Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 11:10 PM EST

PDB ID	:	7UA1
EMDB ID	:	EMD-26412
Title	:	Structure of PKA phosphorylated human RyR2-R2474S in the closed state in the presence of ARM210
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2022-03-11
Resolution	:	2.99 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:

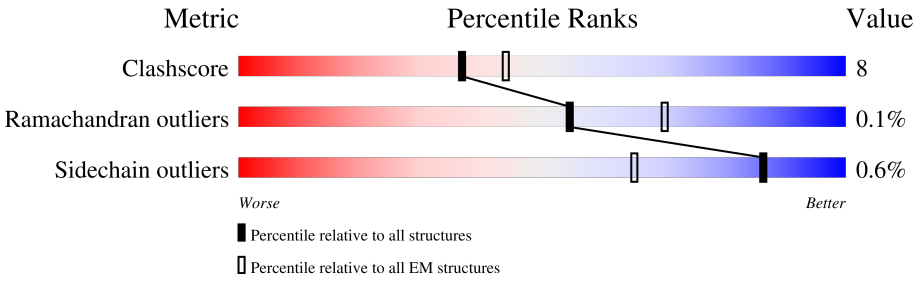
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.99 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4967	6% 67% 18% 15%
1	B	4967	6% 67% 18% 15%
1	C	4967	6% 67% 18% 15%
1	D	4967	6% 67% 18% 15%
2	E	108	78% 21%
2	F	108	78% 21%
2	G	108	78% 21%
2	H	108	78% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	A	5003	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 138680 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 Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4224	Total 33766	C 21513	N 5742	O 6281	S 230	2	0
1	B	4224	Total 33766	C 21513	N 5742	O 6281	S 230	2	0
1	C	4224	Total 33766	C 21513	N 5742	O 6281	S 230	2	0
1	D	4224	Total 33766	C 21513	N 5742	O 6281	S 230	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2474	SER	ARG	variant	UNP Q92736
B	2474	SER	ARG	variant	UNP Q92736
C	2474	SER	ARG	variant	UNP Q92736
D	2474	SER	ARG	variant	UNP Q92736

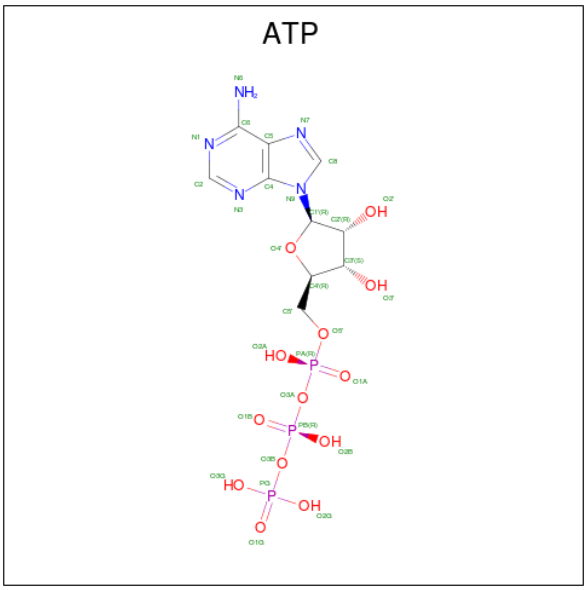
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- 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 1 1	0
3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0

- 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 62 20 10 26 6	0
4	A	1	Total C N O P 62 20 10 26 6	0
4	B	1	Total C N O P 62 20 10 26 6	0
4	B	1	Total C N O P 62 20 10 26 6	0
4	C	1	Total C N O P 62 20 10 26 6	0
4	C	1	Total C N O P 62 20 10 26 6	0
4	D	1	Total C N O P 62 20 10 26 6	0

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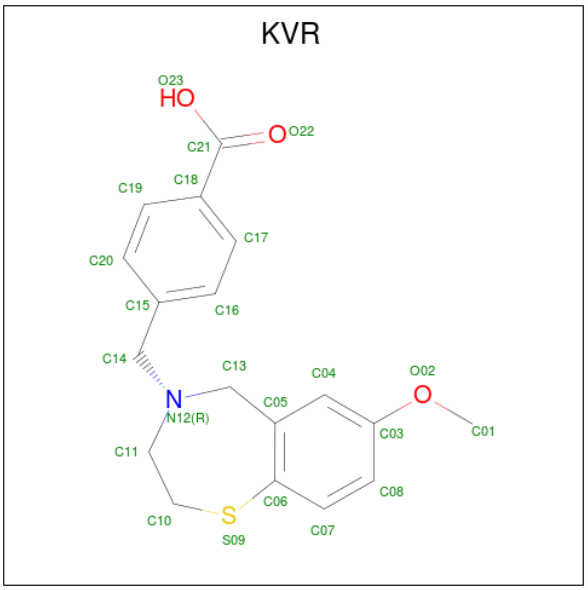
Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			62	20	10	26	6	

- Molecule 5 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (three-letter code: KVR) (formula: $C_{18}H_{19}NO_3S$).



