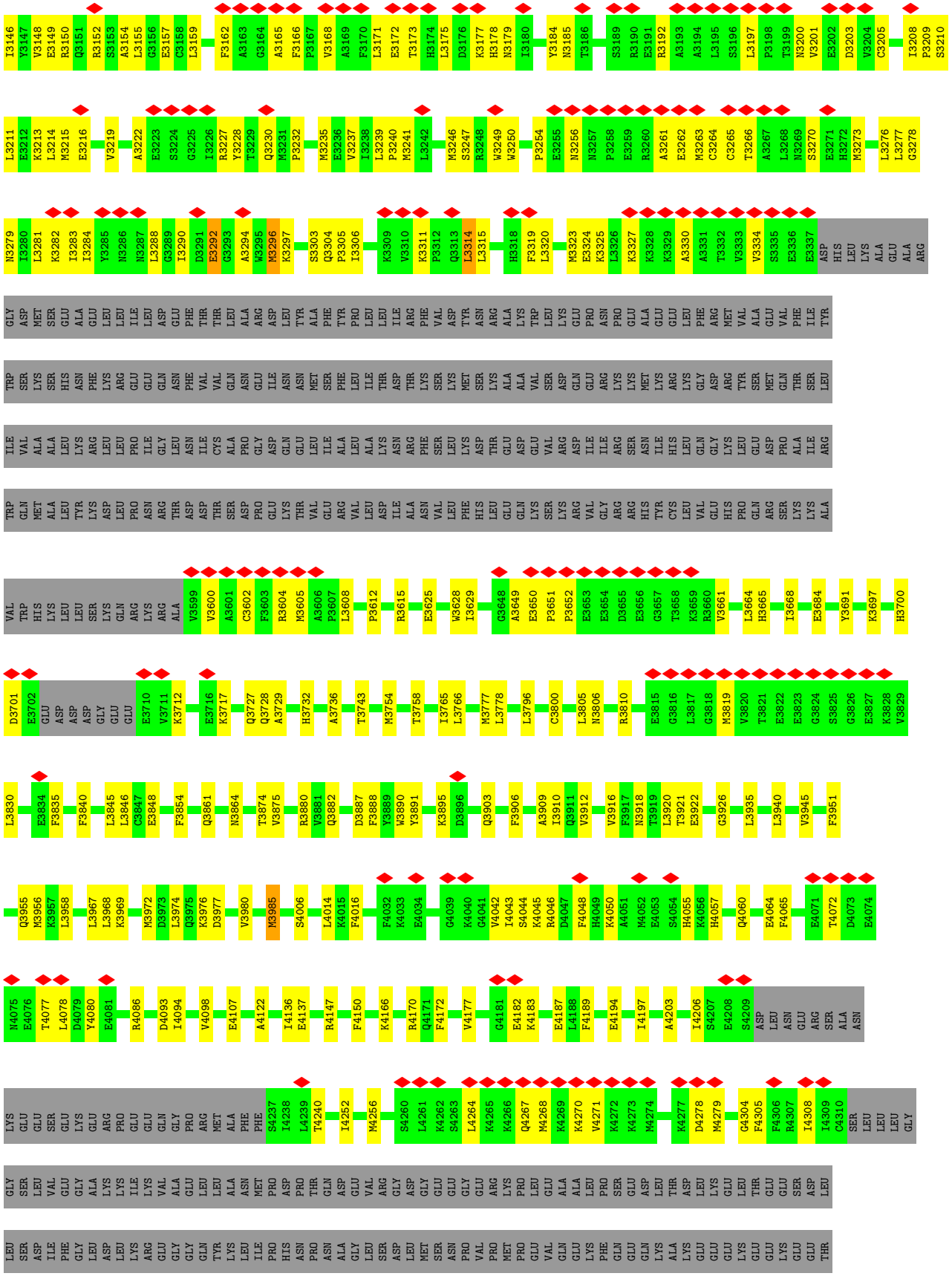
• Molecule 2: Ryanodine receptor 2

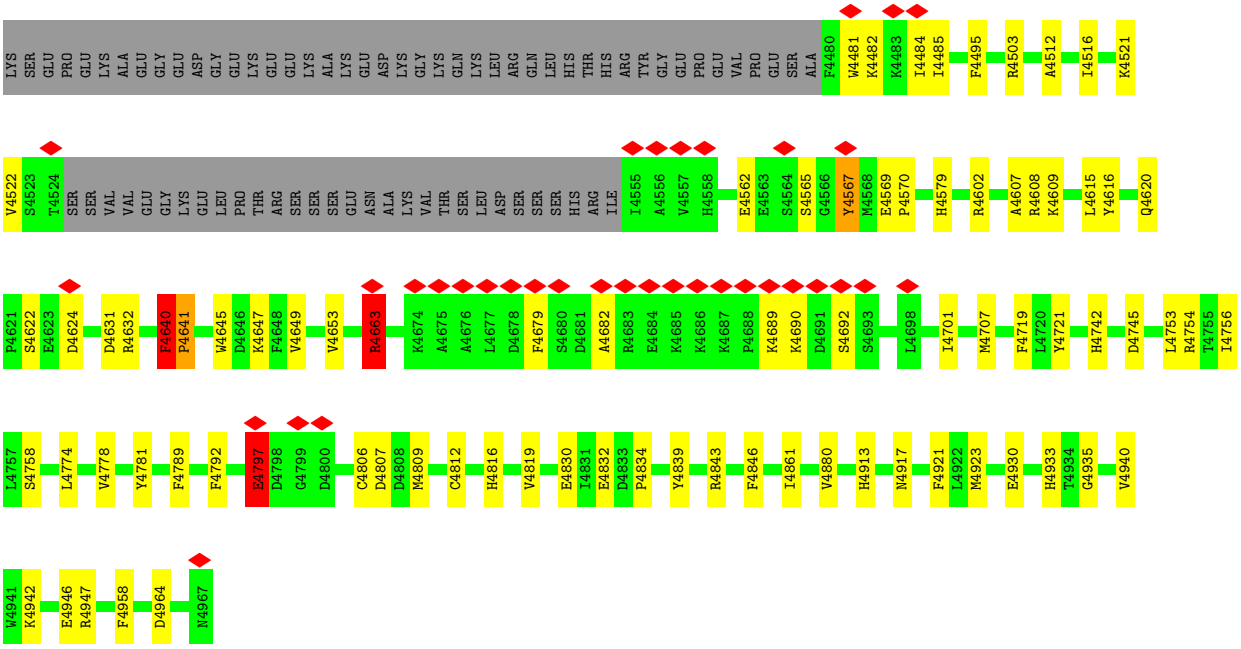
Chain B:




Y670 K671 K672 W673 Y674 Y675 E676 L677 W678 V679 D680 H692 V695 A698 Y703 G709 W713 G717 V718 F723 F727 I737 D752 I755 S756 F768 R769 P774 V775 M778 F779 E780 F788 F789 P790 V791 V792 S793 V800 R801 F802 L803
H808 L814 P815 P816 Y819 E824 L832 H836 E839 Y840 K841 Q842 E843 R844 L851 G852 P853 S856 L857 T858 Q859 A860 P866 T869 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 K884 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899
W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 P921 S922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956 A957 E958 D959 K960
V961 K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 D982 L983 I986 Q992 V996 D997 K998 L999 N1002 V1006 W1007 A1008 R1009 D1010 R1011 Q1014 G1015 W1016 L1020 Q1021 Q1022 R1027 R1028 N1029 P1030 R1031 Y1035 T1036 L1037 L1038 D1039
D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 R1055 Y1062 N1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1086 R1100 W1101 Y1102 E1106 R1114 S1118 R1119 L1128 G1129 A1134 K1141 A1142 Q1143
R1144 W1145 E1150 R1154 M1165 E1180 I1181 L1182 L1183 D1184 D1185 S1188 A1191 D1194 F1195 D1196 D1199 V1204 R1214 E1234 F1239 N1242 M1249 W1250 L1251 P1262 H1265 E1266 H1267 I1268 R1272 I1273 I1277 D1278 C1282 L1283 G1291 S1292 Q1293 N1294
S1295 N1296 R1303 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE
ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418 F1419 L1420 M1421 Q1422 Y1427 Y1428 R1431 Q1436
N1440 G1444 W1445 I1446 R1461 D1471 E1472 K1473 G1474 K1475 M1487 E1492 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 S1515 Q1532 V1533 E1534 A1542 Q1546 S1549 P1550 N1551 V1552 F1553 Q1554 F1555 E1556 R1559 N1562 V1563 M1564 P1565 K1576 N1577 P1578
C1582 R1585 F1590 L1591 S1592 M1599 P1600 N1601 Q1602 F1603 V1608 I1611 R1614 Q1615 L1618 L1630 P1633 E1634 L1644 E1649 L1650 L1651 S1662 L1667 R1671 S1678 D1681 E1682 L1685 M1694 P1695 G1696 L1697 L1698 R1699 Y1702 Y1703 L1706 I1707
D1708 S1712 A1717 R1718 L1719 M1720 M1721 N1722 Y1725 E1731 N1743 K1744 K1745 L1757 P1766 S1767 F1768 E1774 P1780 K1788 L1795 L1804 H1805 A1806 R1807 V1810 E1815 F1816 L1817 F1818 V1819 P1820 L1821 L1824 T1827 L1828 L1829 I1830 I1833 F1834 L1839
I1842 L1843 Q1844 L1845 I1846 E1847 V1850 F1851 K1852 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 Q1895 L1898 V1902 L1910 D1915 F1932
Q1937 R1943 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 K1963 E1964 F1965 R1966 S1967 P1968 Q1972 I1973 F1979 D1982 K1983 S1984 E1985 E1990 E1991 I1992 R1993 D1994 Q1995 L1996 L2003 M2004 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER

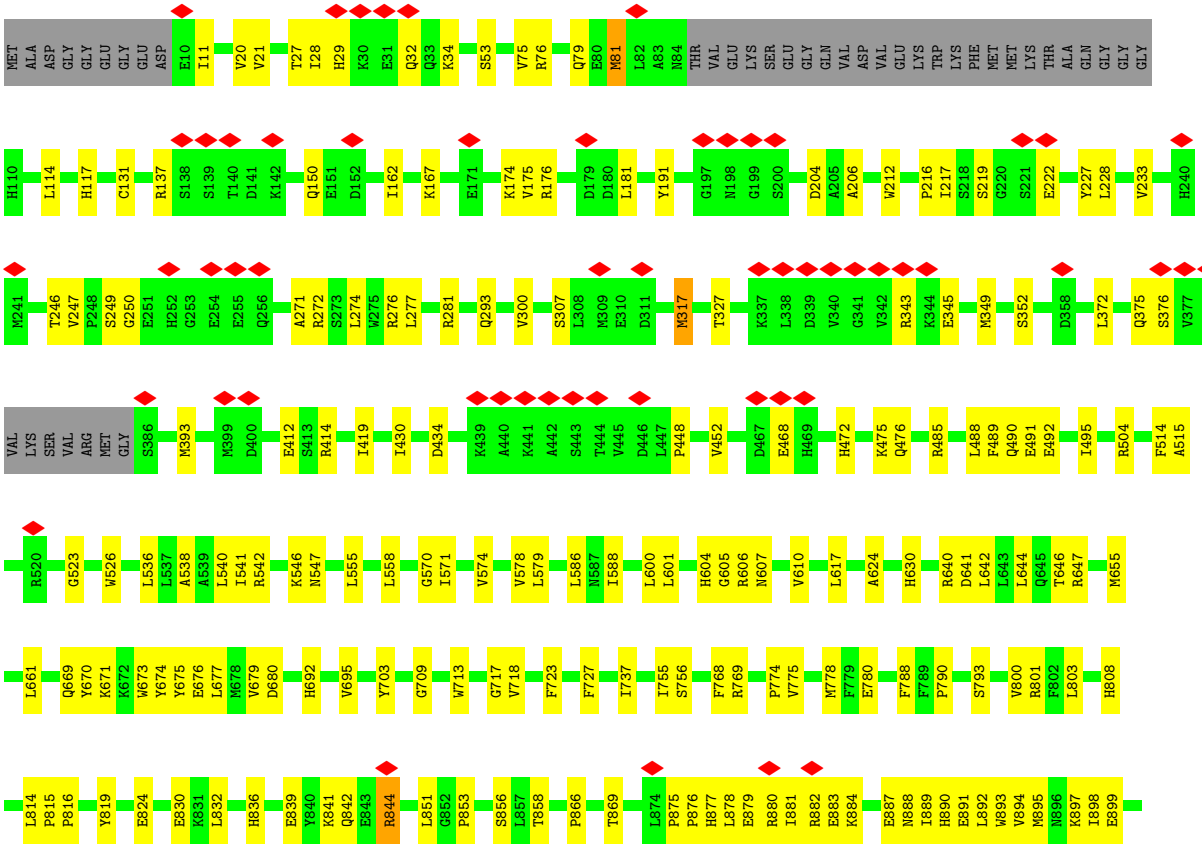


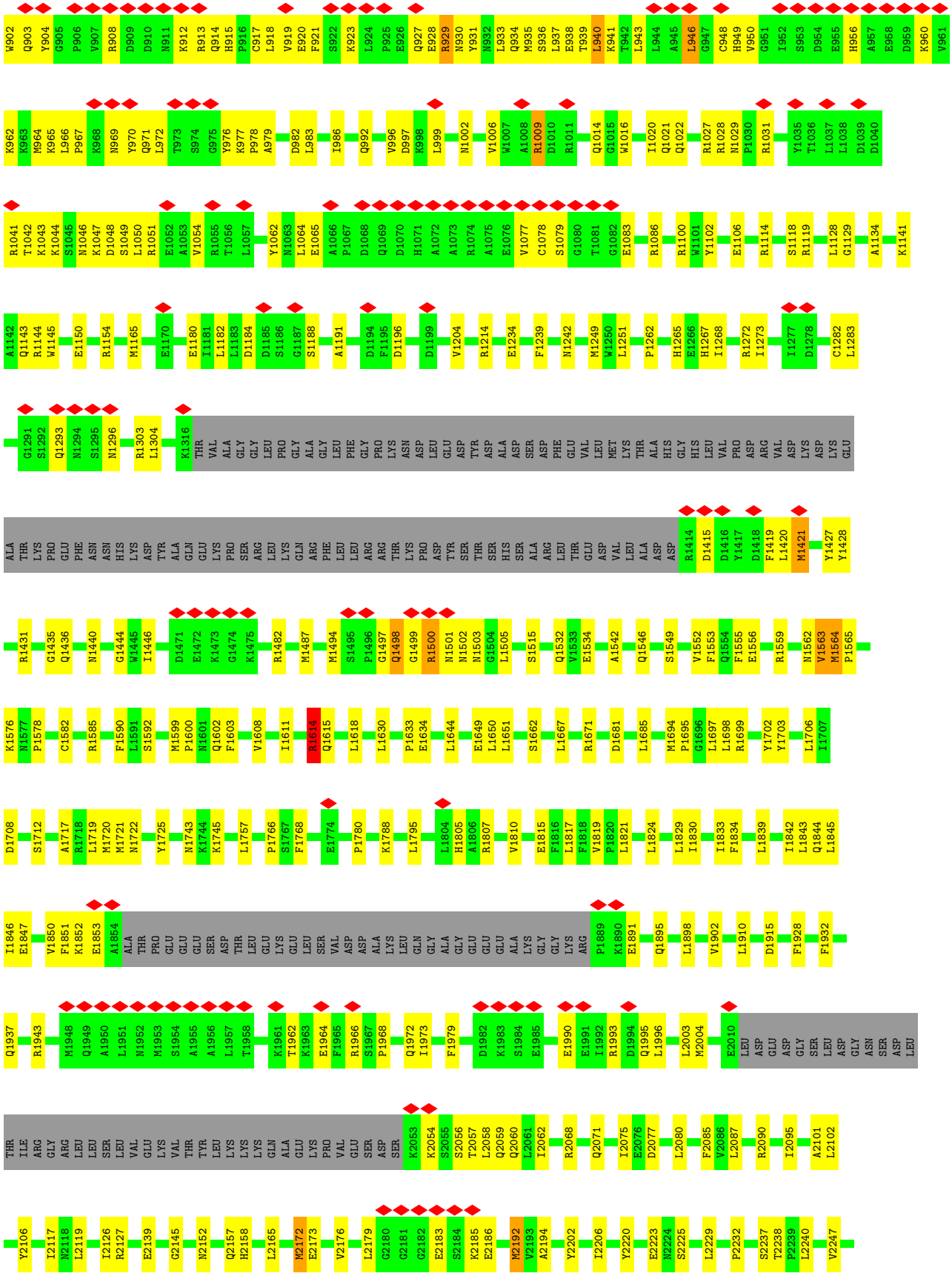


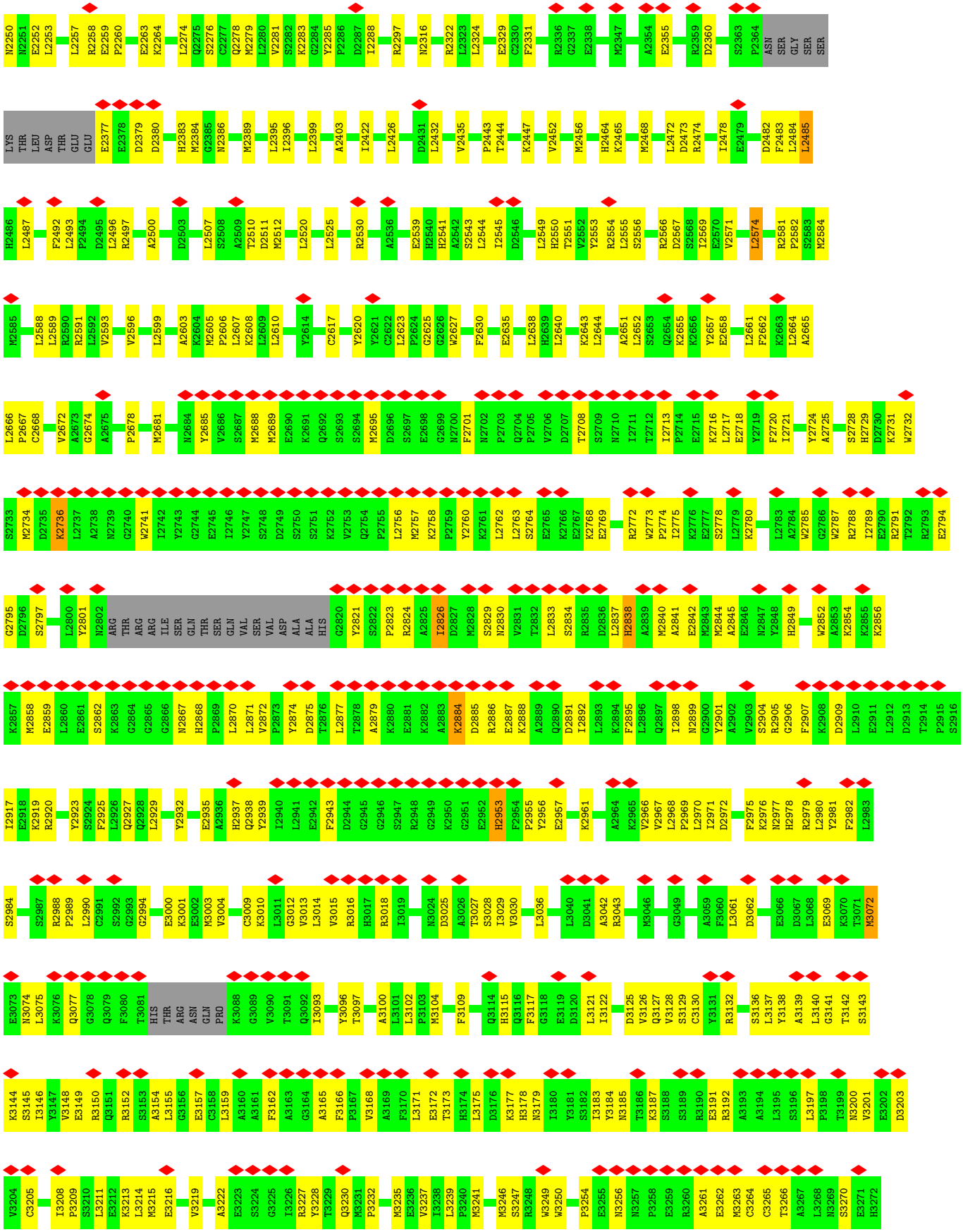


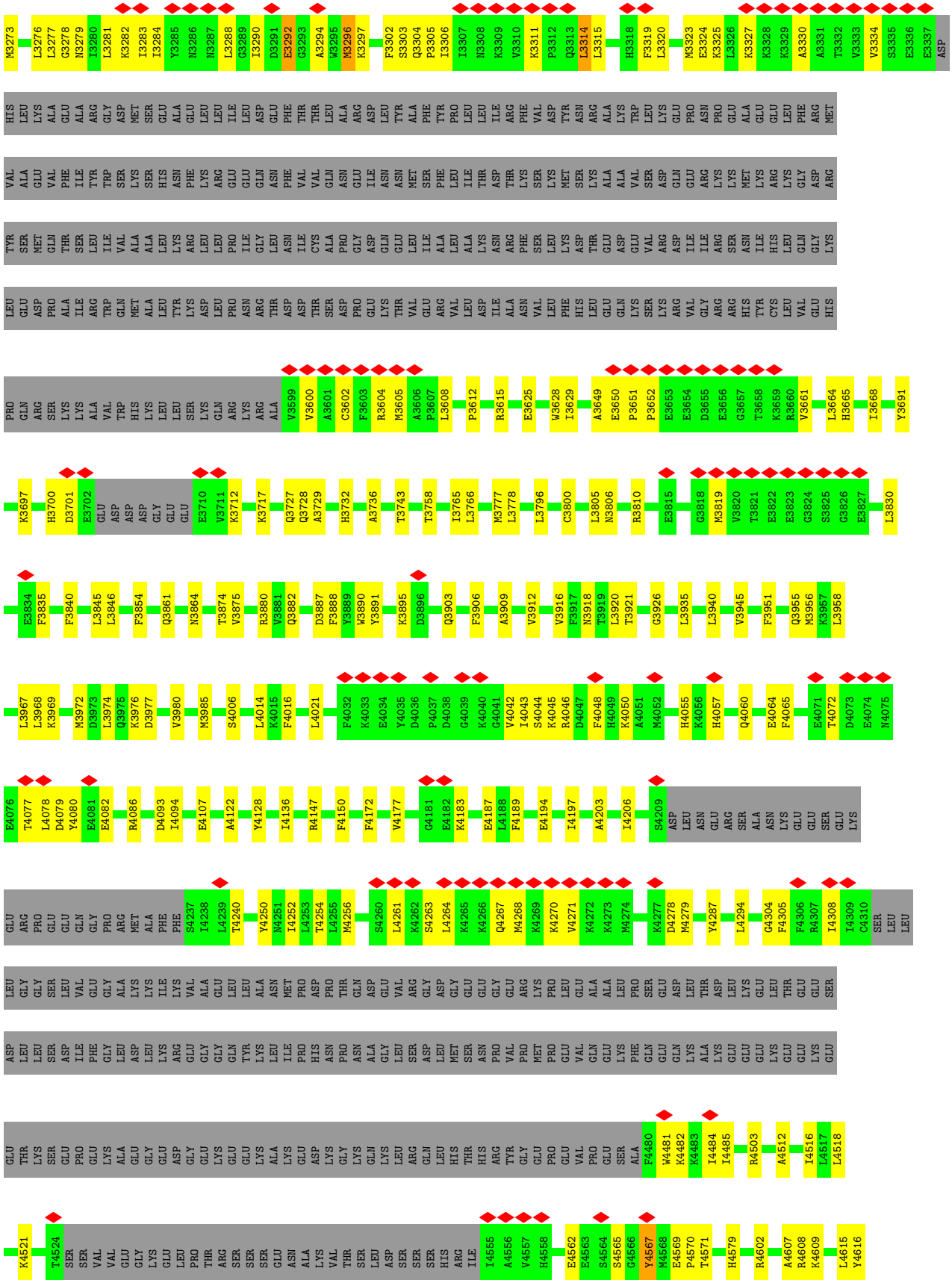
• Molecule 2: Ryanodine receptor 2

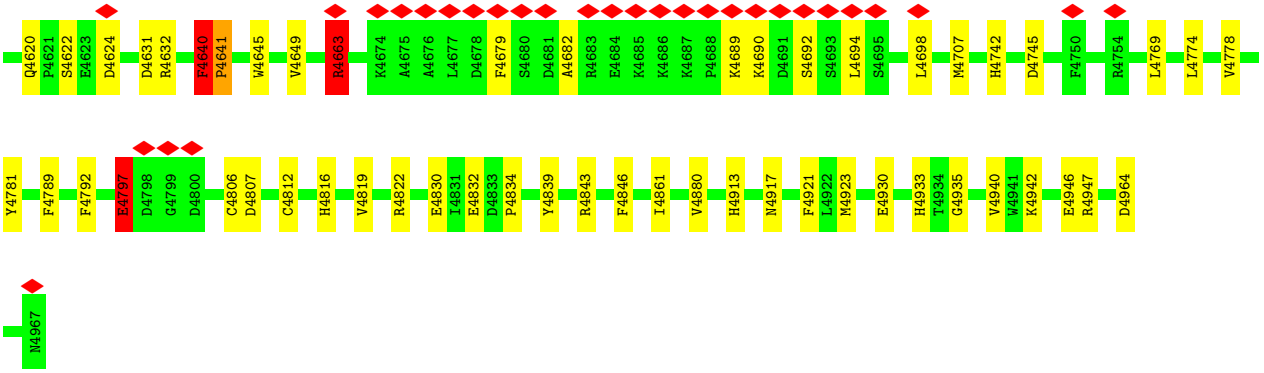
Chain C:




W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956 A957 E958 D959 K960 V961
K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 D982 L983 I986 Q992 V996 D997 K998 L999 N1002 V1006 W1007 A1008 R1009 D1010 R1011 Q1014 G1015 W1016 I1020 Q1021 Q1022 R1027 R1028 N1029 P1030 R1031 Y1035 T1036 L1037 L1038 D1039 D1040
R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 Y1062 N1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1086 R1100 W1101 Y1102 E1106 R1114 S1118 R1119 L1128 G1129 A1134 K1141
A1142 Q1143 R1144 W1145 E1150 R1154 M1165 E1170 E1180 I1181 L1182 L1183 D1184 D1185 S1186 G1187 S1188 A1191 D1194 F1195 D1196 D1199 V1204 R1214 E1234 F1239 N1242 M1249 W1250 L1251 P1262 H1265 E1266 H1267 I1268 R1272 I1273 I1277 D1278 C1282 L1283
G1291 S1292 Q1293 N1294 S1295 N1296 R1303 L1304 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU
ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418 F1419 L1420 M1421 Y1427 Y1428
R1431 G1435 Q1436 N1440 G1444 W1445 I1446 D1471 E1472 K1473 G1474 K1475 R1482 M1487 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 S1515 Q1532 V1533 E1534 A1542 Q1546 S1549 V1552 F1553 Q1554 F1555 E1556 R1559 N1562 V1563 M1564 P1565
K1576 N1577 P1578 C1582 R1585 F1590 L1591 S1592 M1599 P1600 N1601 Q1602 F1603 V1608 I1611 R1614 Q1615 L1618 L1630 P1633 E1634 L1644 E1649 L1650 L1651 S1662 L1667 R1671 D1681 L1685 M1694 P1695 G1696 L1697 L1698 R1699 Y1702 Y1703 L1706 I1707
D1708 S1712 A1717 R1718 L1719 M1720 M1721 N1722 Y1725 N1743 K1744 K1745 L1757 P1766 S1767 F1768 E1774 P1780 K1788 L1795 L1804 H1805 A1806 R1807 V1810 E1815 F1816 L1817 F1818 V1819 P1820 L1821 L1824 L1829 I1830 I1833 F1834 L1839 I1842 L1843 Q1844 L1845
I1846 E1847 V1850 F1851 K1852 E1853 A1854 ALA THR PRO GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 E1891 Q1895 L1898 V1902 L1910 D1915 F1928 F1932
Q1937 R1943 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 K1961 T1962 K1963 E1964 F1965 R1966 S1967 P1968 Q1972 I1973 F1979 D1982 K1983 S1984 E1985 E1990 E1991 I1992 R1993 D1994 Q1995 L1996 L2003 M2004 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU
THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 S2055 S2056 T2057 L2058 Q2059 Q2060 L2061 I2062 R2068 Q2071 I2075 E2076 D2077 L2080 F2085 V2086 L2087 R2090 I2095 A2101 L2102
Y2106 I2117 N2118 L2119 I2126 R2127 E2139 G2145 N2152 Q2157 H2158 L2165 M2172 E2173 V2176 L2179 G2180 G2181 G2182 E2183 S2184 K2185 E2186 M2192 V2193 A2194 Y2202 I2206 Y2220 E2223 N2224 S2225 L2229 P2232 S2237 T2238 P2239 L2240 V2247






Q4620
P4621
S4622
E4623
D4624
D4631
R4632
F4640
P4641
W4645
V4649
R4663
K4674
A4675
A4676
L4677
D4678
F4679
S4680
D4681
A4682
R4683
E4684
K4685
K4686
K4687
P4688
K4689
K4690
D4691
S4692
S4693
L4694
S4695
L4698
M4707
H4742
D4745
F4750
R4754
L4769
L4774
V4778

Y4781
F4789
F4792
E4797
D4798
G4799
D4800
C4806
D4807
C4812
H4816
V4819
R4822
E4830
T4831
E4832
D4833
P4834
V4839
R4843
F4846
I4861
V4880
H4913
N4917
F4921
L4922
M4923
E4930
H4933
T4934
G4935
V4940
W4941
K4942
E4946
R4947
D4964

M4967

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94476	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 ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.590	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	E	0.31	0/834	0.59	1/1123 (0.1%)
1	F	0.31	0/834	0.60	1/1123 (0.1%)
1	G	0.30	0/834	0.59	1/1123 (0.1%)
1	H	0.31	0/834	0.59	1/1123 (0.1%)
2	A	0.26	0/34511	0.53	15/46614 (0.0%)
2	B	0.26	0/34511	0.53	15/46614 (0.0%)
2	C	0.26	0/34511	0.53	15/46614 (0.0%)
2	D	0.26	0/34511	0.53	14/46614 (0.0%)
All	All	0.26	0/141380	0.53	63/190948 (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
2	A	0	2
2	B	0	2
2	C	0	2
2	D	0	2
All	All	0	8

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	4	GLU	CA-CB-CG	8.33	131.72	113.40
1	G	4	GLU	CA-CB-CG	8.31	131.68	113.40
1	H	4	GLU	CA-CB-CG	8.31	131.68	113.40
1	E	4	GLU	CA-CB-CG	8.30	131.66	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2736	LYS	CD-CE-NZ	-7.74	93.90	111.70
2	C	2736	LYS	CD-CE-NZ	-7.74	93.91	111.70
2	D	2736	LYS	CD-CE-NZ	-7.73	93.92	111.70
2	B	2736	LYS	CD-CE-NZ	-7.71	93.97	111.70
2	A	3075	LEU	CA-CB-CG	7.27	132.02	115.30
2	B	3075	LEU	CA-CB-CG	7.27	132.01	115.30
2	D	3075	LEU	CA-CB-CG	7.24	131.94	115.30
2	C	3075	LEU	CA-CB-CG	7.23	131.92	115.30
2	A	317	MET	CA-CB-CG	7.09	125.35	113.30
2	C	317	MET	CA-CB-CG	7.08	125.33	113.30
2	B	317	MET	CA-CB-CG	7.06	125.31	113.30
2	D	317	MET	CA-CB-CG	7.05	125.28	113.30
2	C	4640	PHE	C-N-CD	-6.70	105.86	120.60
2	B	4640	PHE	C-N-CD	-6.69	105.89	120.60
2	A	4640	PHE	C-N-CD	-6.68	105.89	120.60
2	D	4640	PHE	C-N-CD	-6.68	105.91	120.60
2	D	81	MET	CA-CB-CG	6.23	123.89	113.30
2	A	81	MET	CA-CB-CG	6.22	123.87	113.30
2	B	81	MET	CA-CB-CG	6.21	123.86	113.30
2	C	81	MET	CA-CB-CG	6.20	123.84	113.30
2	C	81	MET	CB-CG-SD	6.13	130.78	112.40
2	D	81	MET	CB-CG-SD	6.12	130.78	112.40
2	A	81	MET	CB-CG-SD	6.12	130.77	112.40
2	B	81	MET	CB-CG-SD	6.12	130.77	112.40
2	B	4797	GLU	CA-CB-CG	6.09	126.81	113.40
2	C	4797	GLU	CA-CB-CG	6.09	126.80	113.40
2	A	4797	GLU	CA-CB-CG	6.07	126.75	113.40
2	D	4797	GLU	CA-CB-CG	6.06	126.73	113.40
2	C	1563	VAL	C-N-CA	5.93	136.52	121.70
2	B	1563	VAL	C-N-CA	5.92	136.50	121.70
2	B	2485	LEU	CA-CB-CG	5.92	128.91	115.30
2	C	2485	LEU	CA-CB-CG	5.92	128.91	115.30
2	A	1563	VAL	C-N-CA	5.91	136.48	121.70
2	D	1563	VAL	C-N-CA	5.91	136.48	121.70
2	D	2485	LEU	CA-CB-CG	5.91	128.90	115.30
2	A	2485	LEU	CA-CB-CG	5.91	128.89	115.30
2	B	3296	MET	CB-CG-SD	-5.90	94.70	112.40
2	D	3296	MET	CB-CG-SD	-5.89	94.72	112.40
2	C	3296	MET	CB-CG-SD	-5.88	94.75	112.40
2	A	3296	MET	CB-CG-SD	-5.88	94.75	112.40
2	C	1614	ARG	CA-CB-CG	5.56	125.64	113.40
2	A	1614	ARG	CA-CB-CG	5.56	125.63	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1614	ARG	CA-CB-CG	5.54	125.58	113.40
2	B	1614	ARG	CA-CB-CG	5.53	125.56	113.40
2	A	2574	LEU	CA-CB-CG	5.43	127.79	115.30
2	C	2574	LEU	CA-CB-CG	5.43	127.78	115.30
2	D	2574	LEU	CA-CB-CG	5.41	127.75	115.30
2	B	2574	LEU	CA-CB-CG	5.41	127.75	115.30
2	A	4663	ARG	CG-CD-NE	5.34	123.02	111.80
2	C	4663	ARG	CG-CD-NE	5.33	123.00	111.80
2	B	4663	ARG	CG-CD-NE	5.33	123.00	111.80
2	D	4663	ARG	CG-CD-NE	5.32	122.97	111.80
2	C	1293	GLN	C-N-CA	5.18	134.66	121.70
2	D	1293	GLN	C-N-CA	5.18	134.64	121.70
2	A	1293	GLN	C-N-CA	5.17	134.63	121.70
2	B	1293	GLN	C-N-CA	5.17	134.62	121.70
2	A	844	ARG	CB-CG-CD	5.01	124.63	111.60
2	C	844	ARG	CB-CG-CD	5.01	124.62	111.60
2	B	844	ARG	CB-CG-CD	5.00	124.61	111.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1009	ARG	Sidechain
2	A	4640	PHE	Peptide
2	B	1009	ARG	Sidechain
2	B	4640	PHE	Peptide
2	C	1009	ARG	Sidechain
2	C	4640	PHE	Peptide
2	D	1009	ARG	Sidechain
2	D	4640	PHE	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	E	818	0	821	15	0
1	F	818	0	821	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	818	0	821	16	0
1	H	818	0	821	17	0
2	A	33771	0	33455	816	0
2	B	33771	0	33455	808	0
2	C	33771	0	33455	811	0
2	D	33771	0	33455	819	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	2	0
4	B	62	0	24	2	0
4	C	62	0	24	2	0
4	D	62	0	24	2	0
All	All	138608	0	137200	3223	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 12.