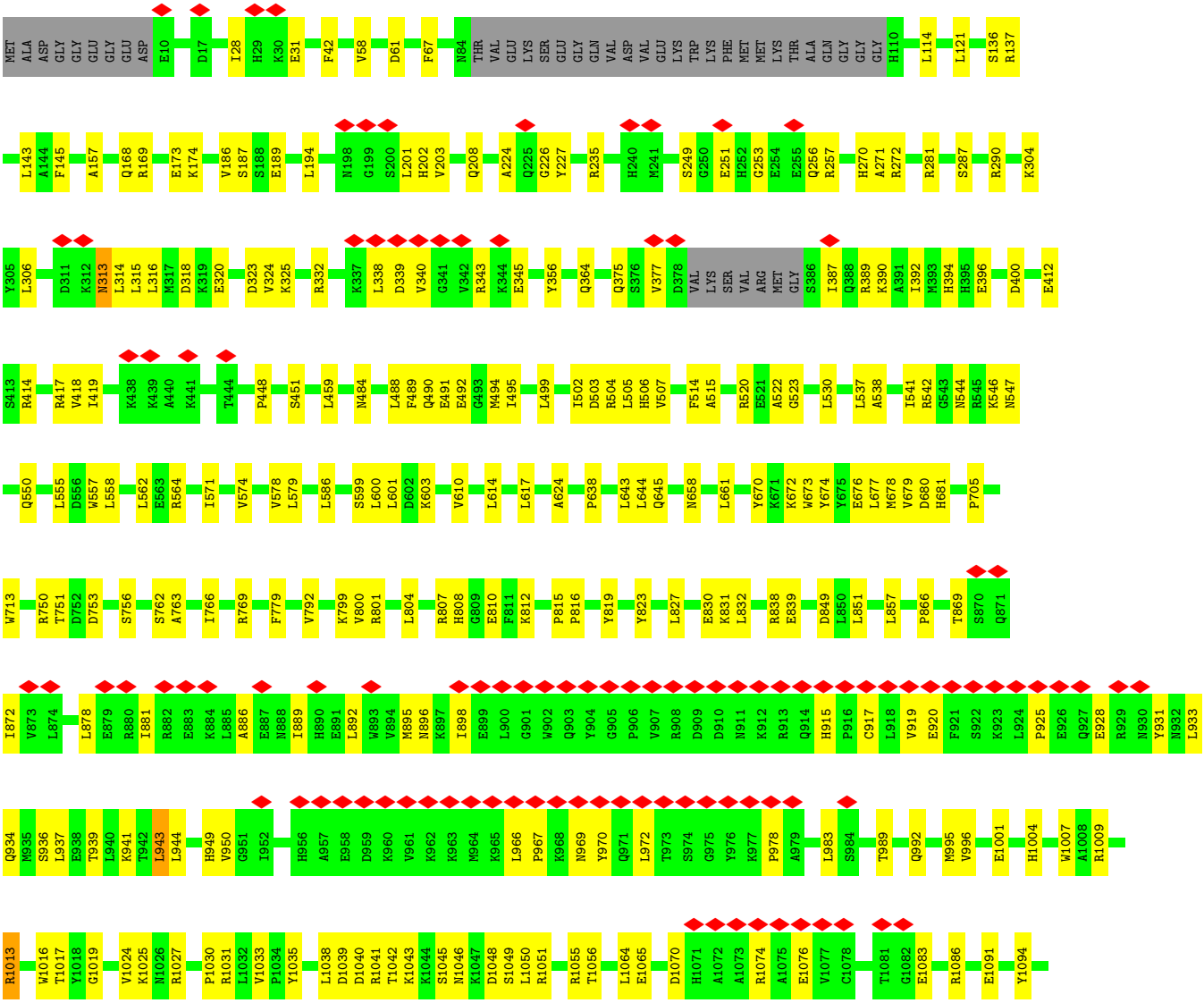
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	B	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	C	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	D	1	Total	C	N	O	S	0
			23	18	1	3	1	

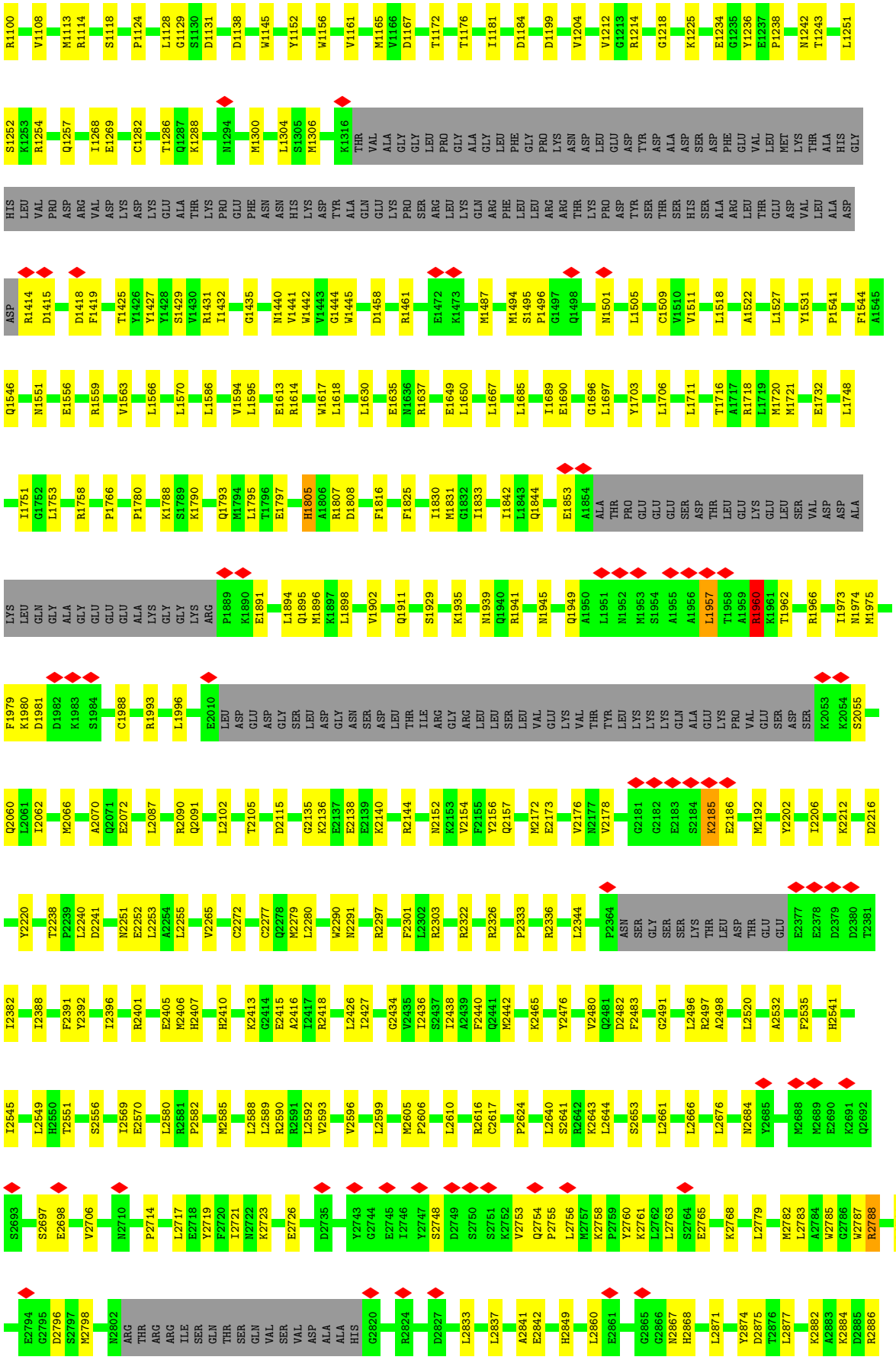
3 Residue-property plots (i)