All (3223) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4663:ARG:HG2	2:C:4663:ARG:HH11	1.37	0.90
2:D:4797:GLU:N	2:D:4797:GLU:OE1	2.07	0.88
2:B:2830:ASN:HB3	2:C:1549:SER:HB2	1.55	0.88
2:C:4797:GLU:OE1	2:C:4797:GLU:N	2.07	0.88
2:B:4797:GLU:OE1	2:B:4797:GLU:N	2.07	0.88
2:B:4663:ARG:HH11	2:B:4663:ARG:HG2	1.37	0.87
2:A:4797:GLU:OE1	2:A:4797:GLU:N	2.07	0.87
2:D:4663:ARG:HG2	2:D:4663:ARG:HH11	1.37	0.87
2:A:4663:ARG:HG2	2:A:4663:ARG:HH11	1.37	0.86
2:D:3171:LEU:HB3	2:D:3211:LEU:HB2	1.58	0.86
2:C:3171:LEU:HB3	2:C:3211:LEU:HB2	1.58	0.85
2:A:3171:LEU:HB3	2:A:3211:LEU:HB2	1.58	0.83
2:B:3171:LEU:HB3	2:B:3211:LEU:HB2	1.58	0.82
2:D:2923:TYR:O	2:D:2927:GLN:NE2	2.13	0.81
2:B:2923:TYR:O	2:B:2927:GLN:NE2	2.14	0.81
2:C:2923:TYR:O	2:C:2927:GLN:NE2	2.14	0.81
2:A:2923:TYR:O	2:A:2927:GLN:NE2	2.14	0.81
2:B:904:TYR:OH	2:B:923:LYS:NZ	2.16	0.79
2:C:904:TYR:OH	2:C:923:LYS:NZ	2.16	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3294:ALA:HA	2:A:3297:LYS:HE2	1.64	0.79
2:B:3294:ALA:HA	2:B:3297:LYS:HE2	1.64	0.79
2:A:904:TYR:OH	2:A:923:LYS:NZ	2.16	0.79
2:D:904:TYR:OH	2:D:923:LYS:NZ	2.16	0.79
2:D:2179:LEU:O	2:D:2183:GLU:HB2	1.83	0.78
2:B:2360:ASP:OD2	2:B:2383:HIS:ND1	2.14	0.78
2:B:2824:ARG:NH1	2:C:1502:ASN:OD1	2.16	0.78
2:C:2179:LEU:O	2:C:2183:GLU:HB2	1.83	0.78
2:C:3294:ALA:HA	2:C:3297:LYS:HE2	1.64	0.78
2:D:3294:ALA:HA	2:D:3297:LYS:HE2	1.64	0.77
2:B:2179:LEU:O	2:B:2183:GLU:HB2	1.84	0.77
2:A:2179:LEU:O	2:A:2183:GLU:HB2	1.84	0.77
2:B:2640:LEU:HD23	2:B:2643:LYS:HZ3	1.49	0.77
2:B:3227:ARG:HE	2:B:3290:ILE:HG12	1.50	0.76
2:A:2953:HIS:ND1	2:A:2953:HIS:O	2.19	0.76
2:A:1498:GLN:HB2	2:D:2794:GLU:HG3	1.67	0.76
2:B:2953:HIS:ND1	2:B:2953:HIS:O	2.19	0.76
2:C:3227:ARG:HE	2:C:3290:ILE:HG12	1.50	0.76
2:A:3227:ARG:HE	2:A:3290:ILE:HG12	1.50	0.76
2:D:3227:ARG:HE	2:D:3290:ILE:HG12	1.50	0.75
2:D:1502:ASN:OD1	2:C:2824:ARG:NH1	2.20	0.75
2:A:3205:CYS:HB2	2:A:3208:ILE:HB	1.69	0.75
2:A:2640:LEU:HD23	2:A:2643:LYS:HZ3	1.52	0.74
2:D:2953:HIS:ND1	2:D:2953:HIS:O	2.19	0.74
2:D:670:TYR:O	2:D:673:TRP:NE1	2.20	0.74
2:B:4481:TRP:HA	2:B:4484:ILE:HG12	1.70	0.74
2:C:2953:HIS:ND1	2:C:2953:HIS:O	2.19	0.74
2:A:670:TYR:O	2:A:673:TRP:NE1	2.20	0.74
2:C:670:TYR:O	2:C:673:TRP:NE1	2.20	0.74
2:A:4481:TRP:HA	2:A:4484:ILE:HG12	1.70	0.74
2:D:2856:LYS:HA	2:D:2859:GLU:HG3	1.70	0.74
2:D:3205:CYS:HB2	2:D:3208:ILE:HB	1.69	0.74
2:B:670:TYR:O	2:B:673:TRP:NE1	2.20	0.74
2:C:2640:LEU:HD23	2:C:2643:LYS:HZ3	1.50	0.74
2:C:3205:CYS:HB2	2:C:3208:ILE:HB	1.69	0.74
2:A:2360:ASP:OD2	2:A:2383:HIS:ND1	2.14	0.74
2:D:1283:LEU:HB2	2:D:1555:PHE:HB2	1.70	0.73
2:D:2360:ASP:OD2	2:D:2383:HIS:ND1	2.14	0.73
2:A:2856:LYS:HA	2:A:2859:GLU:HG3	1.70	0.73
2:D:1788:LYS:HD2	2:D:1833:ILE:HG22	1.71	0.73
2:C:4481:TRP:HA	2:C:4484:ILE:HG12	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2360:ASP:OD2	2:C:2383:HIS:ND1	2.14	0.73
2:A:2830:ASN:HB3	2:B:1549:SER:HB2	1.70	0.73
2:B:2824:ARG:NH2	2:C:1502:ASN:O	2.21	0.73
2:C:1788:LYS:HD2	2:C:1833:ILE:HG22	1.70	0.73
2:A:1129:GLY:HA3	2:A:1145:TRP:HB3	1.71	0.73
2:A:1283:LEU:HB2	2:A:1555:PHE:HB2	1.70	0.73
2:D:491:GLU:OE2	2:D:546:LYS:NZ	2.22	0.73
2:A:1788:LYS:HD2	2:A:1833:ILE:HG22	1.71	0.72
2:B:1283:LEU:HB2	2:B:1555:PHE:HB2	1.70	0.72
2:C:491:GLU:OE2	2:C:546:LYS:NZ	2.22	0.72
2:C:1129:GLY:HA3	2:C:1145:TRP:HB3	1.71	0.72
2:C:2856:LYS:HA	2:C:2859:GLU:HG3	1.70	0.72
2:A:491:GLU:OE2	2:A:546:LYS:NZ	2.22	0.72
1:F:35:LYS:NZ	2:B:640:ARG:O	2.22	0.72
2:D:1129:GLY:HA3	2:D:1145:TRP:HB3	1.71	0.72
2:D:4481:TRP:HA	2:D:4484:ILE:HG12	1.70	0.72
2:B:3205:CYS:HB2	2:B:3208:ILE:HB	1.69	0.72
2:C:2905:ARG:HD2	2:C:2906:GLY:H	1.54	0.72
2:D:281:ARG:NH1	2:D:345:GLU:OE2	2.23	0.72
2:B:491:GLU:OE2	2:B:546:LYS:NZ	2.22	0.72
2:B:1129:GLY:HA3	2:B:1145:TRP:HB3	1.71	0.72
2:A:2905:ARG:HD2	2:A:2906:GLY:H	1.54	0.72
2:C:824:GLU:OE1	2:C:1028:ARG:NH1	2.23	0.72
2:C:1283:LEU:HB2	2:C:1555:PHE:HB2	1.70	0.72
2:C:281:ARG:NH1	2:C:345:GLU:OE2	2.23	0.71
2:A:824:GLU:OE1	2:A:1028:ARG:NH1	2.23	0.71
2:A:2666:LEU:HD11	2:A:2969:PRO:HB2	1.72	0.71
2:B:2856:LYS:HA	2:B:2859:GLU:HG3	1.70	0.71
2:B:3701:ASP:OD2	2:B:3727:GLN:NE2	2.23	0.71
2:B:1788:LYS:HD2	2:B:1833:ILE:HG22	1.70	0.71
2:C:876:PRO:HA	2:C:879:GLU:HG3	1.72	0.71
2:B:281:ARG:NH1	2:B:345:GLU:OE2	2.23	0.71
2:A:281:ARG:NH1	2:A:345:GLU:OE2	2.23	0.71
2:D:3701:ASP:OD2	2:D:3727:GLN:NE2	2.23	0.71
2:D:2905:ARG:HD2	2:D:2906:GLY:H	1.54	0.71
2:B:2905:ARG:HD2	2:B:2906:GLY:H	1.54	0.71
2:C:2935:GLU:HB3	2:C:2939:TYR:HE1	1.56	0.71
2:D:824:GLU:OE1	2:D:1028:ARG:NH1	2.23	0.71
2:D:2935:GLU:HB3	2:D:2939:TYR:HE1	1.56	0.71
2:D:876:PRO:HA	2:D:879:GLU:HG3	1.72	0.70
2:D:2640:LEU:HD23	2:D:2643:LYS:HZ3	1.53	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2666:LEU:HD11	2:D:2969:PRO:HB2	1.72	0.70
2:C:2736:LYS:HG3	2:C:2741:TRP:CD1	2.26	0.70
2:A:2842:GLU:HA	2:A:2886:ARG:HH22	1.56	0.70
2:B:2769:GLU:HA	2:B:2772:ARG:HB2	1.74	0.70
2:D:76:ARG:NH1	2:C:3890:TRP:O	2.25	0.70
2:B:3139:ALA:O	2:B:3143:SER:HB3	1.92	0.70
2:B:3955:GLN:NE2	2:B:3972:MET:SD	2.65	0.70
2:C:3955:GLN:NE2	2:C:3972:MET:SD	2.65	0.70
2:A:3955:GLN:NE2	2:A:3972:MET:SD	2.65	0.70
2:D:2736:LYS:HG3	2:D:2741:TRP:CD1	2.26	0.70
2:A:876:PRO:HA	2:A:879:GLU:HG3	1.72	0.70
2:A:2935:GLU:HB3	2:A:2939:TYR:HE1	1.56	0.70
2:A:3139:ALA:O	2:A:3143:SER:HB3	1.92	0.70
2:A:4579:HIS:CE1	2:A:4742:HIS:CD2	2.80	0.70
2:B:2666:LEU:HD11	2:B:2969:PRO:HB2	1.72	0.70
2:C:2769:GLU:HA	2:C:2772:ARG:HB2	1.74	0.70
2:C:2842:GLU:HA	2:C:2886:ARG:HH22	1.56	0.70
2:A:2769:GLU:HA	2:A:2772:ARG:HB2	1.74	0.70
2:B:876:PRO:HA	2:B:879:GLU:HG3	1.72	0.70
2:C:3139:ALA:O	2:C:3143:SER:HB3	1.92	0.70
2:C:3701:ASP:OD2	2:C:3727:GLN:NE2	2.23	0.70
2:B:2736:LYS:HG3	2:B:2741:TRP:CD1	2.26	0.70
2:D:2769:GLU:HA	2:D:2772:ARG:HB2	1.74	0.69
2:B:2935:GLU:HB3	2:B:2939:TYR:HE1	1.56	0.69
2:A:2736:LYS:HG3	2:A:2741:TRP:CD1	2.26	0.69
2:C:2666:LEU:HD11	2:C:2969:PRO:HB2	1.72	0.69
2:A:1503:ASN:OD1	2:D:2824:ARG:NH2	2.23	0.69
2:D:1503:ASN:OD1	2:C:2824:ARG:NH2	2.24	0.69
2:A:3969:LYS:NZ	2:A:4086:ARG:O	2.26	0.69
2:A:3701:ASP:OD2	2:A:3727:GLN:NE2	2.23	0.69
2:D:3139:ALA:O	2:D:3143:SER:HB3	1.92	0.69
2:B:2842:GLU:HA	2:B:2886:ARG:HH22	1.56	0.69
2:A:3292:GLU:HB2	2:A:3296:MET:HE1	1.75	0.69
2:D:2842:GLU:HA	2:D:2886:ARG:HH22	1.56	0.69
2:D:4521:LYS:HE2	2:D:4562:GLU:HB3	1.75	0.69
2:B:2127:ARG:NH2	2:B:2165:LEU:O	2.26	0.69
2:C:2688:MET:SD	2:C:2905:ARG:NH1	2.66	0.69
2:B:3292:GLU:HB2	2:B:3296:MET:HE1	1.75	0.69
2:A:878:LEU:HD11	2:A:950:VAL:HG11	1.75	0.69
2:D:3955:GLN:NE2	2:D:3972:MET:SD	2.65	0.69
2:D:3969:LYS:NZ	2:D:4086:ARG:O	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2688:MET:SD	2:B:2905:ARG:NH1	2.66	0.69
2:B:3969:LYS:NZ	2:B:4086:ARG:O	2.26	0.69
2:C:3969:LYS:NZ	2:C:4086:ARG:O	2.26	0.69
2:C:2127:ARG:NH2	2:C:2165:LEU:O	2.26	0.68
2:D:2688:MET:SD	2:D:2905:ARG:NH1	2.66	0.68
2:B:824:GLU:OE1	2:B:1028:ARG:NH1	2.23	0.68
2:A:880:ARG:HG3	2:A:881:ILE:HD12	1.75	0.68
2:A:2688:MET:SD	2:A:2905:ARG:NH1	2.66	0.68
2:B:878:LEU:HD11	2:B:950:VAL:HG11	1.75	0.68
2:A:2127:ARG:NH2	2:A:2165:LEU:O	2.26	0.68
2:C:2185:LYS:O	2:C:2186:GLU:HG3	1.94	0.68
2:A:4521:LYS:HE2	2:A:4562:GLU:HB3	1.75	0.68
2:D:880:ARG:HG3	2:D:881:ILE:HD12	1.75	0.68
2:D:2127:ARG:NH2	2:D:2165:LEU:O	2.26	0.68
2:C:880:ARG:HG3	2:C:881:ILE:HD12	1.75	0.68
2:A:2435:VAL:O	2:A:2465:LYS:NZ	2.27	0.68
2:D:1114:ARG:NH1	2:D:1128:LEU:O	2.27	0.68
1:F:22:THR:HG22	1:F:50:ARG:HG2	1.76	0.68
2:D:2185:LYS:O	2:D:2186:GLU:HG3	1.94	0.68
2:D:2435:VAL:O	2:D:2465:LYS:NZ	2.27	0.67
2:B:2826:ILE:HD13	2:C:1501:ASN:HB2	1.77	0.67
2:B:4521:LYS:HE2	2:B:4562:GLU:HB3	1.75	0.67
2:D:878:LEU:HD11	2:D:950:VAL:HG11	1.75	0.67
2:C:4521:LYS:HE2	2:C:4562:GLU:HB3	1.75	0.67
2:B:4834:PRO:HB3	2:B:4843:ARG:HD3	1.76	0.67
2:C:2435:VAL:O	2:C:2465:LYS:NZ	2.27	0.67
2:D:4834:PRO:HB3	2:D:4843:ARG:HD3	1.76	0.67
2:B:880:ARG:HG3	2:B:881:ILE:HD12	1.75	0.67
1:G:22:THR:HG22	1:G:50:ARG:HG2	1.76	0.67
2:B:2185:LYS:O	2:B:2186:GLU:HG3	1.94	0.67
2:B:2435:VAL:O	2:B:2465:LYS:NZ	2.27	0.67
2:C:3926:GLY:HA2	2:C:4935:GLY:HA3	1.77	0.67
2:B:3926:GLY:HA2	2:B:4935:GLY:HA3	1.77	0.67
2:A:1114:ARG:NH1	2:A:1128:LEU:O	2.27	0.67
2:A:1501:ASN:HB2	2:D:2826:ILE:HD13	1.76	0.67
1:E:22:THR:HG22	1:E:50:ARG:HG2	1.76	0.67
2:D:2920:ARG:HH12	2:D:3000:GLU:HG3	1.60	0.67
2:B:2593:VAL:HA	2:B:2644:LEU:HD13	1.77	0.67
2:B:4607:ALA:HB1	2:B:4649:VAL:HG21	1.77	0.67
2:C:878:LEU:HD11	2:C:950:VAL:HG11	1.75	0.67
2:C:2593:VAL:HA	2:C:2644:LEU:HD13	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2185:LYS:O	2:A:2186:GLU:HG3	1.94	0.66
2:C:1114:ARG:NH1	2:C:1128:LEU:O	2.27	0.66
2:D:4622:SER:OG	2:D:4624:ASP:OD2	2.13	0.66
2:C:1031:ARG:HE	2:C:1042:THR:HG21	1.61	0.66
2:B:1031:ARG:HE	2:B:1042:THR:HG21	1.61	0.66
2:A:4834:PRO:HB3	2:A:4843:ARG:HD3	1.76	0.66
2:D:2943:PHE:HZ	2:D:2955:PRO:HD2	1.60	0.66
2:D:4707:MET:HG3	2:C:4252:ILE:HG21	1.77	0.66
2:B:1114:ARG:NH1	2:B:1128:LEU:O	2.27	0.66
2:D:2057:THR:HB	2:D:2060:GLN:HG3	1.78	0.66
2:D:2085:PHE:HB3	2:D:3691:TYR:HE2	1.61	0.66
2:B:2920:ARG:HH12	2:B:3000:GLU:HG3	1.60	0.66
2:D:3926:GLY:HA2	2:D:4935:GLY:HA3	1.77	0.66
2:C:2658:GLU:OE1	2:C:2661:LEU:N	2.25	0.66
2:A:1843:LEU:HD23	2:A:1846:ILE:HD12	1.78	0.66
2:D:2658:GLU:OE1	2:D:2661:LEU:N	2.25	0.66
2:C:2085:PHE:HB3	2:C:3691:TYR:HE2	1.61	0.66
2:A:2920:ARG:HH12	2:A:3000:GLU:HG3	1.60	0.66
2:A:3926:GLY:HA2	2:A:4935:GLY:HA3	1.77	0.66
2:A:1031:ARG:HE	2:A:1042:THR:HG21	1.61	0.66
2:A:2057:THR:HB	2:A:2060:GLN:HG3	1.78	0.66
2:D:1843:LEU:HD23	2:D:1846:ILE:HD12	1.78	0.66
2:B:2943:PHE:HZ	2:B:2955:PRO:HD2	1.60	0.66
2:C:4834:PRO:HB3	2:C:4843:ARG:HD3	1.76	0.66
2:A:1910:LEU:HD13	2:A:2062:ILE:HG12	1.78	0.65
2:C:1910:LEU:HD13	2:C:2062:ILE:HG12	1.78	0.65
2:C:2057:THR:HB	2:C:2060:GLN:HG3	1.78	0.65
2:C:2920:ARG:HH12	2:C:3000:GLU:HG3	1.60	0.65
2:C:2943:PHE:HZ	2:C:2955:PRO:HD2	1.60	0.65
2:A:2085:PHE:HB3	2:A:3691:TYR:HE2	1.61	0.65
2:D:1910:LEU:HD13	2:D:2062:ILE:HG12	1.78	0.65
2:B:1910:LEU:HD13	2:B:2062:ILE:HG12	1.78	0.65
2:B:2057:THR:HB	2:B:2060:GLN:HG3	1.78	0.65
1:H:22:THR:HG22	1:H:50:ARG:HG2	1.76	0.65
2:A:2975:PHE:O	2:A:2979:ARG:NE	2.23	0.65
2:C:842:GLN:HE22	2:C:1602:GLN:HG3	1.62	0.65
2:A:372:LEU:HA	2:A:393:MET:HG2	1.79	0.65
2:D:1501:ASN:HB2	2:C:2826:ILE:HD13	1.77	0.65
2:D:3292:GLU:HB2	2:D:3296:MET:CE	2.27	0.65
2:A:276:ARG:HG3	2:A:300:VAL:HG22	1.79	0.65
2:A:2658:GLU:OE1	2:A:2661:LEU:N	2.25	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:372:LEU:HA	2:D:393:MET:HG2	1.79	0.65
2:C:4622:SER:OG	2:C:4624:ASP:OD2	2.13	0.65
2:A:2593:VAL:HA	2:A:2644:LEU:HD13	1.77	0.65
2:D:2593:VAL:HA	2:D:2644:LEU:HD13	1.77	0.65
2:D:4607:ALA:HB1	2:D:4649:VAL:HG21	1.77	0.65
2:C:4607:ALA:HB1	2:C:4649:VAL:HG21	1.78	0.65
2:B:1843:LEU:HD23	2:B:1846:ILE:HD12	1.78	0.65
2:B:4622:SER:OG	2:B:4624:ASP:OD2	2.13	0.65
2:A:4607:ALA:HB1	2:A:4649:VAL:HG21	1.77	0.65
2:B:276:ARG:HG3	2:B:300:VAL:HG22	1.79	0.65
2:A:2943:PHE:HZ	2:A:2955:PRO:HD2	1.60	0.65
2:A:4622:SER:OG	2:A:4624:ASP:OD2	2.13	0.65
2:D:1757:LEU:HD22	2:D:2117:ILE:HD11	1.79	0.65
2:B:842:GLN:HE22	2:B:1602:GLN:HG3	1.62	0.64
2:B:2975:PHE:HB3	2:B:2979:ARG:HH21	1.62	0.64
2:B:4187:GLU:OE2	2:B:4947:ARG:NH2	2.30	0.64
2:A:842:GLN:HE22	2:A:1602:GLN:HG3	1.62	0.64
2:A:2975:PHE:HB3	2:A:2979:ARG:HH21	1.62	0.64
2:D:842:GLN:HE22	2:D:1602:GLN:HG3	1.62	0.64
2:B:2126:ILE:HD11	2:B:2145:GLY:HA3	1.80	0.64
2:C:2975:PHE:HB3	2:C:2979:ARG:HH21	1.62	0.64
2:A:2651:ALA:O	2:A:2655:LYS:HG2	1.98	0.64
2:A:4852:PHE:HE1	2:D:4862:ILE:HD13	1.63	0.64
2:D:2975:PHE:HB3	2:D:2979:ARG:HH21	1.62	0.64
2:B:3292:GLU:HB2	2:B:3296:MET:CE	2.27	0.64
2:C:1757:LEU:HD22	2:C:2117:ILE:HD11	1.79	0.64
2:A:2126:ILE:HD11	2:A:2145:GLY:HA3	1.80	0.64
2:D:1031:ARG:HE	2:D:1042:THR:HG21	1.61	0.64
2:C:1843:LEU:HD23	2:C:1846:ILE:HD12	1.78	0.64
2:D:2126:ILE:HD11	2:D:2145:GLY:HA3	1.80	0.64
2:D:2651:ALA:O	2:D:2655:LYS:HG2	1.98	0.64
2:C:3292:GLU:HB2	2:C:3296:MET:CE	2.27	0.64
2:A:167:LYS:HE2	2:D:240:HIS:HB3	1.80	0.64
2:A:1757:LEU:HD22	2:A:2117:ILE:HD11	1.79	0.64
2:B:2658:GLU:OE1	2:B:2661:LEU:N	2.25	0.64
2:C:4187:GLU:OE2	2:C:4947:ARG:NH2	2.30	0.64
2:A:3292:GLU:HB2	2:A:3296:MET:CE	2.27	0.64
2:A:4187:GLU:OE2	2:A:4947:ARG:NH2	2.30	0.64
2:D:1043:LYS:HG2	2:D:1047:LYS:HE2	1.79	0.64
2:D:1549:SER:HB2	2:C:2830:ASN:HB3	1.80	0.64
2:B:2085:PHE:HB3	2:B:3691:TYR:HE2	1.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2386:ASN:HA	2:D:2389:MET:HE2	1.79	0.64
2:C:1043:LYS:HG2	2:C:1047:LYS:HE2	1.79	0.64
2:D:276:ARG:HG3	2:D:300:VAL:HG22	1.79	0.64
2:B:2975:PHE:O	2:B:2979:ARG:NE	2.23	0.64
2:D:1795:LEU:HA	2:D:1821:LEU:HD21	1.80	0.64
2:B:1757:LEU:HD22	2:B:2117:ILE:HD11	1.79	0.64
2:B:2541:HIS:HB3	2:B:2544:LEU:HD21	1.80	0.64
2:A:4579:HIS:HE1	2:A:4742:HIS:CD2	2.15	0.63
2:D:1503:ASN:CG	2:C:2824:ARG:HH22	2.02	0.63
2:B:2824:ARG:NH2	2:C:1503:ASN:OD1	2.23	0.63
2:D:4187:GLU:OE2	2:D:4947:ARG:NH2	2.30	0.63
2:C:2126:ILE:HD11	2:C:2145:GLY:HA3	1.80	0.63
2:D:2553:TYR:O	2:D:2556:SER:OG	2.15	0.63
2:B:1043:LYS:HG2	2:B:1047:LYS:HE2	1.79	0.63
2:C:276:ARG:HG3	2:C:300:VAL:HG22	1.79	0.63
2:D:3945:VAL:HG23	2:D:4006:SER:HB3	1.81	0.63
2:B:3945:VAL:HG23	2:B:4006:SER:HB3	1.81	0.63
2:C:2403:ALA:O	2:C:2474:ARG:NH2	2.31	0.63
2:A:3261:ALA:O	2:A:3262:GLU:HG3	1.99	0.63
2:D:2403:ALA:O	2:D:2474:ARG:NH2	2.31	0.63
2:D:3172:GLU:OE2	2:D:3266:THR:OG1	2.17	0.63
2:B:372:LEU:HA	2:B:393:MET:HG2	1.79	0.63
2:C:372:LEU:HA	2:C:393:MET:HG2	1.79	0.63
2:C:3172:GLU:OE2	2:C:3266:THR:OG1	2.17	0.63
2:A:1043:LYS:HG2	2:A:1047:LYS:HE2	1.79	0.63
2:D:3261:ALA:O	2:D:3262:GLU:HG3	1.99	0.63
2:A:1795:LEU:HA	2:A:1821:LEU:HD21	1.80	0.63
2:A:2833:LEU:HB2	2:A:2838[B]:HIS:CE1	2.34	0.63
2:A:3172:GLU:OE2	2:A:3266:THR:OG1	2.17	0.63
2:D:2975:PHE:O	2:D:2979:ARG:NE	2.23	0.63
2:C:1795:LEU:HA	2:C:1821:LEU:HD21	1.80	0.63
2:B:2651:ALA:O	2:B:2655:LYS:HG2	1.98	0.63
2:C:2651:ALA:O	2:C:2655:LYS:HG2	1.98	0.63
2:C:3227:ARG:HB2	2:C:3230:GLN:HG2	1.81	0.63
2:C:3945:VAL:HG23	2:C:4006:SER:HB3	1.81	0.63
2:D:137:ARG:HH12	2:D:204:ASP:HB3	1.64	0.62
2:D:2935:GLU:O	2:D:2939:TYR:HD1	1.82	0.62
2:C:2541:HIS:HB3	2:C:2544:LEU:HD21	1.80	0.62
2:A:137:ARG:HH12	2:A:204:ASP:HB3	1.64	0.62
2:B:2497:ARG:HH12	2:B:2877:LEU:HA	1.65	0.62
2:A:2545:ILE:HD11	2:A:2584:MET:HG2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2545:ILE:HD11	2:D:2584:MET:HG2	1.81	0.62
2:B:2403:ALA:O	2:B:2474:ARG:NH2	2.31	0.62
2:C:2386:ASN:HA	2:C:2389:MET:HE2	1.82	0.62
2:C:3261:ALA:O	2:C:3262:GLU:HG3	1.99	0.62
2:A:2935:GLU:O	2:A:2939:TYR:HD1	1.82	0.62
2:A:3227:ARG:HB2	2:A:3230:GLN:HG2	1.81	0.62
2:C:137:ARG:HH12	2:C:204:ASP:HB3	1.64	0.62
2:A:2541:HIS:HB3	2:A:2544:LEU:HD21	1.80	0.62
2:D:1041:ARG:HA	2:D:1044:LYS:HZ3	1.64	0.62
2:D:2982:PHE:O	2:D:3001:LYS:NZ	2.33	0.62
2:C:2935:GLU:O	2:C:2939:TYR:HD1	1.82	0.62
2:D:2541:HIS:HB3	2:D:2544:LEU:HD21	1.80	0.62
2:B:3728:GLN:HG2	2:B:3765:ILE:HA	1.82	0.62
2:D:3184:TYR:CD1	2:D:3192:ARG:HD3	2.35	0.62
2:B:1795:LEU:HA	2:B:1821:LEU:HD21	1.80	0.62
2:B:2545:ILE:HD11	2:B:2584:MET:HG2	1.81	0.62
2:B:2935:GLU:O	2:B:2939:TYR:HD1	1.82	0.62
2:D:3227:ARG:HB2	2:D:3230:GLN:HG2	1.81	0.62
2:C:2497:ARG:HH12	2:C:2877:LEU:HA	1.65	0.62
2:A:2386:ASN:HA	2:A:2389:MET:HE2	1.82	0.62
2:A:2497:ARG:HH12	2:A:2877:LEU:HA	1.65	0.62
2:A:3945:VAL:HG23	2:A:4006:SER:HB3	1.81	0.62
2:B:3184:TYR:CD1	2:B:3192:ARG:HD3	2.35	0.62
2:A:2982:PHE:O	2:A:3001:LYS:NZ	2.33	0.61
2:A:3184:TYR:CD1	2:A:3192:ARG:HD3	2.35	0.61
2:B:3261:ALA:O	2:B:3262:GLU:HG3	1.99	0.61
2:C:3728:GLN:HG2	2:C:3765:ILE:HA	1.81	0.61
2:A:1844:GLN:NE2	2:A:1851:PHE:O	2.34	0.61
2:A:2553:TYR:O	2:A:2556:SER:OG	2.15	0.61
2:B:3227:ARG:HB2	2:B:3230:GLN:HG2	1.81	0.61
2:C:2982:PHE:O	2:C:3001:LYS:NZ	2.33	0.61
2:A:2403:ALA:O	2:A:2474:ARG:NH2	2.31	0.61
2:A:2826:ILE:HD13	2:B:1501:ASN:HB2	1.82	0.61
2:B:1844:GLN:NE2	2:B:1851:PHE:O	2.34	0.61
2:B:2386:ASN:HA	2:B:2389:MET:HE2	1.82	0.61
2:B:2982:PHE:O	2:B:3001:LYS:NZ	2.33	0.61
2:C:2545:ILE:HD11	2:C:2584:MET:HG2	1.81	0.61
2:A:2623:LEU:HD23	2:A:2625:GLY:H	1.66	0.61
2:A:3004:VAL:HG13	2:A:3036:LEU:HD11	1.82	0.61
2:D:1844:GLN:NE2	2:D:1851:PHE:O	2.34	0.61
2:C:2257:LEU:HB2	2:C:2316:ASN:HD21	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3015:VAL:HB	2:A:3029:ILE:HG21	1.82	0.61
2:D:3004:VAL:HG13	2:D:3036:LEU:HD11	1.82	0.61
2:D:3728:GLN:HG2	2:D:3765:ILE:HA	1.82	0.61
2:B:2257:LEU:HB2	2:B:2316:ASN:HD21	1.66	0.61
2:D:1842:ILE:HD12	2:D:1845:LEU:HD12	1.83	0.61
2:B:137:ARG:HH12	2:B:204:ASP:HB3	1.64	0.61
2:C:1844:GLN:NE2	2:C:1851:PHE:O	2.34	0.61
2:C:2223:GLU:OE2	2:C:2264:LYS:NZ	2.29	0.61
2:C:2732:TRP:CD1	2:C:2736:LYS:NZ	2.67	0.61
2:C:3015:VAL:HB	2:C:3029:ILE:HG21	1.82	0.61
2:C:3141:GLY:O	2:C:3152:ARG:NH2	2.34	0.61
1:H:35:LYS:NZ	2:D:640:ARG:O	2.34	0.61
2:A:2257:LEU:HB2	2:A:2316:ASN:HD21	1.66	0.61
2:A:2824:ARG:NH2	2:B:1503:ASN:OD1	2.28	0.61
2:A:3072:MET:SD	2:A:3136:SER:HA	2.41	0.61
2:D:3015:VAL:HB	2:D:3029:ILE:HG21	1.82	0.61
2:C:3184:TYR:CD1	2:C:3192:ARG:HD3	2.35	0.60
2:D:2623:LEU:HD23	2:D:2625:GLY:H	1.66	0.60
2:B:1842:ILE:HD12	2:B:1845:LEU:HD12	1.83	0.60
2:D:3072:MET:SD	2:D:3136:SER:HA	2.41	0.60
2:B:894:VAL:HA	2:B:915:HIS:HE1	1.67	0.60
2:B:3172:GLU:OE2	2:B:3266:THR:OG1	2.17	0.60
2:C:877:HIS:O	2:C:1062:TYR:OH	2.15	0.60
2:C:2553:TYR:O	2:C:2556:SER:OG	2.15	0.60
2:A:2833:LEU:HB2	2:A:2838[A]:HIS:CE1	2.35	0.60
2:A:4769:LEU:HD22	2:D:4753:LEU:HD21	1.82	0.60
2:B:2789:ILE:HD11	2:B:2901:TYR:HB3	1.83	0.60
2:A:877:HIS:O	2:A:1062:TYR:OH	2.15	0.60
2:D:2497:ARG:HH12	2:D:2877:LEU:HA	1.65	0.60
2:B:3004:VAL:HG13	2:B:3036:LEU:HD11	1.82	0.60
2:C:2778:SER:OG	2:C:2888:LYS:NZ	2.24	0.60
2:A:3728:GLN:HG2	2:A:3765:ILE:HA	1.82	0.60
2:D:2223:GLU:OE2	2:D:2264:LYS:NZ	2.29	0.60
2:B:2708:THR:HB	2:B:2780:LYS:HB3	1.84	0.60
2:C:894:VAL:HA	2:C:915:HIS:HE1	1.67	0.60
2:B:3072:MET:SD	2:B:3136:SER:HA	2.41	0.60
2:C:1842:ILE:HD12	2:C:1845:LEU:HD12	1.83	0.60
2:C:3004:VAL:HG13	2:C:3036:LEU:HD11	1.82	0.60
2:A:3141:GLY:O	2:A:3152:ARG:NH2	2.34	0.60
2:C:2834:SER:O	2:C:2838[A]:HIS:HB2	2.02	0.60
2:D:2257:LEU:HB2	2:D:2316:ASN:HD21	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2599:LEU:HD11	2:B:2652:LEU:HD12	1.84	0.60
2:B:2623:LEU:HD23	2:B:2625:GLY:H	1.66	0.60
2:B:2732:TRP:HH2	2:B:2756:LEU:HB3	1.67	0.60
2:A:972:LEU:HD11	2:A:976:TYR:HB3	1.83	0.60
2:A:2708:THR:HB	2:A:2780:LYS:HB3	1.84	0.60
2:B:3015:VAL:HB	2:B:3029:ILE:HG21	1.82	0.60
2:A:894:VAL:HA	2:A:915:HIS:HE1	1.67	0.59
2:A:1842:ILE:HD12	2:A:1845:LEU:HD12	1.83	0.59
2:D:894:VAL:HA	2:D:915:HIS:HE1	1.66	0.59
2:B:972:LEU:HD11	2:B:976:TYR:HB3	1.83	0.59
2:C:972:LEU:HD11	2:C:976:TYR:HB3	1.83	0.59
2:D:992:GLN:HG2	2:D:1064:LEU:HD11	1.85	0.59
2:D:3130:CYS:HB3	2:D:3162:PHE:HZ	1.67	0.59
2:B:2225:SER:HB2	2:B:2240:LEU:HD13	1.85	0.59
2:B:3043:ARG:NH1	2:B:3115:HIS:O	2.35	0.59
2:C:2500:ALA:HB2	2:C:2555:LEU:HD11	1.84	0.59
2:C:2708:THR:HB	2:C:2780:LYS:HB3	1.84	0.59
2:C:2975:PHE:O	2:C:2979:ARG:NE	2.23	0.59
2:C:3805:LEU:HD11	2:C:3887:ASP:HB3	1.85	0.59
2:D:2789:ILE:HD11	2:D:2901:TYR:HB3	1.83	0.59
2:D:4921:PHE:HE2	2:D:4940:VAL:HG11	1.67	0.59
2:C:2789:ILE:HD11	2:C:2901:TYR:HB3	1.83	0.59
2:C:3072:MET:SD	2:C:3136:SER:HA	2.41	0.59
2:C:2225:SER:HB2	2:C:2240:LEU:HD13	1.85	0.59
2:C:2917:ILE:HB	2:C:2920:ARG:HH21	1.66	0.59
2:C:3043:ARG:NH1	2:C:3115:HIS:O	2.35	0.59
2:A:2789:ILE:HD11	2:A:2901:TYR:HB3	1.83	0.59
2:A:3130:CYS:HB3	2:A:3162:PHE:HZ	1.67	0.59
2:B:3805:LEU:HD11	2:B:3887:ASP:HB3	1.85	0.59
2:C:2623:LEU:HD23	2:C:2625:GLY:H	1.66	0.59
2:A:2599:LEU:HD11	2:A:2652:LEU:HD12	1.84	0.59
2:A:3043:ARG:NH1	2:A:3115:HIS:O	2.35	0.59
2:A:3184:TYR:HD1	2:A:3192:ARG:HD3	1.67	0.59
2:D:972:LEU:HD11	2:D:976:TYR:HB3	1.83	0.59
2:D:2917:ILE:HB	2:D:2920:ARG:HH21	1.67	0.59
2:D:3292:GLU:HB2	2:D:3296:MET:HE1	1.84	0.59
2:B:2917:ILE:HB	2:B:2920:ARG:HH21	1.66	0.59
2:B:3184:TYR:HD1	2:B:3192:ARG:HD3	1.68	0.59
2:C:1041:ARG:HA	2:C:1044:LYS:HZ3	1.67	0.59
2:A:2500:ALA:HB2	2:A:2555:LEU:HD11	1.84	0.59
2:D:996:VAL:HG12	2:D:1051:ARG:NH1	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2732:TRP:HH2	2:D:2756:LEU:HB3	1.67	0.59
2:C:992:GLN:HG2	2:C:1064:LEU:HD11	1.84	0.59
2:A:680:ASP:OD1	2:A:801:ARG:NH2	2.36	0.59
2:A:992:GLN:HG2	2:A:1064:LEU:HD11	1.84	0.59
2:A:2732:TRP:HH2	2:A:2756:LEU:HB3	1.67	0.59
2:D:2708:THR:HB	2:D:2780:LYS:HB3	1.84	0.59
2:D:2732:TRP:CD1	2:D:2736:LYS:NZ	2.67	0.59
2:D:3184:TYR:HD1	2:D:3192:ARG:HD3	1.67	0.59
2:D:3805:LEU:HD11	2:D:3887:ASP:HB3	1.85	0.59
2:C:680:ASP:OD1	2:C:801:ARG:NH2	2.36	0.59
1:H:3:VAL:HG12	1:H:77:CYS:HA	1.84	0.59
2:A:434:ASP:OD1	2:A:504:ARG:NE	2.35	0.59
2:B:2732:TRP:CD1	2:B:2736:LYS:NZ	2.67	0.59
2:A:1503:ASN:CG	2:D:2824:ARG:HH22	2.06	0.58
2:A:1766:PRO:HG3	2:A:1780:PRO:HB3	1.85	0.58
2:A:2225:SER:HB2	2:A:2240:LEU:HD13	1.85	0.58
2:A:2791:ARG:NH1	2:A:2901:TYR:OH	2.36	0.58
2:D:983:LEU:HD13	2:D:986:ILE:HD12	1.85	0.58
2:B:983:LEU:HD13	2:B:986:ILE:HD12	1.85	0.58
2:B:1766:PRO:HG3	2:B:1780:PRO:HB3	1.85	0.58
2:A:2223:GLU:OE2	2:A:2264:LYS:NZ	2.28	0.58
1:G:3:VAL:HG12	1:G:77:CYS:HA	1.84	0.58
2:D:2225:SER:HB2	2:D:2240:LEU:HD13	1.84	0.58
2:D:3043:ARG:NH1	2:D:3115:HIS:O	2.35	0.58
2:B:1119:ARG:NH2	2:B:1196:ASP:OD1	2.36	0.58
2:B:2553:TYR:O	2:B:2556:SER:OG	2.15	0.58
2:B:2791:ARG:NH1	2:B:2901:TYR:OH	2.36	0.58
2:C:983:LEU:HD13	2:C:986:ILE:HD12	1.85	0.58
2:A:3805:LEU:HD11	2:A:3887:ASP:HB3	1.85	0.58
2:D:680:ASP:OD1	2:D:801:ARG:NH2	2.36	0.58
2:D:997:ASP:HA	2:D:1051:ARG:HH12	1.68	0.58
2:B:996:VAL:HG12	2:B:1051:ARG:NH1	2.18	0.58
2:C:997:ASP:HA	2:C:1051:ARG:HH12	1.68	0.58
2:C:2834:SER:O	2:C:2838[B]:HIS:HB2	2.03	0.58
2:C:3130:CYS:HB3	2:C:3162:PHE:HZ	1.67	0.58
2:C:3184:TYR:HD1	2:C:3192:ARG:HD3	1.68	0.58
2:A:2917:ILE:HB	2:A:2920:ARG:HH21	1.67	0.58
2:A:2929:LEU:HD21	2:A:2970:LEU:HD11	1.86	0.58
2:D:4579:HIS:CE1	2:D:4742:HIS:ND1	2.72	0.58
2:C:824:GLU:HA	2:C:1020:ILE:HD12	1.85	0.58
2:C:894:VAL:HG12	2:C:918:LEU:HA	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2599:LEU:HD11	2:C:2652:LEU:HD12	1.84	0.58
2:A:875:PRO:HB2	2:A:878:LEU:HD13	1.85	0.58
2:A:1119:ARG:NH2	2:A:1196:ASP:OD1	2.37	0.58
2:A:4921:PHE:HE2	2:A:4940:VAL:HG11	1.67	0.58
2:D:894:VAL:HG12	2:D:918:LEU:HA	1.85	0.58
2:D:1502:ASN:O	2:C:2824:ARG:NH2	2.37	0.58
2:D:2500:ALA:HB2	2:D:2555:LEU:HD11	1.84	0.58
2:B:3141:GLY:O	2:B:3152:ARG:NH2	2.34	0.58
2:C:3778:LEU:HD13	2:C:3854:PHE:HD1	1.69	0.58
2:A:156:GLU:OE1	2:D:2418:ARG:NH2	2.26	0.58
2:A:983:LEU:HD13	2:A:986:ILE:HD12	1.85	0.58
2:A:1564:MET:HE1	2:A:1578:PRO:HA	1.85	0.58
2:A:2778:SER:OG	2:A:2888:LYS:NZ	2.24	0.58
2:D:2966:VAL:HG12	2:D:2970:LEU:HD23	1.85	0.58
2:D:3192:ARG:HG2	2:D:3197:LEU:HG	1.86	0.58
2:B:2202:TYR:O	2:B:2206:ILE:HG12	2.03	0.58
2:B:3209:PRO:HB2	2:B:3214:LEU:HG	1.86	0.58
2:C:2202:TYR:O	2:C:2206:ILE:HG12	2.04	0.58
2:A:3209:PRO:HB2	2:A:3214:LEU:HG	1.86	0.58
2:D:1766:PRO:HG3	2:D:1780:PRO:HB3	1.85	0.58
2:D:2202:TYR:O	2:D:2206:ILE:HG12	2.04	0.58
2:D:2791:ARG:NH1	2:D:2901:TYR:OH	2.36	0.58
2:B:2701:PHE:HE2	2:B:2867:ASN:HD21	1.52	0.58
2:C:434:ASP:OD1	2:C:504:ARG:NE	2.35	0.58
2:C:555:LEU:HD12	2:C:588:ILE:HD11	1.86	0.58
2:C:1766:PRO:HG3	2:C:1780:PRO:HB3	1.85	0.58
2:C:3315:LEU:HD12	2:C:3319:PHE:CD2	2.39	0.58
2:A:996:VAL:HG12	2:A:1051:ARG:NH1	2.18	0.58
2:A:997:ASP:HA	2:A:1051:ARG:HH12	1.68	0.58
2:A:2202:TYR:O	2:A:2206:ILE:HG12	2.04	0.58
2:A:2966:VAL:HG12	2:A:2970:LEU:HD23	1.86	0.58
2:A:3192:ARG:HG2	2:A:3197:LEU:HG	1.86	0.58
2:D:4055:HIS:CE1	2:D:4057:HIS:HB2	2.39	0.58
2:B:824:GLU:HA	2:B:1020:ILE:HD12	1.85	0.58
2:B:3130:CYS:HB3	2:B:3162:PHE:HZ	1.67	0.58
2:C:2791:ARG:NH1	2:C:2901:TYR:OH	2.36	0.58
2:C:2966:VAL:HG12	2:C:2970:LEU:HD23	1.86	0.58
2:C:3142:THR:O	2:C:3144:LYS:NZ	2.35	0.58
2:A:1041:ARG:HA	2:A:1044:LYS:HZ3	1.68	0.58
2:A:2732:TRP:CD1	2:A:2736:LYS:NZ	2.67	0.58
2:D:2778:SER:OG	2:D:2888:LYS:NZ	2.24	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3209:PRO:HB2	2:D:3214:LEU:HG	1.86	0.58
2:B:894:VAL:HG12	2:B:918:LEU:HA	1.85	0.58
2:B:997:ASP:HA	2:B:1051:ARG:HH12	1.68	0.58
2:B:1415:ASP:OD2	2:B:1559:ARG:NH2	2.37	0.58
2:B:2500:ALA:HB2	2:B:2555:LEU:HD11	1.84	0.58
2:B:2929:LEU:HD21	2:B:2970:LEU:HD11	1.86	0.58
2:B:4579:HIS:CE1	2:B:4742:HIS:ND1	2.72	0.58
2:C:4921:PHE:HE2	2:C:4940:VAL:HG11	1.67	0.58
2:A:2591:ARG:NH2	2:A:2695:MET:HB2	2.19	0.58
2:A:2824:ARG:NH1	2:B:1502:ASN:OD1	2.36	0.58
2:D:1119:ARG:NH2	2:D:1196:ASP:OD1	2.36	0.58
2:D:2599:LEU:HD11	2:D:2652:LEU:HD12	1.84	0.58
2:B:992:GLN:HG2	2:B:1064:LEU:HD11	1.84	0.58
2:C:646:THR:HG21	2:C:1702:TYR:OH	2.04	0.58
2:C:2591:ARG:NH2	2:C:2695:MET:HB2	2.19	0.58
2:C:2732:TRP:HH2	2:C:2756:LEU:HB3	1.67	0.58
2:C:4579:HIS:CE1	2:C:4742:HIS:ND1	2.72	0.58
2:A:3861:GLN:HB3	2:A:3864:ASN:HD22	1.69	0.57
2:D:3142:THR:O	2:D:3144:LYS:NZ	2.35	0.57
2:C:2701:PHE:HE2	2:C:2867:ASN:HD21	1.52	0.57
2:C:2943:PHE:CZ	2:C:2955:PRO:HD2	2.39	0.57
2:A:555:LEU:HD12	2:A:588:ILE:HD11	1.86	0.57
1:E:3:VAL:HG12	1:E:77:CYS:HA	1.84	0.57
2:D:875:PRO:HB2	2:D:878:LEU:HD13	1.85	0.57
2:C:233:VAL:HG12	2:C:274:LEU:HD22	1.87	0.57
2:C:996:VAL:HG12	2:C:1051:ARG:NH1	2.18	0.57
2:C:4930:GLU:HA	2:C:4933:HIS:CE1	2.40	0.57
2:A:1415:ASP:OD2	2:A:1559:ARG:NH2	2.37	0.57
2:A:3315:LEU:HD12	2:A:3319:PHE:CD2	2.39	0.57
1:G:18:LYS:HB2	1:G:18:LYS:NZ	2.19	0.57
2:D:2591:ARG:NH2	2:D:2695:MET:HB2	2.19	0.57
2:B:894:VAL:HB	2:B:972:LEU:HB3	1.86	0.57
2:C:3861:GLN:HB3	2:C:3864:ASN:HD22	1.69	0.57
2:A:4055:HIS:CE1	2:A:4057:HIS:HB2	2.39	0.57
1:F:3:VAL:HG12	1:F:77:CYS:HA	1.84	0.57
2:D:1943:ARG:NH1	2:D:1964:GLU:OE1	2.35	0.57
2:D:2834:SER:O	2:D:2838[A]:HIS:HB2	2.05	0.57
2:D:4930:GLU:HA	2:D:4933:HIS:CE1	2.40	0.57
2:B:3315:LEU:HD12	2:B:3319:PHE:CD2	2.39	0.57
2:B:3861:GLN:HB3	2:B:3864:ASN:HD22	1.69	0.57
2:C:889:ILE:HG22	2:C:893:TRP:CZ3	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2760:TYR:O	2:C:2768:LYS:NZ	2.37	0.57
2:C:2845:ALA:HB1	2:C:2885:ASP:HB3	1.87	0.57
2:C:3192:ARG:HG2	2:C:3197:LEU:HG	1.86	0.57
2:C:3209:PRO:HB2	2:C:3214:LEU:HG	1.86	0.57
2:C:4055:HIS:CE1	2:C:4057:HIS:HB2	2.39	0.57
2:C:4913:HIS:O	4:C:5002:ATP:N6	2.38	0.57
2:B:240:HIS:HB3	2:C:167:LYS:HE2	1.86	0.57
2:B:2845:ALA:HB1	2:B:2885:ASP:HB3	1.87	0.57
2:B:3013:VAL:O	2:B:3018:ARG:NH2	2.37	0.57
2:B:3192:ARG:HG2	2:B:3197:LEU:HG	1.86	0.57
2:C:1415:ASP:OD2	2:C:1559:ARG:NH2	2.37	0.57
2:C:3292:GLU:HB2	2:C:3296:MET:HE1	1.87	0.57
2:A:1515:SER:O	2:A:1532:GLN:NE2	2.37	0.57
2:A:4913:HIS:O	4:A:5002:ATP:N6	2.38	0.57
2:D:1415:ASP:OD2	2:D:1559:ARG:NH2	2.37	0.57
2:B:646:THR:HG21	2:B:1702:TYR:OH	2.04	0.57
2:B:3142:THR:O	2:B:3144:LYS:NZ	2.35	0.57
2:A:824:GLU:HA	2:A:1020:ILE:HD12	1.85	0.57
2:A:839:GLU:HB3	2:A:851:LEU:HD12	1.87	0.57
2:D:1273:ILE:HB	2:D:1282:CYS:HB2	1.87	0.57
2:D:2929:LEU:HD21	2:D:2970:LEU:HD11	1.86	0.57
2:D:3141:GLY:O	2:D:3152:ARG:NH2	2.34	0.57
2:B:875:PRO:HB2	2:B:878:LEU:HD13	1.85	0.57
2:B:2760:TYR:O	2:B:2768:LYS:NZ	2.37	0.57
2:B:2841:ALA:HA	2:B:2844:MET:HG3	1.87	0.57
2:B:3246:MET:SD	2:B:3306:ILE:HD12	2.45	0.57
2:B:4055:HIS:CE1	2:B:4057:HIS:HB2	2.39	0.57
2:C:875:PRO:HB2	2:C:878:LEU:HD13	1.85	0.57
2:C:1273:ILE:HB	2:C:1282:CYS:HB2	1.87	0.57
2:D:646:THR:HG21	2:D:1702:TYR:OH	2.04	0.57
2:D:4913:HIS:O	4:D:5002:ATP:N6	2.38	0.57
2:B:233:VAL:HG12	2:B:274:LEU:HD22	1.87	0.57
2:B:3146:ILE:O	2:B:3150:ARG:NH1	2.38	0.57
2:B:4913:HIS:O	4:B:5002:ATP:N6	2.38	0.57
2:C:1119:ARG:NH2	2:C:1196:ASP:OD1	2.37	0.57
2:C:1515:SER:O	2:C:1532:GLN:NE2	2.37	0.57
2:C:3246:MET:SD	2:C:3306:ILE:HD12	2.45	0.57
2:A:2845:ALA:HB1	2:A:2885:ASP:HB3	1.87	0.57
2:D:1564:MET:HE1	2:D:1578:PRO:HA	1.85	0.57
2:D:2845:ALA:HB1	2:D:2885:ASP:HB3	1.87	0.57
2:D:3013:VAL:O	2:D:3018:ARG:NH2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1515:SER:O	2:B:1532:GLN:NE2	2.37	0.57
2:B:2591:ARG:NH2	2:B:2695:MET:HB2	2.19	0.57
2:A:3013:VAL:O	2:A:3018:ARG:NH2	2.37	0.57
2:D:3173:THR:HG23	2:D:3201:VAL:HG22	1.87	0.57
2:D:4698:LEU:HD11	2:C:4264:LEU:HD21	1.87	0.57
2:B:4806:CYS:HA	2:B:4812:CYS:HB2	1.87	0.57
2:C:3273:MET:O	2:C:3277:LEU:HG	2.05	0.57
2:A:114:LEU:HD12	2:A:117:HIS:HE1	1.70	0.56
2:D:839:GLU:HB3	2:D:851:LEU:HD12	1.87	0.56
2:D:889:ILE:HG22	2:D:893:TRP:CZ3	2.40	0.56
2:D:3315:LEU:HD12	2:D:3319:PHE:CD2	2.39	0.56
2:B:2966:VAL:HG12	2:B:2970:LEU:HD23	1.86	0.56
2:A:2841:ALA:HA	2:A:2844:MET:HG3	1.87	0.56
2:A:2868:HIS:HB3	2:A:2871:LEU:HB2	1.87	0.56
2:D:2868:HIS:HB3	2:D:2871:LEU:HB2	1.87	0.56
2:B:2868:HIS:HB3	2:B:2871:LEU:HB2	1.87	0.56
2:B:3173:THR:HG23	2:B:3201:VAL:HG22	1.87	0.56
2:B:4921:PHE:HE2	2:B:4940:VAL:HG11	1.67	0.56
2:C:3013:VAL:O	2:C:3018:ARG:NH2	2.37	0.56
2:A:3891:TYR:O	2:A:3895:LYS:NZ	2.38	0.56
1:F:36:LYS:HB2	2:B:647:ARG:HH12	1.71	0.56
2:D:894:VAL:HB	2:D:972:LEU:HB3	1.86	0.56
2:D:1440:ASN:HB3	2:D:1546:GLN:HB3	1.88	0.56
2:D:2943:PHE:CZ	2:D:2955:PRO:HD2	2.39	0.56
2:D:3215:MET:SD	2:D:3279:ASN:ND2	2.76	0.56
2:B:430:ILE:HG23	2:B:504:ARG:HD2	1.87	0.56
2:B:836:HIS:HB2	2:B:841:LYS:HE3	1.87	0.56
2:B:2447:LYS:NZ	2:B:2862:SER:O	2.38	0.56
2:B:2549:LEU:HD13	2:B:2588:LEU:HD22	1.87	0.56
2:B:2943:PHE:CZ	2:B:2955:PRO:HD2	2.39	0.56
2:B:3141:GLY:HA3	2:B:3237:VAL:HG11	1.88	0.56
2:B:4930:GLU:HA	2:B:4933:HIS:CE1	2.40	0.56
2:C:839:GLU:HB3	2:C:851:LEU:HD12	1.87	0.56
2:C:894:VAL:HB	2:C:972:LEU:HB3	1.86	0.56
2:C:2868:HIS:HB3	2:C:2871:LEU:HB2	1.87	0.56
2:C:2929:LEU:HD21	2:C:2970:LEU:HD11	1.86	0.56
2:A:894:VAL:HG12	2:A:918:LEU:HA	1.85	0.56
2:A:1721:MET:SD	2:A:2127:ARG:NH1	2.79	0.56
2:A:2447:LYS:NZ	2:A:2862:SER:O	2.38	0.56
2:A:3141:GLY:HA3	2:A:3237:VAL:HG11	1.88	0.56
2:D:233:VAL:HG12	2:D:274:LEU:HD22	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:555:LEU:HD12	2:D:588:ILE:HD11	1.86	0.56
2:D:824:GLU:HA	2:D:1020:ILE:HD12	1.85	0.56
2:D:2596:VAL:HG21	2:D:2610:LEU:HD11	1.88	0.56
2:D:3778:LEU:HD13	2:D:3854:PHE:HD1	1.69	0.56
2:B:889:ILE:HG22	2:B:893:TRP:CZ3	2.40	0.56
2:A:1433:PHE:HB3	2:D:2830:ASN:ND2	2.20	0.56
2:A:2760:TYR:O	2:A:2768:LYS:NZ	2.37	0.56
2:A:2943:PHE:CZ	2:A:2955:PRO:HD2	2.39	0.56
2:A:4930:GLU:HA	2:A:4933:HIS:CE1	2.40	0.56
1:E:18:LYS:HB2	1:E:18:LYS:NZ	2.19	0.56
2:D:2701:PHE:HE2	2:D:2867:ASN:HD21	1.52	0.56
2:D:2834:SER:O	2:D:2838[B]:HIS:HB2	2.06	0.56
2:B:3273:MET:O	2:B:3277:LEU:HG	2.05	0.56
2:B:3778:LEU:HD13	2:B:3854:PHE:HD1	1.69	0.56
2:A:962:LYS:HG3	2:A:982:ASP:H	1.71	0.56
2:A:1273:ILE:HB	2:A:1282:CYS:HB2	1.87	0.56
2:D:962:LYS:HG3	2:D:982:ASP:H	1.71	0.56
2:B:555:LEU:HD12	2:B:588:ILE:HD11	1.86	0.56
2:B:1721:MET:SD	2:B:2127:ARG:NH1	2.79	0.56
2:C:2841:ALA:HA	2:C:2844:MET:HG3	1.87	0.56
1:H:18:LYS:HB2	1:H:18:LYS:NZ	2.19	0.56
1:H:36:LYS:HB2	2:D:647:ARG:HH12	1.71	0.56
2:A:894:VAL:HB	2:A:972:LEU:HB3	1.86	0.56
2:D:2760:TYR:O	2:D:2768:LYS:NZ	2.37	0.56
2:D:3246:MET:SD	2:D:3306:ILE:HD12	2.45	0.56
2:D:3912:VAL:O	2:D:3916:VAL:HG23	2.06	0.56
2:B:3215:MET:SD	2:B:3279:ASN:ND2	2.76	0.56
2:B:3891:TYR:O	2:B:3895:LYS:NZ	2.38	0.56
2:C:3173:THR:HG23	2:C:3201:VAL:HG22	1.87	0.56
2:A:233:VAL:HG12	2:A:274:LEU:HD22	1.87	0.56
2:A:646:THR:HG21	2:A:1702:TYR:OH	2.04	0.56
2:A:889:ILE:HG22	2:A:893:TRP:CZ3	2.40	0.56
2:A:919:VAL:HG11	2:A:923:LYS:HD3	1.88	0.56
2:A:2785:TRP:HB2	2:A:2787:TRP:CD1	2.41	0.56
2:A:4806:CYS:HA	2:A:4812:CYS:HB2	1.87	0.56
2:D:114:LEU:HD12	2:D:117:HIS:HE1	1.71	0.56
2:B:680:ASP:OD1	2:B:801:ARG:NH2	2.36	0.56
2:B:839:GLU:HB3	2:B:851:LEU:HD12	1.87	0.56
2:B:1431:ARG:NE	2:B:1556:GLU:OE2	2.39	0.56
2:C:2106:TYR:OH	2:C:2158:HIS:ND1	2.29	0.56
2:A:1440:ASN:HB3	2:A:1546:GLN:HB3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2549:LEU:HD13	2:A:2588:LEU:HD22	1.87	0.56
2:A:2596:VAL:HG21	2:A:2610:LEU:HD11	1.88	0.56
2:A:2701:PHE:HE2	2:A:2867:ASN:HD21	1.52	0.56
2:A:3200:ASN:HB2	2:A:3203:ASP:HB2	1.88	0.56
2:D:2841:ALA:HA	2:D:2844:MET:HG3	1.87	0.56
2:B:1041:ARG:HA	2:B:1044:LYS:HZ3	1.71	0.56
2:C:1419:PHE:HE2	2:C:1562:ASN:HB3	1.71	0.56
2:C:1431:ARG:NE	2:C:1556:GLU:OE2	2.39	0.56
2:A:430:ILE:HG23	2:A:504:ARG:HD2	1.87	0.56
2:A:2980:LEU:HD21	2:A:2989:PRO:HB3	1.88	0.56
2:A:3173:THR:HG23	2:A:3201:VAL:HG22	1.87	0.56
2:A:3215:MET:SD	2:A:3279:ASN:ND2	2.76	0.56
2:A:4503:ARG:NH1	2:A:4745:ASP:OD2	2.39	0.56
2:D:891:GLU:O	2:D:894:VAL:HG22	2.06	0.56
2:D:1419:PHE:HE2	2:D:1562:ASN:HB3	1.71	0.56
2:D:2549:LEU:HD13	2:D:2588:LEU:HD22	1.87	0.56
2:B:891:GLU:O	2:B:894:VAL:HG22	2.06	0.56
2:B:1273:ILE:HB	2:B:1282:CYS:HB2	1.87	0.56
2:B:3912:VAL:O	2:B:3916:VAL:HG23	2.06	0.56
2:C:114:LEU:HD12	2:C:117:HIS:HE1	1.70	0.56
2:C:2596:VAL:HG21	2:C:2610:LEU:HD11	1.88	0.56
2:C:2785:TRP:HB2	2:C:2787:TRP:CD1	2.41	0.56
2:C:3912:VAL:O	2:C:3916:VAL:HG23	2.06	0.56
2:A:1419:PHE:HE2	2:A:1562:ASN:HB3	1.71	0.55
2:A:3146:ILE:O	2:A:3150:ARG:NH1	2.38	0.55
2:A:3778:LEU:HD13	2:A:3854:PHE:HD1	1.69	0.55
2:D:430:ILE:HG23	2:D:504:ARG:HD2	1.87	0.55
2:D:2829:SER:OG	2:D:2830:ASN:ND2	2.39	0.55
2:D:3141:GLY:HA3	2:D:3237:VAL:HG11	1.88	0.55
2:D:3200:ASN:HB2	2:D:3203:ASP:HB2	1.88	0.55
2:D:3273:MET:O	2:D:3277:LEU:HG	2.05	0.55
2:C:1721:MET:SD	2:C:2127:ARG:NH1	2.79	0.55
2:C:3146:ILE:O	2:C:3150:ARG:NH1	2.38	0.55
2:C:3200:ASN:HB2	2:C:3203:ASP:HB2	1.88	0.55
2:A:2829:SER:OG	2:A:2830:ASN:ND2	2.39	0.55
2:A:3246:MET:SD	2:A:3306:ILE:HD12	2.45	0.55
1:G:35:LYS:NZ	2:C:640:ARG:O	2.39	0.55
2:D:836:HIS:HB2	2:D:841:LYS:HE3	1.87	0.55
2:D:2854:LYS:HG2	2:D:2858:MET:HE1	1.89	0.55
2:D:3891:TYR:O	2:D:3895:LYS:NZ	2.38	0.55
2:B:434:ASP:OD1	2:B:504:ARG:NE	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4503:ARG:NH1	2:B:4745:ASP:OD2	2.39	0.55
2:B:4579:HIS:HE1	2:B:4742:HIS:CE1	2.25	0.55
2:C:2447:LYS:NZ	2:C:2862:SER:O	2.38	0.55
2:C:4579:HIS:HE1	2:C:4742:HIS:CE1	2.25	0.55
2:C:4806:CYS:HA	2:C:4812:CYS:HB2	1.87	0.55
2:D:919:VAL:HG11	2:D:923:LYS:HD3	1.88	0.55
2:D:4809:MET:HG2	2:C:4518:LEU:HA	1.89	0.55
2:B:2377:GLU:OE2	2:B:2383:HIS:NE2	2.40	0.55
2:A:836:HIS:HB2	2:A:841:LYS:HE3	1.88	0.55
2:A:4240:THR:HG22	2:A:4308:ILE:HD12	1.89	0.55
2:D:434:ASP:OD1	2:D:504:ARG:NE	2.35	0.55
2:D:1721:MET:SD	2:D:2127:ARG:NH1	2.79	0.55
2:D:1932:PHE:HZ	2:D:1979:PHE:HE2	1.54	0.55
2:D:2106:TYR:OH	2:D:2158:HIS:ND1	2.29	0.55
2:D:2833:LEU:HB3	2:D:2837:LEU:HD22	1.89	0.55
2:B:919:VAL:HG11	2:B:923:LYS:HD3	1.88	0.55
2:B:927:GLN:NE2	2:B:928:GLU:HG2	2.22	0.55
2:C:962:LYS:HG3	2:C:982:ASP:H	1.71	0.55
2:C:1564:MET:HE3	2:C:1565:PRO:HD2	1.87	0.55
2:C:2833:LEU:HB3	2:C:2837:LEU:HD22	1.89	0.55
2:C:3141:GLY:HA3	2:C:3237:VAL:HG11	1.88	0.55
2:A:1551:ASN:HB2	2:D:2830:ASN:OD1	2.06	0.55
1:F:18:LYS:NZ	1:F:18:LYS:HB2	2.19	0.55
2:D:2980:LEU:HD21	2:D:2989:PRO:HB3	1.88	0.55
2:D:4240:THR:HG22	2:D:4308:ILE:HD12	1.89	0.55
2:D:4806:CYS:HA	2:D:4812:CYS:HB2	1.87	0.55
2:B:114:LEU:HD12	2:B:117:HIS:HE1	1.71	0.55
2:B:4240:THR:HG22	2:B:4308:ILE:HD12	1.89	0.55
2:C:430:ILE:HG23	2:C:504:ARG:HD2	1.87	0.55
2:C:2760:TYR:HA	2:C:2763:LEU:HD13	1.89	0.55
2:A:891:GLU:O	2:A:894:VAL:HG22	2.06	0.55
2:A:1708:ASP:HA	2:A:1712:SER:HB2	1.89	0.55
2:D:2447:LYS:NZ	2:D:2862:SER:O	2.38	0.55
2:D:4503:ARG:NH1	2:D:4745:ASP:OD2	2.39	0.55
2:B:1564:MET:HE1	2:B:1578:PRO:HA	1.87	0.55
2:B:1979:PHE:HB2	2:B:3628:TRP:HZ2	1.72	0.55
2:B:2760:TYR:HA	2:B:2763:LEU:HD13	1.89	0.55
2:B:2785:TRP:HB2	2:B:2787:TRP:CD1	2.41	0.55
2:B:2833:LEU:HB3	2:B:2837:LEU:HD22	1.89	0.55
2:C:836:HIS:HB2	2:C:841:LYS:HE3	1.87	0.55
2:C:891:GLU:O	2:C:894:VAL:HG22	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2980:LEU:HD21	2:C:2989:PRO:HB3	1.88	0.55
2:A:3273:MET:O	2:A:3277:LEU:HG	2.05	0.55
2:D:2785:TRP:HB2	2:D:2787:TRP:CD1	2.41	0.55
2:B:962:LYS:HG3	2:B:982:ASP:H	1.71	0.55
2:B:3200:ASN:HB2	2:B:3203:ASP:HB2	1.88	0.55
2:C:1979:PHE:HB2	2:C:3628:TRP:HZ2	1.72	0.55
2:C:2549:LEU:HD13	2:C:2588:LEU:HD22	1.87	0.55
2:C:4240:THR:HG22	2:C:4308:ILE:HD12	1.89	0.55
2:A:1979:PHE:HB2	2:A:3628:TRP:HZ2	1.72	0.55
2:A:2377:GLU:OE2	2:A:2383:HIS:NE2	2.40	0.55
2:A:3250:TRP:O	2:A:3256:ASN:ND2	2.40	0.55
2:A:3912:VAL:O	2:A:3916:VAL:HG23	2.06	0.55
2:D:1141:LYS:O	2:D:1143:GLN:NE2	2.40	0.55
2:D:1895:GLN:NE2	2:D:2068:ARG:HH22	2.05	0.55
2:B:1440:ASN:HB3	2:B:1546:GLN:HB3	1.88	0.55
2:B:2724:TYR:HD2	2:B:2775:ILE:HG12	1.72	0.55
2:C:927:GLN:NE2	2:C:928:GLU:HG2	2.21	0.55
2:C:1141:LYS:O	2:C:1143:GLN:NE2	2.40	0.55
2:C:1564:MET:HE1	2:C:1578:PRO:HA	1.88	0.55
2:D:1708:ASP:HA	2:D:1712:SER:HB2	1.89	0.55
2:B:2980:LEU:HD21	2:B:2989:PRO:HB3	1.88	0.55
2:B:3250:TRP:O	2:B:3256:ASN:ND2	2.40	0.55
2:B:4620:GLN:OE1	2:B:4632:ARG:NH2	2.34	0.55
2:C:1708:ASP:HA	2:C:1712:SER:HB2	1.89	0.55
2:C:1932:PHE:HZ	2:C:1979:PHE:HE2	1.55	0.55
2:C:1943:ARG:NH1	2:C:1964:GLU:OE1	2.35	0.55
2:C:3891:TYR:O	2:C:3895:LYS:NZ	2.38	0.55
2:C:4792:PHE:HB3	2:C:4843:ARG:HH21	1.72	0.55
2:A:2724:TYR:HD2	2:A:2775:ILE:HG12	1.72	0.55
2:A:4792:PHE:HB3	2:A:4843:ARG:HH21	1.72	0.55
2:D:943:LEU:HD21	2:D:999:LEU:HD11	1.89	0.55
2:D:3254:PRO:HD3	2:D:3266:THR:O	2.08	0.55
2:B:2596:VAL:HG21	2:B:2610:LEU:HD11	1.88	0.55
2:B:4792:PHE:HB3	2:B:4843:ARG:HH21	1.72	0.55
2:C:2713:ILE:HG21	2:C:2721:ILE:HD11	1.89	0.55
2:A:1662:SER:OG	2:A:1708:ASP:OD2	2.22	0.54
2:A:2833:LEU:HB3	2:A:2837:LEU:HD22	1.89	0.54
2:A:4707:MET:HG3	2:D:4252:ILE:HG21	1.89	0.54
2:D:881:ILE:HG23	2:D:884:LYS:HE2	1.89	0.54
2:D:927:GLN:NE2	2:D:928:GLU:HG2	2.22	0.54
2:D:2377:GLU:OE2	2:D:2383:HIS:NE2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4792:PHE:HB3	2:D:4843:ARG:HH21	1.72	0.54
2:B:1564:MET:HE3	2:B:1565:PRO:HD2	1.89	0.54
2:B:2829:SER:OG	2:B:2830:ASN:ND2	2.39	0.54
2:C:1844:GLN:NE2	2:C:1853:GLU:OE1	2.41	0.54
2:C:2605:MET:CG	2:C:2606:PRO:HD3	2.37	0.54
2:C:2829:SER:OG	2:C:2830:ASN:ND2	2.39	0.54
2:A:4517:LEU:O	2:B:4809:MET:HG2	2.06	0.54
2:D:4579:HIS:HE1	2:D:4742:HIS:CE1	2.25	0.54
2:B:938:GLU:HA	2:B:941:LYS:HB2	1.90	0.54
2:B:1708:ASP:HA	2:B:1712:SER:HB2	1.89	0.54
2:B:4252:ILE:HG21	2:C:4707:MET:HG3	1.89	0.54
2:C:866:PRO:HB3	2:C:1002:ASN:OD1	2.07	0.54
2:A:579:LEU:HD22	2:A:586:LEU:HD23	1.90	0.54
2:D:247:VAL:O	2:D:272:ARG:NH1	2.40	0.54
2:D:4707:MET:HG3	2:C:4252:ILE:CG2	2.37	0.54
2:B:1419:PHE:HE2	2:B:1562:ASN:HB3	1.71	0.54
2:B:1564:MET:CE	2:B:1565:PRO:HD2	2.38	0.54
2:B:1895:GLN:HE22	2:B:2068:ARG:HH22	1.55	0.54
2:C:1895:GLN:NE2	2:C:2068:ARG:HH22	2.05	0.54
2:A:927:GLN:NE2	2:A:928:GLU:HG2	2.22	0.54
2:A:938:GLU:HA	2:A:941:LYS:HB2	1.90	0.54
2:D:1564:MET:CE	2:D:1565:PRO:HD2	2.38	0.54
2:B:1895:GLN:NE2	2:B:2068:ARG:HH22	2.05	0.54
2:C:1440:ASN:HB3	2:C:1546:GLN:HB3	1.88	0.54
2:C:2724:TYR:HD2	2:C:2775:ILE:HG12	1.72	0.54
2:A:640:ARG:O	1:E:35:LYS:NZ	2.40	0.54
2:A:4756:ILE:HG23	2:B:4861:ILE:HG21	1.89	0.54
2:B:247:VAL:O	2:B:272:ARG:NH1	2.41	0.54
2:B:2713:ILE:HG21	2:B:2721:ILE:HD11	1.89	0.54
2:C:247:VAL:O	2:C:272:ARG:NH1	2.40	0.54
2:A:866:PRO:HB3	2:A:1002:ASN:OD1	2.07	0.54
2:A:881:ILE:HG23	2:A:884:LYS:HE2	1.89	0.54
2:A:1564:MET:CE	2:A:1565:PRO:HD2	2.38	0.54
2:D:890:HIS:HA	2:D:893:TRP:HE3	1.73	0.54
2:D:3250:TRP:O	2:D:3256:ASN:ND2	2.40	0.54
2:B:2605:MET:CG	2:B:2606:PRO:HD3	2.37	0.54
2:C:943:LEU:HD21	2:C:999:LEU:HD11	1.89	0.54
2:C:1564:MET:CE	2:C:1565:PRO:HD2	2.38	0.54
2:A:943:LEU:HD21	2:A:999:LEU:HD11	1.89	0.54
2:A:1943:ARG:NH1	2:A:1964:GLU:OE1	2.35	0.54
2:A:2713:ILE:HG21	2:A:2721:ILE:HD11	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:866:PRO:HB3	2:D:1002:ASN:OD1	2.07	0.54
2:D:1844:GLN:NE2	2:D:1853:GLU:OE1	2.41	0.54
2:D:4197:ILE:HG23	2:D:4923:MET:HE2	1.89	0.54
2:B:881:ILE:HG23	2:B:884:LYS:HE2	1.89	0.54
2:B:3025:ASP:O	2:B:3028:SER:OG	2.17	0.54
2:C:881:ILE:HG23	2:C:884:LYS:HE2	1.89	0.54
2:A:1141:LYS:O	2:A:1143:GLN:NE2	2.40	0.54
2:A:3254:PRO:HD3	2:A:3266:THR:O	2.08	0.54
2:D:579:LEU:HD22	2:D:586:LEU:HD23	1.90	0.54
2:D:1515:SER:O	2:D:1532:GLN:NE2	2.37	0.54
2:D:2605:MET:CG	2:D:2606:PRO:HD3	2.37	0.54
2:D:4014:LEU:HD13	2:D:4122:ALA:HB2	1.89	0.54
2:B:866:PRO:HB3	2:B:1002:ASN:OD1	2.07	0.54
2:B:890:HIS:HA	2:B:893:TRP:HE3	1.73	0.54
2:B:943:LEU:HD21	2:B:999:LEU:HD11	1.89	0.54
2:B:2232:PRO:HB2	2:B:2379:ASP:HA	1.90	0.54
2:C:3254:PRO:HD3	2:C:3266:THR:O	2.08	0.54
2:A:247:VAL:O	2:A:272:ARG:NH1	2.41	0.54
2:A:890:HIS:HA	2:A:893:TRP:HE3	1.73	0.54
2:A:1420:LEU:HD21	2:A:1559:ARG:HH12	1.73	0.54
2:A:1498:GLN:O	2:A:1500:ARG:NH1	2.41	0.54
2:A:1962:THR:HG23	2:A:1966:ARG:HE	1.73	0.54
2:A:2605:MET:CG	2:A:2606:PRO:HD3	2.37	0.54
2:A:2760:TYR:HA	2:A:2763:LEU:HD13	1.89	0.54
2:A:4867:ILE:HD12	2:D:4867:ILE:HD13	1.90	0.54
2:D:935:MET:O	2:D:939:THR:OG1	2.17	0.54
2:D:938:GLU:HA	2:D:941:LYS:HB2	1.90	0.54
2:D:1431:ARG:NE	2:D:1556:GLU:OE2	2.39	0.54
2:B:877:HIS:O	2:B:1062:TYR:OH	2.15	0.54
2:B:1851:PHE:HZ	2:B:2058:LEU:HD13	1.73	0.54
2:B:2223:GLU:OE2	2:B:2264:LYS:NZ	2.28	0.54
2:B:2824:ARG:CZ	2:C:1502:ASN:O	2.55	0.54
2:A:185:SER:HG	2:A:188:SER:HG	1.51	0.54
2:A:940:LEU:HA	2:A:943:LEU:HD12	1.90	0.54
2:A:1895:GLN:HE22	2:A:2068:ARG:HH22	1.56	0.54
2:A:1932:PHE:HZ	2:A:1979:PHE:HE2	1.55	0.54
2:A:4620:GLN:OE1	2:A:4632:ARG:NH2	2.34	0.54
2:D:2724:TYR:HD2	2:D:2775:ILE:HG12	1.72	0.54
2:B:1141:LYS:O	2:B:1143:GLN:NE2	2.40	0.54
2:B:2834:SER:O	2:B:2838[A]:HIS:HB2	2.08	0.54
2:C:919:VAL:HG11	2:C:923:LYS:HD3	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2854:LYS:HG2	2:C:2858:MET:HE1	1.89	0.54
2:C:4014:LEU:HD13	2:C:4122:ALA:HB2	1.89	0.54
2:A:4484:ILE:HG13	2:A:4485:ILE:HD12	1.90	0.53
2:D:1498:GLN:O	2:D:1500:ARG:NH1	2.41	0.53
2:B:2102:LEU:HD23	2:B:3625:GLU:HB2	1.90	0.53
2:C:713:TRP:HH2	2:C:1251:LEU:HD21	1.73	0.53
2:C:890:HIS:HA	2:C:893:TRP:HE3	1.73	0.53
2:C:1895:GLN:HE22	2:C:2068:ARG:HH22	1.56	0.53
2:C:2102:LEU:HD23	2:C:3625:GLU:HB2	1.90	0.53
2:C:2377:GLU:OE2	2:C:2383:HIS:NE2	2.40	0.53
2:C:3250:TRP:O	2:C:3256:ASN:ND2	2.40	0.53
2:C:4567:TYR:O	2:C:4571:THR:OG1	2.23	0.53
2:A:1851:PHE:HZ	2:A:2058:LEU:HD13	1.73	0.53
2:D:1100:ARG:NH2	2:D:1234:GLU:O	2.42	0.53
2:D:1895:GLN:HE22	2:D:2068:ARG:HH22	1.56	0.53
2:D:2674:GLY:HA3	2:D:2977:ASN:HD22	1.74	0.53
2:D:3146:ILE:O	2:D:3150:ARG:NH1	2.38	0.53
2:C:271:ALA:HB2	2:C:488:LEU:HD22	1.91	0.53
2:C:1100:ARG:NH2	2:C:1234:GLU:O	2.42	0.53
2:C:1498:GLN:O	2:C:1500:ARG:NH1	2.41	0.53
2:C:1962:THR:HG23	2:C:1966:ARG:HE	1.73	0.53
2:A:1895:GLN:NE2	2:A:2068:ARG:HH22	2.05	0.53
2:A:3796:LEU:HD22	2:A:3835:PHE:HZ	1.73	0.53
2:A:4694:LEU:HD21	2:D:4264:LEU:HG	1.90	0.53
2:D:1079:SER:OG	2:D:1083:GLU:O	2.27	0.53
2:D:1979:PHE:HB2	2:D:3628:TRP:HZ2	1.72	0.53
2:B:579:LEU:HD22	2:B:586:LEU:HD23	1.90	0.53
2:B:1844:GLN:NE2	2:B:1853:GLU:OE1	2.41	0.53
2:B:1932:PHE:HZ	2:B:1979:PHE:HE2	1.54	0.53
2:C:4620:GLN:OE1	2:C:4632:ARG:NH2	2.34	0.53
2:A:930:ASN:HA	2:A:933:LEU:HD13	1.91	0.53
2:A:2102:LEU:HD23	2:A:3625:GLU:HB2	1.90	0.53
2:A:3743:THR:HB	2:A:3758:THR:HG21	1.90	0.53
2:A:4283:PHE:HE2	2:B:4495:PHE:HE2	1.57	0.53
2:D:938:GLU:HG3	2:D:941:LYS:HE2	1.91	0.53
2:D:2102:LEU:HD23	2:D:3625:GLU:HB2	1.90	0.53
2:D:2760:TYR:HA	2:D:2763:LEU:HD13	1.89	0.53
2:D:3796:LEU:HD22	2:D:3835:PHE:HZ	1.74	0.53
2:B:713:TRP:HH2	2:B:1251:LEU:HD21	1.73	0.53
2:B:938:GLU:HG3	2:B:941:LYS:HE2	1.91	0.53
2:B:2824:ARG:HH22	2:C:1503:ASN:CG	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3254:PRO:HD3	2:B:3266:THR:O	2.08	0.53
2:C:3025:ASP:O	2:C:3029:ILE:HD12	2.09	0.53
2:C:4503:ARG:NH1	2:C:4745:ASP:OD2	2.39	0.53
2:A:938:GLU:HG3	2:A:941:LYS:HE2	1.91	0.53
2:A:1844:GLN:NE2	2:A:1853:GLU:OE1	2.41	0.53
1:G:36:LYS:HB2	2:C:647:ARG:HH12	1.72	0.53
2:D:2787:TRP:HH2	2:D:2840:MET:HB3	1.74	0.53
2:D:2874:TYR:OH	2:D:2886:ARG:NH2	2.42	0.53
2:D:3025:ASP:O	2:D:3029:ILE:HD12	2.09	0.53
2:D:4484:ILE:HG13	2:D:4485:ILE:HD12	1.90	0.53
2:B:930:ASN:HA	2:B:933:LEU:HD13	1.91	0.53
2:B:1498:GLN:O	2:B:1500:ARG:NH1	2.41	0.53
2:B:1943:ARG:NH1	2:B:1964:GLU:OE1	2.35	0.53
2:B:2627:TRP:HB2	2:B:2630:PHE:HB2	1.91	0.53
2:B:3025:ASP:O	2:B:3029:ILE:HD12	2.09	0.53
2:C:2232:PRO:HB2	2:C:2379:ASP:HA	1.90	0.53
2:C:2627:TRP:HB2	2:C:2630:PHE:HB2	1.91	0.53
2:C:3796:LEU:HD22	2:C:3835:PHE:HZ	1.74	0.53
2:A:883:GLU:OE2	2:A:929:ARG:NH2	2.42	0.53
2:A:1100:ARG:NH2	2:A:1234:GLU:O	2.42	0.53
2:D:930:ASN:HA	2:D:933:LEU:HD13	1.91	0.53
2:D:1420:LEU:HD21	2:D:1559:ARG:HH12	1.73	0.53
2:D:2172:MET:O	2:D:2176:VAL:N	2.38	0.53
2:D:2713:ILE:HG21	2:D:2721:ILE:HD11	1.89	0.53
2:B:2787:TRP:HH2	2:B:2840:MET:HB3	1.74	0.53
2:B:3796:LEU:HD22	2:B:3835:PHE:HZ	1.74	0.53
2:C:579:LEU:HD22	2:C:586:LEU:HD23	1.90	0.53
2:C:915:HIS:NE2	2:C:917:CYS:HB2	2.24	0.53
2:C:930:ASN:HA	2:C:933:LEU:HD13	1.91	0.53
2:C:938:GLU:HA	2:C:941:LYS:HB2	1.90	0.53
2:C:4484:ILE:HG13	2:C:4485:ILE:HD12	1.90	0.53
2:A:915:HIS:NE2	2:A:917:CYS:HB2	2.24	0.53
2:A:1431:ARG:NE	2:A:1556:GLU:OE2	2.39	0.53
2:B:1100:ARG:NH2	2:B:1234:GLU:O	2.42	0.53
2:B:2605:MET:HG2	2:B:2606:PRO:HD3	1.91	0.53
2:B:4484:ILE:HG13	2:B:4485:ILE:HD12	1.90	0.53
2:C:940:LEU:HA	2:C:943:LEU:HD12	1.90	0.53
2:C:2605:MET:HG2	2:C:2606:PRO:HD3	1.91	0.53
2:C:2787:TRP:HH2	2:C:2840:MET:HB3	1.74	0.53
2:C:3292:GLU:HB2	2:C:3296:MET:HE2	1.91	0.53
2:A:2674:GLY:HA3	2:A:2977:ASN:HD22	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2874:TYR:OH	2:A:2886:ARG:NH2	2.42	0.53
2:D:3743:THR:HB	2:D:3758:THR:HG21	1.90	0.53
2:B:1420:LEU:HD21	2:B:1559:ARG:HH12	1.73	0.53
2:B:2778:SER:OG	2:B:2888:LYS:NZ	2.24	0.53
2:C:1420:LEU:HD21	2:C:1559:ARG:HH12	1.73	0.53
2:C:2874:TYR:OH	2:C:2886:ARG:NH2	2.42	0.53
2:A:233:VAL:HG22	2:A:276:ARG:HG2	1.91	0.53
2:A:2854:LYS:HG2	2:A:2858:MET:HE1	1.91	0.53
2:A:4014:LEU:HD13	2:A:4122:ALA:HB2	1.89	0.53
2:D:713:TRP:HH2	2:D:1251:LEU:HD21	1.73	0.53
2:D:887:GLU:O	2:D:976:TYR:OH	2.27	0.53
2:D:915:HIS:NE2	2:D:917:CYS:HB2	2.24	0.53
2:D:4177:VAL:HG11	2:D:4880:VAL:HA	1.91	0.53
2:B:3743:THR:HB	2:B:3758:THR:HG21	1.90	0.53
2:C:679:VAL:HG13	2:C:800:VAL:HG12	1.91	0.53
2:C:938:GLU:HG3	2:C:941:LYS:HE2	1.91	0.53
2:A:2603:ALA:C	2:A:2606:PRO:HD2	2.29	0.53
2:A:2666:LEU:HD13	2:A:2966:VAL:HA	1.91	0.53
2:A:2732:TRP:O	2:A:2736:LYS:NZ	2.41	0.53
2:A:2787:TRP:HH2	2:A:2840:MET:HB3	1.74	0.53
2:D:966:LEU:HD22	2:D:970:TYR:HD2	1.74	0.53
2:B:1144:ARG:NH2	2:B:1191:ALA:O	2.42	0.53
2:B:1962:THR:HG23	2:B:1966:ARG:HE	1.73	0.53
2:B:2603:ALA:C	2:B:2606:PRO:HD2	2.30	0.53
2:C:1144:ARG:NH2	2:C:1191:ALA:O	2.42	0.53
2:C:2935:GLU:HB3	2:C:2939:TYR:CE1	2.43	0.53
2:A:1144:ARG:NH2	2:A:1191:ALA:O	2.42	0.52
2:A:2232:PRO:HB2	2:A:2379:ASP:HA	1.90	0.52
2:A:3145:SER:HB3	2:A:3148:VAL:HG12	1.91	0.52
2:A:3297:LYS:HD2	2:A:3334:VAL:HA	1.91	0.52
2:A:4267:GLN:HG3	2:A:4270:LYS:HZ3	1.74	0.52
2:D:1851:PHE:HZ	2:D:2058:LEU:HD13	1.73	0.52
2:D:2497:ARG:HH22	2:D:2877:LEU:HD13	1.74	0.52
2:D:2666:LEU:HD13	2:D:2966:VAL:HA	1.91	0.52
2:D:3273:MET:HA	2:D:3276:LEU:HG	1.90	0.52
2:B:915:HIS:NE2	2:B:917:CYS:HB2	2.24	0.52
2:B:2666:LEU:HD13	2:B:2966:VAL:HA	1.91	0.52
2:B:2854:LYS:HG2	2:B:2858:MET:HE1	1.90	0.52
2:B:4014:LEU:HD13	2:B:4122:ALA:HB2	1.89	0.52
2:C:1851:PHE:HZ	2:C:2058:LEU:HD13	1.73	0.52
2:A:27:THR:OG1	2:A:32:GLN:OE1	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:966:LEU:HD22	2:A:970:TYR:HD2	1.75	0.52
2:A:1433:PHE:HB3	2:D:2830:ASN:CG	2.29	0.52
2:A:2718:GLU:HA	2:A:2721:ILE:HD12	1.91	0.52
2:A:3284:ILE:O	2:A:3288:LEU:HG	2.10	0.52
2:D:940:LEU:HA	2:D:943:LEU:HD12	1.90	0.52
2:D:1962:THR:HG23	2:D:1966:ARG:HE	1.73	0.52
2:D:2232:PRO:HB2	2:D:2379:ASP:HA	1.90	0.52
2:D:2718:GLU:HA	2:D:2721:ILE:HD12	1.91	0.52
2:D:2895:PHE:O	2:D:2899:ASN:ND2	2.29	0.52
2:D:4267:GLN:HG3	2:D:4270:LYS:HZ3	1.75	0.52
2:D:4579:HIS:CE1	2:D:4742:HIS:CE1	2.98	0.52
2:B:2849:HIS:CD2	2:B:2852:TRP:HE3	2.27	0.52
2:B:3327:LYS:HA	2:B:3330:ALA:HB2	1.91	0.52
2:C:943:LEU:HA	2:C:946:LEU:HD23	1.92	0.52
2:C:2172:MET:O	2:C:2176:VAL:N	2.38	0.52
2:C:2252:GLU:HB2	2:C:3819:MET:SD	2.50	0.52
2:C:2849:HIS:CD2	2:C:2852:TRP:HE3	2.27	0.52
2:A:1071:HIS:CD2	2:D:2986:ALA:HB1	2.45	0.52
2:A:2591:ARG:HH22	2:A:2695:MET:HB2	1.74	0.52
2:D:3284:ILE:O	2:D:3288:LEU:HG	2.10	0.52
2:B:679:VAL:HG13	2:B:800:VAL:HG12	1.91	0.52
2:B:2252:GLU:HB2	2:B:3819:MET:SD	2.50	0.52
2:B:2278:GLN:HA	2:B:2281:VAL:HG22	1.91	0.52
2:B:2544:LEU:HD23	2:B:2544:LEU:H	1.74	0.52
2:B:2834:SER:O	2:B:2838[B]:HIS:HB2	2.09	0.52
2:B:2935:GLU:HB3	2:B:2939:TYR:CE1	2.43	0.52
2:C:966:LEU:HD22	2:C:970:TYR:HD2	1.74	0.52
2:C:1079:SER:OG	2:C:1083:GLU:O	2.27	0.52
2:C:2544:LEU:HD23	2:C:2544:LEU:H	1.74	0.52
2:A:1303:ARG:HA	2:A:1542:ALA:HA	1.91	0.52
2:A:4847:ASP:OD2	2:D:4818:TYR:OH	2.22	0.52
2:D:271:ALA:HB2	2:D:488:LEU:HD22	1.91	0.52
2:D:943:LEU:HA	2:D:946:LEU:HD23	1.92	0.52
2:D:1421:MET:HE1	2:D:1576:LYS:HB3	1.91	0.52
2:D:3297:LYS:HD2	2:D:3334:VAL:HA	1.91	0.52
2:B:940:LEU:HA	2:B:943:LEU:HD12	1.90	0.52
2:B:966:LEU:HD22	2:B:970:TYR:HD2	1.74	0.52
2:B:2874:TYR:OH	2:B:2886:ARG:NH2	2.42	0.52
2:B:3159:LEU:HD12	2:B:3241:MET:SD	2.50	0.52
2:B:3297:LYS:HD2	2:B:3334:VAL:HA	1.91	0.52
2:C:1303:ARG:HA	2:C:1542:ALA:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:271:ALA:HB2	2:A:488:LEU:HD22	1.91	0.52
2:A:943:LEU:HA	2:A:946:LEU:HD23	1.92	0.52
2:A:1047:LYS:O	2:A:1051:ARG:HD3	2.10	0.52
2:A:2593:VAL:HG21	2:A:2640:LEU:HD22	1.92	0.52
2:A:3273:MET:HA	2:A:3276:LEU:HG	1.90	0.52
2:D:883:GLU:OE2	2:D:929:ARG:NH2	2.42	0.52
2:D:934:GLN:HG3	2:D:937:LEU:HD12	1.92	0.52
2:D:1144:ARG:NH2	2:D:1191:ALA:O	2.42	0.52
2:D:2278:GLN:HA	2:D:2281:VAL:HG22	1.91	0.52
2:B:2553:TYR:HE1	2:B:2606:PRO:HG3	1.75	0.52
2:B:3145:SER:HB3	2:B:3148:VAL:HG12	1.91	0.52
2:B:3284:ILE:O	2:B:3288:LEU:HG	2.10	0.52
2:C:233:VAL:HG22	2:C:276:ARG:HG2	1.91	0.52
2:C:1047:LYS:O	2:C:1051:ARG:HD3	2.10	0.52
2:C:1154:ARG:H	2:C:1182:LEU:HD22	1.75	0.52
2:C:2278:GLN:HA	2:C:2281:VAL:HG22	1.91	0.52
2:C:3297:LYS:HD2	2:C:3334:VAL:HA	1.91	0.52
2:C:3327:LYS:HA	2:C:3330:ALA:HB2	1.91	0.52
2:A:2544:LEU:HD23	2:A:2544:LEU:H	1.74	0.52
2:A:2553:TYR:HE1	2:A:2606:PRO:HG3	1.75	0.52
2:A:4177:VAL:HG11	2:A:4880:VAL:HA	1.91	0.52
2:D:3145:SER:HB3	2:D:3148:VAL:HG12	1.91	0.52
2:D:4591:TYR:HD2	2:C:4287:TYR:HH	1.57	0.52
2:B:27:THR:OG1	2:B:32:GLN:OE1	2.27	0.52
2:B:233:VAL:HG22	2:B:276:ARG:HG2	1.91	0.52
2:B:2674:GLY:HA3	2:B:2977:ASN:HD22	1.74	0.52