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: Ryanodine receptor 2

Chain A:

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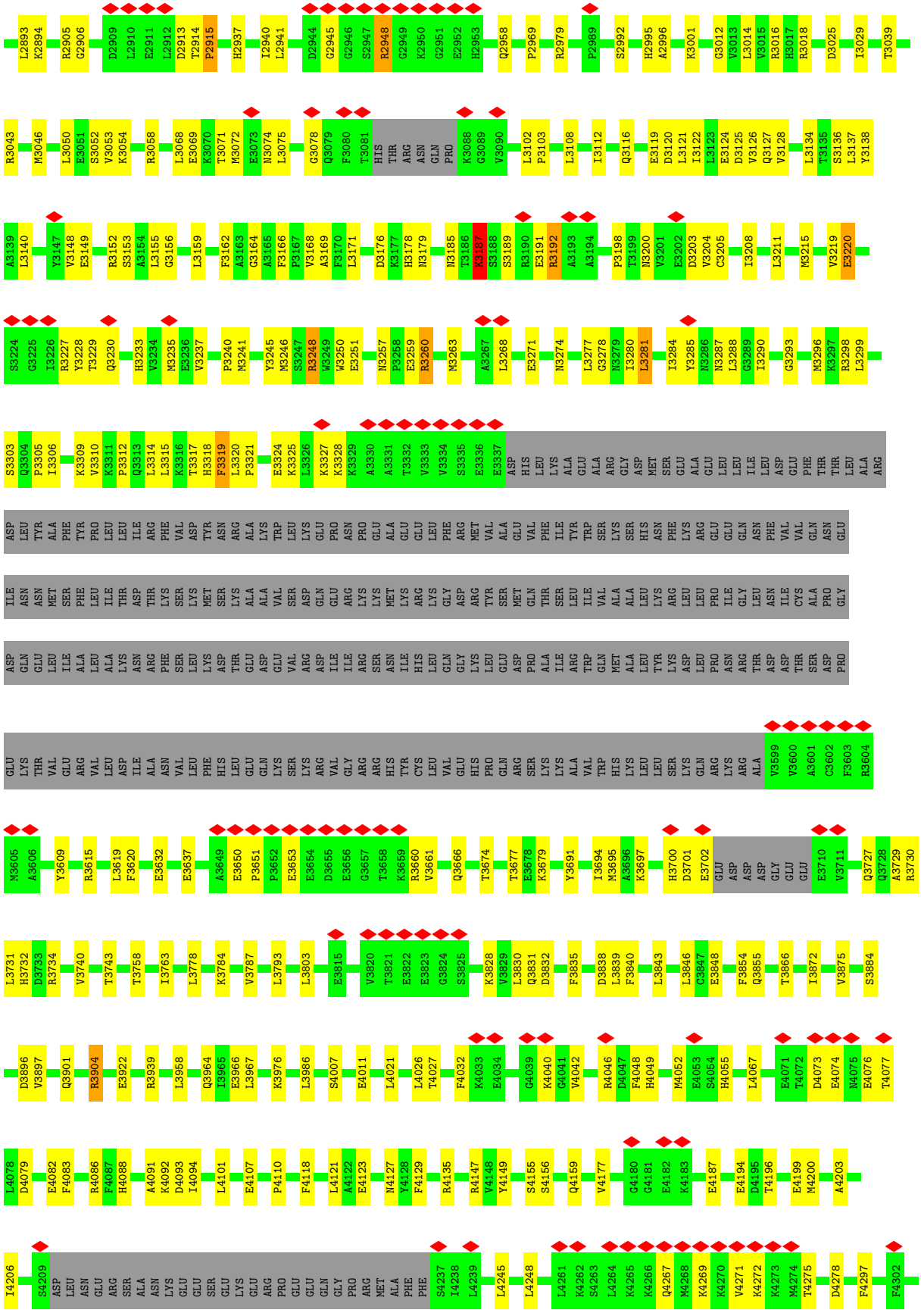
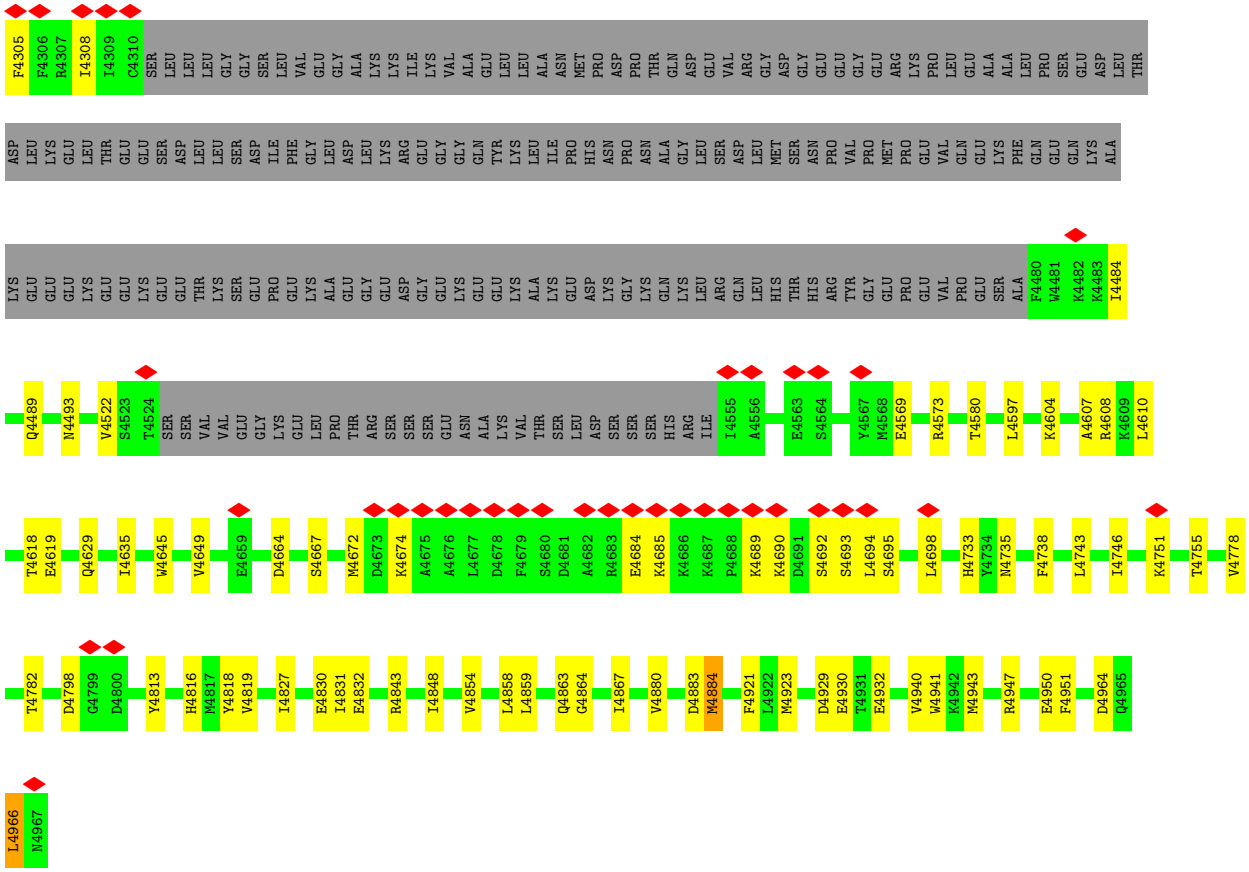
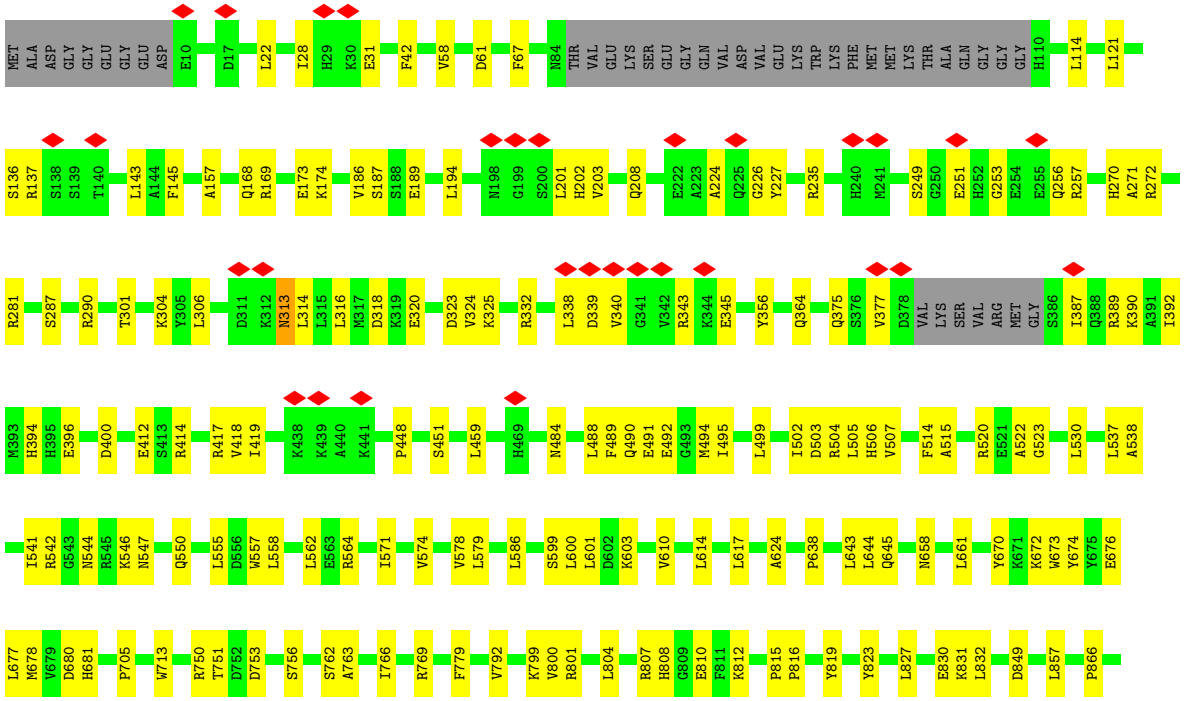
S1252 K1253 R1254 Q1257 I1268 E1269 C1282 T1286 Q1287 K1288 N1294 M1300 L1304 S1305 M1306 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY
HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO 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 LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU VAL ASP LEU LEU ALA ASP
ASP R1414 D1415 D1418 F1419 T1425 Y1426 Y1427 Y1428 S1429 V1430 R1431 I1432 G1435 N1440 V1441 W1442 V1443 G1444 W1445 D1458 R1461 E1472 K1473 M1487 M1494 S1495 P1496 G1497 Q1498 N1501 L1505 C1509 V1510 V1511 L1518 A1522 L1527 Y1531 P1541 F1544 A1545
Q1546 N1551 E1556 R1559 V1563 L1566 L1570 L1586 V1594 L1595 E1613 R1614 W1617 L1618 L1630 E1635 N1636 R1637 E1649 L1650 L1667 L1685 I1689 E1690 G1696 L1697 Y1703 L1706 L1711 T1716 A1717 R1718 L1719 M1720 M1721 E1732 L1748
I1751 G1752 L1753 R1758 P1766 P1780 K1788 S1789 K1790 Q1793 M1794 L1795 T1796 E1797 H1805 A1806 R1807 D1808 F1816 F1825 I1830 M1831 G1832 I1833 I1842 L1843 Q1844 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 E1891 L1894 Q1895 M1896 K1897 L1898 V1902 Q1911 S1929 K1935 N1939 Q1940 R1941 N1945 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 R1966 I1973 N1974 M1975
F1979 K1980 D1981 D1982 K1983 S1984 C1988 R1993 L1996 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU 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
Q2060 L2061 I2062 M2066 A2070 Q2071 E2072 L2087 R2090 Q2091 L2102 T2105 D2115 G2135 K2136 E2137 E2138 E2139 K2140 R2144 N2152 K2153 V2154 F2155 Y2156 Q2157 M2172 E2173 V2176 N2177 V2178 G2181 G2182 E2183 S2184 K2185 E2186 M2192 Y2202 I2206 K2212 D2216
Y2220 T2238 P2239 L2240 D2241 N2251 E2252 L2253 A2254 L2255 V2265 C2272 C2277 Q2278 M2279 L2280 W2290 N2291 R2297 F2301 L2302 R2303 R2322 R2326 P2333 R2336 L2344 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 T2381
I2382 I2388 F2391 Y2392 I2396 R2401 E2405 M2406 H2407 H2410 K2413 G2414 E2415 A2416 I2417 R2418 L2426 I2427 G2434 V2435 I2436 S2437 I2438 A2439 F2440 Q2441 M2442 K2465 Y2476 V2480 Q2481 D2482 F2483 G2491 L2496 R2497 A2498 L2520 A2532 F2535 H2541
I2545 L2549 H2550 T2551 S2556 I2569 E2570 L2580 R2581 P2582 M2585 L2588 L2589 R2590 R2591 L2592 V2593 V2596 L2599 M2605 P2606 L2610 R2616 C2617 P2624 L2640 S2641 R2642 K2643 L2644 S2653 L2661 L2666 L2676 N2684 Y2685 M2688 M2689 E2690 K2691 Q2692
S2693 S2697 E2698 V2706 N2710 P2714 L2717 E2718 Y2719 F2720 I2721 N2722 K2723 E2726 D2735 Y2743 G2744 E2745 I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759 Y2760 K2761 L2762 L2763 S2764 E2765 K2768 L2779 M2782 L2783 A2784 W2785 G2786 W2787 R2788 R2791
E2794 G2795 D2796 S2797 M2798 N2802 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 R2824 D2827 L2833 L2837 A2841 E2842 H2849 L2860 E2861 G2865 G2866 N2867 H2868 L2871 Y2874 D2875 T2876 L2877 K2882 A2883 K2884 D2885 R2886