2:B:4177:VAL:HG11	2:B:4880:VAL:HA	1.91	0.52
2:C:934:GLN:HG3	2:C:937:LEU:HD12	1.92	0.52
2:C:1421:MET:HE1	2:C:1576:LYS:HB3	1.92	0.52
2:C:3273:MET:HA	2:C:3276:LEU:HG	1.90	0.52
2:A:713:TRP:HH2	2:A:1251:LEU:HD21	1.73	0.52
2:A:1079:SER:OG	2:A:1083:GLU:O	2.27	0.52
2:A:3920:LEU:HD22	2:A:3935:LEU:HD21	1.92	0.52
2:A:4616:TYR:HE2	2:A:4632:ARG:HG2	1.75	0.52
2:D:27:THR:OG1	2:D:32:GLN:OE1	2.27	0.52
2:D:4620:GLN:OE1	2:D:4632:ARG:NH2	2.34	0.52
2:B:887:GLU:O	2:B:976:TYR:OH	2.27	0.52
2:B:934:GLN:HG3	2:B:937:LEU:HD12	1.92	0.52
2:B:943:LEU:HA	2:B:946:LEU:HD23	1.92	0.52
2:B:3273:MET:HA	2:B:3276:LEU:HG	1.90	0.52
2:C:27:THR:OG1	2:C:32:GLN:OE1	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2593:VAL:HG21	2:C:2640:LEU:HD22	1.92	0.52
2:C:2603:ALA:C	2:C:2606:PRO:HD2	2.29	0.52
2:C:2674:GLY:HA3	2:C:2977:ASN:HD22	1.74	0.52
2:C:3159:LEU:HD12	2:C:3241:MET:SD	2.50	0.52
2:C:3743:THR:HB	2:C:3758:THR:HG21	1.90	0.52
2:A:412:GLU:HG3	2:A:488:LEU:HD11	1.92	0.52
2:A:2497:ARG:HH22	2:A:2877:LEU:HD13	1.74	0.52
2:A:2935:GLU:HB3	2:A:2939:TYR:CE1	2.42	0.52
2:D:233:VAL:HG22	2:D:276:ARG:HG2	1.91	0.52
2:D:1047:LYS:O	2:D:1051:ARG:HD3	2.10	0.52
2:D:2544:LEU:HD23	2:D:2544:LEU:H	1.74	0.52
2:D:2593:VAL:HG21	2:D:2640:LEU:HD22	1.92	0.52
2:B:2681:MET:HE3	2:B:2919:LYS:HE2	1.92	0.52
2:C:2666:LEU:HD13	2:C:2966:VAL:HA	1.91	0.52
2:A:34:LYS:N	2:A:53:SER:OG	2.37	0.52
2:A:2678:PRO:HD3	2:A:2978:HIS:NE2	2.25	0.52
2:D:2603:ALA:C	2:D:2606:PRO:HD2	2.29	0.52
2:D:2605:MET:HG2	2:D:2606:PRO:HD3	1.91	0.52
2:D:3159:LEU:HD12	2:D:3241:MET:SD	2.50	0.52
2:B:412:GLU:HG3	2:B:488:LEU:HD11	1.92	0.52
2:B:1047:LYS:O	2:B:1051:ARG:HD3	2.10	0.52
2:B:2593:VAL:HG21	2:B:2640:LEU:HD22	1.92	0.52
2:C:891:GLU:HA	2:C:894:VAL:HG22	1.92	0.52
2:C:2553:TYR:HE1	2:C:2606:PRO:HG3	1.75	0.52
1:H:83:TYR:OH	2:D:1768:PHE:O	2.19	0.52
2:A:2605:MET:HG2	2:A:2606:PRO:HD3	1.91	0.52
1:E:22:THR:OG1	1:E:108:GLU:HG3	2.10	0.52
2:D:679:VAL:HG13	2:D:800:VAL:HG12	1.91	0.52
2:D:2591:ARG:HH22	2:D:2695:MET:HB2	1.74	0.52
2:D:2678:PRO:HD3	2:D:2978:HIS:NE2	2.25	0.52
2:B:1303:ARG:HA	2:B:1542:ALA:HA	1.91	0.52
2:B:4689:LYS:HG3	2:B:4690:LYS:H	1.75	0.52
2:C:2718:GLU:HA	2:C:2721:ILE:HD12	1.91	0.52
2:A:934:GLN:HG3	2:A:937:LEU:HD12	1.92	0.51
2:A:2252:GLU:HB2	2:A:3819:MET:SD	2.50	0.51
2:A:2627:TRP:HB2	2:A:2630:PHE:HB2	1.91	0.51
2:A:3025:ASP:O	2:A:3029:ILE:HD12	2.09	0.51
2:D:2627:TRP:HB2	2:D:2630:PHE:HB2	1.91	0.51
2:D:2935:GLU:HB3	2:D:2939:TYR:CE1	2.43	0.51
2:B:676:GLU:HB3	2:B:803:LEU:HB2	1.92	0.51
2:B:883:GLU:OE2	2:B:929:ARG:NH2	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1154:ARG:H	2:B:1182:LEU:HD22	1.75	0.51
2:B:2497:ARG:HH22	2:B:2877:LEU:HD13	1.74	0.51
2:B:3920:LEU:HD22	2:B:3935:LEU:HD21	1.92	0.51
2:B:4616:TYR:HE2	2:B:4632:ARG:HG2	1.75	0.51
2:C:883:GLU:OE2	2:C:929:ARG:NH2	2.42	0.51
2:C:4177:VAL:HG11	2:C:4880:VAL:HA	1.91	0.51
2:C:4689:LYS:HG3	2:C:4690:LYS:H	1.75	0.51
2:A:2250:ASN:HB3	2:A:2253:LEU:HB2	1.92	0.51
2:D:2252:GLU:HB2	2:D:3819:MET:SD	2.50	0.51
2:C:2732:TRP:O	2:C:2736:LYS:NZ	2.41	0.51
2:A:891:GLU:HA	2:A:894:VAL:HG22	1.92	0.51
2:A:2172:MET:O	2:A:2176:VAL:N	2.38	0.51
2:A:3159:LEU:HD12	2:A:3241:MET:SD	2.50	0.51
2:D:1788:LYS:HE3	2:D:1834:PHE:HA	1.93	0.51
2:B:271:ALA:HB2	2:B:488:LEU:HD22	1.91	0.51
2:B:2591:ARG:HH22	2:B:2695:MET:HB2	1.74	0.51
2:A:679:VAL:HG13	2:A:800:VAL:HG12	1.91	0.51
1:G:22:THR:OG1	1:G:108:GLU:HG3	2.10	0.51
2:D:2581:ARG:HG2	2:D:2630:PHE:CE1	2.46	0.51
2:D:2732:TRP:O	2:D:2736:LYS:NZ	2.41	0.51
2:D:4616:TYR:HE2	2:D:4632:ARG:HG2	1.75	0.51
2:B:2250:ASN:HB3	2:B:2253:LEU:HB2	1.92	0.51
2:B:4579:HIS:CE1	2:B:4742:HIS:CE1	2.98	0.51
2:C:2591:ARG:HH22	2:C:2695:MET:HB2	1.74	0.51
2:A:3327:LYS:HA	2:A:3330:ALA:HB2	1.91	0.51
2:D:412:GLU:HG3	2:D:488:LEU:HD11	1.92	0.51
2:D:877:HIS:O	2:D:1062:TYR:OH	2.15	0.51
2:D:1303:ARG:HA	2:D:1542:ALA:HA	1.91	0.51
2:D:2054:LYS:NZ	2:D:2056:SER:OG	2.31	0.51
2:D:3270:SER:HA	2:D:3273:MET:HG3	1.93	0.51
2:D:3324:GLU:OE2	2:D:3325:LYS:HG3	2.10	0.51
2:B:2718:GLU:HA	2:B:2721:ILE:HD12	1.91	0.51
2:C:3145:SER:HB3	2:C:3148:VAL:HG12	1.91	0.51
2:C:3284:ILE:O	2:C:3288:LEU:HG	2.10	0.51
2:C:3920:LEU:HD22	2:C:3935:LEU:HD21	1.92	0.51
2:C:4579:HIS:CE1	2:C:4742:HIS:CE1	2.98	0.51
2:A:887:GLU:O	2:A:976:TYR:OH	2.27	0.51
2:A:1788:LYS:HE3	2:A:1834:PHE:HA	1.93	0.51
2:A:2794:GLU:HG3	2:B:1498:GLN:HB2	1.91	0.51
2:A:3324:GLU:OE2	2:A:3325:LYS:HG3	2.10	0.51
2:D:878:LEU:HD23	2:D:940:LEU:HD22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1154:ARG:H	2:D:1182:LEU:HD22	1.75	0.51
2:D:2553:TYR:HE1	2:D:2606:PRO:HG3	1.75	0.51
2:D:4689:LYS:HG3	2:D:4690:LYS:H	1.75	0.51
2:D:4720:LEU:HD23	2:C:4294:LEU:HD21	1.92	0.51
2:B:808:HIS:CE1	2:B:832:LEU:HB3	2.46	0.51
2:B:3729:ALA:HA	2:B:3732:HIS:CD2	2.46	0.51
2:C:3215:MET:SD	2:C:3279:ASN:ND2	2.76	0.51
2:A:808:HIS:CE1	2:A:832:LEU:HB3	2.46	0.51
2:D:536:LEU:O	2:D:540:LEU:HG	2.11	0.51
2:D:2250:ASN:HB3	2:D:2253:LEU:HB2	1.92	0.51
2:D:3327:LYS:HA	2:D:3330:ALA:HB2	1.91	0.51
2:D:4267:GLN:HG3	2:D:4270:LYS:NZ	2.26	0.51
2:C:878:LEU:HD23	2:C:940:LEU:HD22	1.93	0.51
2:A:1154:ARG:H	2:A:1182:LEU:HD22	1.75	0.51
2:A:1184:ASP:OD2	2:A:1188:SER:OG	2.29	0.51
2:A:2849:HIS:CD2	2:A:2852:TRP:HE3	2.27	0.51
2:A:3977:ASP:HA	2:A:3980:VAL:HG12	1.92	0.51
2:A:4689:LYS:HG3	2:A:4690:LYS:H	1.76	0.51
2:D:808:HIS:CE1	2:D:832:LEU:HB3	2.46	0.51
2:D:1184:ASP:OD2	2:D:1188:SER:OG	2.29	0.51
2:D:2849:HIS:CD2	2:D:2852:TRP:HE3	2.27	0.51
2:C:676:GLU:HB3	2:C:803:LEU:HB2	1.92	0.51
2:C:1184:ASP:OD2	2:C:1188:SER:OG	2.29	0.51
2:C:2274:LEU:HD21	2:C:2329:GLU:HG2	1.93	0.51
2:C:3069:GLU:O	2:C:3072:MET:HB2	2.11	0.51
2:A:3270:SER:HA	2:A:3273:MET:HG3	1.93	0.51
2:A:4197:ILE:HG23	2:A:4923:MET:HE2	1.92	0.51
1:F:22:THR:OG1	1:F:108:GLU:HG3	2.10	0.51
2:D:3729:ALA:HA	2:D:3732:HIS:CD2	2.46	0.51
2:B:515:ALA:HB2	2:B:523:GLY:HA3	1.93	0.51
2:B:891:GLU:HA	2:B:894:VAL:HG22	1.92	0.51
2:B:3324:GLU:OE2	2:B:3325:LYS:HG3	2.10	0.51
2:C:2497:ARG:HH22	2:C:2877:LEU:HD13	1.74	0.51
2:C:2717:LEU:O	2:C:2721:ILE:HG13	2.11	0.51
2:C:3324:GLU:OE2	2:C:3325:LYS:HG3	2.10	0.51
2:A:536:LEU:O	2:A:540:LEU:HG	2.11	0.51
2:A:2824:ARG:NH2	2:B:1502:ASN:O	2.44	0.51
2:D:2119:LEU:HB2	2:D:2152:ASN:ND2	2.26	0.51
2:D:3920:LEU:HD22	2:D:3935:LEU:HD21	1.92	0.51
2:C:412:GLU:HG3	2:C:488:LEU:HD11	1.92	0.51
1:H:22:THR:OG1	1:H:108:GLU:HG3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2119:LEU:HB2	2:A:2152:ASN:ND2	2.27	0.50
2:A:2278:GLN:HA	2:A:2281:VAL:HG22	1.91	0.50
2:D:2274:LEU:HD21	2:D:2329:GLU:HG2	1.93	0.50
2:B:1079:SER:OG	2:B:1083:GLU:O	2.27	0.50
2:C:1788:LYS:HE3	2:C:1834:PHE:HA	1.93	0.50
2:C:3729:ALA:HA	2:C:3732:HIS:CD2	2.46	0.50
2:A:2581:ARG:HG2	2:A:2630:PHE:CE1	2.46	0.50
2:A:3250:TRP:HE1	2:A:3270:SER:HA	1.76	0.50
2:A:3264:CYS:SG	2:A:3265:CYS:N	2.84	0.50
2:D:249:SER:OG	2:D:250:GLY:N	2.44	0.50
2:C:2119:LEU:HB2	2:C:2152:ASN:ND2	2.27	0.50
2:A:515:ALA:HB2	2:A:523:GLY:HA3	1.93	0.50
2:A:2176:VAL:HG22	2:A:2220:TYR:CE2	2.47	0.50
2:A:3142:THR:O	2:A:3144:LYS:NZ	2.35	0.50
2:D:1016:TRP:CE3	2:D:1029:ASN:HB2	2.47	0.50
2:D:2496:LEU:HD13	2:D:2520:LEU:HD13	1.94	0.50
2:D:3250:TRP:HE1	2:D:3270:SER:HA	1.76	0.50
2:B:1184:ASP:OD2	2:B:1188:SER:OG	2.29	0.50
2:B:2119:LEU:HB2	2:B:2152:ASN:ND2	2.27	0.50
2:B:2432:LEU:HB3	2:B:2472:LEU:HD21	1.94	0.50
2:B:2830:ASN:HB2	2:C:1435:GLY:HA3	1.94	0.50
2:B:3977:ASP:HA	2:B:3980:VAL:HG12	1.93	0.50
2:C:515:ALA:HB2	2:C:523:GLY:HA3	1.93	0.50
2:C:1016:TRP:CE3	2:C:1029:ASN:HB2	2.47	0.50
2:C:2250:ASN:HB3	2:C:2253:LEU:HB2	1.92	0.50
2:C:2678:PRO:HD3	2:C:2978:HIS:NE2	2.25	0.50
2:C:3977:ASP:HA	2:C:3980:VAL:HG12	1.92	0.50
2:C:4267:GLN:HG3	2:C:4270:LYS:NZ	2.26	0.50
2:A:2456:MET:SD	2:A:2456:MET:N	2.76	0.50
2:A:3729:ALA:HA	2:A:3732:HIS:CD2	2.46	0.50
2:A:3958:LEU:HB2	2:A:3968:LEU:HD13	1.93	0.50
2:D:676:GLU:HB3	2:D:803:LEU:HB2	1.92	0.50
2:B:2176:VAL:HG22	2:B:2220:TYR:CE2	2.47	0.50
2:B:2456:MET:SD	2:B:2456:MET:N	2.76	0.50
2:C:249:SER:OG	2:C:250:GLY:N	2.44	0.50
2:A:676:GLU:HB3	2:A:803:LEU:HB2	1.92	0.50
2:A:695:VAL:O	2:A:727:PHE:N	2.44	0.50
2:D:703:TYR:HD2	2:D:858:THR:HA	1.77	0.50
2:D:2176:VAL:HG22	2:D:2220:TYR:CE2	2.47	0.50
2:D:2971:ILE:HG23	2:D:2975:PHE:CE2	2.47	0.50
2:D:3069:GLU:O	2:D:3072:MET:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:965:LYS:HA	2:B:977:LYS:HZ1	1.75	0.50
2:B:2717:LEU:O	2:B:2721:ILE:HG13	2.11	0.50
2:B:3270:SER:HA	2:B:3273:MET:HG3	1.93	0.50
2:B:4267:GLN:HG3	2:B:4270:LYS:NZ	2.26	0.50
2:C:448:PRO:HB2	2:C:452:VAL:HG23	1.94	0.50
2:C:2176:VAL:HG22	2:C:2220:TYR:CE2	2.47	0.50
2:C:4616:TYR:HE2	2:C:4632:ARG:HG2	1.75	0.50
2:A:899:GLU:HB2	2:A:970:TYR:HD1	1.76	0.50
2:A:965:LYS:HA	2:A:977:LYS:HZ1	1.75	0.50
2:A:4194:GLU:HG2	2:A:4645:TRP:HZ3	1.77	0.50
2:D:1144:ARG:HG2	2:D:1150:GLU:O	2.11	0.50
2:D:1435:GLY:HA3	2:C:2830:ASN:HB2	1.94	0.50
2:D:2541:HIS:HB3	2:D:2544:LEU:CD2	2.42	0.50
2:D:3292:GLU:HB2	2:D:3296:MET:HE2	1.93	0.50
2:B:1144:ARG:HG2	2:B:1150:GLU:O	2.11	0.50
2:B:2581:ARG:HG2	2:B:2630:PHE:CE1	2.46	0.50
2:B:2678:PRO:HD3	2:B:2978:HIS:NE2	2.25	0.50
2:B:3264:CYS:SG	2:B:3265:CYS:N	2.84	0.50
2:B:3319:PHE:O	2:B:3323:MET:N	2.39	0.50
2:B:3875:VAL:HG21	2:B:3940:LEU:HB2	1.93	0.50
2:B:4194:GLU:HG2	2:B:4645:TRP:HZ3	1.77	0.50
2:C:536:LEU:O	2:C:540:LEU:HG	2.11	0.50
2:A:1016:TRP:CE3	2:A:1029:ASN:HB2	2.47	0.50
2:A:3875:VAL:HG21	2:A:3940:LEU:HB2	1.93	0.50
2:D:448:PRO:HB2	2:D:452:VAL:HG23	1.94	0.50
2:D:2432:LEU:HB3	2:D:2472:LEU:HD21	1.94	0.50
2:D:2484:LEU:O	2:D:2487:LEU:HG	2.11	0.50
2:B:1016:TRP:CE3	2:B:1029:ASN:HB2	2.47	0.50
2:B:1788:LYS:HE3	2:B:1834:PHE:HA	1.93	0.50
2:C:935:MET:O	2:C:939:THR:OG1	2.17	0.50
2:C:2432:LEU:HB3	2:C:2472:LEU:HD21	1.94	0.50
2:A:2274:LEU:HD21	2:A:2329:GLU:HG2	1.93	0.50
2:A:2541:HIS:HB3	2:A:2544:LEU:CD2	2.42	0.50
2:D:891:GLU:HA	2:D:894:VAL:HG22	1.92	0.50
2:D:965:LYS:HA	2:D:977:LYS:HZ1	1.76	0.50
2:D:2157:GLN:O	2:D:3615:ARG:NH2	2.38	0.50
2:D:2717:LEU:O	2:D:2721:ILE:HG13	2.11	0.50
2:D:3977:ASP:HA	2:D:3980:VAL:HG12	1.93	0.50
2:D:4194:GLU:HG2	2:D:4645:TRP:HZ3	1.77	0.50
2:B:2971:ILE:HG23	2:B:2975:PHE:CE2	2.47	0.50
2:C:2541:HIS:HB3	2:C:2544:LEU:CD2	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2581:ARG:HG2	2:C:2630:PHE:CE1	2.46	0.50
2:C:2756:LEU:HD13	2:C:2758:LYS:HE3	1.94	0.50
2:C:3958:LEU:HB2	2:C:3968:LEU:HD13	1.93	0.50
2:C:4194:GLU:HG2	2:C:4645:TRP:HZ3	1.77	0.50
2:A:1144:ARG:HG2	2:A:1150:GLU:O	2.11	0.50
2:A:2496:LEU:HD13	2:A:2520:LEU:HD13	1.94	0.50
2:A:2717:LEU:O	2:A:2721:ILE:HG13	2.11	0.50
2:A:3069:GLU:O	2:A:3072:MET:HB2	2.11	0.50
2:D:1614:ARG:HD2	2:D:1614:ARG:O	2.12	0.50
2:D:2582:PRO:HG3	2:D:2617:CYS:SG	2.52	0.50
2:D:3958:LEU:HB2	2:D:3968:LEU:HD13	1.93	0.50
2:B:249:SER:OG	2:B:250:GLY:N	2.44	0.50
2:B:899:GLU:HB2	2:B:970:TYR:HD1	1.76	0.50
2:B:2484:LEU:O	2:B:2487:LEU:HG	2.11	0.50
2:C:891:GLU:HB3	2:C:978:PRO:HB3	1.94	0.50
2:C:908:ARG:NH2	4:C:5003:ATP:O1A	2.43	0.50
2:C:2681:MET:HE3	2:C:2919:LYS:HE2	1.94	0.50
2:A:75:VAL:O	2:A:79:GLN:HG2	2.12	0.49
2:A:878:LEU:HD23	2:A:940:LEU:HD22	1.93	0.49
2:A:1703:TYR:OH	2:A:1824:LEU:HB3	2.12	0.49
2:A:2432:LEU:HB3	2:A:2472:LEU:HD21	1.94	0.49
2:A:2484:LEU:O	2:A:2487:LEU:HG	2.11	0.49
2:A:2980:LEU:O	2:A:2984:SER:N	2.44	0.49
2:A:4860:ALA:HB2	2:D:4863:GLN:OE1	2.11	0.49
1:F:36:LYS:NZ	2:B:1681:ASP:OD2	2.32	0.49
2:D:3664:LEU:O	2:D:3668:ILE:HG13	2.11	0.49
2:B:703:TYR:HD2	2:B:858:THR:HA	1.77	0.49
2:B:1614:ARG:HD2	2:B:1614:ARG:O	2.12	0.49
2:B:1685:LEU:HD22	2:B:1706:LEU:HB2	1.94	0.49
2:B:2106:TYR:OH	2:B:2158:HIS:ND1	2.29	0.49
2:C:703:TYR:HD2	2:C:858:THR:HA	1.77	0.49
2:C:887:GLU:O	2:C:976:TYR:OH	2.27	0.49
2:C:1144:ARG:HG2	2:C:1150:GLU:O	2.11	0.49
2:C:3664:LEU:O	2:C:3668:ILE:HG13	2.11	0.49
2:A:76:ARG:NH1	2:D:3890:TRP:O	2.44	0.49
2:A:1990:GLU:HA	2:A:1993:ARG:HB2	1.94	0.49
2:B:448:PRO:HB2	2:B:452:VAL:HG23	1.94	0.49
2:B:536:LEU:O	2:B:540:LEU:HG	2.11	0.49
2:C:808:HIS:CE1	2:C:832:LEU:HB3	2.46	0.49
2:C:965:LYS:HA	2:C:977:LYS:HZ1	1.76	0.49
2:C:2484:LEU:O	2:C:2487:LEU:HG	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:908:ARG:NH2	4:A:5003:ATP:O1A	2.44	0.49
2:A:2937:HIS:HB2	2:A:3014:LEU:HD21	1.94	0.49
2:A:3664:LEU:O	2:A:3668:ILE:HG13	2.11	0.49
2:D:1703:TYR:OH	2:D:1824:LEU:HB3	2.12	0.49
2:D:3264:CYS:SG	2:D:3265:CYS:N	2.84	0.49
2:B:897:LYS:HA	2:B:902:TRP:HE3	1.78	0.49
2:B:898:ILE:HG23	2:B:969:ASN:O	2.13	0.49
2:B:931:TYR:O	2:B:935:MET:HG2	2.12	0.49
2:B:2895:PHE:O	2:B:2899:ASN:ND2	2.29	0.49
2:B:3958:LEU:HB2	2:B:3968:LEU:HD13	1.93	0.49
2:C:1614:ARG:O	2:C:1614:ARG:HD2	2.12	0.49
2:A:3145:SER:O	2:A:3149:GLU:HG2	2.13	0.49
2:D:898:ILE:HG23	2:D:969:ASN:O	2.13	0.49
2:D:1662:SER:OG	2:D:1708:ASP:OD2	2.21	0.49
2:D:1990:GLU:HA	2:D:1993:ARG:HB2	1.94	0.49
2:D:3025:ASP:O	2:D:3028:SER:OG	2.17	0.49
2:D:3145:SER:O	2:D:3149:GLU:HG2	2.13	0.49
2:B:878:LEU:HD23	2:B:940:LEU:HD22	1.93	0.49
2:B:1703:TYR:OH	2:B:1824:LEU:HB3	2.12	0.49
2:B:2496:LEU:HD13	2:B:2520:LEU:HD13	1.94	0.49
2:B:2980:LEU:O	2:B:2984:SER:N	2.44	0.49
2:C:768:PHE:O	2:C:775:VAL:HG12	2.13	0.49
2:C:2259:GLU:O	2:C:2263:GLU:HG2	2.13	0.49
2:C:2980:LEU:O	2:C:2984:SER:N	2.44	0.49
2:C:3264:CYS:SG	2:C:3265:CYS:N	2.84	0.49
2:C:3270:SER:HA	2:C:3273:MET:HG3	1.93	0.49
2:A:891:GLU:HB3	2:A:978:PRO:HB3	1.94	0.49
2:A:897:LYS:HA	2:A:902:TRP:HE3	1.78	0.49
2:A:898:ILE:HG23	2:A:969:ASN:O	2.13	0.49
2:A:3888:PHE:HD2	2:A:3906:PHE:CE1	2.31	0.49
2:D:75:VAL:O	2:D:79:GLN:HG2	2.12	0.49
2:D:897:LYS:HA	2:D:902:TRP:HE3	1.78	0.49
2:D:3216:GLU:HA	2:D:3219:VAL:HG22	1.94	0.49
2:B:2582:PRO:HG3	2:B:2617:CYS:SG	2.52	0.49
2:C:34:LYS:N	2:C:53:SER:OG	2.37	0.49
2:C:899:GLU:HB2	2:C:970:TYR:HD1	1.77	0.49
2:C:3250:TRP:HE1	2:C:3270:SER:HA	1.76	0.49
2:A:703:TYR:HD2	2:A:858:THR:HA	1.77	0.49
2:A:1006:VAL:HG22	2:A:1009:ARG:HH12	1.78	0.49
2:A:2717:LEU:HD21	2:A:2789:ILE:HG21	1.94	0.49
2:D:515:ALA:HB2	2:D:523:GLY:HA3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2591:ARG:HH12	2:D:2695:MET:HA	1.78	0.49
2:B:3213:LYS:HA	2:B:3216:GLU:HG3	1.94	0.49
2:B:3250:TRP:HE1	2:B:3270:SER:HA	1.76	0.49
2:B:3664:LEU:O	2:B:3668:ILE:HG13	2.11	0.49
2:C:897:LYS:HA	2:C:902:TRP:HE3	1.78	0.49
2:C:898:ILE:HG23	2:C:969:ASN:O	2.13	0.49
2:C:3875:VAL:HG21	2:C:3940:LEU:HB2	1.93	0.49
2:A:448:PRO:HB2	2:A:452:VAL:HG23	1.94	0.49
2:A:555:LEU:HD11	2:A:578:VAL:HG11	1.94	0.49
2:A:935:MET:O	2:A:939:THR:OG1	2.17	0.49
2:A:2285:TYR:HD2	2:A:2384:MET:HE1	1.78	0.49
2:A:2756:LEU:HD13	2:A:2758:LYS:HE3	1.94	0.49
2:A:2971:ILE:HG23	2:A:2975:PHE:CE2	2.47	0.49
2:D:1428:TYR:OH	2:D:1444:GLY:O	2.31	0.49
2:D:3888:PHE:HD2	2:D:3906:PHE:CE1	2.31	0.49
2:B:2274:LEU:HD21	2:B:2329:GLU:HG2	1.93	0.49
2:C:876:PRO:HA	2:C:879:GLU:CG	2.42	0.49
2:C:931:TYR:O	2:C:935:MET:HG2	2.12	0.49
2:C:2496:LEU:HD13	2:C:2520:LEU:HD13	1.94	0.49
2:A:2582:PRO:HG3	2:A:2617:CYS:SG	2.52	0.49
2:A:2591:ARG:HH12	2:A:2695:MET:HA	1.78	0.49
2:D:899:GLU:HB2	2:D:970:TYR:HD1	1.77	0.49
2:D:2259:GLU:O	2:D:2263:GLU:HG2	2.13	0.49
2:D:2756:LEU:HD13	2:D:2758:LYS:HE3	1.94	0.49
2:D:3213:LYS:HA	2:D:3216:GLU:HG3	1.95	0.49
2:B:1990:GLU:HA	2:B:1993:ARG:HB2	1.94	0.49
2:C:1644:LEU:HD23	2:C:1651:LEU:HA	1.95	0.49
2:C:2591:ARG:HH12	2:C:2695:MET:HA	1.78	0.49
2:C:2937:HIS:HB2	2:C:3014:LEU:HD21	1.94	0.49
2:C:2971:ILE:HG23	2:C:2975:PHE:CE2	2.47	0.49
2:A:249:SER:OG	2:A:250:GLY:N	2.44	0.49
2:A:1614:ARG:O	2:A:1614:ARG:HD2	2.12	0.49
2:A:3179:ASN:O	2:A:3185:ASN:ND2	2.46	0.49
2:D:3009:CYS:O	2:D:3013:VAL:HG23	2.13	0.49
2:D:3875:VAL:HG21	2:D:3940:LEU:HB2	1.93	0.49
2:B:75:VAL:O	2:B:79:GLN:HG2	2.12	0.49
2:B:768:PHE:O	2:B:775:VAL:HG12	2.13	0.49
2:B:2756:LEU:HD13	2:B:2758:LYS:HE3	1.94	0.49
2:B:3069:GLU:O	2:B:3072:MET:HB2	2.11	0.49
2:C:75:VAL:O	2:C:79:GLN:HG2	2.12	0.49
2:C:1703:TYR:OH	2:C:1824:LEU:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1990:GLU:HA	2:C:1993:ARG:HB2	1.94	0.49
2:C:4942:LYS:O	2:C:4946:GLU:HG3	2.13	0.49
2:A:902:TRP:HA	2:A:913:ARG:HB3	1.95	0.49
2:A:4267:GLN:HG3	2:A:4270:LYS:NZ	2.26	0.49
1:E:78:THR:HG22	1:E:81:VAL:HG22	1.95	0.49
2:D:1644:LEU:HD23	2:D:1651:LEU:HA	1.95	0.49
2:D:2937:HIS:HB2	2:D:3014:LEU:HD21	1.94	0.49
2:B:902:TRP:HA	2:B:913:ARG:HB3	1.95	0.49
2:B:1006:VAL:HG22	2:B:1009:ARG:HH12	1.78	0.49
2:C:816:PRO:HB2	2:C:819:TYR:CD1	2.48	0.49
2:C:3216:GLU:HA	2:C:3219:VAL:HG22	1.94	0.49
2:C:4203:ALA:HA	2:C:4206:ILE:HG12	1.95	0.49
1:H:78:THR:HG22	1:H:81:VAL:HG22	1.95	0.48
2:A:768:PHE:O	2:A:775:VAL:HG12	2.13	0.48
2:A:1644:LEU:HD23	2:A:1651:LEU:HA	1.95	0.48
2:A:4045:LYS:HE3	2:A:4078:LEU:HD22	1.96	0.48
1:G:78:THR:HG22	1:G:81:VAL:HG22	1.95	0.48
2:B:1239:PHE:O	2:B:1807:ARG:NH1	2.45	0.48
2:B:3216:GLU:HA	2:B:3219:VAL:HG22	1.94	0.48
2:B:3888:PHE:HD2	2:B:3906:PHE:CE1	2.31	0.48
2:C:695:VAL:O	2:C:727:PHE:N	2.44	0.48
2:C:3009:CYS:O	2:C:3013:VAL:HG23	2.13	0.48
2:C:3145:SER:O	2:C:3149:GLU:HG2	2.13	0.48
2:A:2106:TYR:OH	2:A:2158:HIS:ND1	2.29	0.48
2:A:4042:VAL:HG12	2:A:4077:THR:HB	1.95	0.48
2:A:4203:ALA:HA	2:A:4206:ILE:HG12	1.95	0.48
2:A:4690:LYS:HG3	2:A:4692:SER:H	1.78	0.48
1:F:78:THR:HG22	1:F:81:VAL:HG22	1.95	0.48
2:D:931:TYR:O	2:D:935:MET:HG2	2.12	0.48
2:D:1685:LEU:HD22	2:D:1706:LEU:HB2	1.94	0.48
2:D:4042:VAL:HG12	2:D:4077:THR:HB	1.95	0.48
2:D:4579:HIS:HE1	2:D:4742:HIS:ND1	2.12	0.48
2:B:1743:ASN:HB3	2:B:1745:LYS:HD3	1.96	0.48
2:B:2259:GLU:O	2:B:2263:GLU:HG2	2.13	0.48
2:B:2717:LEU:HD21	2:B:2789:ILE:HG21	1.94	0.48
2:B:3145:SER:O	2:B:3149:GLU:HG2	2.13	0.48
2:B:3179:ASN:O	2:B:3185:ASN:ND2	2.46	0.48
2:B:4690:LYS:HG3	2:B:4692:SER:H	1.78	0.48
2:B:4942:LYS:O	2:B:4946:GLU:HG3	2.13	0.48
2:C:2582:PRO:HG3	2:C:2617:CYS:SG	2.52	0.48
2:C:3179:ASN:O	2:C:3185:ASN:ND2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3213:LYS:HA	2:C:3216:GLU:HG3	1.95	0.48
2:A:931:TYR:O	2:A:935:MET:HG2	2.12	0.48
2:A:996:VAL:HG12	2:A:1051:ARG:HH11	1.78	0.48
2:A:3216:GLU:HA	2:A:3219:VAL:HG22	1.94	0.48
2:A:4044:SER:HA	2:A:4077:THR:HG22	1.95	0.48
2:D:768:PHE:O	2:D:775:VAL:HG12	2.13	0.48
2:D:902:TRP:HA	2:D:913:ARG:HB3	1.95	0.48
2:D:3179:ASN:O	2:D:3185:ASN:ND2	2.46	0.48
2:D:4569:GLU:HB3	2:D:4570:PRO:HD3	1.95	0.48
2:B:876:PRO:HA	2:B:879:GLU:CG	2.42	0.48
2:B:966:LEU:HB3	2:B:971:GLN:HB2	1.95	0.48
2:B:4044:SER:HA	2:B:4077:THR:HG22	1.96	0.48
2:B:4754:ARG:O	2:B:4758:SER:OG	2.27	0.48
2:C:1428:TYR:OH	2:C:1444:GLY:O	2.31	0.48
2:C:3888:PHE:HD2	2:C:3906:PHE:CE1	2.31	0.48
2:A:2259:GLU:O	2:A:2263:GLU:HG2	2.13	0.48
2:A:2905:ARG:NH2	2:A:2907:PHE:O	2.47	0.48
2:D:3166:PHE:CE2	2:D:3168:VAL:HB	2.49	0.48
2:B:227:TYR:CG	2:B:352:SER:HB3	2.49	0.48
2:B:695:VAL:O	2:B:727:PHE:N	2.44	0.48
2:B:891:GLU:HB3	2:B:978:PRO:HB3	1.94	0.48
2:B:1446:ILE:HG12	2:B:1542:ALA:HB2	1.95	0.48
2:B:1644:LEU:HD23	2:B:1651:LEU:HA	1.95	0.48
2:B:2473:ASP:OD2	2:B:2530:ARG:NH2	2.47	0.48
2:B:4569:GLU:HB3	2:B:4570:PRO:HD3	1.95	0.48
2:C:555:LEU:HD11	2:C:578:VAL:HG11	1.94	0.48
2:C:2905:ARG:NH2	2:C:2907:PHE:O	2.47	0.48
2:C:3840:PHE:HE1	2:C:3874:THR:HG23	1.79	0.48
2:A:1046:ASN:OD1	2:A:1047:LYS:N	2.47	0.48
2:A:3166:PHE:CE2	2:A:3168:VAL:HB	2.49	0.48
2:D:2355:GLU:OE1	2:D:2355:GLU:N	2.47	0.48
2:D:2607:LEU:HD22	2:D:2664:LEU:HB3	1.95	0.48
2:D:2657:TYR:HA	2:D:2662:PHE:CZ	2.49	0.48
2:B:908:ARG:NH2	4:B:5003:ATP:O1A	2.43	0.48
2:B:1428:TYR:OH	2:B:1444:GLY:O	2.31	0.48
2:B:2591:ARG:HH12	2:B:2695:MET:HA	1.78	0.48
2:B:3320:LEU:O	2:B:3323:MET:HB2	2.13	0.48
2:B:3890:TRP:O	2:C:76:ARG:NH1	2.45	0.48
2:B:4579:HIS:HE1	2:B:4742:HIS:ND1	2.12	0.48
2:C:915:HIS:HD1	2:C:918:LEU:HD13	1.78	0.48
2:C:996:VAL:HG12	2:C:1051:ARG:HH11	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:227:TYR:CG	2:A:352:SER:HB3	2.49	0.48
2:A:1428:TYR:OH	2:A:1444:GLY:O	2.31	0.48
2:A:2355:GLU:OE1	2:A:2355:GLU:N	2.47	0.48
2:A:4569:GLU:HB3	2:A:4570:PRO:HD3	1.96	0.48
2:D:1006:VAL:HG22	2:D:1009:ARG:HH12	1.78	0.48
2:D:1743:ASN:HB3	2:D:1745:LYS:HD3	1.96	0.48
2:D:3012:GLY:O	2:D:3016:ARG:HG3	2.14	0.48
2:D:3184:TYR:HE2	2:D:3201:VAL:HA	1.78	0.48
2:D:4851:PHE:CD2	2:C:4822:ARG:HG2	2.48	0.48
2:B:2607:LEU:HD22	2:B:2664:LEU:HB3	1.95	0.48
2:B:4197:ILE:HG23	2:B:4923:MET:HE2	1.95	0.48
2:C:1685:LEU:HD22	2:C:1706:LEU:HB2	1.94	0.48
2:C:1743:ASN:HB3	2:C:1745:LYS:HD3	1.96	0.48
2:C:2717:LEU:HD21	2:C:2789:ILE:HG21	1.94	0.48
2:C:3012:GLY:O	2:C:3016:ARG:HG3	2.14	0.48
2:C:3166:PHE:CE2	2:C:3168:VAL:HB	2.49	0.48
2:A:966:LEU:HB3	2:A:971:GLN:HB2	1.95	0.48
2:A:2895:PHE:O	2:A:2899:ASN:ND2	2.29	0.48
2:A:3319:PHE:O	2:A:3323:MET:N	2.39	0.48
2:A:3320:LEU:O	2:A:3323:MET:HB2	2.14	0.48
1:G:36:LYS:NZ	2:C:1681:ASP:OD2	2.36	0.48
2:D:2057:THR:HG22	2:D:2059:GLN:H	1.78	0.48
2:B:555:LEU:HD11	2:B:578:VAL:HG11	1.94	0.48
2:B:915:HIS:HD1	2:B:918:LEU:HD13	1.78	0.48
2:B:936:SER:O	2:B:940:LEU:HD12	2.14	0.48
2:B:2157:GLN:O	2:B:3615:ARG:NH2	2.38	0.48
2:B:2937:HIS:HB2	2:B:3014:LEU:HD21	1.94	0.48
2:C:1662:SER:OG	2:C:1708:ASP:OD2	2.22	0.48
2:C:3184:TYR:HE2	2:C:3201:VAL:HA	1.78	0.48
2:A:647:ARG:HH12	1:E:36:LYS:HB2	1.79	0.48
2:A:3906:PHE:HD2	2:A:3967:LEU:HD21	1.79	0.48
2:D:891:GLU:HB3	2:D:978:PRO:HB3	1.94	0.48
2:D:4942:LYS:O	2:D:4946:GLU:HG3	2.13	0.48
2:B:2057:THR:HG22	2:B:2059:GLN:H	1.78	0.48
2:B:3012:GLY:O	2:B:3016:ARG:HG3	2.14	0.48
2:B:3166:PHE:CE2	2:B:3168:VAL:HB	2.49	0.48
2:C:966:LEU:HB3	2:C:971:GLN:HB2	1.95	0.48
2:C:1006:VAL:HG22	2:C:1009:ARG:HH12	1.78	0.48
2:C:2736:LYS:HG3	2:C:2741:TRP:NE1	2.29	0.48
2:C:3290:ILE:O	2:C:3292:GLU:N	2.47	0.48
2:A:11:ILE:HG12	2:A:176:ARG:HH11	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:162:ILE:HD12	2:A:175:VAL:HG21	1.96	0.48
2:A:1446:ILE:HG12	2:A:1542:ALA:HB2	1.95	0.48
2:A:2681:MET:HE3	2:A:2919:LYS:HE2	1.96	0.48
2:A:2824:ARG:HH22	2:B:1503:ASN:CG	2.16	0.48
2:A:3009:CYS:O	2:A:3013:VAL:HG23	2.13	0.48
2:A:3213:LYS:HA	2:A:3216:GLU:HG3	1.95	0.48
2:A:4271:VAL:HG23	2:A:4278:ASP:OD1	2.14	0.48
2:D:1046:ASN:OD1	2:D:1047:LYS:N	2.47	0.48
2:D:2717:LEU:HD21	2:D:2789:ILE:HG21	1.95	0.48
2:D:2905:ARG:NH2	2:D:2907:PHE:O	2.47	0.48
2:D:4609:LYS:HD2	2:D:4615:LEU:HD22	1.96	0.48
2:B:816:PRO:HB2	2:B:819:TYR:CD1	2.48	0.48
2:B:2657:TYR:HA	2:B:2662:PHE:CZ	2.49	0.48
2:B:3290:ILE:O	2:B:3292:GLU:N	2.47	0.48
2:C:162:ILE:HD12	2:C:175:VAL:HG21	1.96	0.48
2:C:936:SER:O	2:C:940:LEU:HD12	2.14	0.48
2:C:4569:GLU:HB3	2:C:4570:PRO:HD3	1.95	0.48
2:A:490:GLN:HG2	2:A:495:ILE:HG13	1.96	0.48
2:A:1421:MET:HE1	2:A:1576:LYS:HB3	1.94	0.48
2:A:1685:LEU:HD22	2:A:1706:LEU:HB2	1.94	0.48
2:A:2854:LYS:HG2	2:A:2858:MET:CE	2.44	0.48
2:D:769:ARG:HG2	2:D:774:PRO:HA	1.96	0.48
2:D:3840:PHE:HE1	2:D:3874:THR:HG23	1.78	0.48
2:D:4203:ALA:HA	2:D:4206:ILE:HG12	1.95	0.48
2:B:996:VAL:HG12	2:B:1051:ARG:HH11	1.78	0.48
2:B:1662:SER:OG	2:B:1708:ASP:OD2	2.22	0.48
2:B:2355:GLU:N	2:B:2355:GLU:OE1	2.47	0.48
2:B:2854:LYS:HG2	2:B:2858:MET:CE	2.44	0.48
2:B:2905:ARG:NH2	2:B:2907:PHE:O	2.47	0.48
2:B:4271:VAL:HG23	2:B:4278:ASP:OD1	2.14	0.48
2:C:2379:ASP:OD1	2:C:2380:ASP:N	2.47	0.48
2:C:2984:SER:OG	2:C:2994:GLY:O	2.28	0.48
2:C:3320:LEU:O	2:C:3323:MET:HB2	2.14	0.48
2:A:769:ARG:HG2	2:A:774:PRO:HA	1.96	0.47
2:A:2468:MET:O	2:A:2472:LEU:HD23	2.14	0.47
2:A:2607:LEU:HD22	2:A:2664:LEU:HB3	1.95	0.47
2:A:3012:GLY:O	2:A:3016:ARG:HG3	2.14	0.47
2:A:3184:TYR:HE2	2:A:3201:VAL:HA	1.78	0.47
2:D:28:ILE:HG22	2:D:29:HIS:CD2	2.49	0.47
2:D:816:PRO:HB2	2:D:819:TYR:CD1	2.48	0.47
2:D:966:LEU:HB3	2:D:971:GLN:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:966:LEU:HD12	2:B:978:PRO:HD2	1.96	0.47
2:B:1046:ASN:OD1	2:B:1047:LYS:N	2.47	0.47
2:B:2541:HIS:HB3	2:B:2544:LEU:CD2	2.42	0.47
2:B:4203:ALA:HA	2:B:4206:ILE:HG12	1.95	0.47
2:B:4819:VAL:HG12	2:B:4830:GLU:HG3	1.96	0.47
2:C:1046:ASN:OD1	2:C:1047:LYS:N	2.47	0.47
2:C:1937:GLN:NE2	2:C:3608:LEU:O	2.46	0.47
2:C:2607:LEU:HD22	2:C:2664:LEU:HB3	1.95	0.47
2:C:3906:PHE:HD2	2:C:3967:LEU:HD21	1.79	0.47
2:C:4609:LYS:HD2	2:C:4615:LEU:HD22	1.96	0.47
2:A:28:ILE:HG22	2:A:29:HIS:CD2	2.49	0.47
2:A:661:LEU:O	2:A:788:PHE:N	2.47	0.47
2:A:966:LEU:HD12	2:A:978:PRO:HD2	1.97	0.47
2:A:1427:TYR:HB2	2:A:1563:VAL:HG11	1.96	0.47
2:A:1720:MET:SD	2:A:2127:ARG:HB3	2.55	0.47
2:A:1743:ASN:HB3	2:A:1745:LYS:HD3	1.96	0.47
2:A:3213:LYS:O	2:A:3216:GLU:HG3	2.15	0.47
2:D:2980:LEU:O	2:D:2984:SER:N	2.44	0.47
2:D:4044:SER:HA	2:D:4077:THR:HG22	1.96	0.47
2:B:2259:GLU:OE2	2:B:3806:ASN:ND2	2.47	0.47
2:B:2736:LYS:HG3	2:B:2741:TRP:NE1	2.29	0.47
2:C:902:TRP:HA	2:C:913:ARG:HB3	1.95	0.47
2:C:1041:ARG:HA	2:C:1044:LYS:NZ	2.29	0.47
2:C:1446:ILE:HG12	2:C:1542:ALA:HB2	1.95	0.47
2:C:3712:LYS:O	2:C:3717:LYS:NZ	2.46	0.47
2:C:4045:LYS:HE3	2:C:4078:LEU:HD22	1.96	0.47
2:A:307:SER:HB3	2:A:327:THR:HG22	1.96	0.47
2:A:816:PRO:HB2	2:A:819:TYR:CD1	2.48	0.47
2:A:936:SER:O	2:A:940:LEU:HD12	2.14	0.47
2:A:1937:GLN:NE2	2:A:3608:LEU:O	2.46	0.47
2:A:2473:ASP:OD2	2:A:2530:ARG:NH2	2.47	0.47
2:D:555:LEU:HD11	2:D:578:VAL:HG11	1.94	0.47
2:D:936:SER:O	2:D:940:LEU:HD12	2.14	0.47
2:D:2259:GLU:OE2	2:D:3806:ASN:ND2	2.47	0.47
2:D:2854:LYS:HG2	2:D:2858:MET:CE	2.44	0.47
2:D:4045:LYS:HE3	2:D:4078:LEU:HD22	1.95	0.47
2:B:1421:MET:HE2	2:B:1576:LYS:HD2	1.95	0.47
2:B:3009:CYS:O	2:B:3013:VAL:HG23	2.13	0.47
2:B:3184:TYR:HE2	2:B:3201:VAL:HA	1.78	0.47
2:B:3840:PHE:HE1	2:B:3874:THR:HG23	1.78	0.47
2:C:692:HIS:HE1	2:C:717:GLY:HA3	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2057:THR:HG22	2:C:2059:GLN:H	1.78	0.47
2:C:2355:GLU:OE1	2:C:2355:GLU:N	2.47	0.47
2:C:2468:MET:O	2:C:2472:LEU:HD23	2.14	0.47
2:C:3650:GLU:HB2	2:C:3651:PRO:HD3	1.96	0.47
2:A:2259:GLU:OE2	2:A:3806:ASN:ND2	2.47	0.47
2:A:2830:ASN:OD1	2:B:1551:ASN:HB2	2.13	0.47
2:D:34:LYS:N	2:D:53:SER:OG	2.37	0.47
2:D:162:ILE:HD12	2:D:175:VAL:HG21	1.96	0.47
2:D:227:TYR:CG	2:D:352:SER:HB3	2.49	0.47
2:D:490:GLN:HG2	2:D:495:ILE:HG13	1.96	0.47
2:D:2468:MET:O	2:D:2472:LEU:HD23	2.14	0.47
2:D:2478:ILE:HG21	2:D:2484:LEU:HD13	1.96	0.47
2:D:2681:MET:HE3	2:D:2919:LYS:HE2	1.96	0.47
2:D:3290:ILE:O	2:D:3292:GLU:N	2.47	0.47
2:D:4048:PHE:HZ	2:D:4080:TYR:HB3	1.80	0.47
2:B:2859:GLU:O	2:B:2862:SER:OG	2.27	0.47
2:C:490:GLN:HG2	2:C:495:ILE:HG13	1.96	0.47
2:C:661:LEU:O	2:C:788:PHE:N	2.47	0.47
2:C:2854:LYS:HG2	2:C:2858:MET:CE	2.44	0.47
2:C:3213:LYS:O	2:C:3216:GLU:HG3	2.14	0.47
2:C:4044:SER:HA	2:C:4077:THR:HG22	1.96	0.47
2:C:4690:LYS:HG3	2:C:4692:SER:H	1.78	0.47
2:A:877:HIS:HA	2:A:880:ARG:NH1	2.30	0.47
2:A:915:HIS:HD1	2:A:918:LEU:HD13	1.78	0.47
2:A:1041:ARG:HA	2:A:1044:LYS:NZ	2.29	0.47
2:A:2492:PHE:O	2:A:2496:LEU:N	2.45	0.47
2:A:2657:TYR:HA	2:A:2662:PHE:CZ	2.49	0.47
2:A:4259:LEU:HD21	2:B:4701:ILE:HD13	1.96	0.47
2:A:4819:VAL:HG12	2:A:4830:GLU:HG3	1.96	0.47
2:D:307:SER:HB3	2:D:327:THR:HG22	1.96	0.47
2:D:3712:LYS:O	2:D:3717:LYS:NZ	2.46	0.47
2:B:3072:MET:HE3	2:B:3072:MET:HB3	1.70	0.47
2:B:3213:LYS:O	2:B:3216:GLU:HG3	2.15	0.47
2:C:4197:ILE:HG23	2:C:4923:MET:HE2	1.95	0.47
2:A:2179:LEU:O	2:A:2183:GLU:CB	2.60	0.47
2:A:2872:VAL:HG23	2:A:2877:LEU:HD22	1.96	0.47
2:A:3013:VAL:HA	2:A:3016:ARG:HD3	1.97	0.47
2:D:11:ILE:HG12	2:D:176:ARG:HH11	1.79	0.47
2:D:842:GLN:HB2	2:D:1603:PHE:HB2	1.97	0.47
2:D:1446:ILE:HG12	2:D:1542:ALA:HB2	1.95	0.47
2:B:11:ILE:HG12	2:B:176:ARG:HH11	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:ILE:HG22	2:B:29:HIS:CD2	2.49	0.47
2:B:2172:MET:O	2:B:2176:VAL:N	2.38	0.47
2:B:2379:ASP:OD1	2:B:2380:ASP:N	2.47	0.47
2:B:2635:GLU:HA	2:B:2638:LEU:HB2	1.96	0.47
2:B:3042:ALA:HB1	2:B:3121:LEU:HB2	1.97	0.47
2:B:4045:LYS:HE3	2:B:4078:LEU:HD22	1.95	0.47
2:C:227:TYR:CG	2:C:352:SER:HB3	2.49	0.47
2:C:4789:PHE:HE1	2:C:4839:TYR:HB3	1.80	0.47
2:A:1239:PHE:O	2:A:1807:ARG:NH1	2.45	0.47
2:A:2478:ILE:HG21	2:A:2484:LEU:HD13	1.96	0.47
2:A:3042:ALA:HB1	2:A:3121:LEU:HB2	1.96	0.47
2:A:3840:PHE:HE1	2:A:3874:THR:HG23	1.79	0.47
2:A:4609:LYS:HD2	2:A:4615:LEU:HD22	1.96	0.47
2:A:4942:LYS:O	2:A:4946:GLU:HG3	2.13	0.47
2:D:877:HIS:HA	2:D:880:ARG:NH1	2.30	0.47
2:D:915:HIS:HD1	2:D:918:LEU:HD13	1.78	0.47
2:D:1720:MET:SD	2:D:2127:ARG:HB3	2.55	0.47
2:D:1968:PRO:O	2:D:1972:GLN:HG3	2.15	0.47
2:D:2456:MET:SD	2:D:2456:MET:N	2.76	0.47
2:D:2984:SER:HA	2:D:2989:PRO:HB2	1.97	0.47
2:D:4690:LYS:HG3	2:D:4692:SER:H	1.78	0.47
2:D:4789:PHE:HE1	2:D:4839:TYR:HB3	1.80	0.47
2:B:162:ILE:HD12	2:B:175:VAL:HG21	1.96	0.47
2:B:490:GLN:HG2	2:B:495:ILE:HG13	1.96	0.47
2:B:692:HIS:HE1	2:B:717:GLY:HA3	1.80	0.47
2:B:713:TRP:CE2	2:B:1600:PRO:HD3	2.50	0.47
2:B:877:HIS:HA	2:B:880:ARG:NH1	2.30	0.47
2:B:2331:PHE:HD1	2:B:2395:LEU:HD21	1.80	0.47
2:B:2468:MET:O	2:B:2472:LEU:HD23	2.14	0.47
2:B:3650:GLU:HB2	2:B:3651:PRO:HD3	1.96	0.47
2:B:4774:LEU:O	2:B:4778:VAL:HG23	2.15	0.47
2:C:713:TRP:CE2	2:C:1600:PRO:HD3	2.50	0.47
2:C:2259:GLU:OE2	2:C:3806:ASN:ND2	2.47	0.47
2:C:2473:ASP:OD2	2:C:2530:ARG:NH2	2.47	0.47
2:C:2657:TYR:HA	2:C:2662:PHE:CZ	2.49	0.47
2:C:2664:LEU:O	2:C:2667:PRO:HD2	2.15	0.47
2:C:4271:VAL:HG23	2:C:4278:ASP:OD1	2.14	0.47
2:C:4819:VAL:HG12	2:C:4830:GLU:HG3	1.96	0.47
1:H:26:HIS:NE2	1:H:41:ARG:HG2	2.30	0.47
2:A:2057:THR:HG22	2:A:2059:GLN:H	1.78	0.47
2:A:3143:SER:O	2:A:3152:ARG:NH1	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:ILE:HG12	2:D:176:ARG:HD2	1.97	0.47
2:D:962:LYS:HD2	2:D:982:ASP:HB2	1.97	0.47
2:D:1498:GLN:HB2	2:C:2794:GLU:HG3	1.96	0.47
2:D:4271:VAL:HG23	2:D:4278:ASP:OD1	2.14	0.47
2:D:4512:ALA:O	2:D:4516:ILE:HG13	2.15	0.47
2:B:962:LYS:HD2	2:B:982:ASP:HB2	1.97	0.47
2:B:1041:ARG:HA	2:B:1044:LYS:NZ	2.29	0.47
2:B:4267:GLN:HG3	2:B:4270:LYS:HZ3	1.80	0.47
2:C:28:ILE:HG22	2:C:29:HIS:CD2	2.49	0.47
2:C:1427:TYR:HB2	2:C:1563:VAL:HG11	1.96	0.47
2:A:2331:PHE:HD1	2:A:2395:LEU:HD21	1.80	0.47
1:F:26:HIS:NE2	1:F:41:ARG:HG2	2.30	0.47
2:D:1552:VAL:HG12	2:D:1553:PHE:HD2	1.80	0.47
2:D:2635:GLU:HA	2:D:2638:LEU:HB2	1.96	0.47
2:D:2664:LEU:O	2:D:2667:PRO:HD2	2.15	0.47
2:D:2872:VAL:HG23	2:D:2877:LEU:HD22	1.96	0.47
2:D:3320:LEU:O	2:D:3323:MET:HB2	2.14	0.47
2:B:1500:ARG:HG2	2:B:1505:LEU:HG	1.97	0.47
2:B:1720:MET:SD	2:B:2127:ARG:HB3	2.55	0.47
2:B:2478:ILE:HG21	2:B:2484:LEU:HD13	1.96	0.47
2:C:1500:ARG:HG2	2:C:1505:LEU:HG	1.97	0.47
2:C:2925:PHE:HZ	2:C:2970:LEU:HD13	1.80	0.47
2:C:4512:ALA:O	2:C:4516:ILE:HG13	2.15	0.47
2:A:2482:ASP:OD1	2:A:2483:PHE:N	2.48	0.47
2:A:2635:GLU:HA	2:A:2638:LEU:HB2	1.96	0.47
2:A:3712:LYS:O	2:A:3717:LYS:NZ	2.46	0.47
2:D:713:TRP:CE2	2:D:1600:PRO:HD3	2.50	0.47
2:D:996:VAL:HG12	2:D:1051:ARG:HH11	1.78	0.47
2:D:2473:ASP:OD2	2:D:2530:ARG:NH2	2.47	0.47
2:D:3100:ALA:O	2:D:3104:MET:HG3	2.15	0.47
2:B:4512:ALA:O	2:B:4516:ILE:HG13	2.15	0.47
2:C:11:ILE:HG12	2:C:176:ARG:HH11	1.79	0.47
2:C:1239:PHE:O	2:C:1807:ARG:NH1	2.45	0.47
2:C:3100:ALA:O	2:C:3104:MET:HG3	2.15	0.47
2:C:3155:LEU:O	2:C:3159:LEU:HD23	2.15	0.47
2:A:1154:ARG:NH2	2:A:1180:GLU:OE2	2.48	0.46
2:A:1552:VAL:HG12	2:A:1553:PHE:HD2	1.80	0.46
2:A:4774:LEU:O	2:A:4778:VAL:HG23	2.15	0.46
2:D:222:GLU:HB3	2:D:349:MET:HG3	1.97	0.46
2:D:661:LEU:O	2:D:788:PHE:N	2.47	0.46
2:D:908:ARG:NH2	4:D:5003:ATP:O1A	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:842:GLN:HB2	2:B:1603:PHE:HB2	1.97	0.46
2:B:2884:LYS:HA	2:B:2887:GLU:HG3	1.97	0.46
2:B:2925:PHE:HZ	2:B:2970:LEU:HD13	1.80	0.46
2:B:3100:ALA:O	2:B:3104:MET:HG3	2.15	0.46
2:B:3903:GLN:HG3	2:B:3967:LEU:HD22	1.96	0.46
2:B:3906:PHE:HD2	2:B:3967:LEU:HD21	1.79	0.46
2:B:4042:VAL:HG12	2:B:4077:THR:HB	1.95	0.46
2:B:4789:PHE:HE1	2:B:4839:TYR:HB3	1.80	0.46
2:C:842:GLN:HB2	2:C:1603:PHE:HB2	1.97	0.46
2:C:877:HIS:HA	2:C:880:ARG:NH1	2.30	0.46
2:C:2872:VAL:HG23	2:C:2877:LEU:HD22	1.96	0.46
2:C:4042:VAL:HG12	2:C:4077:THR:HB	1.95	0.46
2:A:11:ILE:HG12	2:A:176:ARG:HD2	1.97	0.46
2:A:114:LEU:HB2	2:A:117:HIS:CE1	2.51	0.46
2:A:713:TRP:CE2	2:A:1600:PRO:HD3	2.50	0.46
2:A:897:LYS:HB3	2:A:902:TRP:HB2	1.98	0.46
2:A:1549:SER:HB2	2:D:2830:ASN:HB3	1.96	0.46
2:A:4789:PHE:HE1	2:A:4839:TYR:HB3	1.80	0.46
1:F:4:GLU:C	1:F:4:GLU:OE1	2.54	0.46
2:D:674:TYR:CE1	2:D:756:SER:HB2	2.51	0.46
2:D:2736:LYS:HG3	2:D:2741:TRP:NE1	2.29	0.46
2:D:2971:ILE:HG23	2:D:2975:PHE:CD2	2.51	0.46
2:D:3074:ASN:HA	2:D:3077:GLN:HG3	1.98	0.46
2:D:3155:LEU:O	2:D:3159:LEU:HD23	2.15	0.46
2:D:3906:PHE:HD2	2:D:3967:LEU:HD21	1.79	0.46
2:D:4832:GLU:O	2:D:4843:ARG:NH2	2.48	0.46
2:B:1154:ARG:NH2	2:B:1180:GLU:OE2	2.48	0.46
2:C:11:ILE:HG12	2:C:176:ARG:HD2	1.97	0.46
2:C:769:ARG:HG2	2:C:774:PRO:HA	1.96	0.46
2:C:1118:SER:HA	2:C:1134:ALA:HA	1.97	0.46
2:C:2478:ILE:HG21	2:C:2484:LEU:HD13	1.96	0.46
2:C:2984:SER:HA	2:C:2989:PRO:HB2	1.97	0.46
2:C:3074:ASN:HA	2:C:3077:GLN:HG3	1.98	0.46
2:C:3177:LYS:HE2	2:C:3178:HIS:CE1	2.51	0.46
2:C:3903:GLN:HG3	2:C:3967:LEU:HD22	1.96	0.46
2:C:4832:GLU:O	2:C:4843:ARG:NH2	2.48	0.46
2:A:1421:MET:HE2	2:A:1576:LYS:HD2	1.98	0.46
2:A:2607:LEU:HD11	2:A:2665:ALA:HA	1.97	0.46
2:A:2720:PHE:HB2	2:A:2901:TYR:CE2	2.51	0.46
2:A:2724:TYR:CD2	2:A:2775:ILE:HG12	2.51	0.46
2:A:2834:SER:O	2:A:2838[A]:HIS:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2856:LYS:HA	2:A:2859:GLU:CG	2.44	0.46
2:A:4048:PHE:HZ	2:A:4080:TYR:HB3	1.80	0.46
2:A:4512:ALA:O	2:A:4516:ILE:HG13	2.15	0.46
2:D:692:HIS:HE1	2:D:717:GLY:HA3	1.80	0.46
2:D:1590:PHE:CE2	2:D:1592:SER:HB3	2.51	0.46
2:D:2482:ASP:OD1	2:D:2483:PHE:N	2.48	0.46
2:D:3013:VAL:HA	2:D:3016:ARG:HD3	1.97	0.46
2:D:3213:LYS:O	2:D:3216:GLU:HG3	2.15	0.46
2:D:3650:GLU:HB2	2:D:3651:PRO:HD3	1.96	0.46
2:B:1968:PRO:O	2:B:1972:GLN:HG3	2.15	0.46
2:B:2482:ASP:OD1	2:B:2483:PHE:N	2.48	0.46
2:B:2664:LEU:O	2:B:2667:PRO:HD2	2.15	0.46
2:B:2872:VAL:HG23	2:B:2877:LEU:HD22	1.96	0.46
2:B:4609:LYS:HD2	2:B:4615:LEU:HD22	1.96	0.46
2:B:4832:GLU:O	2:B:4843:ARG:NH2	2.48	0.46
2:C:962:LYS:HD2	2:C:982:ASP:HB2	1.97	0.46
2:C:1552:VAL:HG12	2:C:1553:PHE:HD2	1.80	0.46
2:C:2635:GLU:HA	2:C:2638:LEU:HB2	1.97	0.46
2:C:3805:LEU:HD21	2:C:3888:PHE:HA	1.98	0.46
2:C:4482:LYS:N	2:C:4482:LYS:HD2	2.31	0.46
2:C:4774:LEU:O	2:C:4778:VAL:HG23	2.15	0.46
2:A:222:GLU:HB3	2:A:349:MET:HG3	1.97	0.46
2:A:240:HIS:HB3	2:B:167:LYS:HE2	1.97	0.46
2:A:962:LYS:HD2	2:A:982:ASP:HB2	1.97	0.46
2:A:2664:LEU:O	2:A:2667:PRO:HD2	2.15	0.46
2:A:2984:SER:OG	2:A:2994:GLY:O	2.28	0.46
2:A:3100:ALA:O	2:A:3104:MET:HG3	2.15	0.46
2:D:869:THR:OG1	2:D:941:LYS:HB3	2.15	0.46
2:D:2797:SER:HB3	2:D:2801:TYR:CE2	2.51	0.46
2:D:3042:ALA:HB1	2:D:3121:LEU:HB2	1.96	0.46
2:D:3235:MET:HA	2:D:3239:LEU:HD23	1.97	0.46
2:D:4774:LEU:O	2:D:4778:VAL:HG23	2.15	0.46
2:B:114:LEU:HB2	2:B:117:HIS:CE1	2.51	0.46
2:B:307:SER:HB3	2:B:327:THR:HG22	1.96	0.46
2:B:601:LEU:HB3	2:B:642:LEU:HD11	1.98	0.46
2:B:2980:LEU:CD2	2:B:2990:LEU:HG	2.46	0.46
2:B:4640:PHE:CD2	2:B:4641:PRO:HD3	2.51	0.46
2:C:1932:PHE:CZ	2:C:1996:LEU:HB2	2.51	0.46
2:C:4107:GLU:OE1	2:C:4147:ARG:NH1	2.43	0.46
2:C:4579:HIS:HE1	2:C:4742:HIS:ND1	2.12	0.46
1:H:4:GLU:C	1:H:4:GLU:OE1	2.54	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:692:HIS:HE1	2:A:717:GLY:HA3	1.80	0.46
2:A:1590:PHE:CE2	2:A:1592:SER:HB3	2.51	0.46
2:A:1844:GLN:HE22	2:A:1852:LYS:HA	1.81	0.46
2:A:3650:GLU:HB2	2:A:3651:PRO:HD3	1.96	0.46
2:A:4640:PHE:CD2	2:A:4641:PRO:HD3	2.51	0.46
1:E:4:GLU:OE1	1:E:4:GLU:C	2.54	0.46
2:D:1154:ARG:NH2	2:D:1180:GLU:OE2	2.48	0.46
2:D:2720:PHE:HB2	2:D:2901:TYR:CE2	2.51	0.46
2:D:2980:LEU:CD2	2:D:2990:LEU:HG	2.46	0.46
2:D:4482:LYS:HD2	2:D:4482:LYS:N	2.31	0.46
2:D:4819:VAL:HG12	2:D:4830:GLU:HG3	1.96	0.46
2:B:2984:SER:OG	2:B:2994:GLY:O	2.28	0.46
2:B:3122:ILE:HD11	2:B:3127:GLN:HA	1.98	0.46
2:C:1720:MET:SD	2:C:2127:ARG:HB3	2.55	0.46
2:C:3013:VAL:HA	2:C:3016:ARG:HD3	1.97	0.46
2:C:3042:ALA:HB1	2:C:3121:LEU:HB2	1.96	0.46
2:C:4640:PHE:CD2	2:C:4641:PRO:HD3	2.51	0.46
2:A:842:GLN:HB2	2:A:1603:PHE:HB2	1.97	0.46
2:A:1968:PRO:O	2:A:1972:GLN:HG3	2.15	0.46
2:A:2379:ASP:OD1	2:A:2380:ASP:N	2.47	0.46
2:A:2925:PHE:HZ	2:A:2970:LEU:HD13	1.80	0.46
2:A:3122:ILE:HD11	2:A:3127:GLN:HA	1.98	0.46
2:A:3290:ILE:O	2:A:3292:GLU:N	2.47	0.46
2:A:3903:GLN:HG3	2:A:3967:LEU:HD22	1.96	0.46
2:A:4294:LEU:HD22	2:B:4719:PHE:CE2	2.50	0.46
1:E:26:HIS:NE2	1:E:41:ARG:HG2	2.30	0.46
1:G:91:VAL:HG21	2:C:1768:PHE:CE1	2.51	0.46
2:D:897:LYS:HB3	2:D:902:TRP:HB2	1.98	0.46
2:D:1500:ARG:HG2	2:D:1505:LEU:HG	1.97	0.46
2:D:1694:MET:SD	2:D:1695:PRO:HD2	2.56	0.46
2:B:769:ARG:HG2	2:B:774:PRO:HA	1.96	0.46
2:B:1118:SER:HA	2:B:1134:ALA:HA	1.97	0.46
2:B:1844:GLN:HE22	2:B:1852:LYS:HA	1.81	0.46
2:B:3074:ASN:HA	2:B:3077:GLN:HG3	1.98	0.46
2:C:307:SER:HB3	2:C:327:THR:HG22	1.96	0.46
2:C:1154:ARG:NH2	2:C:1180:GLU:OE2	2.48	0.46
2:C:1829:LEU:HD11	2:C:1839:LEU:HD13	1.97	0.46
2:C:2482:ASP:OD1	2:C:2483:PHE:N	2.48	0.46
2:C:2797:SER:HB3	2:C:2801:TYR:CE2	2.51	0.46
2:C:4048:PHE:HZ	2:C:4080:TYR:HB3	1.80	0.46
2:C:4267:GLN:HG3	2:C:4270:LYS:HZ3	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:674:TYR:CE1	2:A:756:SER:HB2	2.51	0.46
2:A:3074:ASN:HA	2:A:3077:GLN:HG3	1.98	0.46
2:A:4194:GLU:CD	2:A:4608:ARG:HH22	2.19	0.46
2:D:114:LEU:HB2	2:D:117:HIS:CE1	2.51	0.46
2:D:2316:ASN:OD1	2:D:3810:ARG:NH1	2.49	0.46
2:D:2724:TYR:CD2	2:D:2775:ILE:HG12	2.51	0.46
2:D:4640:PHE:CD2	2:D:4641:PRO:HD3	2.51	0.46
2:B:1427:TYR:HB2	2:B:1563:VAL:HG11	1.96	0.46
2:B:1910:LEU:HD22	2:B:2062:ILE:HD11	1.97	0.46
2:B:2316:ASN:OD1	2:B:3810:ARG:NH1	2.49	0.46
2:B:3155:LEU:O	2:B:3159:LEU:HD23	2.15	0.46
2:B:3712:LYS:O	2:B:3717:LYS:NZ	2.46	0.46
2:C:114:LEU:HB2	2:C:117:HIS:CE1	2.51	0.46
2:C:695:VAL:HG11	2:C:755:ILE:HG21	1.98	0.46
2:C:869:THR:OG1	2:C:941:LYS:HB3	2.15	0.46
2:C:1590:PHE:CE2	2:C:1592:SER:HB3	2.51	0.46
2:C:1968:PRO:O	2:C:1972:GLN:HG3	2.15	0.46
2:C:2157:GLN:O	2:C:3615:ARG:NH2	2.38	0.46
2:C:2331:PHE:HD1	2:C:2395:LEU:HD21	1.80	0.46
2:C:2724:TYR:CD2	2:C:2775:ILE:HG12	2.51	0.46
2:A:1500:ARG:HG2	2:A:1505:LEU:HG	1.97	0.46
2:A:1932:PHE:CZ	2:A:1996:LEU:HB2	2.51	0.46
2:A:2736:LYS:HG3	2:A:2741:TRP:NE1	2.29	0.46
2:A:2895:PHE:HA	2:A:2898:ILE:HG22	1.98	0.46
2:D:966:LEU:HD12	2:D:978:PRO:HD2	1.97	0.46
2:D:1427:TYR:HB2	2:D:1563:VAL:HG11	1.96	0.46
2:D:2285:TYR:HD2	2:D:2384:MET:HE1	1.80	0.46
2:D:2331:PHE:HD1	2:D:2395:LEU:HD21	1.80	0.46
2:D:3805:LEU:HD21	2:D:3888:PHE:HA	1.98	0.46
2:D:4652:LYS:NZ	2:D:4945:GLN:OE1	2.35	0.46
2:B:34:LYS:N	2:B:53:SER:OG	2.37	0.46
2:B:756:SER:OG	2:B:769:ARG:HB2	2.16	0.46
2:B:869:THR:OG1	2:B:941:LYS:HB3	2.15	0.46
2:B:2984:SER:HA	2:B:2989:PRO:HB2	1.97	0.46
2:C:756:SER:OG	2:C:769:ARG:HB2	2.16	0.46
2:C:2068:ARG:HA	2:C:2071:GLN:HG2	1.98	0.46
2:A:1829:LEU:HD11	2:A:1839:LEU:HD13	1.97	0.46
2:A:2316:ASN:OD1	2:A:3810:ARG:NH1	2.49	0.46
2:A:2971:ILE:HG23	2:A:2975:PHE:CD2	2.51	0.46
2:A:2980:LEU:CD2	2:A:2990:LEU:HG	2.46	0.46
2:A:3025:ASP:O	2:A:3028:SER:OG	2.17	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4832:GLU:O	2:A:4843:ARG:NH2	2.48	0.46
2:D:541:ILE:HG22	2:D:547:ASN:HB3	1.98	0.46
2:D:1065:GLU:O	2:D:1065:GLU:HG2	2.16	0.46
2:D:1910:LEU:HD22	2:D:2062:ILE:HD11	1.98	0.46
2:D:2068:ARG:HA	2:D:2071:GLN:HG2	1.98	0.46
2:D:2736:LYS:HD3	2:D:2736:LYS:N	2.31	0.46
2:D:3903:GLN:HG3	2:D:3967:LEU:HD22	1.96	0.46
2:D:4194:GLU:CD	2:D:4608:ARG:HH22	2.19	0.46
2:B:897:LYS:HB3	2:B:902:TRP:HB2	1.98	0.46
2:C:966:LEU:HD12	2:C:978:PRO:HD2	1.97	0.46
2:C:1106:GLU:HB3	2:C:1214:ARG:HB2	1.98	0.46
2:C:2856:LYS:HA	2:C:2859:GLU:CG	2.44	0.46
2:C:2884:LYS:HA	2:C:2887:GLU:HG3	1.97	0.46
2:C:4778:VAL:HG12	2:C:4816:HIS:HB3	1.98	0.46
2:A:869:THR:OG1	2:A:941:LYS:HB3	2.15	0.46
2:A:1694:MET:SD	2:A:1695:PRO:HD2	2.56	0.46
2:A:3152:ARG:HA	2:A:3155:LEU:HD12	1.98	0.46
2:A:3235:MET:HA	2:A:3239:LEU:HD23	1.98	0.46
2:A:4482:LYS:N	2:A:4482:LYS:HD2	2.31	0.46
2:D:1829:LEU:HD11	2:D:1839:LEU:HD13	1.97	0.46
2:D:2379:ASP:OD1	2:D:2380:ASP:N	2.47	0.46
2:D:3122:ILE:HD11	2:D:3127:GLN:HA	1.98	0.46
2:B:1590:PHE:CE2	2:B:1592:SER:HB3	2.51	0.46
2:B:1932:PHE:CZ	2:B:1996:LEU:HB2	2.51	0.46
2:B:2396:ILE:HD11	2:B:2432:LEU:HD21	1.98	0.46
2:B:2736:LYS:HD3	2:B:2736:LYS:N	2.31	0.46
2:B:3235:MET:HA	2:B:3239:LEU:HD23	1.97	0.46
2:B:4482:LYS:HD2	2:B:4482:LYS:N	2.31	0.46
2:C:2736:LYS:HD3	2:C:2736:LYS:N	2.31	0.46
2:C:2895:PHE:HA	2:C:2898:ILE:HG22	1.98	0.46
2:C:3918:ASN:HA	2:C:3921:THR:HG22	1.98	0.46
2:A:601:LEU:HB3	2:A:642:LEU:HD11	1.98	0.45
2:A:756:SER:OG	2:A:769:ARG:HB2	2.16	0.45
1:G:4:GLU:C	1:G:4:GLU:OE1	2.54	0.45
2:D:1118:SER:HA	2:D:1134:ALA:HA	1.97	0.45
2:D:2075:ILE:HG22	2:D:2077:ASP:H	1.81	0.45
2:D:2238:THR:HG22	2:D:2240:LEU:H	1.82	0.45
2:D:2247:VAL:HG11	2:D:2257:LEU:HD21	1.98	0.45
2:D:2925:PHE:HZ	2:D:2970:LEU:HD13	1.80	0.45
2:D:3143:SER:O	2:D:3152:ARG:NH1	2.48	0.45
2:D:3177:LYS:HE2	2:D:3178:HIS:CE1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:ILE:HG12	2:B:176:ARG:HD2	1.97	0.45
2:B:1106:GLU:HB3	2:B:1214:ARG:HB2	1.98	0.45
2:B:2068:ARG:HA	2:B:2071:GLN:HG2	1.98	0.45
2:B:2797:SER:HB3	2:B:2801:TYR:CE2	2.51	0.45
2:B:2895:PHE:HA	2:B:2898:ILE:HG22	1.98	0.45
2:B:3013:VAL:HA	2:B:3016:ARG:HD3	1.97	0.45
2:C:1694:MET:SD	2:C:1695:PRO:HD2	2.56	0.45
2:C:2247:VAL:HG11	2:C:2257:LEU:HD21	1.98	0.45
2:C:2607:LEU:HD11	2:C:2665:ALA:HA	1.97	0.45
2:C:2732:TRP:CH2	2:C:2756:LEU:HB3	2.51	0.45
2:C:3074:ASN:HD21	2:C:3093:ILE:HD11	1.81	0.45
1:H:8:ILE:HA	2:D:730:LEU:HD11	1.97	0.45
2:A:661:LEU:HD12	2:A:673:TRP:CD1	2.51	0.45
2:A:695:VAL:HG11	2:A:755:ILE:HG21	1.98	0.45
2:A:1979:PHE:HB2	2:A:3628:TRP:CZ2	2.51	0.45
2:A:2238:THR:HG22	2:A:2240:LEU:H	1.82	0.45
2:A:2443:PRO:HD3	2:A:2512:MET:HG3	1.97	0.45
2:A:2797:SER:HB3	2:A:2801:TYR:CE2	2.51	0.45
1:G:26:HIS:NE2	1:G:41:ARG:HG2	2.30	0.45
2:D:1041:ARG:HA	2:D:1044:LYS:NZ	2.29	0.45
2:D:2179:LEU:O	2:D:2183:GLU:CB	2.60	0.45
2:D:2895:PHE:HA	2:D:2898:ILE:HG22	1.98	0.45
2:B:222:GLU:HB3	2:B:349:MET:HG3	1.97	0.45
2:B:674:TYR:CE1	2:B:756:SER:HB2	2.51	0.45
2:B:1829:LEU:HD11	2:B:1839:LEU:HD13	1.97	0.45
2:B:2551:THR:O	2:B:2555:LEU:HD13	2.16	0.45
2:B:2720:PHE:HB2	2:B:2901:TYR:CE2	2.51	0.45
2:B:3985:MET:HA	2:B:3985:MET:HE3	1.98	0.45
2:C:1242:ASN:HB3	2:C:1807:ARG:HG3	1.99	0.45
2:C:1649:GLU:HG2	2:C:1650:LEU:N	2.32	0.45
2:C:2285:TYR:HD2	2:C:2384:MET:HE1	1.80	0.45
2:C:2396:ILE:HD11	2:C:2432:LEU:HD21	1.98	0.45
2:C:2720:PHE:HB2	2:C:2901:TYR:CE2	2.51	0.45
1:H:54:GLN:HG3	1:H:58:LYS:NZ	2.32	0.45
2:A:605:GLY:HA2	2:A:1585:ARG:HG3	1.99	0.45
2:A:1065:GLU:O	2:A:1065:GLU:HG2	2.16	0.45
2:A:2258:ARG:HH22	2:A:3810:ARG:HD2	1.82	0.45
1:E:54:GLN:HG3	1:E:58:LYS:NZ	2.32	0.45
2:D:1937:GLN:NE2	2:D:3608:LEU:O	2.46	0.45
2:D:2258:ARG:HH22	2:D:3810:ARG:HD2	1.82	0.45
2:D:2757:MET:SD	2:D:2757:MET:N	2.90	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4046:ARG:HG3	2:D:4050:LYS:NZ	2.32	0.45
2:B:605:GLY:HA2	2:B:1585:ARG:HG3	1.99	0.45
2:B:892:LEU:HD22	2:B:895:MET:HE3	1.99	0.45
2:B:2716:LYS:HG3	2:B:2717:LEU:HD12	1.99	0.45
2:B:3143:SER:O	2:B:3152:ARG:NH1	2.48	0.45
2:B:3805:LEU:HD21	2:B:3888:PHE:HA	1.98	0.45
2:C:1065:GLU:HG2	2:C:1065:GLU:O	2.16	0.45
2:C:2981:TYR:O	2:C:2984:SER:OG	2.34	0.45
2:C:3062:ASP:OD1	2:C:3132:ARG:NH2	2.50	0.45
2:C:3235:MET:HA	2:C:3239:LEU:HD23	1.97	0.45
2:A:2884:LYS:HA	2:A:2887:GLU:HG3	1.98	0.45
2:D:644:LEU:HB3	2:D:1630:LEU:HD11	1.99	0.45
2:D:1979:PHE:HB2	2:D:3628:TRP:CZ2	2.51	0.45
2:D:2607:LEU:HD11	2:D:2665:ALA:HA	1.97	0.45
2:D:2981:TYR:O	2:D:2984:SER:OG	2.34	0.45
2:B:935:MET:O	2:B:939:THR:OG1	2.17	0.45
2:B:1552:VAL:HG12	2:B:1553:PHE:HD2	1.80	0.45
2:B:1694:MET:SD	2:B:1695:PRO:HD2	2.56	0.45
2:B:1937:GLN:NE2	2:B:3608:LEU:O	2.46	0.45
2:B:2247:VAL:HG11	2:B:2257:LEU:HD21	1.98	0.45
2:B:2443:PRO:HD3	2:B:2512:MET:HG3	1.97	0.45
2:B:2724:TYR:CD2	2:B:2775:ILE:HG12	2.51	0.45
2:B:2830:ASN:HB3	2:C:1549:SER:CB	2.39	0.45
2:C:2075:ILE:HG22	2:C:2077:ASP:H	1.81	0.45
2:C:2980:LEU:CD2	2:C:2990:LEU:HG	2.46	0.45
2:C:3025:ASP:O	2:C:3028:SER:OG	2.17	0.45
2:C:3143:SER:O	2:C:3152:ARG:NH1	2.48	0.45
2:A:541:ILE:HG22	2:A:547:ASN:HB3	1.98	0.45
2:A:2543:SER:HB3	2:A:2879:ALA:HB2	1.99	0.45
2:A:4906:GLU:OE2	2:B:4182:GLU:HG3	2.17	0.45
1:G:54:GLN:HG3	1:G:58:LYS:NZ	2.32	0.45
2:D:1844:GLN:HE22	2:D:1852:LYS:HA	1.81	0.45
2:D:2283:LYS:HD3	2:D:2285:TYR:HE1	1.82	0.45
2:D:2443:PRO:HD3	2:D:2512:MET:HG3	1.98	0.45
2:D:2821:TYR:O	2:D:2823:PRO:HD3	2.17	0.45
2:D:3918:ASN:HA	2:D:3921:THR:HG22	1.98	0.45
2:B:921:PHE:HB3	2:B:929:ARG:HG3	1.98	0.45
2:B:1649:GLU:HG2	2:B:1650:LEU:N	2.32	0.45
2:B:2507:LEU:HA	2:B:2510:THR:HG23	1.99	0.45
2:B:2550:HIS:CE1	2:B:2875:ASP:HB3	2.52	0.45
2:B:2607:LEU:HD11	2:B:2665:ALA:HA	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4048:PHE:HZ	2:B:4080:TYR:HB3	1.80	0.45
2:B:4778:VAL:HG12	2:B:4816:HIS:HB3	1.98	0.45
2:C:674:TYR:CE1	2:C:756:SER:HB2	2.51	0.45
2:C:4046:ARG:HG3	2:C:4050:LYS:NZ	2.32	0.45
2:A:2068:ARG:HA	2:A:2071:GLN:HG2	1.98	0.45
2:A:2736:LYS:HD3	2:A:2736:LYS:N	2.31	0.45
2:A:2757:MET:N	2:A:2757:MET:SD	2.90	0.45
2:A:3155:LEU:O	2:A:3159:LEU:HD23	2.15	0.45
2:D:1932:PHE:CZ	2:D:1996:LEU:HB2	2.51	0.45
2:D:2444:THR:O	2:D:2452:VAL:N	2.42	0.45
2:D:2884:LYS:HA	2:D:2887:GLU:HG3	1.97	0.45
2:D:3319:PHE:O	2:D:3323:MET:N	2.39	0.45
2:B:274:LEU:HD23	2:B:274:LEU:HA	1.85	0.45
2:B:661:LEU:O	2:B:788:PHE:N	2.47	0.45
2:B:695:VAL:HG11	2:B:755:ILE:HG21	1.98	0.45
2:B:888:ASN:O	2:B:892:LEU:HD23	2.17	0.45
2:B:1242:ASN:ND2	2:B:1805:HIS:O	2.50	0.45
2:B:4264:LEU:HD21	2:C:4698:LEU:HD11	1.99	0.45
2:C:222:GLU:HB3	2:C:349:MET:HG3	1.97	0.45
2:C:605:GLY:HA2	2:C:1585:ARG:HG3	1.99	0.45
2:C:2316:ASN:OD1	2:C:3810:ARG:NH1	2.49	0.45
2:C:2895:PHE:O	2:C:2899:ASN:ND2	2.29	0.45
2:C:2932:TYR:CD2	2:C:2967:VAL:HG21	2.51	0.45
2:A:2172:MET:O	2:A:2176:VAL:HG23	2.17	0.45
2:A:3125:ASP:O	2:A:3128:VAL:HG12	2.17	0.45
2:A:3177:LYS:HE2	2:A:3178:HIS:CE1	2.51	0.45
2:D:756:SER:OG	2:D:769:ARG:HB2	2.16	0.45
2:D:888:ASN:HA	2:D:891:GLU:HB2	1.99	0.45
2:D:943:LEU:O	2:D:948:CYS:N	2.43	0.45
2:D:967:PRO:O	2:D:971:GLN:HB3	2.17	0.45
2:D:1239:PHE:O	2:D:1807:ARG:NH1	2.45	0.45
2:D:1242:ASN:HB3	2:D:1807:ARG:HG3	1.99	0.45
2:D:1262:PRO:HD3	2:D:1590:PHE:HE1	1.82	0.45
2:D:1962:THR:O	2:D:1966:ARG:HG3	2.17	0.45
2:D:2543:SER:HB3	2:D:2879:ALA:HB2	1.99	0.45
2:D:3152:ARG:HA	2:D:3155:LEU:HD12	1.98	0.45
2:B:541:ILE:HG22	2:B:547:ASN:HB3	1.98	0.45
2:B:661:LEU:HD12	2:B:673:TRP:CD1	2.51	0.45
2:B:2172:MET:O	2:B:2176:VAL:HG23	2.17	0.45
2:B:2324:LEU:HD23	2:B:2399:LEU:HD21	1.98	0.45
2:B:2757:MET:N	2:B:2757:MET:SD	2.90	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2788:ARG:HB2	2:B:2904:SER:OG	2.17	0.45
2:B:2971:ILE:HG23	2:B:2975:PHE:CD2	2.51	0.45
2:B:3152:ARG:HA	2:B:3155:LEU:HD12	1.98	0.45
2:B:3177:LYS:HE2	2:B:3178:HIS:CE1	2.50	0.45
2:C:601:LEU:HB3	2:C:642:LEU:HD11	1.98	0.45
2:C:644:LEU:HB3	2:C:1630:LEU:HD11	1.99	0.45
2:C:778:MET:HG3	2:C:780:GLU:OE2	2.17	0.45
2:C:888:ASN:HA	2:C:891:GLU:HB2	1.99	0.45
2:C:897:LYS:HB3	2:C:902:TRP:HB2	1.98	0.45
2:C:1719:LEU:HD21	2:C:1830:ILE:HD12	1.99	0.45
2:C:1844:GLN:HE22	2:C:1852:LYS:HA	1.81	0.45
2:C:2238:THR:HG22	2:C:2240:LEU:H	1.82	0.45
2:C:2324:LEU:HD23	2:C:2399:LEU:HD21	1.98	0.45
2:C:2971:ILE:HG23	2:C:2975:PHE:CD2	2.51	0.45
2:A:644:LEU:HB3	2:A:1630:LEU:HD11	1.99	0.45
2:A:1118:SER:HA	2:A:1134:ALA:HA	1.97	0.45
2:A:1962:THR:O	2:A:1966:ARG:HG3	2.17	0.45
2:A:2075:ILE:HG22	2:A:2077:ASP:H	1.81	0.45
2:A:2550:HIS:CE1	2:A:2875:ASP:HB3	2.52	0.45
2:A:2932:TYR:CD2	2:A:2967:VAL:HG21	2.51	0.45
2:A:3805:LEU:HD21	2:A:3888:PHE:HA	1.98	0.45
2:D:601:LEU:HB3	2:D:642:LEU:HD11	1.98	0.45
2:D:1242:ASN:ND2	2:D:1805:HIS:O	2.50	0.45
2:D:3074:ASN:HD21	2:D:3093:ILE:HD11	1.81	0.45
2:B:181:LEU:N	2:B:212:TRP:O	2.39	0.45
2:B:1719:LEU:HD21	2:B:1830:ILE:HD12	1.99	0.45
2:B:1898:LEU:HD22	2:B:1902:VAL:HG11	1.99	0.45
2:B:2422:ILE:O	2:B:2426:LEU:HG	2.17	0.45
2:B:2935:GLU:O	2:B:2939:TYR:CD1	2.67	0.45
2:B:3062:ASP:OD1	2:B:3132:ARG:NH2	2.50	0.45
2:B:4194:GLU:CD	2:B:4608:ARG:HH22	2.19	0.45
2:C:888:ASN:O	2:C:892:LEU:HD23	2.17	0.45
2:C:956:HIS:O	2:C:960:LYS:HG3	2.17	0.45
2:C:1910:LEU:HD22	2:C:2062:ILE:HD11	1.97	0.45
2:C:2443:PRO:HD3	2:C:2512:MET:HG3	1.98	0.45
2:C:2507:LEU:HA	2:C:2510:THR:HG23	1.99	0.45
2:C:2716:LYS:HG3	2:C:2717:LEU:HD12	1.99	0.45
2:C:4044:SER:O	2:C:4048:PHE:HD2	2.00	0.45
2:A:876:PRO:HA	2:A:879:GLU:CG	2.42	0.45
2:A:892:LEU:HD22	2:A:895:MET:HE3	1.99	0.45
2:A:956:HIS:O	2:A:960:LYS:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1242:ASN:HB3	2:A:1807:ARG:HG3	1.99	0.45
2:A:2247:VAL:HG11	2:A:2257:LEU:HD21	1.98	0.45
2:A:2324:LEU:HD23	2:A:2399:LEU:HD21	1.98	0.45
2:A:2824:ARG:HA	2:A:2824:ARG:HD2	1.64	0.45
2:A:2984:SER:HA	2:A:2989:PRO:HB2	1.97	0.45
2:A:4046:ARG:HG3	2:A:4050:LYS:NZ	2.32	0.45
2:A:4652:LYS:NZ	2:A:4945:GLN:OE1	2.35	0.45
1:F:54:GLN:HG3	1:F:58:LYS:NZ	2.31	0.45
2:D:605:GLY:HA2	2:D:1585:ARG:HG3	1.99	0.45
2:D:2324:LEU:HD23	2:D:2399:LEU:HD21	1.98	0.45
2:D:4778:VAL:HG12	2:D:4816:HIS:HB3	1.98	0.45
2:B:778:MET:HG3	2:B:780:GLU:OE2	2.17	0.45
2:B:1962:THR:O	2:B:1966:ARG:HG3	2.17	0.45
2:B:1979:PHE:HB2	2:B:3628:TRP:CZ2	2.52	0.45
2:B:2238:THR:HG22	2:B:2240:LEU:H	1.82	0.45
2:B:4044:SER:O	2:B:4048:PHE:HD2	2.00	0.45
2:C:892:LEU:HD22	2:C:895:MET:HE3	1.99	0.45
2:C:2551:THR:O	2:C:2555:LEU:HD13	2.17	0.45
2:C:2824:ARG:HA	2:C:2824:ARG:HD2	1.64	0.45
2:A:778:MET:HG3	2:A:780:GLU:OE2	2.17	0.45
2:A:1719:LEU:HD21	2:A:1830:ILE:HD12	1.99	0.45
2:A:1910:LEU:HD22	2:A:2062:ILE:HD11	1.97	0.45
2:A:2054:LYS:NZ	2:A:2056:SER:OG	2.31	0.45
2:A:2283:LYS:HD3	2:A:2285:TYR:HE1	1.82	0.45
2:A:2716:LYS:HG3	2:A:2717:LEU:HD12	1.99	0.45
2:D:375:GLN:O	2:D:376:SER:OG	2.33	0.45
2:D:778:MET:HG3	2:D:780:GLU:OE2	2.17	0.45
2:D:1719:LEU:HD21	2:D:1830:ILE:HD12	1.99	0.45
2:D:2551:THR:O	2:D:2555:LEU:HD13	2.16	0.45
2:D:3972:MET:HE3	2:D:4094:ILE:HD12	1.98	0.45
2:B:644:LEU:HB3	2:B:1630:LEU:HD11	1.99	0.45
2:B:853:PRO:HD3	2:B:1086:ARG:HB2	1.99	0.45
2:B:1065:GLU:O	2:B:1065:GLU:HG2	2.16	0.45
2:B:2525:LEU:HD12	2:B:2569:ILE:HG22	1.99	0.45
2:B:2589:LEU:O	2:B:2593:VAL:HG13	2.17	0.45
2:B:2605:MET:HA	2:B:2608:LYS:HE2	1.99	0.45
2:C:1262:PRO:HD3	2:C:1590:PHE:HE1	1.82	0.45
2:C:1962:THR:O	2:C:1966:ARG:HG3	2.17	0.45
2:C:2492:PHE:O	2:C:2496:LEU:N	2.45	0.45
2:C:2657:TYR:HA	2:C:2662:PHE:CE2	2.52	0.45