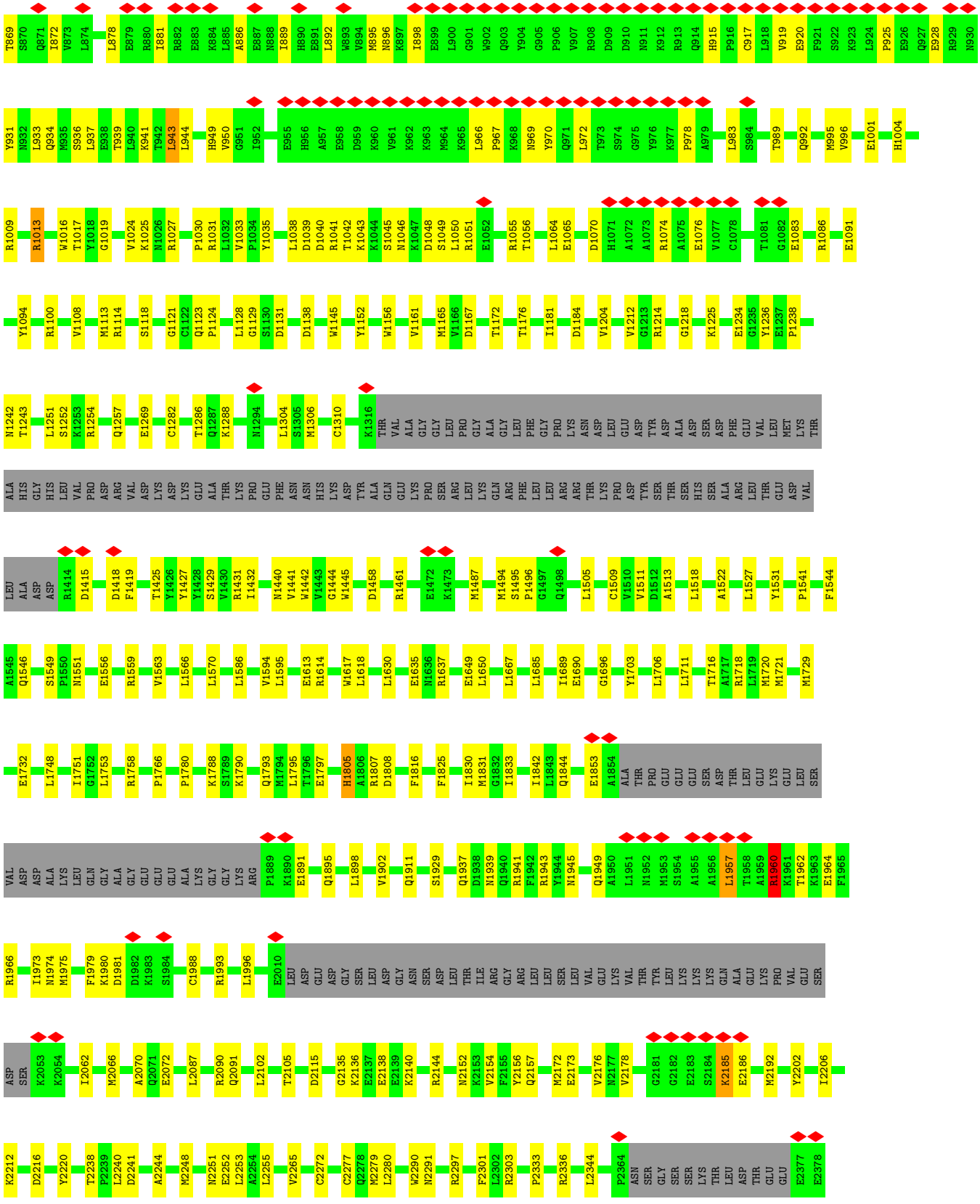




• Molecule 1: Ryanodine receptor 2

Chain B:

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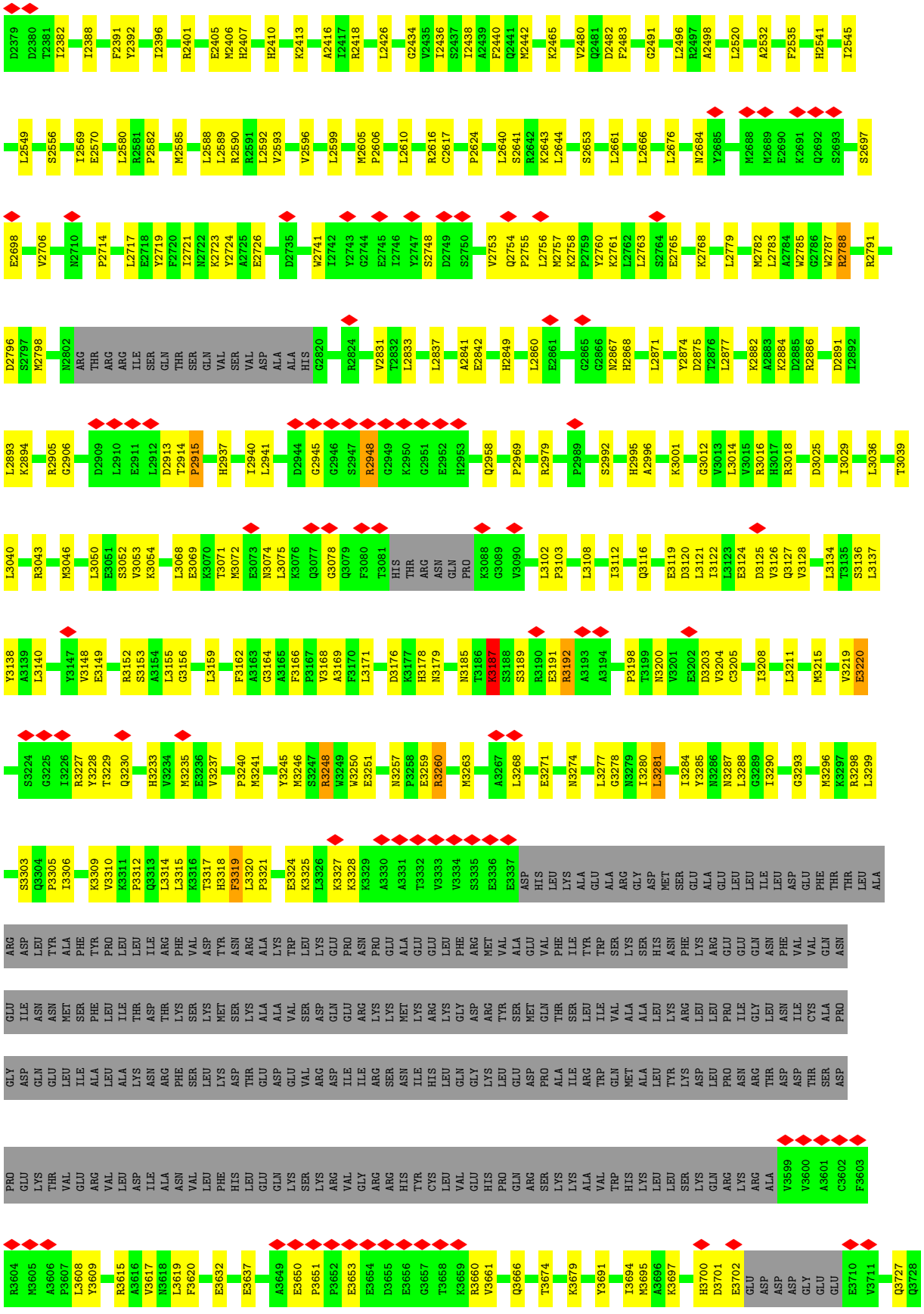
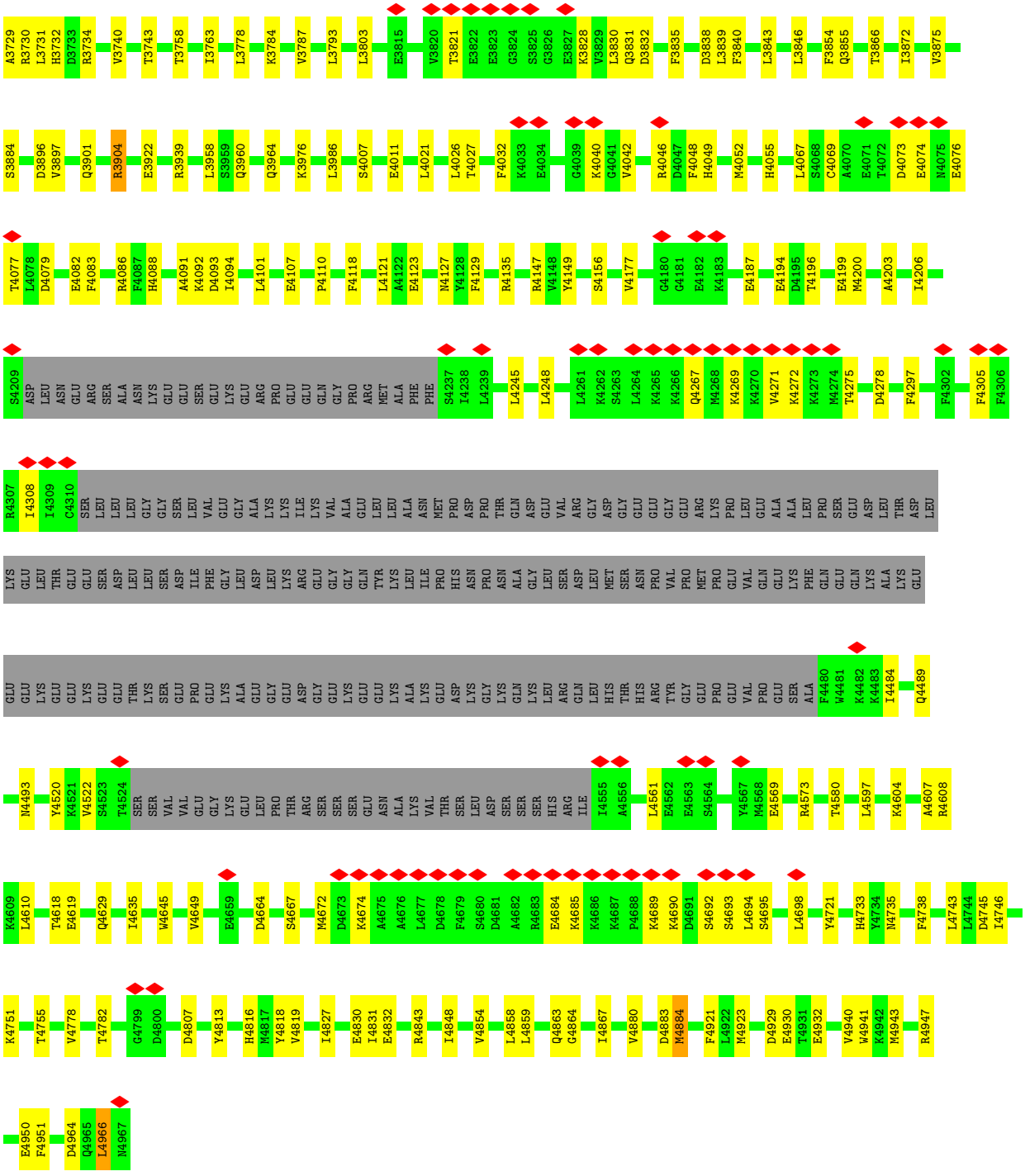
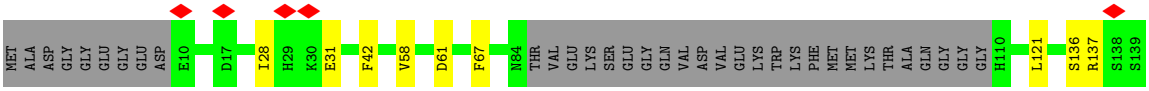
Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 H949 V950 G951 I952 E955 H956 A957 E958 D959 K960 V961 K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 L983 S984 T989 Q992 M995 V996 E1001 H1004
R1009 R1013 W1016 T1017 Y1018 G1019 V1024 K1025 N1026 R1027 P1030 R1031 L1032 V1033 P1034 Y1035 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 R1055 T1056 L1064 E1065 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 T1081 G1082 E1083 R1086 E1091
Y1094 R1100 V1108 M1113 R1114 S1118 G1121 C1122 Q1123 P1124 L1128 G1129 S1130 D1131 D1138 W1145 Y1152 W1156 V1161 M1165 V1166 D1167 T1172 T1176 I1181 D1184 V1204 V1212 G1213 R1214 G1218 K1225 E1234 G1235 Y1236 E1237 P1238
N1242 T1243 L1251 S1252 K1253 R1254 Q1257 E1269 C1282 T1286 Q1287 K1288 N1294 L1304 S1305 M1306 C1310 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 D1418 F1419 T1425 Y1426 Y1427 Y1428 S1429 V1430 R1431 I1432 N1440 V1441 W1442 V1443 G1444 W1445 D1458 R1461 E1472 K1473 M1487 M1494 S1495 P1496 G1497 Q1498 L1505 C1509 V1510 V1511 D1512 A1513 L1518 A1522 L1527 Y1531 P1541 F1544