2:C:2757:MET:N	2:C:2757:MET:SD	2.90	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2821:TYR:O	2:C:2823:PRO:HD3	2.17	0.45
2:C:3122:ILE:HD11	2:C:3127:GLN:HA	1.98	0.45
2:C:3976:LYS:HD2	2:C:4093:ASP:OD2	2.17	0.45
2:A:219:SER:H	2:A:349:MET:CE	2.30	0.44
2:A:888:ASN:HA	2:A:891:GLU:HB2	1.99	0.44
2:A:1649:GLU:HG2	2:A:1650:LEU:N	2.32	0.44
2:A:2173:GLU:HA	2:A:2176:VAL:HB	2.00	0.44
2:A:2500:ALA:HB1	2:A:2554:ARG:HH22	1.82	0.44
2:A:2525:LEU:HD12	2:A:2569:ILE:HG22	2.00	0.44
2:A:2605:MET:HA	2:A:2608:LYS:HE2	1.99	0.44
2:A:2729:HIS:CD2	2:A:2760:TYR:HB2	2.52	0.44
2:A:2981:TYR:O	2:A:2984:SER:OG	2.34	0.44
2:A:3074:ASN:HD21	2:A:3093:ILE:HD11	1.81	0.44
2:A:3976:LYS:HD2	2:A:4093:ASP:OD2	2.17	0.44
2:A:4183:LYS:HB3	2:D:4906:GLU:OE2	2.17	0.44
2:A:4778:VAL:HG12	2:A:4816:HIS:HB3	1.98	0.44
2:D:661:LEU:HD12	2:D:673:TRP:CD1	2.51	0.44
2:D:695:VAL:HG11	2:D:755:ILE:HG21	1.98	0.44
2:D:2456:MET:CE	2:D:2511:ASP:HB2	2.48	0.44
2:D:3976:LYS:HD2	2:D:4093:ASP:OD2	2.17	0.44
2:B:472:HIS:O	2:B:476:GLN:HG2	2.17	0.44
2:B:888:ASN:HA	2:B:891:GLU:HB2	1.99	0.44
2:B:1419:PHE:CE2	2:B:1562:ASN:HB3	2.52	0.44
2:B:2075:ILE:HG22	2:B:2077:ASP:H	1.81	0.44
2:B:2731:LYS:O	2:B:2734:MET:HG2	2.17	0.44
2:C:181:LEU:N	2:C:212:TRP:O	2.39	0.44
2:C:661:LEU:HD12	2:C:673:TRP:CD1	2.51	0.44
2:C:853:PRO:HD3	2:C:1086:ARG:HB2	1.99	0.44
2:C:904:TYR:HB2	2:C:918:LEU:HD23	1.99	0.44
2:C:934:GLN:HA	2:C:937:LEU:HD12	1.99	0.44
2:C:1077:VAL:O	2:C:1077:VAL:HG13	2.18	0.44
2:C:1697:LEU:HD23	2:C:1697:LEU:HA	1.87	0.44
2:C:2422:ILE:O	2:C:2426:LEU:HG	2.17	0.44
2:C:3125:ASP:O	2:C:3128:VAL:HG12	2.17	0.44
2:C:3178:HIS:CD2	2:C:3263:MET:HA	2.53	0.44
2:C:4194:GLU:CD	2:C:4608:ARG:HH22	2.19	0.44
1:H:91:VAL:HG21	2:D:1768:PHE:CE1	2.52	0.44
2:A:967:PRO:O	2:A:971:GLN:HB3	2.17	0.44
2:A:1262:PRO:HD3	2:A:1590:PHE:HE1	1.82	0.44
2:A:1501:ASN:CB	2:D:2826:ILE:HD13	2.45	0.44
2:A:1553:PHE:HE1	2:A:1555:PHE:CE2	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2456:MET:CE	2:A:2511:ASP:HB2	2.48	0.44
2:A:2551:THR:O	2:A:2555:LEU:HD13	2.16	0.44
2:A:2821:TYR:O	2:A:2823:PRO:HD3	2.17	0.44
2:D:1077:VAL:O	2:D:1077:VAL:HG13	2.18	0.44
2:D:1106:GLU:HB3	2:D:1214:ARG:HB2	1.98	0.44
2:D:1553:PHE:HE1	2:D:1555:PHE:CE2	2.35	0.44
2:D:1717:ALA:HA	2:D:1720:MET:HE2	2.00	0.44
2:D:2525:LEU:HD12	2:D:2569:ILE:HG22	1.99	0.44
2:D:2550:HIS:CE1	2:D:2875:ASP:HB3	2.52	0.44
2:D:2731:LYS:O	2:D:2734:MET:HG2	2.17	0.44
2:C:921:PHE:HB3	2:C:929:ARG:HG3	1.98	0.44
2:C:2543:SER:HB3	2:C:2879:ALA:HB2	1.99	0.44
2:C:2550:HIS:CE1	2:C:2875:ASP:HB3	2.52	0.44
2:C:2685:TYR:HB2	2:C:2909:ASP:OD1	2.17	0.44
2:A:472:HIS:O	2:A:476:GLN:HG2	2.17	0.44
2:A:1717:ALA:HA	2:A:1720:MET:HE2	1.99	0.44
2:A:1898:LEU:HD22	2:A:1902:VAL:HG11	1.99	0.44
2:A:2422:ILE:O	2:A:2426:LEU:HG	2.17	0.44
2:A:3918:ASN:HA	2:A:3921:THR:HG22	1.98	0.44
2:A:4044:SER:O	2:A:4048:PHE:HD2	2.00	0.44
2:D:219:SER:H	2:D:349:MET:CE	2.30	0.44
2:D:228:LEU:HD21	2:D:277:LEU:HD13	1.99	0.44
2:D:246:THR:HG22	2:D:247:VAL:O	2.17	0.44
2:D:586:LEU:HD22	2:D:617:LEU:HD23	2.00	0.44
2:D:904:TYR:HB2	2:D:918:LEU:HD23	1.99	0.44
2:D:921:PHE:HB3	2:D:929:ARG:HG3	1.98	0.44
2:D:2396:ILE:HD11	2:D:2432:LEU:HD21	1.98	0.44
2:D:2500:ALA:HB1	2:D:2554:ARG:HH22	1.82	0.44
2:D:3125:ASP:O	2:D:3128:VAL:HG12	2.17	0.44
2:B:967:PRO:O	2:B:971:GLN:HB3	2.17	0.44
2:B:2732:TRP:O	2:B:2736:LYS:NZ	2.41	0.44
2:B:2821:TYR:O	2:B:2823:PRO:HD3	2.17	0.44
2:B:3918:ASN:HA	2:B:3921:THR:HG22	1.98	0.44
2:B:4046:ARG:HG3	2:B:4050:LYS:NZ	2.32	0.44
2:C:607:ASN:HB3	2:C:610:VAL:HG23	2.00	0.44
2:C:1553:PHE:HE1	2:C:1555:PHE:CE2	2.35	0.44
2:C:2172:MET:O	2:C:2176:VAL:HG23	2.17	0.44
2:C:2258:ARG:HH22	2:C:3810:ARG:HD2	1.82	0.44
2:C:2589:LEU:O	2:C:2593:VAL:HG13	2.17	0.44
2:C:2788:ARG:HB2	2:C:2904:SER:OG	2.17	0.44
2:C:3109:PHE:O	2:C:3165:ALA:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3697:LYS:HG3	2:C:3700:HIS:HE2	1.83	0.44
2:A:228:LEU:HD21	2:A:277:LEU:HD13	1.99	0.44
2:A:246:THR:HG22	2:A:247:VAL:O	2.18	0.44
2:A:607:ASN:HB3	2:A:610:VAL:HG23	2.00	0.44
2:A:2507:LEU:HA	2:A:2510:THR:HG23	1.99	0.44
2:D:1649:GLU:HG2	2:D:1650:LEU:N	2.32	0.44
2:D:3062:ASP:OD1	2:D:3132:ARG:NH2	2.50	0.44
2:B:246:THR:HG22	2:B:247:VAL:O	2.18	0.44
2:B:2567:ASP:O	2:B:2571:VAL:HG23	2.18	0.44
2:B:2657:TYR:HA	2:B:2662:PHE:CE2	2.52	0.44
2:B:2728:SER:HA	2:B:2731:LYS:NZ	2.33	0.44
2:B:2981:TYR:O	2:B:2984:SER:OG	2.34	0.44
2:B:3137:LEU:HA	2:B:3140:LEU:HD12	1.99	0.44
2:C:2003:LEU:HG	2:C:2004:MET:HE1	2.00	0.44
2:C:2179:LEU:O	2:C:2183:GLU:CB	2.60	0.44
2:C:2444:THR:O	2:C:2452:VAL:N	2.42	0.44
2:C:3072:MET:HE3	2:C:3072:MET:HB3	1.72	0.44
2:C:3152:ARG:HA	2:C:3155:LEU:HD12	1.98	0.44
2:A:586:LEU:HD22	2:A:617:LEU:HD23	2.00	0.44
2:A:888:ASN:O	2:A:892:LEU:HD23	2.17	0.44
2:A:2396:ILE:HD11	2:A:2432:LEU:HD21	1.98	0.44
2:A:2589:LEU:O	2:A:2593:VAL:HG13	2.17	0.44
2:A:4060:GLN:O	2:A:4064:GLU:OE1	2.36	0.44
2:A:4172:PHE:CZ	2:A:4189:PHE:HA	2.53	0.44
2:D:641:ASP:OD2	2:D:641:ASP:N	2.51	0.44
2:D:934:GLN:HA	2:D:937:LEU:HD12	1.99	0.44
2:D:2507:LEU:HA	2:D:2510:THR:HG23	1.99	0.44
2:D:2657:TYR:HA	2:D:2662:PHE:CE2	2.52	0.44
2:D:2788:ARG:HB2	2:D:2904:SER:OG	2.17	0.44
2:D:2932:TYR:CD2	2:D:2967:VAL:HG21	2.52	0.44
2:D:3697:LYS:HG3	2:D:3700:HIS:HE2	1.83	0.44
2:D:4964:ASP:OD1	2:D:4964:ASP:N	2.50	0.44
2:B:1262:PRO:HD3	2:B:1590:PHE:HE1	1.82	0.44
2:B:2456:MET:CE	2:B:2511:ASP:HB2	2.48	0.44
2:B:2456:MET:HE2	2:B:2511:ASP:HB2	1.99	0.44
2:B:2932:TYR:CD2	2:B:2967:VAL:HG21	2.51	0.44
2:B:3125:ASP:O	2:B:3128:VAL:HG12	2.17	0.44
2:C:912:LYS:HZ3	2:C:914:GLN:HG3	1.82	0.44
2:C:967:PRO:O	2:C:971:GLN:HB3	2.17	0.44
2:C:1436:GLN:NE2	2:C:1546:GLN:O	2.51	0.44
2:C:2456:MET:SD	2:C:2456:MET:N	2.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2525:LEU:HD12	2:C:2569:ILE:HG22	2.00	0.44
2:A:3228:TYR:CE1	2:A:3232:PRO:HB3	2.53	0.44
2:A:4522:VAL:HG12	2:B:4807:ASP:O	2.18	0.44
2:D:1419:PHE:CE2	2:D:1562:ASN:HB3	2.52	0.44
2:D:2003:LEU:HG	2:D:2004:MET:HE1	2.00	0.44
2:D:2567:ASP:O	2:D:2571:VAL:HG23	2.18	0.44
2:D:2716:LYS:HG3	2:D:2717:LEU:HD12	1.99	0.44
2:D:2729:HIS:CD2	2:D:2760:TYR:HB2	2.52	0.44
2:D:3109:PHE:O	2:D:3165:ALA:HB2	2.17	0.44
2:D:3178:HIS:CD2	2:D:3263:MET:HA	2.53	0.44
2:D:3668:ILE:HD13	2:D:3736:ALA:HB2	1.99	0.44
2:D:4044:SER:O	2:D:4048:PHE:HD2	2.00	0.44
2:D:4641:PRO:O	2:D:4647:LYS:NZ	2.35	0.44
2:B:586:LEU:HD22	2:B:617:LEU:HD23	2.00	0.44
2:B:655:MET:HE1	2:B:836:HIS:HA	2.00	0.44
2:B:934:GLN:HA	2:B:937:LEU:HD12	2.00	0.44
2:B:943:LEU:O	2:B:948:CYS:N	2.43	0.44
2:B:2258:ARG:HH22	2:B:3810:ARG:HD2	1.82	0.44
2:B:2497:ARG:NH2	2:B:2870:LEU:HA	2.33	0.44
2:B:2852:TRP:O	2:B:2856:LYS:HE2	2.17	0.44
2:B:3668:ILE:HD13	2:B:3736:ALA:HB2	1.98	0.44
2:C:2620:TYR:HB2	2:C:2627:TRP:CD1	2.53	0.44
2:C:2764:SER:O	2:C:2768:LYS:HG3	2.18	0.44
2:C:3148:VAL:O	2:C:3152:ARG:HG3	2.18	0.44
2:C:3319:PHE:O	2:C:3323:MET:N	2.39	0.44
2:C:4172:PHE:CZ	2:C:4189:PHE:HA	2.53	0.44
2:A:669:GLN:HE22	2:A:671:LYS:HG2	1.83	0.44
2:A:853:PRO:HD3	2:A:1086:ARG:HB2	2.00	0.44
2:A:921:PHE:HB3	2:A:929:ARG:HG3	1.98	0.44
2:A:1106:GLU:HB3	2:A:1214:ARG:HB2	1.98	0.44
2:A:1242:ASN:ND2	2:A:1805:HIS:O	2.50	0.44
2:A:2003:LEU:HG	2:A:2004:MET:HE1	2.00	0.44
2:A:2567:ASP:O	2:A:2571:VAL:HG23	2.18	0.44
2:D:181:LEU:N	2:D:212:TRP:O	2.39	0.44
2:D:888:ASN:O	2:D:892:LEU:HD23	2.17	0.44
2:D:892:LEU:HD22	2:D:895:MET:HE3	1.99	0.44
2:D:2668:CYS:O	2:D:2672:VAL:HG23	2.18	0.44
2:B:1242:ASN:HB3	2:B:1807:ARG:HG3	1.99	0.44
2:B:1553:PHE:HE1	2:B:1555:PHE:CE2	2.35	0.44
2:B:2003:LEU:HG	2:B:2004:MET:HE1	2.00	0.44
2:B:2492:PHE:O	2:B:2496:LEU:N	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2685:TYR:HB2	2:B:2909:ASP:OD1	2.17	0.44
2:B:3926:GLY:CA	2:B:4935:GLY:HA3	2.47	0.44
2:C:472:HIS:O	2:C:476:GLN:HG2	2.17	0.44
2:C:541:ILE:HG22	2:C:547:ASN:HB3	1.98	0.44
2:C:1242:ASN:ND2	2:C:1805:HIS:O	2.50	0.44
2:C:1419:PHE:CE2	2:C:1562:ASN:HB3	2.52	0.44
2:C:1651:LEU:HD12	2:C:1698:LEU:HG	2.00	0.44
2:C:2500:ALA:HB1	2:C:2554:ARG:NH2	2.33	0.44
2:C:2605:MET:HA	2:C:2608:LYS:HE2	1.99	0.44
2:C:2731:LYS:O	2:C:2734:MET:HG2	2.17	0.44
2:A:903:GLN:O	2:A:915:HIS:N	2.51	0.44
2:A:2657:TYR:HA	2:A:2662:PHE:CE2	2.52	0.44
2:A:2666:LEU:HB3	2:A:2667:PRO:HD3	2.00	0.44
2:A:2678:PRO:HB2	2:A:2981:TYR:CE2	2.53	0.44
2:A:2852:TRP:O	2:A:2856:LYS:HE2	2.17	0.44
1:F:63:GLY:HA3	1:F:75:LEU:HD21	2.00	0.44
1:G:63:GLY:HA3	1:G:75:LEU:HD21	2.00	0.44
2:D:655:MET:HE1	2:D:836:HIS:HA	2.00	0.44
2:D:3228:TYR:CE1	2:D:3232:PRO:HB3	2.53	0.44
2:B:293:GLN:HB2	2:B:343:ARG:HH22	1.83	0.44
2:B:607:ASN:HB3	2:B:610:VAL:HG23	2.00	0.44
2:B:669:GLN:HE22	2:B:671:LYS:HG2	1.83	0.44
2:B:904:TYR:HB2	2:B:918:LEU:HD23	1.99	0.44
2:B:1717:ALA:HA	2:B:1720:MET:HE2	1.99	0.44
2:B:2173:GLU:HA	2:B:2176:VAL:HB	2.00	0.44
2:B:2543:SER:HB3	2:B:2879:ALA:HB2	1.99	0.44
2:B:3148:VAL:O	2:B:3152:ARG:HG3	2.18	0.44
2:B:3976:LYS:HD2	2:B:4093:ASP:OD2	2.17	0.44
2:C:219:SER:H	2:C:349:MET:CE	2.30	0.44
2:C:669:GLN:HE22	2:C:671:LYS:HG2	1.83	0.44
2:C:1898:LEU:HD22	2:C:1902:VAL:HG11	1.98	0.44
2:C:2668:CYS:O	2:C:2672:VAL:HG23	2.18	0.44
2:C:2678:PRO:HB2	2:C:2981:TYR:CE2	2.53	0.44
1:H:63:GLY:HA3	1:H:75:LEU:HD21	2.00	0.44
2:A:293:GLN:HB2	2:A:343:ARG:HH22	1.83	0.44
2:A:2728:SER:HA	2:A:2731:LYS:NZ	2.33	0.44
2:A:2731:LYS:O	2:A:2734:MET:HG2	2.17	0.44
2:A:2788:ARG:HB2	2:A:2904:SER:OG	2.17	0.44
2:A:2834:SER:O	2:A:2838[B]:HIS:HB2	2.17	0.44
2:A:3137:LEU:HA	2:A:3140:LEU:HD12	1.99	0.44
2:D:607:ASN:HB3	2:D:610:VAL:HG23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:956:HIS:O	2:D:960:LYS:HG3	2.17	0.44
2:D:1421:MET:HE2	2:D:1576:LYS:HD2	2.00	0.44
2:D:1725:TYR:CE2	2:D:2101:ALA:HB1	2.53	0.44
2:D:1847:GLU:HG3	2:D:1850:VAL:H	1.83	0.44
2:D:1898:LEU:HD22	2:D:1902:VAL:HG11	1.98	0.44
2:D:2422:ILE:O	2:D:2426:LEU:HG	2.17	0.44
2:D:2685:TYR:HB2	2:D:2909:ASP:OD1	2.17	0.44
2:D:2764:SER:O	2:D:2768:LYS:HG3	2.18	0.44
2:D:2984:SER:OG	2:D:2994:GLY:O	2.28	0.44
2:B:903:GLN:O	2:B:915:HIS:N	2.51	0.44
2:B:3061:LEU:HD13	2:B:3126:VAL:HG13	2.00	0.44
2:B:3178:HIS:CD2	2:B:3263:MET:HA	2.53	0.44
2:B:4197:ILE:HG12	2:B:4923:MET:HE2	2.00	0.44
2:C:228:LEU:HD21	2:C:277:LEU:HD13	2.00	0.44
2:C:570:GLY:O	2:C:574:VAL:HG23	2.18	0.44
2:C:655:MET:HE1	2:C:836:HIS:HA	2.00	0.44
2:C:2456:MET:CE	2:C:2511:ASP:HB2	2.48	0.44
2:C:2728:SER:HA	2:C:2731:LYS:NZ	2.33	0.44
2:C:2935:GLU:O	2:C:2939:TYR:CD1	2.67	0.44
2:C:4616:TYR:CE2	2:C:4632:ARG:HG2	2.53	0.44
2:A:2849:HIS:HD2	2:A:2852:TRP:HE3	1.65	0.43
2:A:3062:ASP:OD1	2:A:3132:ARG:NH2	2.50	0.43
2:A:3246:MET:HE2	2:A:3276:LEU:HD21	2.00	0.43
2:A:3668:ILE:HD13	2:A:3736:ALA:HB2	1.98	0.43
2:D:876:PRO:HA	2:D:879:GLU:CG	2.42	0.43
2:D:903:GLN:O	2:D:915:HIS:N	2.51	0.43
2:D:1760:ARG:HE	2:D:1760:ARG:HB3	1.68	0.43
2:D:2279:MET:HE3	2:D:2279:MET:HB2	1.84	0.43
2:D:2589:LEU:O	2:D:2593:VAL:HG13	2.17	0.43
2:D:2605:MET:HA	2:D:2608:LYS:HE2	1.99	0.43
2:D:2620:TYR:HB2	2:D:2627:TRP:CD1	2.53	0.43
2:D:2678:PRO:HB2	2:D:2981:TYR:CE2	2.53	0.43
2:B:1651:LEU:HD12	2:B:1698:LEU:HG	2.00	0.43
2:B:1847:GLU:HG3	2:B:1850:VAL:H	1.83	0.43
2:B:2283:LYS:HD3	2:B:2285:TYR:HE1	1.82	0.43
2:B:2285:TYR:HD2	2:B:2384:MET:HE1	1.82	0.43
2:B:2729:HIS:CD2	2:B:2760:TYR:HB2	2.52	0.43
2:B:4060:GLN:O	2:B:4064:GLU:OE1	2.36	0.43
2:B:4304:GLY:O	2:B:4308:ILE:HG12	2.18	0.43
2:C:897:LYS:HB2	2:C:915:HIS:CE1	2.53	0.43
2:C:903:GLN:O	2:C:915:HIS:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2852:TRP:O	2:C:2856:LYS:HE2	2.17	0.43
2:C:2927:GLN:OE1	2:C:3003:MET:HG2	2.18	0.43
2:C:2967:VAL:HA	2:C:2970:LEU:HG	2.00	0.43
2:C:3228:TYR:CE1	2:C:3232:PRO:HB3	2.53	0.43
2:A:897:LYS:HB2	2:A:915:HIS:CE1	2.53	0.43
2:A:1077:VAL:O	2:A:1077:VAL:HG13	2.18	0.43
2:A:1502:ASN:OD1	2:D:2824:ARG:NH1	2.51	0.43
2:A:1699:ARG:O	2:A:1703:TYR:HB2	2.18	0.43
2:A:1703:TYR:HH	2:A:1824:LEU:H	1.66	0.43
2:A:2456:MET:HE2	2:A:2511:ASP:HB2	1.99	0.43
2:A:2497:ARG:NH2	2:A:2870:LEU:HA	2.33	0.43
2:A:3016:ARG:O	2:A:3018:ARG:NH1	2.51	0.43
2:A:3061:LEU:HD13	2:A:3126:VAL:HG13	2.00	0.43
2:A:3109:PHE:O	2:A:3165:ALA:HB2	2.18	0.43
2:D:189:GLU:OE2	2:C:2322:ARG:NH2	2.44	0.43
2:D:669:GLN:HE22	2:D:671:LYS:HG2	1.83	0.43
2:D:1118:SER:HB3	2:D:1204:VAL:HG11	2.00	0.43
2:D:1651:LEU:HD12	2:D:1698:LEU:HG	2.00	0.43
2:D:1915:ASP:OD1	2:D:2090:ARG:NH1	2.51	0.43
2:D:2500:ALA:HB1	2:D:2554:ARG:NH2	2.33	0.43
2:B:1421:MET:HE1	2:B:1576:LYS:HB3	1.99	0.43
2:B:2179:LEU:O	2:B:2183:GLU:CB	2.60	0.43
2:B:2678:PRO:HB2	2:B:2981:TYR:CE2	2.53	0.43
2:B:2764:SER:O	2:B:2768:LYS:HG3	2.18	0.43
2:B:3109:PHE:O	2:B:3165:ALA:HB2	2.17	0.43
2:C:2283:LYS:HD3	2:C:2285:TYR:HE1	1.82	0.43
2:C:2497:ARG:NH2	2:C:2870:LEU:HA	2.33	0.43
2:C:2975:PHE:CE2	2:C:3036:LEU:HD13	2.53	0.43
2:C:3137:LEU:HA	2:C:3140:LEU:HD12	1.99	0.43
2:C:4060:GLN:O	2:C:4064:GLU:OE1	2.36	0.43
2:C:4565:SER:HB2	2:C:4567:TYR:CD2	2.54	0.43
2:A:655:MET:HE1	2:A:836:HIS:HA	2.00	0.43
2:A:904:TYR:HB2	2:A:918:LEU:HD23	1.99	0.43
2:A:2967:VAL:HA	2:A:2970:LEU:HG	2.01	0.43
2:A:3178:HIS:CD2	2:A:3263:MET:HA	2.53	0.43
2:D:853:PRO:HD3	2:D:1086:ARG:HB2	1.99	0.43
2:D:3016:ARG:O	2:D:3018:ARG:NH1	2.51	0.43
2:D:4177:VAL:HB	2:D:4880:VAL:HG22	2.00	0.43
2:B:219:SER:H	2:B:349:MET:CE	2.30	0.43
2:B:219:SER:H	2:B:349:MET:HE3	1.83	0.43
2:B:2500:ALA:HB1	2:B:2554:ARG:NH2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2666:LEU:HB3	2:B:2667:PRO:HD3	2.00	0.43
2:B:2975:PHE:CE2	2:B:3036:LEU:HD13	2.53	0.43
2:B:3228:TYR:CE1	2:B:3232:PRO:HB3	2.53	0.43
2:C:641:ASP:OD2	2:C:641:ASP:N	2.51	0.43
2:C:1421:MET:HE2	2:C:1576:LYS:HD2	1.99	0.43
2:C:1725:TYR:CE2	2:C:2101:ALA:HB1	2.53	0.43
2:C:2500:ALA:HB1	2:C:2554:ARG:HH22	1.83	0.43
2:C:2729:HIS:CD2	2:C:2760:TYR:HB2	2.52	0.43
2:C:3061:LEU:HD13	2:C:3126:VAL:HG13	2.00	0.43
2:A:641:ASP:N	2:A:641:ASP:OD2	2.51	0.43
2:A:1725:TYR:CE2	2:A:2101:ALA:HB1	2.53	0.43
2:A:2685:TYR:HB2	2:A:2909:ASP:OD1	2.17	0.43
2:A:3148:VAL:O	2:A:3152:ARG:HG3	2.18	0.43
2:A:3846:LEU:HD13	2:A:3854:PHE:CZ	2.53	0.43
1:E:63:GLY:HA3	1:E:75:LEU:HD21	2.00	0.43
2:D:114:LEU:HA	2:D:174:LYS:HA	2.00	0.43
2:D:1810:VAL:HB	2:D:1817:LEU:HD13	2.00	0.43
2:D:3148:VAL:O	2:D:3152:ARG:HG3	2.18	0.43
2:D:4565:SER:HB2	2:D:4567:TYR:CD2	2.54	0.43
2:B:114:LEU:HA	2:B:174:LYS:HA	2.00	0.43
2:B:956:HIS:O	2:B:960:LYS:HG3	2.17	0.43
2:B:1077:VAL:HG13	2:B:1077:VAL:O	2.18	0.43
2:B:1725:TYR:CE2	2:B:2101:ALA:HB1	2.53	0.43
2:B:2620:TYR:HB2	2:B:2627:TRP:CD1	2.53	0.43
2:B:2927:GLN:OE1	2:B:3003:MET:HG2	2.18	0.43
2:B:3278:GLY:O	2:B:3281:LEU:HG	2.19	0.43
2:B:3777:MET:SD	2:B:3846:LEU:HD21	2.59	0.43
2:B:3846:LEU:HD13	2:B:3854:PHE:CZ	2.53	0.43
2:C:1979:PHE:HB2	2:C:3628:TRP:CZ2	2.52	0.43
2:C:2791:ARG:HA	2:C:2901:TYR:HA	2.01	0.43
2:C:3926:GLY:CA	2:C:4935:GLY:HA3	2.47	0.43
2:C:4177:VAL:HB	2:C:4880:VAL:HG22	1.99	0.43
2:A:934:GLN:HA	2:A:937:LEU:HD12	1.99	0.43
2:A:3278:GLY:O	2:A:3281:LEU:HG	2.19	0.43
2:A:3777:MET:SD	2:A:3846:LEU:HD21	2.59	0.43
2:A:4304:GLY:O	2:A:4308:ILE:HG12	2.18	0.43
2:D:570:GLY:O	2:D:574:VAL:HG23	2.18	0.43
2:D:897:LYS:HB2	2:D:915:HIS:CE1	2.53	0.43
2:D:2728:SER:HA	2:D:2731:LYS:NZ	2.33	0.43
2:D:3061:LEU:HD13	2:D:3126:VAL:HG13	2.00	0.43
2:D:3316:LYS:O	2:D:3317:THR:OG1	2.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:LEU:HD21	2:B:277:LEU:HD13	2.00	0.43
2:B:2791:ARG:HE	2:B:2795:GLY:C	2.22	0.43
2:B:3074:ASN:HD21	2:B:3093:ILE:HD11	1.81	0.43
2:C:246:THR:HG22	2:C:247:VAL:O	2.18	0.43
2:C:2567:ASP:O	2:C:2571:VAL:HG23	2.18	0.43
2:C:2791:ARG:HE	2:C:2795:GLY:C	2.22	0.43
2:C:3846:LEU:HD13	2:C:3854:PHE:CZ	2.54	0.43
2:C:4197:ILE:HG12	2:C:4923:MET:HE2	2.00	0.43
2:C:4304:GLY:O	2:C:4308:ILE:HG12	2.18	0.43
2:A:1436:GLN:NE2	2:A:1546:GLN:O	2.51	0.43
2:A:1810:VAL:HB	2:A:1817:LEU:HD13	2.00	0.43
2:A:2500:ALA:HB1	2:A:2554:ARG:NH2	2.33	0.43
2:A:3612:PRO:HG2	2:A:3615:ARG:HG3	2.01	0.43
2:A:4045:LYS:NZ	2:A:4072:THR:HA	2.34	0.43
2:D:472:HIS:O	2:D:476:GLN:HG2	2.17	0.43
2:D:1815:GLU:O	2:D:1819:VAL:HB	2.19	0.43
2:D:2852:TRP:O	2:D:2856:LYS:HE2	2.17	0.43
2:D:2967:VAL:HA	2:D:2970:LEU:HG	2.01	0.43
2:D:3138:TYR:CZ	2:D:3209:PRO:HD3	2.54	0.43
2:D:3278:GLY:O	2:D:3281:LEU:HG	2.19	0.43
2:D:3846:LEU:HD13	2:D:3854:PHE:CZ	2.54	0.43
2:D:4172:PHE:CZ	2:D:4189:PHE:HA	2.53	0.43
2:B:2668:CYS:O	2:B:2672:VAL:HG23	2.18	0.43
2:B:2791:ARG:HA	2:B:2901:TYR:HA	2.01	0.43
2:B:3138:TYR:CZ	2:B:3209:PRO:HD3	2.54	0.43
2:B:4781:TYR:HD1	2:B:4846:PHE:CE1	2.37	0.43
2:C:1717:ALA:HA	2:C:1720:MET:HE2	2.01	0.43
2:C:2758:LYS:HB2	2:C:2762:LEU:HB2	2.01	0.43
2:A:1815:GLU:O	2:A:1819:VAL:HB	2.19	0.43
2:A:1847:GLU:HG3	2:A:1850:VAL:H	1.83	0.43
2:A:2444:THR:O	2:A:2452:VAL:N	2.42	0.43
2:A:2668:CYS:O	2:A:2672:VAL:HG23	2.18	0.43
2:A:2764:SER:O	2:A:2768:LYS:HG3	2.18	0.43
2:A:2975:PHE:CE2	2:A:3036:LEU:HD13	2.53	0.43
2:A:4252:ILE:HG21	2:B:4707:MET:HG3	2.01	0.43
2:D:558:LEU:HG	2:D:571:ILE:HG23	2.01	0.43
2:D:737:ILE:HG21	2:D:1534:GLU:OE1	2.19	0.43
2:D:2172:MET:O	2:D:2176:VAL:HG23	2.17	0.43
2:D:3649:ALA:C	2:D:3652:PRO:HD2	2.39	0.43
2:D:3956:MET:HG2	2:D:4065:PHE:CZ	2.54	0.43
2:D:4060:GLN:O	2:D:4064:GLU:OE1	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2856:LYS:HA	2:B:2859:GLU:CG	2.44	0.43
2:B:3129:SER:HA	2:B:3132:ARG:HE	1.84	0.43
2:B:4172:PHE:CZ	2:B:4189:PHE:HA	2.53	0.43
2:B:4565:SER:HB2	2:B:4567:TYR:CD2	2.53	0.43
2:C:114:LEU:HA	2:C:174:LYS:HA	2.00	0.43
2:C:293:GLN:HB2	2:C:343:ARG:HH22	1.83	0.43
2:C:586:LEU:HD22	2:C:617:LEU:HD23	2.00	0.43
2:C:943:LEU:O	2:C:948:CYS:N	2.43	0.43
2:C:1282:CYS:SG	2:C:1556:GLU:HG2	2.59	0.43
2:C:3138:TYR:CZ	2:C:3209:PRO:HD3	2.54	0.43
2:C:4045:LYS:NZ	2:C:4072:THR:HA	2.34	0.43
2:C:4136:ILE:HG23	2:C:4150:PHE:HE1	1.83	0.43
2:A:274:LEU:HD23	2:A:274:LEU:HA	1.85	0.43
2:A:2833:LEU:HB2	2:A:2838[B]:HIS:ND1	2.33	0.43
2:A:4283:PHE:HE2	2:B:4495:PHE:CE2	2.36	0.43
2:D:20:VAL:HG12	2:D:216:PRO:HA	2.00	0.43
2:D:1282:CYS:SG	2:D:1556:GLU:HG2	2.59	0.43
2:D:3137:LEU:HA	2:D:3140:LEU:HD12	1.99	0.43
2:D:4136:ILE:HG23	2:D:4150:PHE:HE1	1.83	0.43
2:D:4304:GLY:O	2:D:4308:ILE:HG12	2.18	0.43
2:B:485:ARG:O	2:B:489:PHE:HB2	2.18	0.43
2:B:2967:VAL:HA	2:B:2970:LEU:HG	2.01	0.43
2:C:485:ARG:O	2:C:489:PHE:HB2	2.18	0.43
2:C:3016:ARG:O	2:C:3018:ARG:NH1	2.51	0.43
2:C:3668:ILE:HD13	2:C:3736:ALA:HB2	1.99	0.43
2:C:4781:TYR:HD1	2:C:4846:PHE:CE1	2.37	0.43
2:A:485:ARG:O	2:A:489:PHE:HB2	2.18	0.43
2:A:570:GLY:O	2:A:574:VAL:HG23	2.18	0.43
2:A:737:ILE:HG21	2:A:1534:GLU:OE1	2.19	0.43
2:A:1282:CYS:SG	2:A:1556:GLU:HG2	2.59	0.43
2:A:1651:LEU:HD12	2:A:1698:LEU:HG	2.00	0.43
2:A:2229:LEU:HD12	2:A:2297:ARG:HB3	2.01	0.43
2:A:2925:PHE:CZ	2:A:2970:LEU:HD13	2.54	0.43
2:A:3016:ARG:HA	2:A:3096:TYR:OH	2.19	0.43
2:A:3129:SER:HA	2:A:3132:ARG:HE	1.84	0.43
2:A:3800:CYS:O	2:A:3880:ARG:NH2	2.52	0.43
2:A:4177:VAL:HB	2:A:4880:VAL:HG22	2.00	0.43
2:D:485:ARG:O	2:D:489:PHE:HB2	2.18	0.43
2:D:675:TYR:CE1	2:D:790:PRO:HB3	2.54	0.43
2:D:1699:ARG:O	2:D:1703:TYR:HB2	2.18	0.43
2:D:2229:LEU:HD12	2:D:2297:ARG:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2638:LEU:HD23	2:D:2638:LEU:HA	1.83	0.43
2:D:2791:ARG:HA	2:D:2901:TYR:HA	2.01	0.43
2:D:2849:HIS:HD2	2:D:2852:TRP:HE3	1.65	0.43
2:D:3016:ARG:HA	2:D:3096:TYR:OH	2.19	0.43
2:D:3612:PRO:HG2	2:D:3615:ARG:HG3	2.01	0.43
2:D:4107:GLU:OE1	2:D:4147:ARG:NH1	2.43	0.43
2:B:20:VAL:HG12	2:B:216:PRO:HA	2.00	0.43
2:B:570:GLY:O	2:B:574:VAL:HG23	2.18	0.43
2:B:675:TYR:CE1	2:B:790:PRO:HB3	2.54	0.43
2:B:897:LYS:HB2	2:B:915:HIS:CE1	2.53	0.43
2:B:1118:SER:HB3	2:B:1204:VAL:HG11	2.00	0.43
2:B:2500:ALA:HB1	2:B:2554:ARG:HH22	1.82	0.43
2:B:2849:HIS:HD2	2:B:2852:TRP:HE3	1.65	0.43
2:B:3697:LYS:HG3	2:B:3700:HIS:HE2	1.83	0.43
2:B:4045:LYS:NZ	2:B:4072:THR:HA	2.34	0.43
2:B:4964:ASP:N	2:B:4964:ASP:OD1	2.50	0.43
2:C:675:TYR:CE1	2:C:790:PRO:HB3	2.54	0.43
2:C:1699:ARG:O	2:C:1703:TYR:HB2	2.18	0.43
2:C:2666:LEU:HB3	2:C:2667:PRO:HD3	2.00	0.43
2:C:2925:PHE:CZ	2:C:2970:LEU:HD13	2.54	0.43
2:A:114:LEU:HA	2:A:174:LYS:HA	2.00	0.43
2:A:2791:ARG:HA	2:A:2901:TYR:HA	2.01	0.43
2:A:2975:PHE:HB3	2:A:2979:ARG:NH2	2.32	0.43
2:A:3956:MET:HG2	2:A:4065:PHE:CZ	2.54	0.43
2:D:293:GLN:HB2	2:D:343:ARG:HH22	1.83	0.43
2:D:1433:PHE:HB3	2:C:2830:ASN:ND2	2.34	0.43
2:D:2640:LEU:HA	2:D:2643:LYS:HZ3	1.82	0.43
2:D:2666:LEU:HB3	2:D:2667:PRO:HD3	2.00	0.43
2:D:3830:LEU:HD11	2:D:3909:ALA:HB2	2.01	0.43
2:B:1979:PHE:CD1	2:B:1993:ARG:HG2	2.54	0.43
2:B:2054:LYS:NZ	2:B:2056:SER:OG	2.31	0.43
2:B:3612:PRO:HG2	2:B:3615:ARG:HG3	2.01	0.43
2:B:4177:VAL:HB	2:B:4880:VAL:HG22	2.00	0.43
2:C:2173:GLU:HA	2:C:2176:VAL:HB	2.00	0.43
2:C:3232:PRO:HA	2:C:3235:MET:HE2	2.01	0.43
2:C:3777:MET:SD	2:C:3846:LEU:HD21	2.59	0.43
2:A:1048:ASP:OD1	2:A:1049:SER:N	2.52	0.42
2:A:2758:LYS:HB2	2:A:2762:LEU:HB2	2.00	0.42
2:A:3011:LEU:HD23	2:A:3011:LEU:HA	1.94	0.42
2:A:3697:LYS:HG3	2:A:3700:HIS:HE2	1.83	0.42
2:A:3890:TRP:O	2:B:76:ARG:NH1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:468:GLU:HA	2:D:475:LYS:NZ	2.34	0.42
2:D:898:ILE:HD13	2:D:918:LEU:HD21	2.01	0.42
2:D:1048:ASP:OD1	2:D:1049:SER:N	2.52	0.42
2:D:2492:PHE:O	2:D:2496:LEU:N	2.45	0.42
2:D:2497:ARG:NH2	2:D:2870:LEU:HA	2.33	0.42
2:D:2975:PHE:CE2	2:D:3036:LEU:HD13	2.53	0.42
2:B:558:LEU:HG	2:B:571:ILE:HG23	2.01	0.42
2:B:1048:ASP:OD1	2:B:1049:SER:N	2.52	0.42
2:B:2758:LYS:HB2	2:B:2762:LEU:HB2	2.00	0.42
2:B:3016:ARG:HA	2:B:3096:TYR:OH	2.19	0.42
2:B:3800:CYS:O	2:B:3880:ARG:NH2	2.52	0.42
2:B:3956:MET:HG2	2:B:4065:PHE:CZ	2.54	0.42
2:B:4107:GLU:OE1	2:B:4147:ARG:NH1	2.43	0.42
2:B:4264:LEU:HG	2:C:4694:LEU:HD21	2.00	0.42
2:C:20:VAL:HG12	2:C:216:PRO:HA	1.99	0.42
2:C:274:LEU:HD23	2:C:274:LEU:HA	1.85	0.42
2:C:1048:ASP:OD1	2:C:1049:SER:N	2.52	0.42
2:C:2729:HIS:O	2:C:2732:TRP:HB3	2.19	0.42
2:C:3830:LEU:HD11	2:C:3909:ALA:HB2	2.01	0.42
2:A:20:VAL:HG12	2:A:216:PRO:HA	2.00	0.42
2:A:1973:ILE:HB	2:A:3608:LEU:HD21	2.01	0.42
2:A:4136:ILE:HG23	2:A:4150:PHE:HE1	1.83	0.42
2:A:4807:ASP:O	2:D:4522:VAL:HG12	2.18	0.42
2:A:4834:PRO:HB3	2:A:4843:ARG:HH11	1.85	0.42
2:A:4964:ASP:N	2:A:4964:ASP:OD1	2.50	0.42
2:D:2758:LYS:HB2	2:D:2762:LEU:HB2	2.00	0.42
2:D:4043:ILE:HG23	2:D:4048:PHE:CE2	2.55	0.42
2:B:3016:ARG:O	2:B:3018:ARG:NH1	2.51	0.42
2:C:1847:GLU:HG3	2:C:1850:VAL:H	1.83	0.42
2:C:1915:ASP:OD1	2:C:2090:ARG:NH1	2.51	0.42
2:C:1979:PHE:CD1	2:C:1993:ARG:HG2	2.54	0.42
2:C:2773:TRP:HB3	2:C:2774:PRO:HD3	2.02	0.42
2:C:2968:LEU:HB2	2:C:2969:PRO:HD3	2.01	0.42
2:C:3972:MET:O	2:C:4094:ILE:HD11	2.20	0.42
2:A:606:ARG:HH21	2:A:1633:PRO:HD2	1.84	0.42
2:A:814:LEU:HD12	2:A:815:PRO:HD2	2.02	0.42
2:A:3027:THR:HA	2:A:3030:VAL:HG12	2.02	0.42
2:A:3649:ALA:C	2:A:3652:PRO:HD2	2.39	0.42
2:A:3830:LEU:HD11	2:A:3909:ALA:HB2	2.01	0.42
2:A:4107:GLU:OE1	2:A:4147:ARG:NH1	2.43	0.42
2:A:4565:SER:HB2	2:A:4567:TYR:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2173:GLU:HA	2:D:2176:VAL:HB	2.00	0.42
2:D:2732:TRP:CH2	2:D:2756:LEU:HB3	2.51	0.42
2:D:2791:ARG:HE	2:D:2795:GLY:C	2.22	0.42
2:D:3296:MET:HE3	2:D:3296:MET:HB2	1.98	0.42
2:D:4136:ILE:HG22	2:D:4917:ASN:HB3	2.01	0.42
2:D:4616:TYR:CE2	2:D:4632:ARG:HG2	2.53	0.42
2:D:4781:TYR:HD1	2:D:4846:PHE:CE1	2.37	0.42
2:B:2729:HIS:O	2:B:2732:TRP:HB3	2.19	0.42
2:C:630:HIS:CE1	2:C:1671:ARG:HE	2.38	0.42
2:C:3016:ARG:HA	2:C:3096:TYR:OH	2.19	0.42
2:A:2620:TYR:HB2	2:A:2627:TRP:CD1	2.53	0.42
2:A:4616:TYR:CE2	2:A:4632:ARG:HG2	2.53	0.42
2:D:630:HIS:CE1	2:D:1671:ARG:HE	2.38	0.42
2:D:695:VAL:O	2:D:727:PHE:N	2.44	0.42
2:D:1973:ILE:HB	2:D:3608:LEU:HD21	2.02	0.42
2:D:2927:GLN:OE1	2:D:3003:MET:HG2	2.18	0.42
2:D:3228:TYR:H	2:D:3290:ILE:HG21	1.85	0.42
2:B:814:LEU:HD12	2:B:815:PRO:HD2	2.02	0.42
2:B:1699:ARG:O	2:B:1703:TYR:HB2	2.19	0.42
2:B:3304:GLN:HB3	2:B:3305:PRO:HD3	2.01	0.42
2:B:3649:ALA:C	2:B:3652:PRO:HD2	2.39	0.42
2:C:1118:SER:HB3	2:C:1204:VAL:HG11	2.00	0.42
2:C:1272:ARG:NH2	2:C:1582:CYS:SG	2.93	0.42
2:C:3027:THR:HA	2:C:3030:VAL:HG12	2.02	0.42
2:C:3602:CYS:HA	2:C:3605:MET:CE	2.50	0.42
2:C:3612:PRO:HG2	2:C:3615:ARG:HG3	2.01	0.42
2:C:3956:MET:HG2	2:C:4065:PHE:CZ	2.54	0.42
2:A:558:LEU:HG	2:A:571:ILE:HG23	2.00	0.42
2:A:675:TYR:CE1	2:A:790:PRO:HB3	2.54	0.42
2:A:2258:ARG:HB3	2:A:2260:PRO:HD2	2.02	0.42
2:A:3010:LYS:O	2:A:3014:LEU:HD23	2.20	0.42
2:A:3175:LEU:O	2:A:3175:LEU:HD23	2.19	0.42
2:A:4136:ILE:HG22	2:A:4917:ASN:HB3	2.01	0.42
2:A:4781:TYR:HD1	2:A:4846:PHE:CE1	2.37	0.42
1:E:63:GLY:O	1:E:67:MET:HG2	2.20	0.42
2:D:856:SER:HB3	2:D:1078:CYS:SG	2.60	0.42
2:D:881:ILE:HD13	2:D:1062:TYR:CZ	2.55	0.42
2:D:2773:TRP:HB3	2:D:2774:PRO:HD3	2.02	0.42
2:D:4048:PHE:CZ	2:D:4080:TYR:HB3	2.55	0.42
2:B:538:ALA:O	2:B:542:ARG:HB2	2.20	0.42
2:B:2840:MET:HB3	2:B:2840:MET:HE3	1.98	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2925:PHE:CZ	2:B:2970:LEU:HD13	2.54	0.42
2:B:3602:CYS:HA	2:B:3605:MET:CE	2.50	0.42
2:B:4043:ILE:HG23	2:B:4048:PHE:CE2	2.55	0.42
2:C:856:SER:HB3	2:C:1078:CYS:SG	2.60	0.42
2:C:881:ILE:HD13	2:C:1062:TYR:CZ	2.55	0.42
2:C:2935:GLU:O	2:C:2938:GLN:N	2.53	0.42
2:C:3010:LYS:O	2:C:3014:LEU:HD23	2.20	0.42
2:C:3175:LEU:HD23	2:C:3175:LEU:O	2.19	0.42
2:A:2935:GLU:O	2:A:2938:GLN:N	2.53	0.42
2:A:3222:ALA:HB1	2:A:3282:LYS:HG2	2.02	0.42
2:A:3972:MET:O	2:A:4094:ILE:HD11	2.19	0.42
1:E:19:LYS:HD3	1:E:19:LYS:HA	1.85	0.42
2:D:814:LEU:HD12	2:D:815:PRO:HD2	2.01	0.42
2:D:1979:PHE:CD1	2:D:1993:ARG:HG2	2.54	0.42
2:D:3129:SER:HA	2:D:3132:ARG:HE	1.84	0.42
2:D:3777:MET:SD	2:D:3846:LEU:HD21	2.59	0.42
2:B:131:CYS:SG	2:B:150:GLN:HB2	2.60	0.42
2:B:641:ASP:OD2	2:B:641:ASP:N	2.51	0.42
2:B:718:VAL:HG23	2:B:793:SER:HB3	2.01	0.42
2:B:1973:ILE:HB	2:B:3608:LEU:HD21	2.02	0.42
2:B:3175:LEU:O	2:B:3175:LEU:HD23	2.19	0.42
2:B:3972:MET:O	2:B:4094:ILE:HD11	2.20	0.42
2:B:4616:TYR:CE2	2:B:4632:ARG:HG2	2.53	0.42
2:C:2638:LEU:HD23	2:C:2638:LEU:HA	1.83	0.42
2:C:3129:SER:HA	2:C:3132:ARG:HE	1.84	0.42
2:C:3304:GLN:HB3	2:C:3305:PRO:HD3	2.01	0.42
2:C:3972:MET:HE3	2:C:4094:ILE:HD12	2.02	0.42
2:A:1249:MET:HB2	2:A:1599:MET:HB3	2.02	0.42
2:A:1272:ARG:NH2	2:A:1582:CYS:SG	2.93	0.42
2:A:2729:HIS:O	2:A:2732:TRP:HB3	2.19	0.42
2:A:2927:GLN:OE1	2:A:3003:MET:HG2	2.18	0.42
2:A:3138:TYR:CZ	2:A:3209:PRO:HD3	2.54	0.42
1:F:63:GLY:O	1:F:67:MET:HG2	2.20	0.42
2:D:2925:PHE:CZ	2:D:2970:LEU:HD13	2.54	0.42
2:D:3187:LYS:O	2:D:3191:GLU:HB2	2.20	0.42
2:B:630:HIS:CE1	2:B:1671:ARG:HE	2.38	0.42
2:B:737:ILE:HG21	2:B:1534:GLU:OE1	2.19	0.42
2:B:2258:ARG:HB3	2:B:2260:PRO:HD2	2.02	0.42
2:B:3222:ALA:HB1	2:B:3282:LYS:HG2	2.02	0.42
2:B:3600:VAL:O	2:B:3604:ARG:HD3	2.20	0.42
2:C:919:VAL:HG12	2:C:920:GLU:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2849:HIS:HD2	2:C:2852:TRP:HE3	1.65	0.42
2:C:3649:ALA:C	2:C:3652:PRO:HD2	2.39	0.42
2:A:468:GLU:HA	2:A:475:LYS:NZ	2.34	0.42
2:A:630:HIS:CE1	2:A:1671:ARG:HE	2.38	0.42
2:A:1697:LEU:HD23	2:A:1697:LEU:HA	1.87	0.42
2:A:1839:LEU:HA	2:A:1842:ILE:HG22	2.02	0.42
2:A:1979:PHE:CD1	2:A:1993:ARG:HG2	2.54	0.42
2:A:2791:ARG:HE	2:A:2795:GLY:C	2.22	0.42
2:A:3159:LEU:HB3	2:A:3241:MET:HG2	2.02	0.42
2:A:3602:CYS:HA	2:A:3605:MET:CE	2.50	0.42
2:A:3955:GLN:HG2	2:A:4016:PHE:CE2	2.55	0.42
2:A:4602:ARG:NH1	2:A:4631:ASP:OD1	2.53	0.42
2:A:4872:GLU:CD	2:D:4874:ARG:HD2	2.40	0.42
2:D:1272:ARG:NH2	2:D:1582:CYS:SG	2.93	0.42
2:D:1304:LEU:HD23	2:D:1304:LEU:HA	1.92	0.42
2:D:2935:GLU:O	2:D:2938:GLN:N	2.53	0.42
2:D:3027:THR:HA	2:D:3030:VAL:HG12	2.02	0.42
2:D:3961:ASP:OD2	2:D:3963:SER:OG	2.32	0.42
2:D:4045:LYS:NZ	2:D:4072:THR:HA	2.34	0.42
2:B:919:VAL:HG12	2:B:920:GLU:N	2.34	0.42
2:B:1719:LEU:HA	2:B:1722:ASN:HB2	2.02	0.42
2:B:2571:VAL:HA	2:B:2574:LEU:CD2	2.50	0.42
2:B:3159:LEU:HB3	2:B:3241:MET:HG2	2.02	0.42
2:B:3830:LEU:HD11	2:B:3909:ALA:HB2	2.01	0.42
2:B:4136:ILE:HG22	2:B:4917:ASN:HB3	2.01	0.42
2:B:4136:ILE:HG23	2:B:4150:PHE:HE1	1.83	0.42
2:C:737:ILE:HG21	2:C:1534:GLU:OE1	2.19	0.42
2:C:814:LEU:HD12	2:C:815:PRO:HD2	2.02	0.42
2:C:1719:LEU:HA	2:C:1722:ASN:HB2	2.02	0.42
2:C:1819:VAL:HG23	2:C:1902:VAL:HG22	2.01	0.42
2:C:3159:LEU:HB3	2:C:3241:MET:HG2	2.02	0.42
2:C:3228:TYR:H	2:C:3290:ILE:HG21	1.85	0.42
2:C:3600:VAL:O	2:C:3604:ARG:HD3	2.20	0.42
2:C:3800:CYS:O	2:C:3880:ARG:NH2	2.52	0.42
2:A:1014:GLN:O	2:A:1027:ARG:NH2	2.53	0.42
2:A:1118:SER:HB3	2:A:1204:VAL:HG11	2.00	0.42
2:A:2095:ILE:HD11	2:A:3629:ILE:HG23	2.02	0.42
2:A:2571:VAL:HA	2:A:2574:LEU:CD2	2.50	0.42
2:A:2772:ARG:HA	2:A:2772:ARG:HD3	1.90	0.42
2:A:2935:GLU:O	2:A:2939:TYR:CD1	2.67	0.42
2:D:2729:HIS:O	2:D:2732:TRP:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2935:GLU:O	2:D:2939:TYR:CD1	2.67	0.42
2:D:3042:ALA:HB3	2:D:3117:PHE:HB3	2.02	0.42
2:D:3972:MET:O	2:D:4094:ILE:HD11	2.19	0.42
2:D:4602:ARG:NH1	2:D:4631:ASP:OD1	2.53	0.42
2:B:1819:VAL:HG23	2:B:1902:VAL:HG22	2.02	0.42
2:B:2139:GLU:O	2:B:2192:MET:HE3	2.20	0.42
2:B:2539:GLU:HB2	2:B:2581:ARG:HD3	2.02	0.42
2:B:3027:THR:HA	2:B:3030:VAL:HG12	2.02	0.42
2:C:558:LEU:HG	2:C:571:ILE:HG23	2.00	0.42
2:C:898:ILE:HD13	2:C:918:LEU:HD21	2.01	0.42
2:C:1810:VAL:HB	2:C:1817:LEU:HD13	2.00	0.42
2:C:1973:ILE:HB	2:C:3608:LEU:HD21	2.01	0.42
2:C:4048:PHE:CZ	2:C:4080:TYR:HB3	2.55	0.42
2:C:4602:ARG:NH1	2:C:4631:ASP:OD1	2.53	0.42
2:A:943:LEU:O	2:A:948:CYS:N	2.43	0.42
2:A:2732:TRP:CH2	2:A:2756:LEU:HB3	2.51	0.42
2:A:2773:TRP:HB3	2:A:2774:PRO:HD3	2.02	0.42
2:A:2930:ILE:HG23	2:A:3010:LYS:HZ1	1.85	0.42
1:G:26:HIS:CD2	1:G:41:ARG:HG2	2.55	0.42
2:D:606:ARG:HH21	2:D:1633:PRO:HD2	1.84	0.42
2:D:919:VAL:HG12	2:D:920:GLU:N	2.34	0.42
2:D:2139:GLU:O	2:D:2192:MET:HE3	2.20	0.42
2:D:3955:GLN:HG2	2:D:4016:PHE:CE2	2.55	0.42
2:B:709:GLY:HA3	2:B:723:PHE:CD1	2.55	0.42
2:B:881:ILE:HD13	2:B:1062:TYR:CZ	2.55	0.42
2:B:1272:ARG:NH2	2:B:1582:CYS:SG	2.93	0.42
2:B:1810:VAL:HB	2:B:1817:LEU:HD13	2.00	0.42
2:B:2095:ILE:HD11	2:B:3629:ILE:HG23	2.02	0.42
2:B:2773:TRP:HB3	2:B:2774:PRO:HD3	2.02	0.42
2:B:3138:TYR:CG	2:B:3208:ILE:HG13	2.55	0.42
2:C:538:ALA:O	2:C:542:ARG:HB2	2.20	0.42
2:C:1021:GLN:NE2	2:C:1022:GLN:O	2.53	0.42
2:C:1815:GLU:O	2:C:1819:VAL:HB	2.19	0.42
2:C:2095:ILE:HD11	2:C:3629:ILE:HG23	2.02	0.42
2:C:3955:GLN:HG2	2:C:4016:PHE:CE2	2.55	0.42
1:H:63:GLY:O	1:H:67:MET:HG2	2.20	0.41
2:A:709:GLY:HA3	2:A:723:PHE:CD1	2.55	0.41
2:A:856:SER:HB3	2:A:1078:CYS:SG	2.60	0.41
2:A:881:ILE:HD13	2:A:1062:TYR:CZ	2.55	0.41
2:A:1497:GLY:O	2:A:1499:GLY:N	2.53	0.41
2:A:1719:LEU:HA	2:A:1722:ASN:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4043:ILE:HG23	2:A:4048:PHE:CE2	2.55	0.41
1:G:63:GLY:O	1:G:67:MET:HG2	2.20	0.41
2:D:1014:GLN:O	2:D:1027:ARG:NH2	2.53	0.41
2:D:1265:HIS:CE1	2:D:1268:ILE:HG13	2.55	0.41
2:D:1839:LEU:HA	2:D:1842:ILE:HG22	2.02	0.41
2:D:2389:MET:HG3	2:D:2464:HIS:CE1	2.55	0.41
2:D:2891:ASP:OD1	2:D:2892:ILE:N	2.53	0.41
2:D:3600:VAL:O	2:D:3604:ARG:HD3	2.20	0.41
2:D:3800:CYS:O	2:D:3880:ARG:NH2	2.52	0.41
2:B:419:ILE:HG21	2:B:492:GLU:HG3	2.02	0.41
2:B:1497:GLY:O	2:B:1499:GLY:N	2.53	0.41
2:B:1815:GLU:O	2:B:1819:VAL:HB	2.19	0.41
2:B:1839:LEU:HA	2:B:1842:ILE:HG22	2.02	0.41
2:B:3228:TYR:H	2:B:3290:ILE:HG21	1.85	0.41
2:B:4602:ARG:NH1	2:B:4631:ASP:OD1	2.53	0.41
2:C:468:GLU:HA	2:C:475:LYS:NZ	2.34	0.41
2:C:514:PHE:HD2	2:C:526:TRP:HB2	1.85	0.41
2:C:1014:GLN:O	2:C:1027:ARG:NH2	2.53	0.41
2:C:2772:ARG:HA	2:C:2772:ARG:HD3	1.90	0.41
2:C:3187:LYS:O	2:C:3191:GLU:HB2	2.20	0.41
2:C:4964:ASP:N	2:C:4964:ASP:OD1	2.50	0.41
2:A:375:GLN:O	2:A:376:SER:OG	2.32	0.41
2:A:538:ALA:O	2:A:542:ARG:HB2	2.20	0.41
2:A:600:LEU:O	2:A:604:HIS:HB2	2.20	0.41
2:A:1265:HIS:CE1	2:A:1268:ILE:HG13	2.55	0.41
2:A:2891:ASP:OD1	2:A:2892:ILE:N	2.53	0.41
2:A:2968:LEU:HB2	2:A:2969:PRO:HD3	2.01	0.41
2:A:3237:VAL:O	2:A:3240:PRO:HD2	2.21	0.41
2:A:3249:TRP:HE3	2:A:3266:THR:HG21	1.86	0.41
2:A:3279:ASN:O	2:A:3283:ILE:HD12	2.21	0.41
2:D:600:LEU:O	2:D:604:HIS:HB2	2.20	0.41
2:D:1249:MET:HB2	2:D:1599:MET:HB3	2.02	0.41
2:D:1497:GLY:O	2:D:1499:GLY:N	2.53	0.41
2:D:1719:LEU:HA	2:D:1722:ASN:HB2	2.02	0.41
2:D:2689:MET:HG3	2:D:2689:MET:O	2.20	0.41
2:D:3304:GLN:HB3	2:D:3305:PRO:HD3	2.01	0.41
2:B:468:GLU:HA	2:B:475:LYS:NZ	2.34	0.41
2:B:606:ARG:HH21	2:B:1633:PRO:HD2	1.84	0.41
2:B:2935:GLU:O	2:B:2938:GLN:N	2.53	0.41
2:B:2939:TYR:CD2	2:B:2956:TYR:CD2	3.09	0.41
2:B:3246:MET:SD	2:B:3247:SER:N	2.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3279:ASN:O	2:B:3283:ILE:HD12	2.21	0.41
2:C:131:CYS:SG	2:C:150:GLN:HB2	2.60	0.41
2:C:2229:LEU:HD12	2:C:2297:ARG:HB3	2.01	0.41
2:C:2721:ILE:HG22	2:C:2772:ARG:HH11	1.85	0.41
2:C:3138:TYR:CG	2:C:3208:ILE:HG13	2.55	0.41
2:C:3246:MET:SD	2:C:3247:SER:N	2.93	0.41
2:C:4043:ILE:HG23	2:C:4048:PHE:CE2	2.55	0.41
2:C:4305:PHE:HA	2:C:4308:ILE:HG12	2.03	0.41
2:A:898:ILE:HD13	2:A:918:LEU:HD21	2.01	0.41
2:A:919:VAL:HG12	2:A:920:GLU:N	2.35	0.41
2:A:1021:GLN:NE2	2:A:1022:GLN:O	2.53	0.41
2:D:538:ALA:O	2:D:542:ARG:HB2	2.20	0.41
2:D:718:VAL:HG23	2:D:793:SER:HB3	2.01	0.41
2:D:977:LYS:NZ	2:D:979:ALA:HB2	2.36	0.41
2:D:2095:ILE:HD11	2:D:3629:ILE:HG23	2.02	0.41
2:D:2571:VAL:HA	2:D:2574:LEU:CD2	2.50	0.41
2:D:3249:TRP:HE3	2:D:3266:THR:HG21	1.86	0.41
2:B:2389:MET:HG3	2:B:2464:HIS:CE1	2.55	0.41
2:B:2721:ILE:HG22	2:B:2772:ARG:HH11	1.85	0.41
2:B:3010:LYS:O	2:B:3014:LEU:HD23	2.20	0.41
2:B:3249:TRP:HE3	2:B:3266:THR:HG21	1.86	0.41
2:C:419:ILE:HG21	2:C:492:GLU:HG3	2.02	0.41
2:C:606:ARG:HH21	2:C:1633:PRO:HD2	1.84	0.41
2:C:964:MET:O	2:C:977:LYS:NZ	2.53	0.41
2:C:977:LYS:NZ	2:C:979:ALA:HB2	2.36	0.41
2:C:1839:LEU:HA	2:C:1842:ILE:HG22	2.02	0.41
2:C:2389:MET:HG3	2:C:2464:HIS:CE1	2.55	0.41
2:C:2689:MET:O	2:C:2689:MET:HG3	2.20	0.41
2:C:2716:LYS:O	2:C:2901:TYR:OH	2.39	0.41
2:C:3278:GLY:O	2:C:3281:LEU:HG	2.19	0.41
1:H:26:HIS:CD2	1:H:41:ARG:HG2	2.55	0.41
2:A:718:VAL:HG23	2:A:793:SER:HB3	2.01	0.41
2:A:1102:TYR:HD1	2:A:1165:MET:HG2	1.85	0.41
2:A:2539:GLU:HB2	2:A:2581:ARG:HD3	2.02	0.41
2:A:2566:ARG:HA	2:A:2569:ILE:HG12	2.02	0.41
2:A:2640:LEU:HA	2:A:2643:LYS:HZ3	1.86	0.41
2:A:2760:TYR:HD1	2:A:2763:LEU:HD22	1.86	0.41
2:A:3304:GLN:HB3	2:A:3305:PRO:HD3	2.01	0.41
2:D:21:VAL:HG13	2:D:217:ILE:HG13	2.02	0.41
2:D:419:ILE:HG21	2:D:492:GLU:HG3	2.02	0.41
2:D:1021:GLN:NE2	2:D:1022:GLN:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1585:ARG:NE	2:D:1634:GLU:OE1	2.53	0.41
2:D:2062:ILE:HG21	2:D:2087:LEU:HG	2.02	0.41
2:D:2566:ARG:HA	2:D:2569:ILE:HG12	2.02	0.41
2:D:2968:LEU:HB2	2:D:2969:PRO:HD3	2.01	0.41
2:D:3154:ALA:O	2:D:3157:GLU:HG3	2.21	0.41
2:D:3246:MET:SD	2:D:3247:SER:N	2.93	0.41
2:D:4305:PHE:HA	2:D:4308:ILE:HG12	2.03	0.41
2:B:856:SER:HB3	2:B:1078:CYS:SG	2.60	0.41
2:B:1021:GLN:NE2	2:B:1022:GLN:O	2.53	0.41
2:B:1436:GLN:NE2	2:B:1546:GLN:O	2.51	0.41
2:B:1915:ASP:OD1	2:B:2090:ARG:NH1	2.51	0.41
2:B:2229:LEU:HD12	2:B:2297:ARG:HB3	2.01	0.41
2:B:2566:ARG:HA	2:B:2569:ILE:HG12	2.03	0.41
2:B:2968:LEU:HB2	2:B:2969:PRO:HD3	2.01	0.41
2:B:3154:ALA:O	2:B:3157:GLU:HG3	2.21	0.41
2:B:3684:GLU:OE1	2:B:3754:MET:HG3	2.21	0.41
2:C:2054:LYS:NZ	2:C:2056:SER:OG	2.31	0.41
2:C:2725:ALA:HB1	2:C:2760:TYR:CZ	2.56	0.41
2:C:2939:TYR:CD2	2:C:2956:TYR:CD2	3.09	0.41
2:A:1419:PHE:CE2	2:A:1562:ASN:HB3	2.52	0.41
2:A:2725:ALA:HB1	2:A:2760:TYR:CZ	2.56	0.41
2:A:3246:MET:HG2	2:A:3276:LEU:HD22	2.02	0.41
2:A:3600:VAL:O	2:A:3604:ARG:HD3	2.20	0.41
2:A:4166:LYS:O	2:A:4170:ARG:HG3	2.21	0.41
2:D:514:PHE:HD2	2:D:526:TRP:HB2	1.85	0.41
2:D:709:GLY:HA3	2:D:723:PHE:CD1	2.55	0.41
2:D:882:ARG:CZ	2:D:933:LEU:HD23	2.51	0.41
2:D:2539:GLU:HB2	2:D:2581:ARG:HD3	2.02	0.41
2:D:2716:LYS:O	2:D:2901:TYR:OH	2.39	0.41
2:D:2760:TYR:HD1	2:D:2763:LEU:HD22	1.86	0.41
2:D:2859:GLU:O	2:D:2862:SER:OG	2.27	0.41
2:D:3159:LEU:HB3	2:D:3241:MET:HG2	2.02	0.41
2:D:3602:CYS:HA	2:D:3605:MET:CE	2.50	0.41
2:D:4261:LEU:HG	2:D:4263:SER:HB2	2.03	0.41
2:B:191:TYR:N	2:B:206:ALA:O	2.54	0.41
2:B:882:ARG:CZ	2:B:933:LEU:HD23	2.51	0.41
2:B:1064:LEU:HD12	2:B:1064:LEU:O	2.21	0.41
2:B:1102:TYR:HD1	2:B:1165:MET:HG2	1.85	0.41
2:B:1585:ARG:NE	2:B:1634:GLU:OE1	2.53	0.41
2:B:4048:PHE:CZ	2:B:4080:TYR:HB3	2.55	0.41
2:C:999:LEU:HD12	2:C:1050:LEU:HD21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1102:TYR:HD1	2:C:1165:MET:HG2	1.85	0.41
2:C:2566:ARG:HA	2:C:2569:ILE:HG12	2.03	0.41
2:C:2785:TRP:HE3	2:C:2787:TRP:NE1	2.19	0.41
2:A:1611:ILE:CG2	2:A:1615:GLN:HG3	2.50	0.41
2:A:2279:MET:HE2	2:A:2279:MET:HB2	1.83	0.41
2:A:2363:SER:O	2:A:2363:SER:OG	2.38	0.41
2:A:4261:LEU:HG	2:A:4263:SER:HB2	2.03	0.41
1:E:26:HIS:CD2	1:E:41:ARG:HG2	2.55	0.41
1:F:26:HIS:CD2	1:F:41:ARG:HG2	2.55	0.41
2:D:131:CYS:SG	2:D:150:GLN:HB2	2.60	0.41
2:D:1611:ILE:CG2	2:D:1615:GLN:HG3	2.51	0.41
2:D:2172:MET:HB2	2:D:2172:MET:HE2	1.85	0.41
2:D:2258:ARG:HB3	2:D:2260:PRO:HD2	2.01	0.41
2:D:2276:SER:HB2	2:D:2288:ILE:O	2.21	0.41
2:D:2721:ILE:HG22	2:D:2772:ARG:HH11	1.85	0.41
2:D:2725:ALA:HB1	2:D:2760:TYR:CZ	2.56	0.41
2:D:2785:TRP:HE3	2:D:2787:TRP:NE1	2.19	0.41
2:D:3175:LEU:O	2:D:3175:LEU:HD23	2.19	0.41
2:D:4679:PHE:O	2:D:4682:ALA:C	2.59	0.41
2:D:4834:PRO:HB3	2:D:4843:ARG:HH11	1.85	0.41
2:B:898:ILE:HD13	2:B:918:LEU:HD21	2.01	0.41
2:B:1265:HIS:CE1	2:B:1268:ILE:HG13	2.56	0.41
2:B:1282:CYS:SG	2:B:1556:GLU:HG2	2.59	0.41
2:B:2785:TRP:HE3	2:B:2787:TRP:NE1	2.19	0.41
2:B:3011:LEU:HD23	2:B:3011:LEU:HA	1.94	0.41
2:B:3237:VAL:O	2:B:3240:PRO:HD2	2.21	0.41
2:B:3955:GLN:HG2	2:B:4016:PHE:CE2	2.55	0.41
2:B:4166:LYS:O	2:B:4170:ARG:HG3	2.21	0.41
2:B:4834:PRO:HB3	2:B:4843:ARG:HH11	1.85	0.41
2:C:21:VAL:HG13	2:C:217:ILE:HG13	2.02	0.41
2:C:2571:VAL:HA	2:C:2574:LEU:CD2	2.50	0.41
2:C:4834:PRO:HB3	2:C:4843:ARG:HH11	1.85	0.41
2:A:21:VAL:HG13	2:A:217:ILE:HG13	2.02	0.41
2:A:514:PHE:HD2	2:A:526:TRP:HB2	1.85	0.41
2:A:1585:ARG:NE	2:A:1634:GLU:OE1	2.53	0.41
2:A:2276:SER:HB2	2:A:2288:ILE:O	2.21	0.41
2:A:2389:MET:HG3	2:A:2464:HIS:CE1	2.55	0.41
2:A:2939:TYR:CD2	2:A:2956:TYR:CD2	3.09	0.41
2:A:3246:MET:SD	2:A:3247:SER:N	2.93	0.41
2:A:3684:GLU:OE1	2:A:3754:MET:HG3	2.21	0.41
2:D:999:LEU:HD12	2:D:1050:LEU:HD21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1064:LEU:O	2:D:1064:LEU:HD12	2.21	0.41
2:D:1102:TYR:HD1	2:D:1165:MET:HG2	1.85	0.41
2:D:1819:VAL:HG23	2:D:1902:VAL:HG22	2.01	0.41
2:D:3010:LYS:O	2:D:3014:LEU:HD23	2.20	0.41
2:D:3138:TYR:CG	2:D:3208:ILE:HG13	2.55	0.41
2:D:3324:GLU:CD	2:D:3325:LYS:HG3	2.41	0.41
2:B:514:PHE:HD2	2:B:526:TRP:HB2	1.85	0.41
2:B:2276:SER:HB2	2:B:2288:ILE:O	2.21	0.41
2:B:3311:LYS:H	2:B:3314:LEU:HD23	1.86	0.41
2:C:624:ALA:HB2	2:C:1667:LEU:HD12	2.02	0.41
2:C:718:VAL:HG23	2:C:793:SER:HB3	2.01	0.41
2:C:2176:VAL:HG22	2:C:2220:TYR:CZ	2.56	0.41
2:C:3042:ALA:HB3	2:C:3117:PHE:HB3	2.02	0.41
2:C:3178:HIS:NE2	2:C:3263:MET:HA	2.36	0.41
2:C:3324:GLU:CD	2:C:3325:LYS:HG3	2.41	0.41
2:A:882:ARG:CZ	2:A:933:LEU:HD23	2.51	0.41
2:A:964:MET:O	2:A:977:LYS:NZ	2.53	0.41
2:A:1819:VAL:HG23	2:A:1902:VAL:HG22	2.02	0.41
2:A:1979:PHE:HD1	2:A:1986:CYS:HG	1.69	0.41
2:A:2604:LYS:HB3	2:A:2608:LYS:HZ3	1.86	0.41
2:A:3187:LYS:O	2:A:3191:GLU:HB2	2.20	0.41
2:A:3311:LYS:H	2:A:3314:LEU:HD23	1.86	0.41
2:A:3324:GLU:CD	2:A:3325:LYS:HG3	2.41	0.41
2:A:4650:LYS:HG2	2:A:4670:LEU:HD22	2.03	0.41
1:F:43:ARG:HA	2:B:1682:GLU:OE1	2.21	0.41
2:D:964:MET:O	2:D:977:LYS:NZ	2.53	0.41
2:D:1245:ARG:HD3	2:D:1692:LYS:HB3	2.03	0.41
2:D:1436:GLN:NE2	2:D:1546:GLN:O	2.51	0.41
2:D:2176:VAL:HG22	2:D:2220:TYR:CZ	2.55	0.41
2:D:3279:ASN:O	2:D:3283:ILE:HD12	2.20	0.41
2:D:3985:MET:HA	2:D:3985:MET:HE3	2.03	0.41
2:B:992:GLN:O	2:B:996:VAL:HG23	2.21	0.41
2:B:2176:VAL:HG22	2:B:2220:TYR:CZ	2.56	0.41
2:B:2732:TRP:CH2	2:B:2756:LEU:HB3	2.50	0.41
2:B:2826:ILE:HD13	2:C:1501:ASN:CB	2.48	0.41
2:B:3114:GLN:HE22	2:B:3115:HIS:CE1	2.39	0.41
2:B:3246:MET:HG2	2:B:3276:LEU:HD22	2.03	0.41
2:B:4641:PRO:O	2:B:4647:LYS:NZ	2.35	0.41
2:C:737:ILE:HD13	2:C:1482:ARG:HD3	2.03	0.41
2:C:2139:GLU:O	2:C:2192:MET:HE3	2.20	0.41
2:C:2891:ASP:OD1	2:C:2892:ILE:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3137:LEU:HB3	2:C:3159:LEU:HD11	2.03	0.41
2:C:3154:ALA:O	2:C:3157:GLU:HG3	2.21	0.41
2:C:3222:ALA:HB1	2:C:3282:LYS:HG2	2.02	0.41
2:A:131:CYS:SG	2:A:150:GLN:HB2	2.60	0.41
2:A:419:ILE:HG21	2:A:492:GLU:HG3	2.02	0.41
2:A:624:ALA:HB2	2:A:1667:LEU:HD12	2.02	0.41
2:A:677:LEU:HD12	2:A:801:ARG:O	2.21	0.41
2:A:977:LYS:NZ	2:A:979:ALA:HB2	2.36	0.41
2:A:2241:ASP:CG	2:A:2297:ARG:HH22	2.24	0.41
2:A:2638:LEU:HD23	2:A:2638:LEU:HA	1.83	0.41
2:A:2785:TRP:HE3	2:A:2787:TRP:NE1	2.19	0.41
2:A:3042:ALA:HB3	2:A:3117:PHE:HB3	2.02	0.41
2:A:3138:TYR:CG	2:A:3208:ILE:HG13	2.55	0.41
2:A:3154:ALA:O	2:A:3157:GLU:HG3	2.21	0.41
2:A:3228:TYR:H	2:A:3290:ILE:HG21	1.85	0.41
2:A:3661:VAL:HB	2:A:3665:HIS:HB3	2.03	0.41
2:A:3715:GLU:O	2:A:3719:MET:HG2	2.21	0.41
2:A:4649:VAL:O	2:A:4653:VAL:HG23	2.21	0.41
2:A:4679:PHE:O	2:A:4682:ALA:C	2.59	0.41
2:D:737:ILE:HD13	2:D:1482:ARG:HD3	2.03	0.41
2:D:1564:MET:HE3	2:D:1565:PRO:HD2	2.01	0.41
2:D:1891:GLU:HB3	2:D:1895:GLN:HB2	2.03	0.41
2:D:2972:ASP:O	2:D:2976:LYS:HG2	2.21	0.41
2:D:4187:GLU:OE1	2:D:4949:TRP:NE1	2.46	0.41
2:D:4649:VAL:O	2:D:4653:VAL:HG23	2.21	0.41
2:B:600:LEU:O	2:B:604:HIS:HB2	2.20	0.41
2:B:677:LEU:HD12	2:B:801:ARG:O	2.21	0.41
2:B:933:LEU:O	2:B:937:LEU:HG	2.21	0.41
2:B:999:LEU:HD12	2:B:1050:LEU:HD21	2.03	0.41
2:B:1014:GLN:O	2:B:1027:ARG:NH2	2.53	0.41
2:B:1267:HIS:CE1	2:B:1296:ASN:H	2.39	0.41
2:B:1444:GLY:HA3	2:B:1487:MET:HA	2.03	0.41
2:B:2062:ILE:HG21	2:B:2087:LEU:HG	2.02	0.41
2:B:2363:SER:O	2:B:2363:SER:OG	2.38	0.41
2:B:2785:TRP:HB2	2:B:2787:TRP:HD1	1.85	0.41
2:B:3042:ALA:HB3	2:B:3117:PHE:HB3	2.02	0.41
2:B:3324:GLU:CD	2:B:3325:LYS:HG3	2.41	0.41
2:B:3848:GLU:HA	2:B:3922:GLU:OE2	2.21	0.41
2:B:4305:PHE:HA	2:B:4308:ILE:HG12	2.03	0.41
2:C:219:SER:H	2:C:349:MET:HE3	1.86	0.41
2:C:882:ARG:CZ	2:C:933:LEU:HD23	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1064:LEU:HD12	2:C:1064:LEU:O	2.21	0.41
2:C:1249:MET:HB2	2:C:1599:MET:HB3	2.02	0.41
2:C:1494:MET:HG3	2:C:1500:ARG:HD2	2.03	0.41
2:C:2062:ILE:HG21	2:C:2087:LEU:HG	2.02	0.41
2:C:2258:ARG:HB3	2:C:2260:PRO:HD2	2.02	0.41
2:C:2276:SER:HB2	2:C:2288:ILE:O	2.21	0.41
2:C:2972:ASP:O	2:C:2976:LYS:HG2	2.21	0.41
2:C:3183:ILE:HD11	2:C:3187:LYS:HE2	2.03	0.41
2:C:3249:TRP:HE3	2:C:3266:THR:HG21	1.85	0.41
2:C:3279:ASN:O	2:C:3283:ILE:HD12	2.20	0.41
1:H:85:ALA:O	1:H:94:PRO:HB3	2.21	0.41
2:A:992:GLN:O	2:A:996:VAL:HG23	2.21	0.41
2:A:1245:ARG:HD3	2:A:1692:LYS:HB3	2.03	0.41
2:A:2721:ILE:HG22	2:A:2772:ARG:HH11	1.85	0.41
2:A:3846:LEU:HB3	2:A:3854:PHE:CE2	2.56	0.41
2:A:3926:GLY:CA	2:A:4935:GLY:HA3	2.47	0.41
1:E:85:ALA:O	1:E:94:PRO:HB3	2.21	0.41
2:D:2456:MET:HE2	2:D:2511:ASP:HB2	2.03	0.41
2:D:2939:TYR:CD2	2:D:2956:TYR:CD2	3.09	0.41
2:D:3222:ALA:HB1	2:D:3282:LYS:HG2	2.02	0.41
2:D:4250:TYR:O	2:D:4254:THR:HG23	2.21	0.41
2:B:964:MET:O	2:B:977:LYS:NZ	2.53	0.41
2:B:1427:TYR:HB2	2:B:1563:VAL:CG1	2.51	0.41
2:B:2194:ALA:HA	2:B:2237:SER:HB3	2.03	0.41
2:B:4522:VAL:HG12	2:C:4807:ASP:O	2.21	0.41
2:C:191:TYR:N	2:C:206:ALA:O	2.54	0.41
2:C:709:GLY:HA3	2:C:723:PHE:CD1	2.55	0.41
2:C:893:TRP:HD1	2:C:897:LYS:HZ3	1.66	0.41
2:C:992:GLN:O	2:C:996:VAL:HG23	2.21	0.41
2:C:1608:VAL:HA	2:C:1618:LEU:O	2.21	0.41
2:C:1928:PHE:HE1	2:C:1995:GLN:HG2	1.86	0.41
2:C:2077:ASP:HB3	2:C:2080:LEU:HB3	2.03	0.41
2:C:2760:TYR:HD1	2:C:2763:LEU:HD22	1.86	0.41
2:C:3766:LEU:O	2:C:3845:LEU:HD22	2.21	0.41
2:C:4136:ILE:HG22	2:C:4917:ASN:HB3	2.01	0.41
2:A:1064:LEU:HD12	2:A:1064:LEU:O	2.21	0.40
2:A:1427:TYR:HB2	2:A:1563:VAL:CG1	2.51	0.40
1:G:85:ALA:O	1:G:94:PRO:HB3	2.21	0.40
2:D:2241:ASP:CG	2:D:2297:ARG:HH22	2.24	0.40
2:D:3302:PHE:O	2:D:3305:PRO:HD2	2.22	0.40
2:D:3715:GLU:O	2:D:3719:MET:HG2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4650:LYS:HG2	2:D:4670:LEU:HD22	2.03	0.40
2:B:1707:ILE:HG23	2:B:1827:THR:HG21	2.03	0.40
2:B:2077:ASP:HB3	2:B:2080:LEU:HB3	2.03	0.40
2:B:2604:LYS:HB3	2:B:2608:LYS:HZ3	1.86	0.40
2:B:2891:ASP:OD1	2:B:2892:ILE:N	2.53	0.40
2:B:2972:ASP:O	2:B:2976:LYS:HG2	2.21	0.40
2:B:3661:VAL:HB	2:B:3665:HIS:HB3	2.03	0.40
2:B:4094:ILE:O	2:B:4098:VAL:HG23	2.21	0.40
2:B:4756:ILE:HG23	2:C:4861:ILE:HG21	2.02	0.40
2:C:600:LEU:O	2:C:604:HIS:HB2	2.20	0.40
2:C:1304:LEU:HD23	2:C:1304:LEU:HA	1.92	0.40
2:C:2194:ALA:HA	2:C:2237:SER:HB3	2.03	0.40
2:C:4021:LEU:HD22	2:C:4128:TYR:CE2	2.56	0.40
2:C:4079:ASP:HB3	2:C:4082:GLU:HG3	2.03	0.40
2:C:4261:LEU:HG	2:C:4263:SER:HB2	2.03	0.40
2:C:4663:ARG:HG2	2:C:4663:ARG:NH1	2.17	0.40
2:A:1291:GLY:HA2	2:D:2835:ARG:HH12	1.85	0.40
2:A:2689:MET:O	2:A:2689:MET:HG3	2.20	0.40
2:A:3910:ILE:HG23	2:A:3974:LEU:HB2	2.03	0.40
2:A:4021:LEU:HD22	2:A:4128:TYR:CE2	2.56	0.40
2:A:4305:PHE:HA	2:A:4308:ILE:HG12	2.02	0.40
2:D:677:LEU:HD12	2:D:801:ARG:O	2.21	0.40
2:D:992:GLN:O	2:D:996:VAL:HG23	2.21	0.40
2:D:2939:TYR:HD2	2:D:2956:TYR:HD2	1.70	0.40
2:D:3011:LEU:HD23	2:D:3011:LEU:HA	1.94	0.40
2:D:3246:MET:HG2	2:D:3276:LEU:HD22	2.02	0.40
2:D:3684:GLU:OE1	2:D:3754:MET:HG3	2.21	0.40
2:D:4021:LEU:HD22	2:D:4128:TYR:CE2	2.56	0.40
2:B:21:VAL:HG13	2:B:217:ILE:HG13	2.02	0.40
2:B:375:GLN:O	2:B:376:SER:OG	2.33	0.40
2:B:624:ALA:HB2	2:B:1667:LEU:HD12	2.02	0.40
2:B:698:ALA:HB2	2:B:791:VAL:HG11	2.03	0.40
2:B:977:LYS:NZ	2:B:979:ALA:HB2	2.35	0.40
2:B:1611:ILE:CG2	2:B:1615:GLN:HG3	2.51	0.40
2:B:1697:LEU:HD23	2:B:1697:LEU:HA	1.87	0.40
2:B:2833:LEU:HB2	2:B:2838[B]:HIS:CE1	2.55	0.40
2:B:3766:LEU:O	2:B:3845:LEU:HD22	2.21	0.40
2:B:4679:PHE:O	2:B:4682:ALA:C	2.59	0.40
2:B:4753:LEU:HD21	2:C:4769:LEU:HD22	2.03	0.40
2:C:1497:GLY:O	2:C:1499:GLY:N	2.53	0.40
2:C:1891:GLU:HB3	2:C:1895:GLN:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2939:TYR:HD2	2:C:2956:TYR:HD2	1.70	0.40
2:C:3661:VAL:HB	2:C:3665:HIS:HB3	2.03	0.40
2:C:3846:LEU:HB3	2:C:3854:PHE:CE2	2.56	0.40
2:C:3846:LEU:HD23	2:C:3846:LEU:HA	1.96	0.40
2:A:219:SER:H	2:A:349:MET:HE3	1.87	0.40
2:A:698:ALA:HB2	2:A:791:VAL:HG11	2.03	0.40
2:A:1444:GLY:HA3	2:A:1487:MET:HA	2.03	0.40
2:A:1494:MET:HG3	2:A:1500:ARG:HD2	2.03	0.40
2:A:2139:GLU:O	2:A:2192:MET:HE3	2.20	0.40
2:A:2605:MET:HG3	2:A:2606:PRO:HD3	2.04	0.40
2:A:3137:LEU:HB3	2:A:3159:LEU:HD11	2.03	0.40
2:A:3302:PHE:O	2:A:3305:PRO:HD2	2.22	0.40
2:A:3766:LEU:O	2:A:3845:LEU:HD22	2.21	0.40
2:A:3986:LEU:HD22	2:A:3989:ASN:ND2	2.37	0.40
2:A:4048:PHE:CZ	2:A:4080:TYR:HB3	2.55	0.40
2:A:4250:TYR:O	2:A:4254:THR:HG23	2.21	0.40
1:F:85:ALA:O	1:F:94:PRO:HB3	2.21	0.40
2:D:698:ALA:HB2	2:D:791:VAL:HG11	2.04	0.40
2:D:933:LEU:O	2:D:937:LEU:HG	2.21	0.40
2:D:3097:THR:HG22	2:D:3102:LEU:HG	2.04	0.40
2:D:3237:VAL:O	2:D:3240:PRO:HD2	2.21	0.40
2:D:3661:VAL:HB	2:D:3665:HIS:HB3	2.03	0.40
2:D:3840:PHE:CE1	2:D:3874:THR:HG23	2.56	0.40
2:D:3910:ILE:HG23	2:D:3974:LEU:HB2	2.03	0.40
2:B:1249:MET:HB2	2:B:1599:MET:HB3	2.02	0.40
2:B:1608:VAL:HA	2:B:1618:LEU:O	2.21	0.40
2:B:3292:GLU:HB2	2:B:3296:MET:HE2	2.02	0.40
2:B:3951:PHE:HZ	2:B:3974:LEU:HG	1.87	0.40
2:B:4649:VAL:O	2:B:4653:VAL:HG23	2.21	0.40
2:C:677:LEU:HD12	2:C:801:ARG:O	2.21	0.40
2:C:1265:HIS:CE1	2:C:1268:ILE:HG13	2.55	0.40
2:C:1267:HIS:CE1	2:C:1296:ASN:H	2.40	0.40
2:C:1444:GLY:HA3	2:C:1487:MET:HA	2.03	0.40
2:C:1611:ILE:CG2	2:C:1615:GLN:HG3	2.51	0.40
2:C:3303:SER:HA	2:C:3306:ILE:CG1	2.52	0.40
2:A:737:ILE:HD13	2:A:1482:ARG:HD3	2.03	0.40
2:A:967:PRO:O	2:A:971:GLN:CB	2.70	0.40
2:A:2176:VAL:HG22	2:A:2220:TYR:CZ	2.56	0.40
2:A:2957:GLU:O	2:A:2961:LYS:HG2	2.22	0.40
2:A:3644:LEU:HD23	2:A:3644:LEU:HA	1.94	0.40
2:D:274:LEU:HD23	2:D:274:LEU:HA	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:891:GLU:HG2	2:D:978:PRO:HG3	2.03	0.40
2:D:1494:MET:HG3	2:D:1500:ARG:HD2	2.03	0.40
2:D:2785:TRP:HB2	2:D:2787:TRP:HD1	1.85	0.40
2:D:2856:LYS:HA	2:D:2859:GLU:CG	2.44	0.40
2:D:3229:THR:HA	2:D:3232:PRO:HG3	2.04	0.40
2:D:3232:PRO:HA	2:D:3235:MET:HE2	2.04	0.40
2:B:1678:SER:HB2	2:B:1768:PHE:CE2	2.57	0.40
2:B:2725:ALA:HB1	2:B:2760:TYR:CZ	2.55	0.40
2:B:2760:TYR:HD1	2:B:2763:LEU:HD22	1.86	0.40
2:B:2833:LEU:HB2	2:B:2838[A]:HIS:CE1	2.56	0.40
2:B:3910:ILE:HG23	2:B:3974:LEU:HB2	2.04	0.40
2:B:4137:GLU:OE1	2:B:4958:PHE:HB2	2.22	0.40
2:C:830:GLU:OE1	2:C:830:GLU:N	2.54	0.40
2:C:967:PRO:O	2:C:971:GLN:CB	2.70	0.40
2:C:2539:GLU:HB2	2:C:2581:ARG:HD3	2.02	0.40
2:C:2957:GLU:O	2:C:2961:LYS:HG2	2.22	0.40
2:C:3302:PHE:O	2:C:3305:PRO:HD2	2.22	0.40
2:C:4250:TYR:O	2:C:4254:THR:HG23	2.21	0.40
2:C:4679:PHE:O	2:C:4682:ALA:C	2.59	0.40
2:A:933:LEU:O	2:A:937:LEU:HG	2.21	0.40
2:A:999:LEU:HD12	2:A:1050:LEU:HD21	2.03	0.40
2:A:1081:THR:HG23	2:A:1082:GLY:H	1.86	0.40
2:A:1685:LEU:HD23	2:A:1685:LEU:HA	1.95	0.40
2:A:2062:ILE:HG21	2:A:2087:LEU:HG	2.02	0.40
2:A:3178:HIS:NE2	2:A:3263:MET:HA	2.36	0.40
2:A:4481:TRP:CG	2:A:4484:ILE:HD11	2.56	0.40
2:D:624:ALA:HB2	2:D:1667:LEU:HD12	2.02	0.40
2:D:1608:VAL:HA	2:D:1618:LEU:O	2.21	0.40
2:D:2824:ARG:HA	2:D:2824:ARG:HD2	1.64	0.40
2:D:3926:GLY:CA	2:D:4935:GLY:HA3	2.47	0.40
2:D:4079:ASP:HB3	2:D:4082:GLU:HG3	2.03	0.40
2:D:4481:TRP:CG	2:D:4484:ILE:HD11	2.56	0.40
2:D:4503:ARG:NH2	2:D:4721:TYR:HE2	2.20	0.40
2:B:3171:LEU:HD23	2:B:3171:LEU:HA	1.93	0.40
2:B:3210:SER:OG	2:B:3213:LYS:NZ	2.48	0.40
2:B:3303:SER:HA	2:B:3306:ILE:CG1	2.52	0.40
2:B:3846:LEU:HB3	2:B:3854:PHE:CE2	2.56	0.40
2:B:3846:LEU:HD23	2:B:3846:LEU:HA	1.96	0.40
2:B:4503:ARG:NH2	2:B:4721:TYR:HE2	2.20	0.40
2:C:375:GLN:O	2:C:376:SER:OG	2.33	0.40
2:C:996:VAL:HG22	2:C:1054:VAL:HG21	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1427:TYR:HB2	2:C:1563:VAL:CG1	2.51	0.40
2:C:1585:ARG:NE	2:C:1634:GLU:OE1	2.53	0.40
2:C:3097:THR:HG22	2:C:3102:LEU:HG	2.04	0.40
2:C:3246:MET:HG2	2:C:3276:LEU:HD22	2.02	0.40
2:C:3311:LYS:H	2:C:3314:LEU:HD23	1.86	0.40
2:C:3951:PHE:HZ	2:C:3974:LEU:HG	1.87	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	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	A	4198/4967 (84%)	4052 (96%)	142 (3%)	4 (0%)	51	83
2	B	4198/4967 (84%)	4052 (96%)	142 (3%)	4 (0%)	51	83
2	C	4198/4967 (84%)	4052 (96%)	142 (3%)	4 (0%)	51	83
2	D	4198/4967 (84%)	4050 (96%)	144 (3%)	4 (0%)	51	83
All	All	17212/20300 (85%)	16618 (96%)	578 (3%)	16 (0%)	54	83

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	2988	ARG
2	A	3292	GLU
2	A	4641	PRO
2	D	2988	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	3292	GLU
2	D	4641	PRO
2	B	2988	ARG
2	B	3292	GLU
2	B	4641	PRO
2	C	2988	ARG
2	C	3292	GLU
2	C	4641	PRO
2	A	1498	GLN
2	D	1498	GLN
2	B	1498	GLN
2	C	1498	GLN

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	E	88/89 (99%)	85 (97%)	3 (3%)	37	68
1	F	88/89 (99%)	85 (97%)	3 (3%)	37	68
1	G	88/89 (99%)	85 (97%)	3 (3%)	37	68
1	H	88/89 (99%)	85 (97%)	3 (3%)	37	68
2	A	3708/4358 (85%)	3675 (99%)	33 (1%)	78	91
2	B	3708/4358 (85%)	3675 (99%)	33 (1%)	78	91
2	C	3708/4358 (85%)	3675 (99%)	33 (1%)	78	91
2	D	3708/4358 (85%)	3675 (99%)	33 (1%)	78	91
All	All	15184/17788 (85%)	15040 (99%)	144 (1%)	79	91

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	4	GLU
1	H	18	LYS
1	H	19	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	81	MET
2	A	317	MET
2	A	414	ARG
2	A	844	ARG
2	A	929	ARG
2	A	940	LEU
2	A	946	LEU
2	A	949	HIS
2	A	1421	MET
2	A	1500	ARG
2	A	1564	MET
2	A	1614	ARG
2	A	2172	MET
2	A	2192	MET
2	A	2279	MET
2	A	2485	LEU
2	A	2493	LEU
2	A	2826	ILE
2	A	2838[A]	HIS
2	A	2838[B]	HIS
2	A	2884	LYS
2	A	2953	HIS
2	A	3072	MET
2	A	3314	LEU
2	A	3882	GLN
2	A	3985	MET
2	A	4183	LYS
2	A	4256	MET
2	A	4268	MET
2	A	4279	MET
2	A	4567	TYR
2	A	4663	ARG
2	A	4797	GLU
1	E	4	GLU
1	E	18	LYS
1	E	19	LYS
1	F	4	GLU
1	F	18	LYS
1	F	19	LYS
1	G	4	GLU
1	G	18	LYS
1	G	19	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	81	MET
2	D	317	MET
2	D	414	ARG
2	D	844	ARG
2	D	929	ARG
2	D	940	LEU
2	D	946	LEU
2	D	949	HIS
2	D	1421	MET
2	D	1500	ARG
2	D	1564	MET
2	D	1614	ARG
2	D	2172	MET
2	D	2192	MET
2	D	2279	MET
2	D	2485	LEU
2	D	2493	LEU
2	D	2826	ILE
2	D	2838[A]	HIS
2	D	2838[B]	HIS
2	D	2884	LYS
2	D	2953	HIS
2	D	3072	MET
2	D	3314	LEU
2	D	3882	GLN
2	D	3985	MET
2	D	4183	LYS
2	D	4256	MET
2	D	4268	MET
2	D	4279	MET
2	D	4567	TYR
2	D	4663	ARG
2	D	4797	GLU
2	B	81	MET
2	B	317	MET
2	B	414	ARG
2	B	844	ARG
2	B	929	ARG
2	B	940	LEU
2	B	946	LEU
2	B	949	HIS
2	B	1421	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1500	ARG
2	B	1564	MET
2	B	1614	ARG
2	B	2172	MET
2	B	2192	MET
2	B	2279	MET
2	B	2485	LEU
2	B	2493	LEU
2	B	2826	ILE
2	B	2838[A]	HIS
2	B	2838[B]	HIS
2	B	2884	LYS
2	B	2953	HIS
2	B	3072	MET
2	B	3314	LEU
2	B	3882	GLN
2	B	3985	MET
2	B	4183	LYS
2	B	4256	MET
2	B	4268	MET
2	B	4279	MET
2	B	4567	TYR
2	B	4663	ARG
2	B	4797	GLU
2	C	81	MET
2	C	317	MET
2	C	414	ARG
2	C	844	ARG
2	C	929	ARG
2	C	940	LEU
2	C	946	LEU
2	C	949	HIS
2	C	1421	MET
2	C	1500	ARG
2	C	1564	MET
2	C	1614	ARG
2	C	2172	MET
2	C	2192	MET
2	C	2279	MET
2	C	2485	LEU
2	C	2493	LEU
2	C	2826	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	2838[A]	HIS
2	C	2838[B]	HIS
2	C	2884	LYS
2	C	2953	HIS
2	C	3072	MET
2	C	3314	LEU
2	C	3882	GLN
2	C	3985	MET
2	C	4183	LYS
2	C	4256	MET
2	C	4268	MET
2	C	4279	MET
2	C	4567	TYR
2	C	4663	ARG
2	C	4797	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	117	HIS
2	A	669	GLN
2	A	927	GLN
2	A	1071	HIS
2	A	1844	GLN
2	A	1974	ASN
2	A	2217	HIS
2	A	2410	HIS
2	A	2540	HIS
2	A	2830	ASN
2	A	3114	GLN
2	A	3256	ASN
2	A	3864	ASN
2	A	4579	HIS
2	A	4742	HIS
2	A	4936	GLN
2	D	117	HIS
2	D	669	GLN
2	D	927	GLN
2	D	1974	ASN
2	D	2217	HIS
2	D	2410	HIS
2	D	2540	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	2830	ASN
2	D	3114	GLN
2	D	3256	ASN
2	D	3864	ASN
2	D	4579	HIS
2	D	4936	GLN
2	B	117	HIS
2	B	669	GLN
2	B	927	GLN
2	B	1844	GLN
2	B	2217	HIS
2	B	2410	HIS
2	B	2540	HIS
2	B	2830	ASN
2	B	3114	GLN
2	B	3256	ASN
2	B	3864	ASN
2	B	4579	HIS
2	B	4936	GLN
2	C	117	HIS
2	C	669	GLN
2	C	927	GLN
2	C	1844	GLN
2	C	2217	HIS
2	C	2410	HIS
2	C	2540	HIS
2	C	2830	ASN
2	C	2977	ASN
2	C	3114	GLN
2	C	3256	ASN
2	C	3864	ASN
2	C	4579	HIS
2	C	4936	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	B	5002	-	26,33,33	0.60	0	31,52,52	0.80	2 (6%)
4	ATP	D	5003	-	26,33,33	0.59	0	31,52,52	0.75	2 (6%)
4	ATP	C	5002	-	26,33,33	0.60	0	31,52,52	0.80	2 (6%)
4	ATP	A	5003	-	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
4	ATP	B	5003	-	26,33,33	0.59	0	31,52,52	0.75	2 (6%)
4	ATP	C	5003	-	26,33,33	0.58	0	31,52,52	0.75	2 (6%)
4	ATP	A	5002	-	26,33,33	0.59	0	31,52,52	0.80	2 (6%)
4	ATP	D	5002	-	26,33,33	0.59	0	31,52,52	0.80	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	D	5003	-	-	8/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	8/18/38/38	0/3/3/3
4	ATP	B	5003	-	-	8/18/38/38	0/3/3/3
4	ATP	C	5003	-	-	8/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	5/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	5002	ATP	C5-C6-N6	2.32	123.88	120.35
4	A	5002	ATP	C5-C6-N6	2.31	123.87	120.35
4	C	5003	ATP	C5-C6-N6	2.31	123.86	120.35
4	B	5002	ATP	C5-C6-N6	2.30	123.84	120.35
4	B	5003	ATP	C5-C6-N6	2.30	123.84	120.35
4	A	5003	ATP	C5-C6-N6	2.29	123.83	120.35
4	D	5003	ATP	C5-C6-N6	2.27	123.80	120.35
4	C	5002	ATP	C5-C6-N6	2.27	123.80	120.35
4	A	5003	ATP	PB-O3B-PG	2.04	139.84	132.83
4	B	5003	ATP	PB-O3B-PG	2.04	139.84	132.83
4	C	5003	ATP	PB-O3B-PG	2.04	139.82	132.83
4	D	5003	ATP	PB-O3B-PG	2.03	139.80	132.83
4	B	5002	ATP	PB-O3B-PG	2.02	139.77	132.83
4	C	5002	ATP	PB-O3B-PG	2.02	139.77	132.83
4	D	5002	ATP	PB-O3B-PG	2.02	139.75	132.83
4	A	5002	ATP	PB-O3B-PG	2.01	139.73	132.83