A1545 Q1546 S1549 P1550 N1551 E1556 R1559 V1563 L1566 L1570 L1586 V1594 L1595 E1613 R1614 W1617 L1618 L1630 E1635 N1636 R1637 E1649 L1650 L1667 L1685 I1689 E1690 G1696 Y1703 L1706 L1711 T1716 A1717 R1718 L1719 M1720 M1721 M1729
E1732 L1748 I1751 G1752 L1753 R1758 P1766 P1780 K1788 S1789 K1790 Q1793 M1794 L1795 T1796 E1797 H1805 A1806 R1807 D1808 F1816 F1825 I1830 M1831 G1832 I1833 I1842 L1843 Q1844 E1853 A1854 ALA THR PRO GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER
VAL ASP ASP ALA LYS LEU GLN GLY GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 E1891 Q1895 L1898 V1902 Q1911 S1929 Q1937 D1938 N1939 Q1940 R1941 F1942 R1943 Y1944 N1945 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 K1963 E1964 F1965
R1966 I1973 N1974 M1975 F1979 K1980 D1981 D1982 K1983 S1984 C1988 R1993 L1996 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 I2062 M2066 A2070 Q2071 E2072 L2087 R2090 Q2091 L2102 T2105 D2115 G2135 K2136 E2137 E2138 E2139 K2140 R2144 N2152 K2153 V2154 F2155 Y2156 Q2157 M2172 E2173 V2176 N2177 V2178 G2181 G2182 E2183 S2184 K2185 E2186 M2192 Y2202 I2206
K2212 D2216 Y2220 T2238 P2239 L2240 D2241 A2244 M2248 N2251 E2252 L2253 A2254 L2255 V2265 C2272 C2277 Q2278 M2279 L2280 W2290 N2291 R2297 F2301 L2302 R2303 P2333 R2336 L2344 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378