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	O4'-C4'-C5'-O5'
4	A	5002	ATP	C3'-C4'-C5'-O5'
4	A	5003	ATP	C5'-O5'-PA-O1A
4	D	5002	ATP	O4'-C4'-C5'-O5'
4	D	5002	ATP	C3'-C4'-C5'-O5'
4	D	5003	ATP	C5'-O5'-PA-O1A
4	B	5002	ATP	O4'-C4'-C5'-O5'
4	B	5002	ATP	C3'-C4'-C5'-O5'
4	B	5003	ATP	C5'-O5'-PA-O1A
4	C	5002	ATP	O4'-C4'-C5'-O5'
4	C	5002	ATP	C3'-C4'-C5'-O5'
4	C	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	PG-O3B-PB-O3A
4	D	5003	ATP	PG-O3B-PB-O3A
4	B	5003	ATP	PG-O3B-PB-O3A
4	C	5003	ATP	PG-O3B-PB-O3A
4	A	5002	ATP	PB-O3A-PA-O5'
4	A	5003	ATP	PB-O3A-PA-O5'
4	D	5002	ATP	PB-O3A-PA-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	5003	ATP	PB-O3A-PA-O5'
4	B	5002	ATP	PB-O3A-PA-O5'
4	B	5003	ATP	PB-O3A-PA-O5'
4	C	5002	ATP	PB-O3A-PA-O5'
4	C	5003	ATP	PB-O3A-PA-O5'
4	A	5003	ATP	PA-O3A-PB-O2B
4	D	5003	ATP	PA-O3A-PB-O2B
4	B	5003	ATP	PA-O3A-PB-O2B
4	C	5003	ATP	PA-O3A-PB-O2B
4	A	5003	ATP	C5'-O5'-PA-O2A
4	D	5003	ATP	C5'-O5'-PA-O2A
4	B	5003	ATP	C5'-O5'-PA-O2A
4	C	5003	ATP	C5'-O5'-PA-O2A
4	A	5002	ATP	PG-O3B-PB-O3A
4	D	5002	ATP	PG-O3B-PB-O3A
4	C	5002	ATP	PG-O3B-PB-O3A
4	B	5002	ATP	PG-O3B-PB-O3A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	D	5003	ATP	C5'-O5'-PA-O3A
4	B	5003	ATP	C5'-O5'-PA-O3A
4	C	5003	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	O4'-C4'-C5'-O5'
4	D	5003	ATP	O4'-C4'-C5'-O5'
4	B	5003	ATP	O4'-C4'-C5'-O5'
4	C	5003	ATP	O4'-C4'-C5'-O5'
4	A	5002	ATP	PG-O3B-PB-O1B
4	A	5003	ATP	PG-O3B-PB-O1B
4	D	5002	ATP	PG-O3B-PB-O1B
4	D	5003	ATP	PG-O3B-PB-O1B
4	B	5002	ATP	PG-O3B-PB-O1B
4	B	5003	ATP	PG-O3B-PB-O1B
4	C	5002	ATP	PG-O3B-PB-O1B
4	C	5003	ATP	PG-O3B-PB-O1B

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5002	ATP	1	0
4	D	5003	ATP	1	0
4	C	5002	ATP	1	0
4	A	5003	ATP	1	0

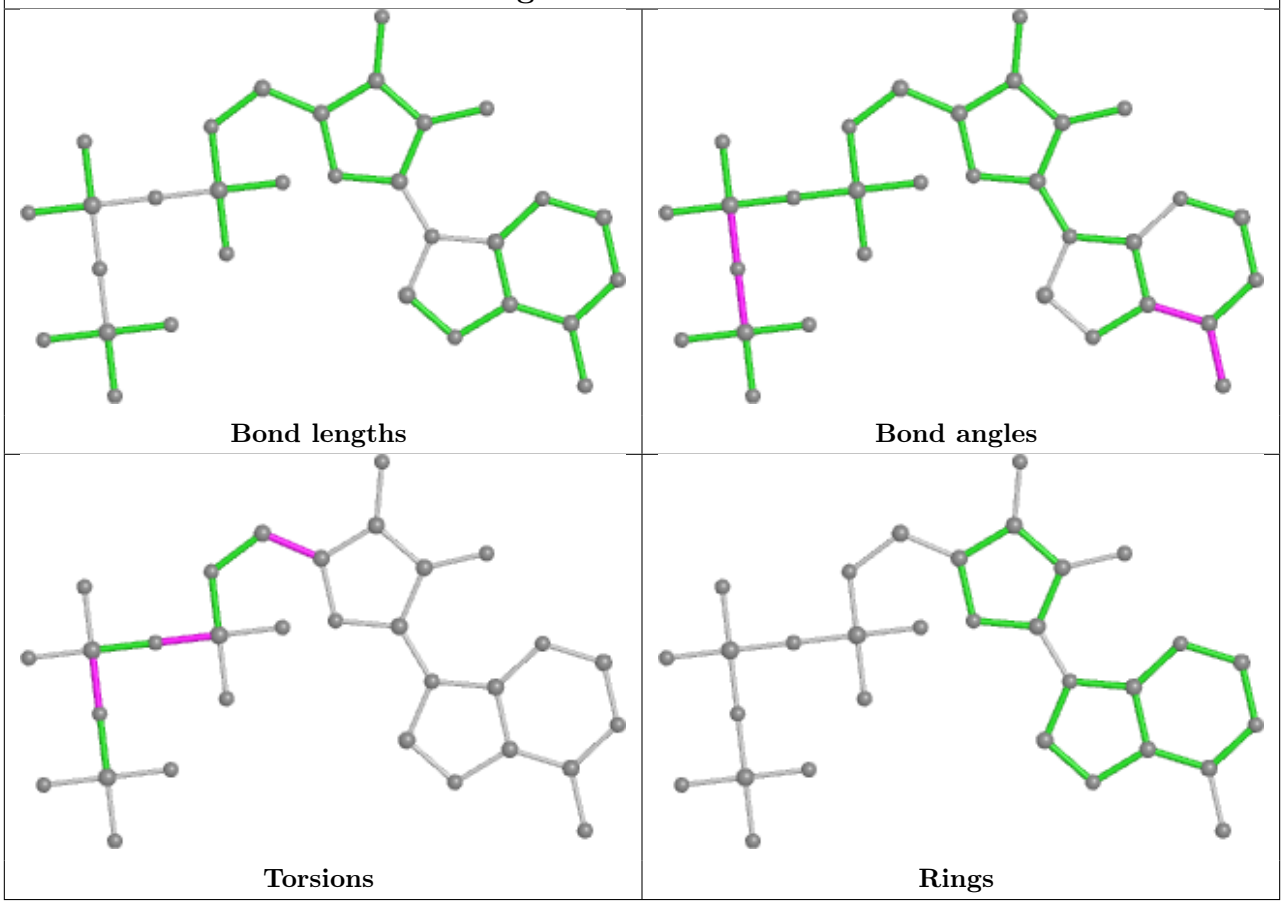
Continued on next page...

Continued from previous page...

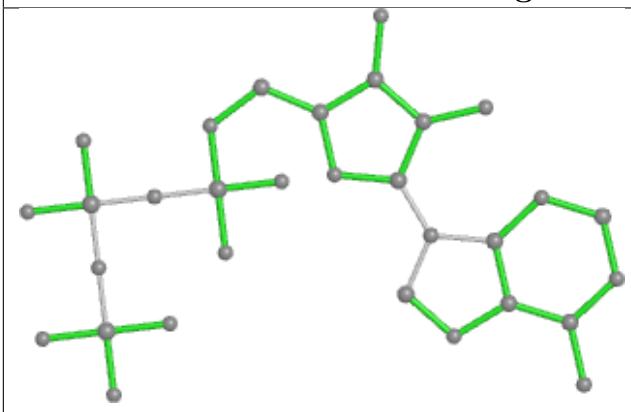
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5003	ATP	1	0
4	C	5003	ATP	1	0
4	A	5002	ATP	1	0
4	D	5002	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

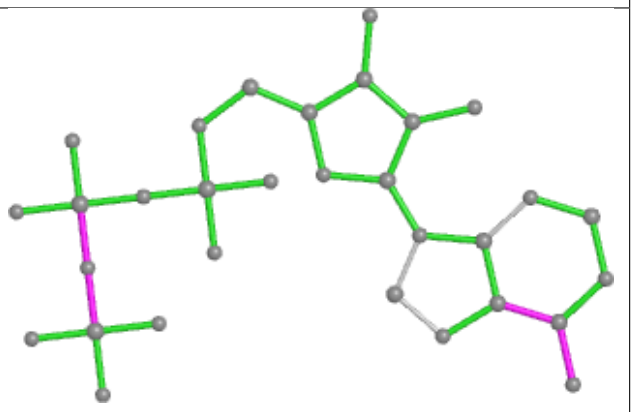
Ligand ATP B 5002



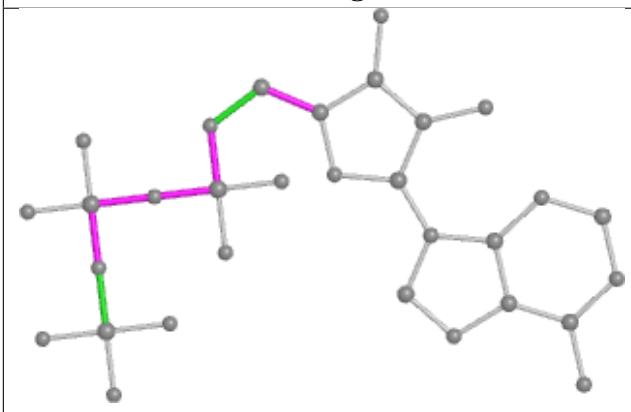
Ligand ATP D 5003



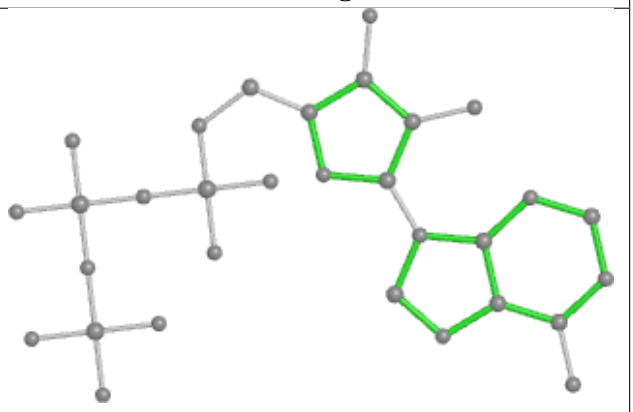
Bond lengths



Bond angles

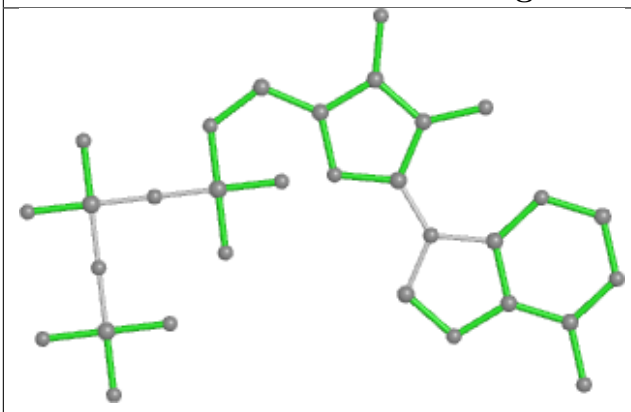


Torsions

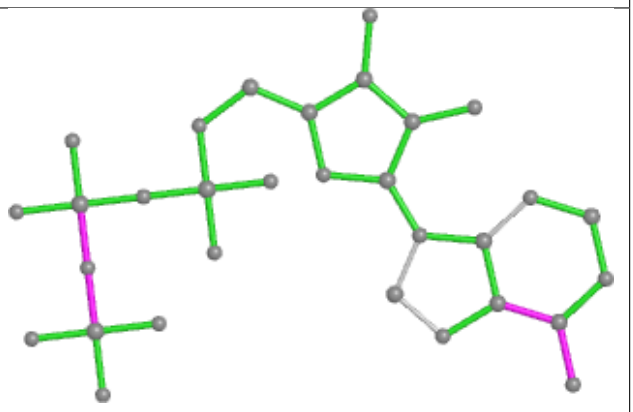


Rings

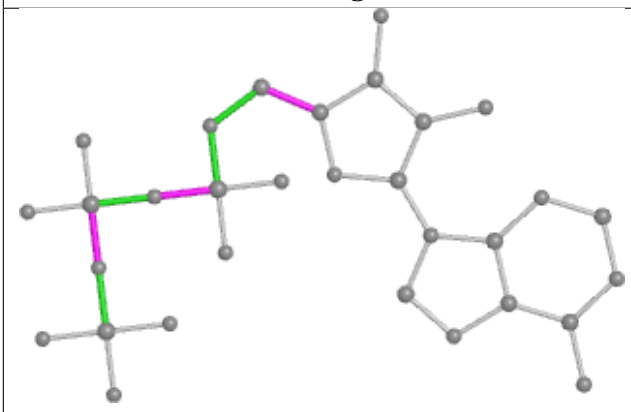
Ligand ATP C 5002



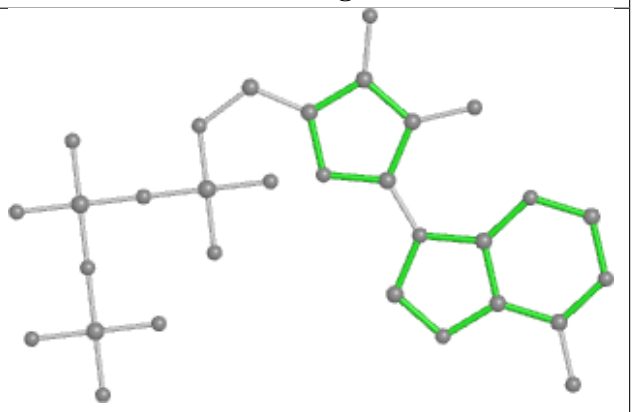
Bond lengths



Bond angles

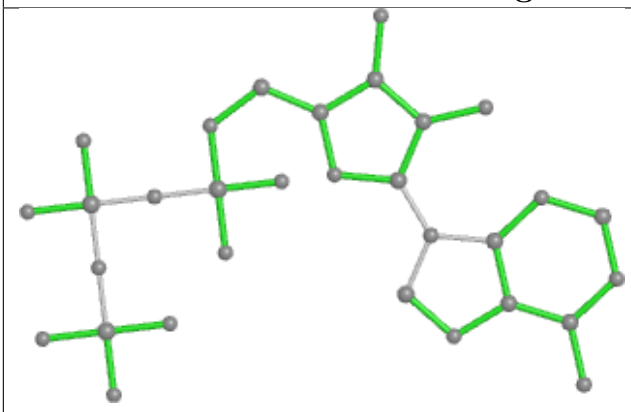


Torsions

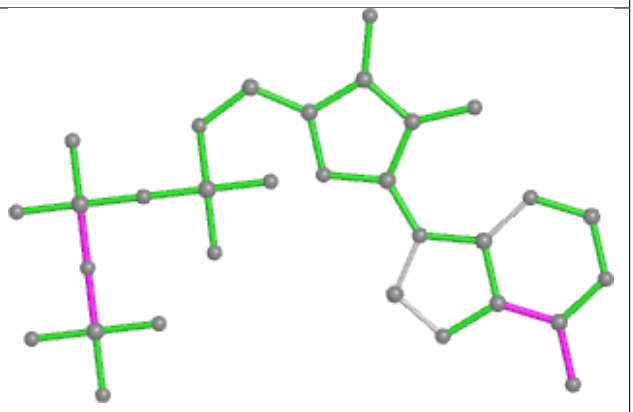


Rings

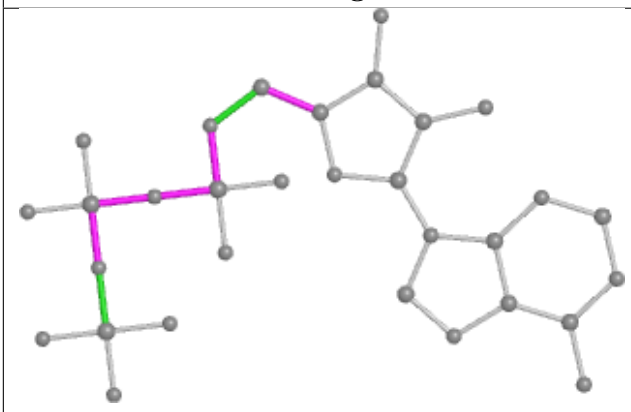
Ligand ATP A 5003



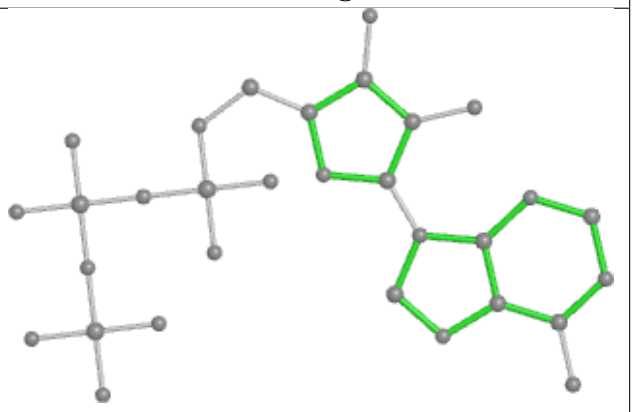
Bond lengths



Bond angles

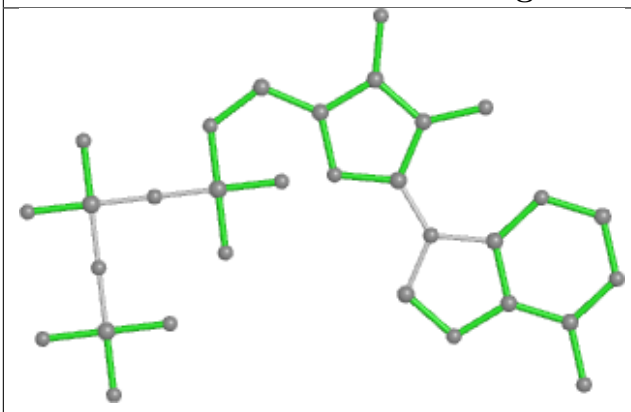


Torsions

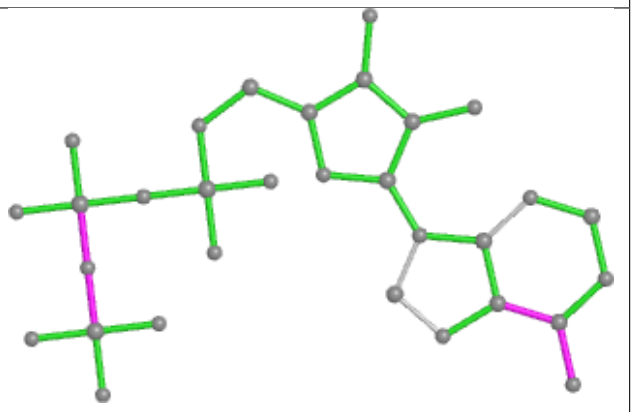


Rings

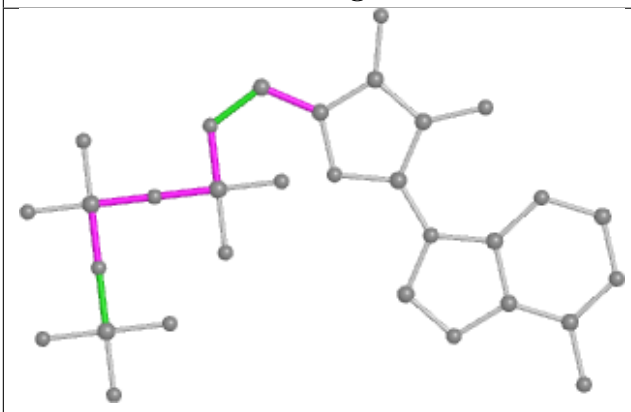
Ligand ATP B 5003



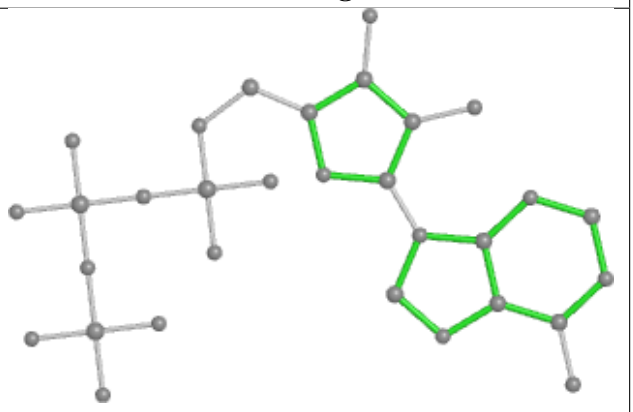
Bond lengths



Bond angles

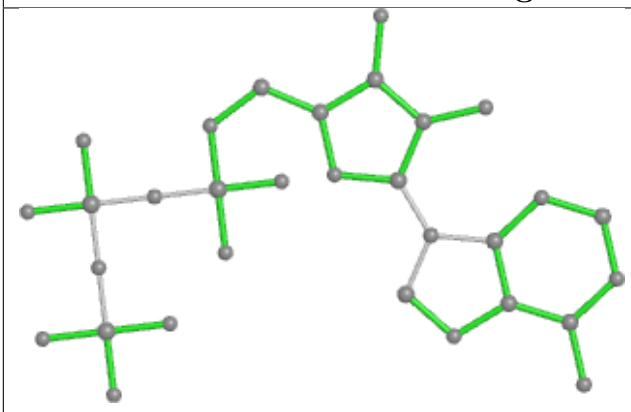


Torsions

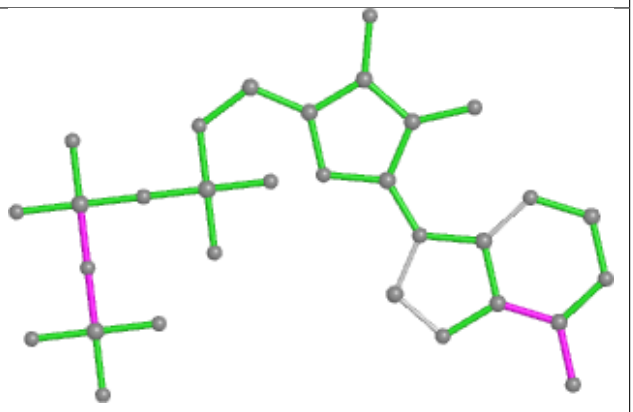


Rings

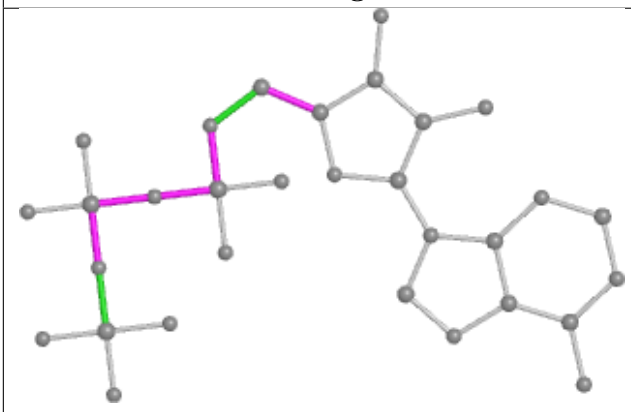
Ligand ATP C 5003



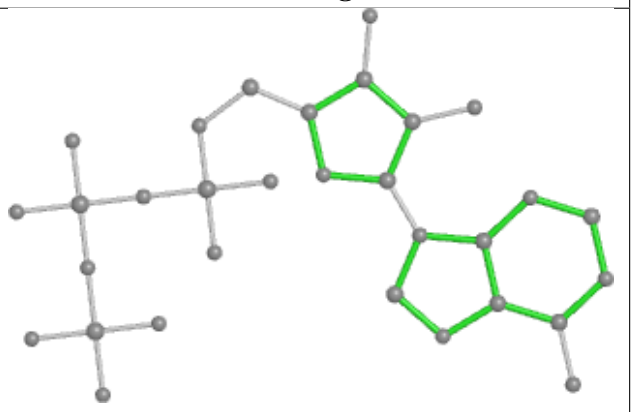
Bond lengths



Bond angles

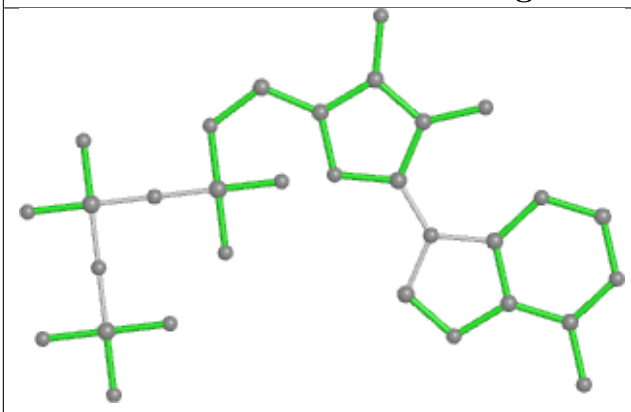


Torsions

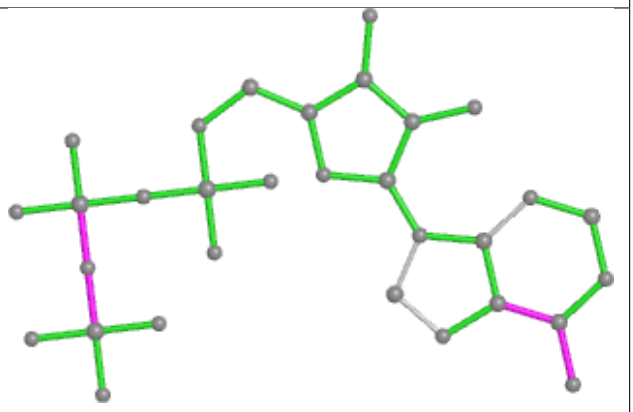


Rings

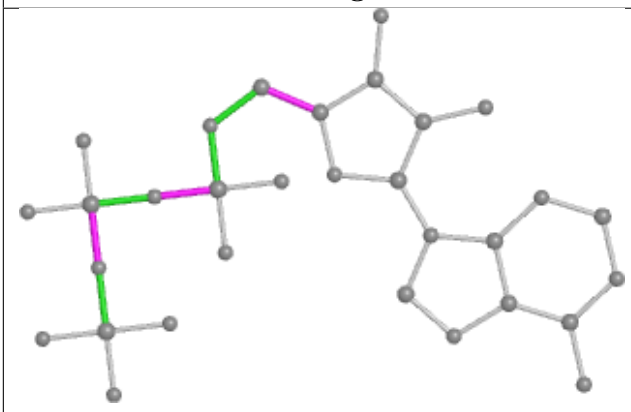
Ligand ATP A 5002



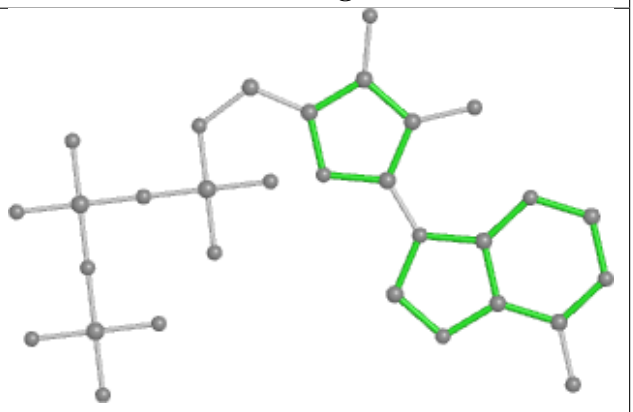
Bond lengths



Bond angles

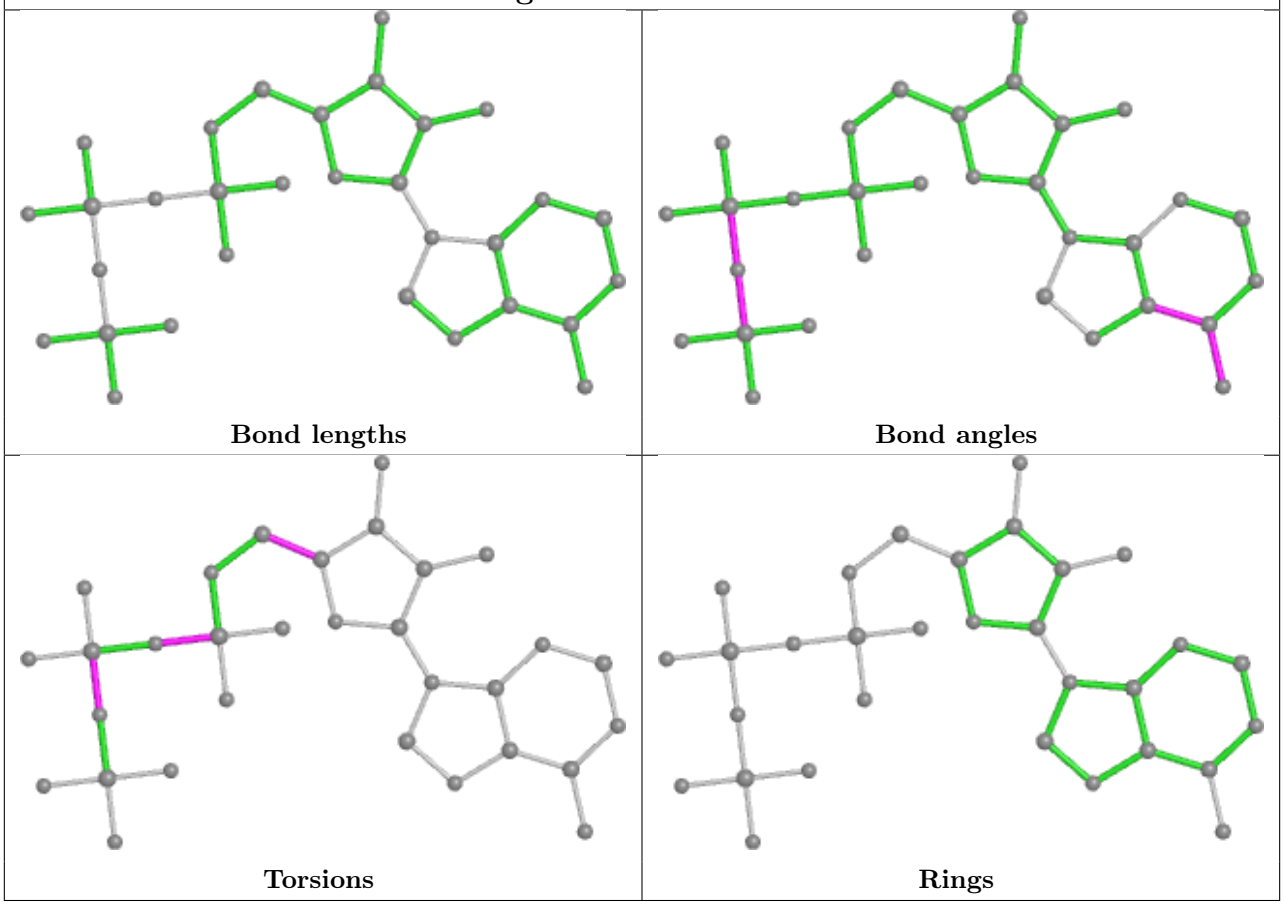


Torsions



Rings

Ligand ATP D 5002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

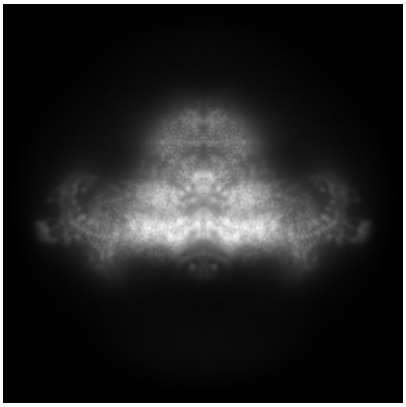
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26405. These allow visual inspection of the internal detail of the map and identification of artifacts.

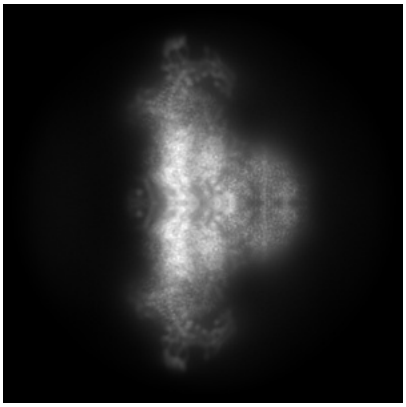
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

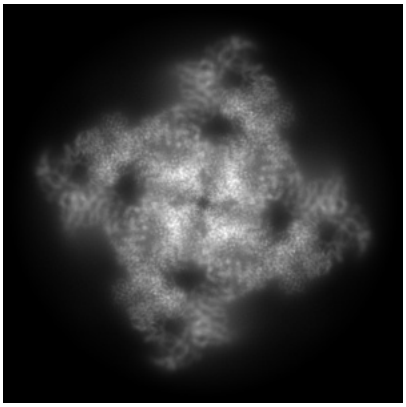
6.1.1 Primary map



X



Y

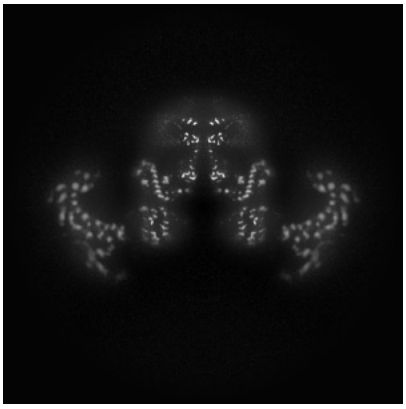


Z

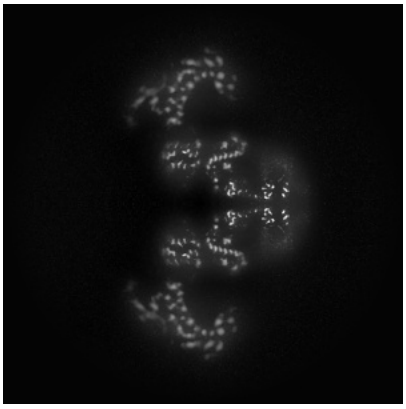
The images above show the map projected in three orthogonal directions.

6.2 Central slices

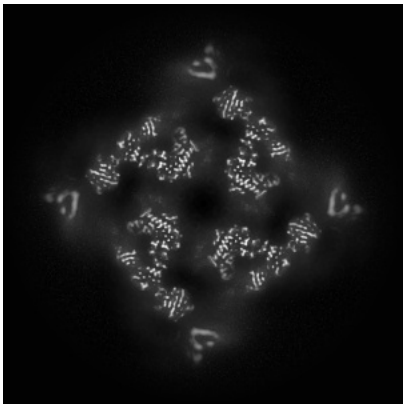
6.2.1 Primary map



X Index: 256



Y Index: 256

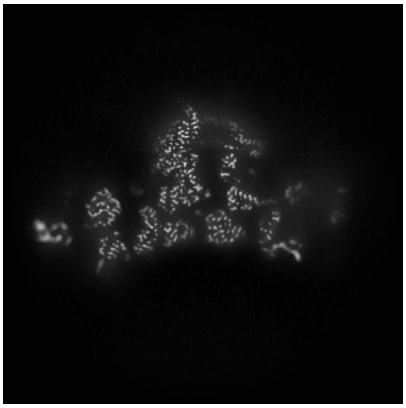


Z Index: 256

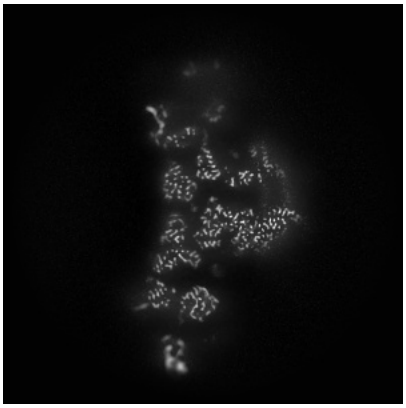
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

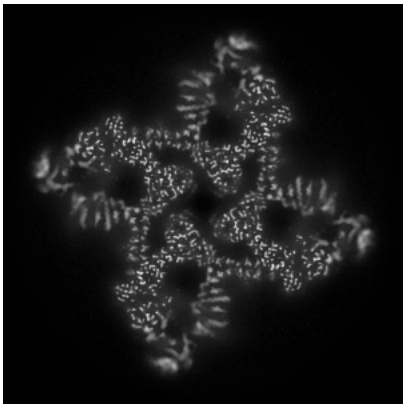
6.3.1 Primary map



X Index: 219



Y Index: 293



Z Index: 224

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 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

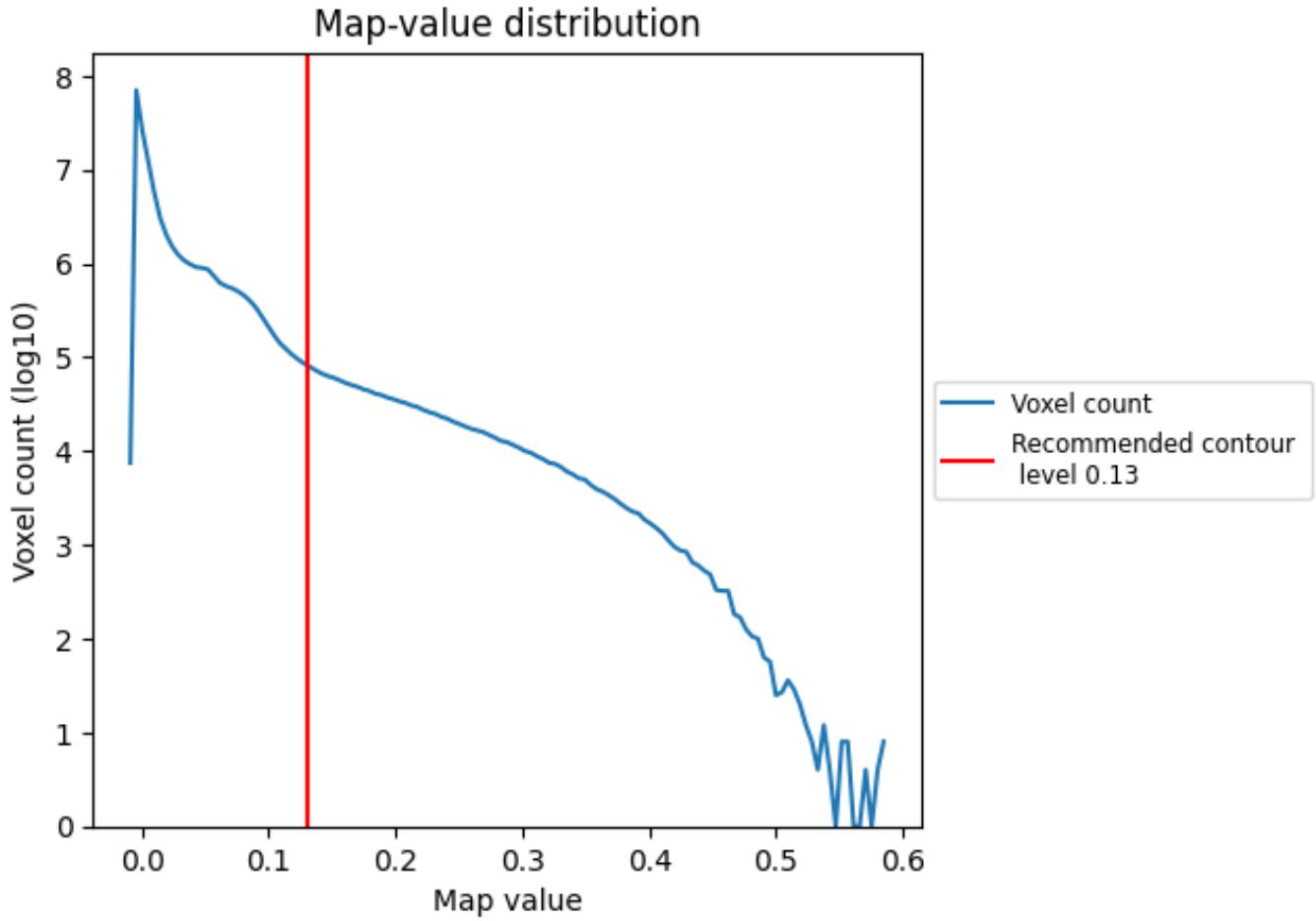
6.5 Mask visualisation (i)

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

7 Map analysis

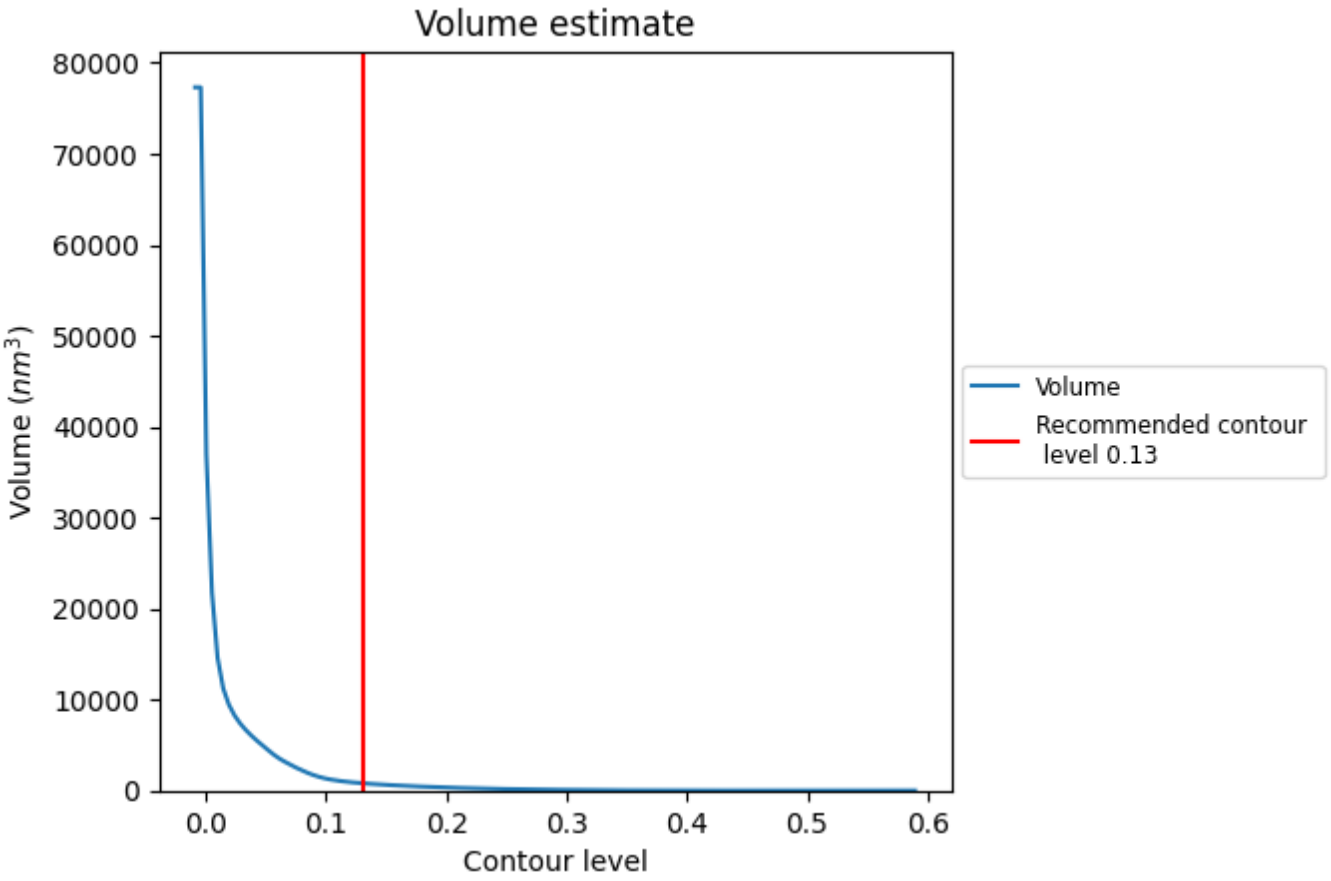
This section contains the results of statistical analysis of the map.

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.

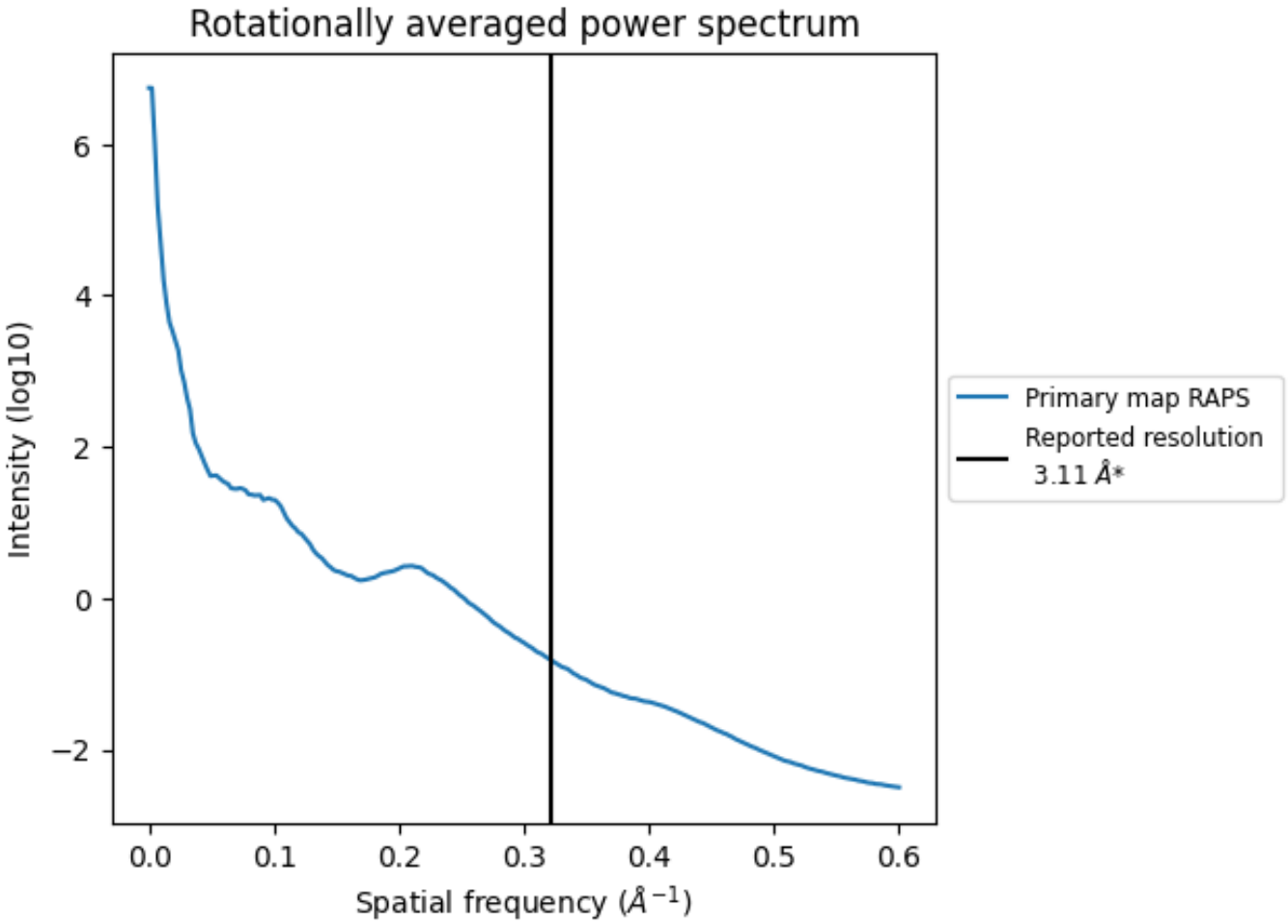
7.2 Volume estimate



The volume at the recommended contour level is 805 nm^3; this corresponds to an approximate mass of 728 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 0.322 Å^{-1}

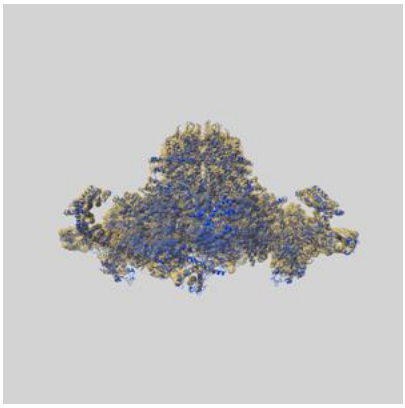
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

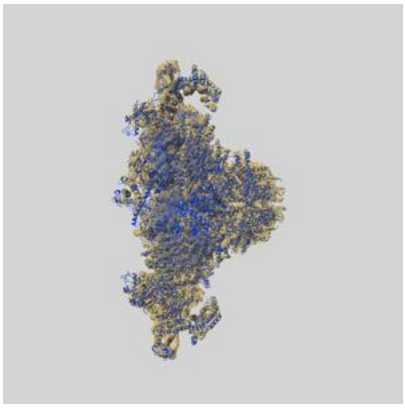
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26405 and PDB model 7U9Q. Per-residue inclusion information can be found in section 3 on page 5.

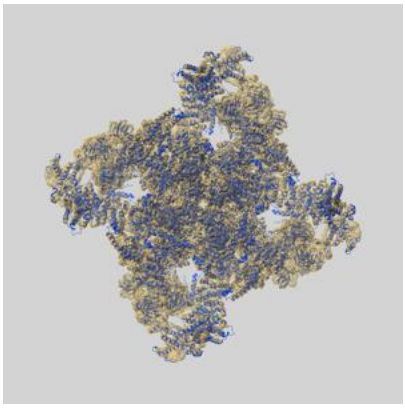
9.1 Map-model overlay



X



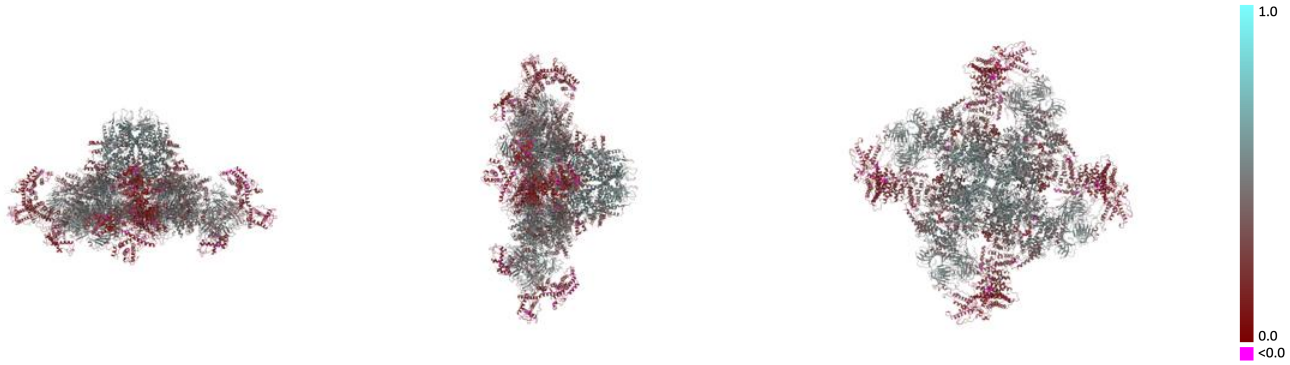
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

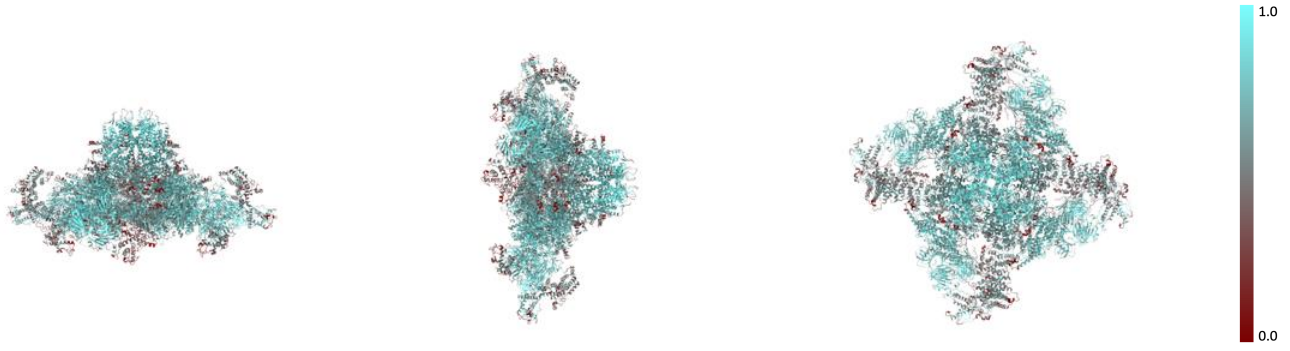
9.2 Q-score mapped to coordinate model



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.

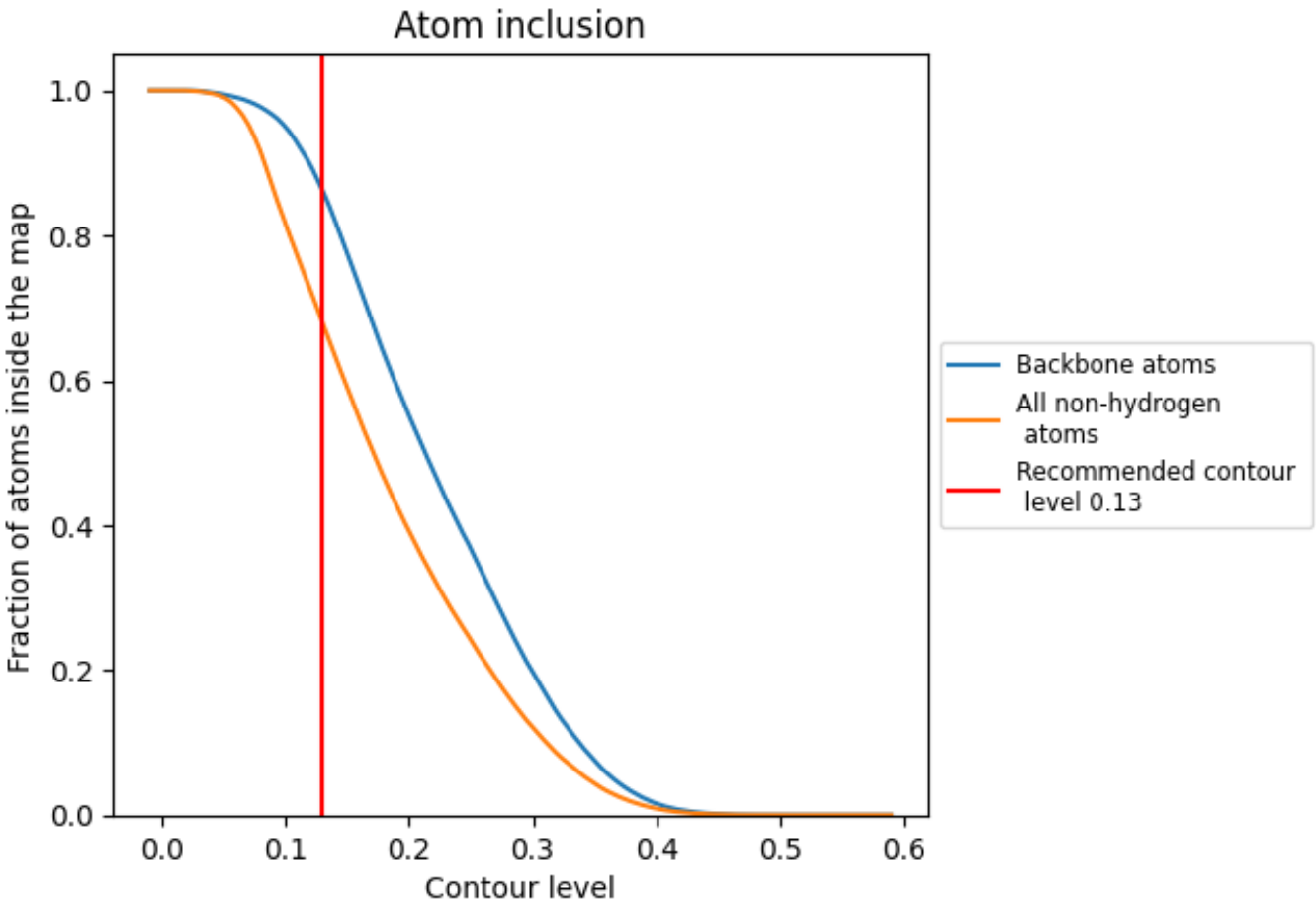
9.3 Atom inclusion mapped to coordinate model



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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 68% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6809	0.3770
A	0.6833	0.3810
B	0.6703	0.3640
C	0.6807	0.3790
D	0.6780	0.3740
E	0.7978	0.4950
F	0.7866	0.4900
G	0.7891	0.5020
H	0.8089	0.5130