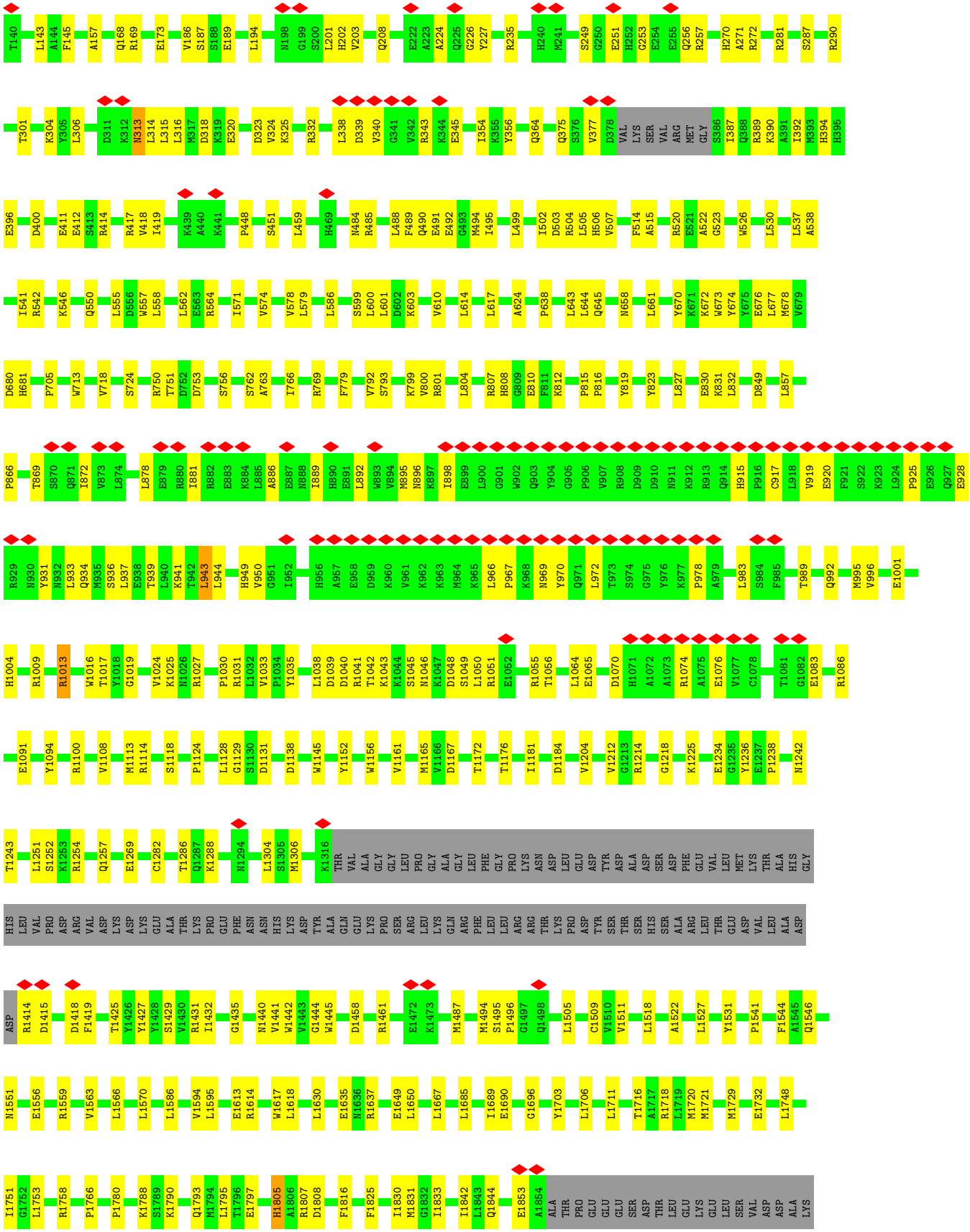




• Molecule 1: Ryanodine receptor 2

Chain C:

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T301 K304 Y305 L306 D311 K312 N313 L314 L315 L316 M317 D318 K319 E320 D323 V324 K325 R332 L338 D339 V340 G341 V342 K343 K344 E345 I354 K355 Y356 Q364 Q375 S376 V377 D378 VAL LYS SER VAL ARG MET GLY S386 I387 Q388 R389 K390 A391 I392 K393 H394 H395
E396 D400 E411 E412 S413 R414 R417 V418 I419 K439 A440 K441 P448 S451 L459 H469 N484 R485 L488 F489 Q490 E491 E492 G493 M494 I495 L499 I502 D503 R504 L505 H506 V507 F514 A515 R520 E521 A522 G523 W526 L530 L537 A538
I541 R542 K546 Q550 L555 D556 W557 L558 L562 E563 R564 I571 V574 V578 L579 L586 S599 L600 L601 D602 K603 V610 L614 L617 A624 P638 L643 L644 Q645 N658 L661 Y670 K671 K672 W673 Y674 Y675 E676 L677 M678 V679
D680 H681 P705 W713 V718 S724 R750 T751 D752 D753 S756 S762 A763 I766 R769 F779 V792 S793 K799 V800 R801 L804 R807 H808 G809 E810 F811 K812 P815 P816 Y819 Y823 L827 E830 K831 L832 D849 L857
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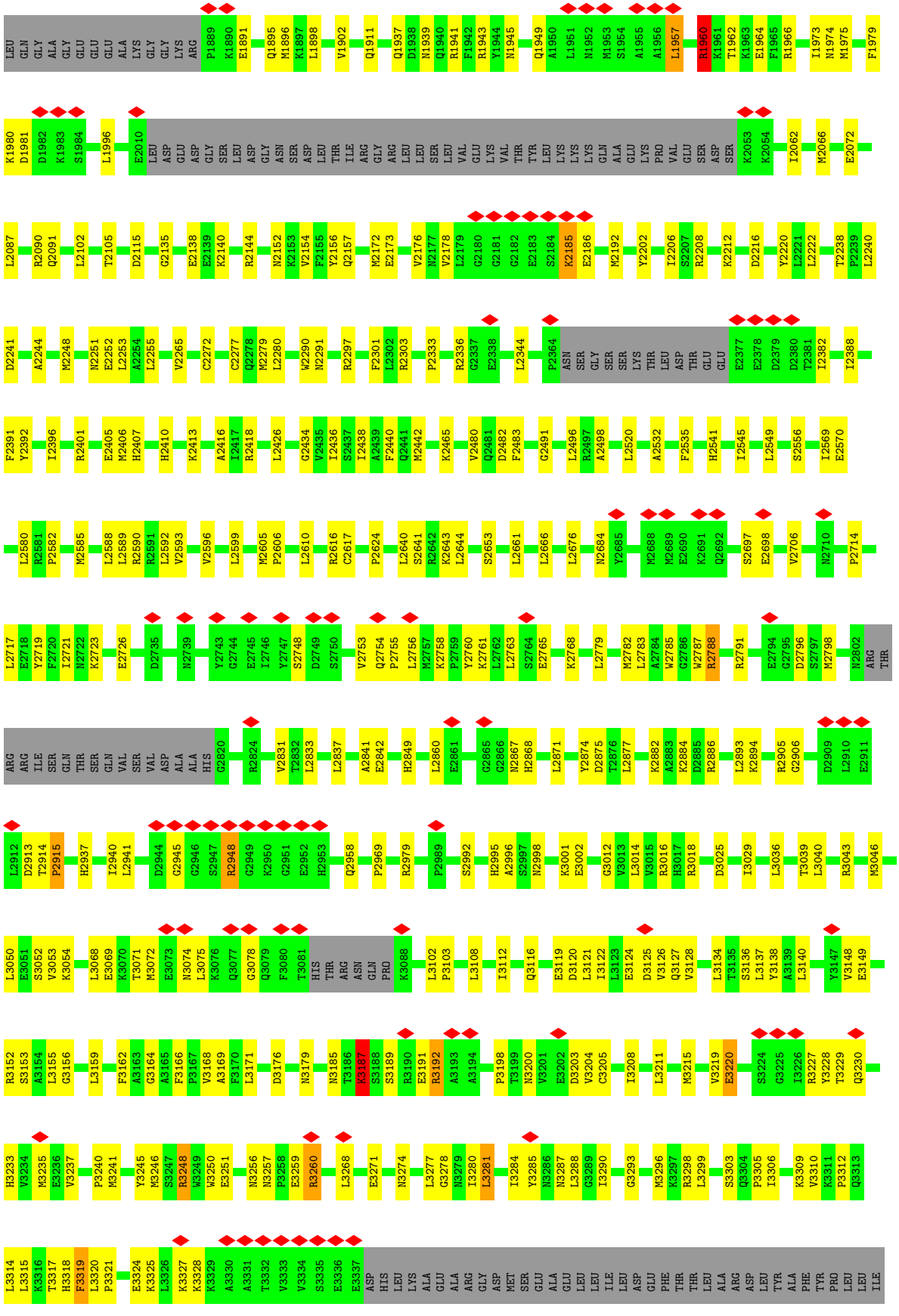
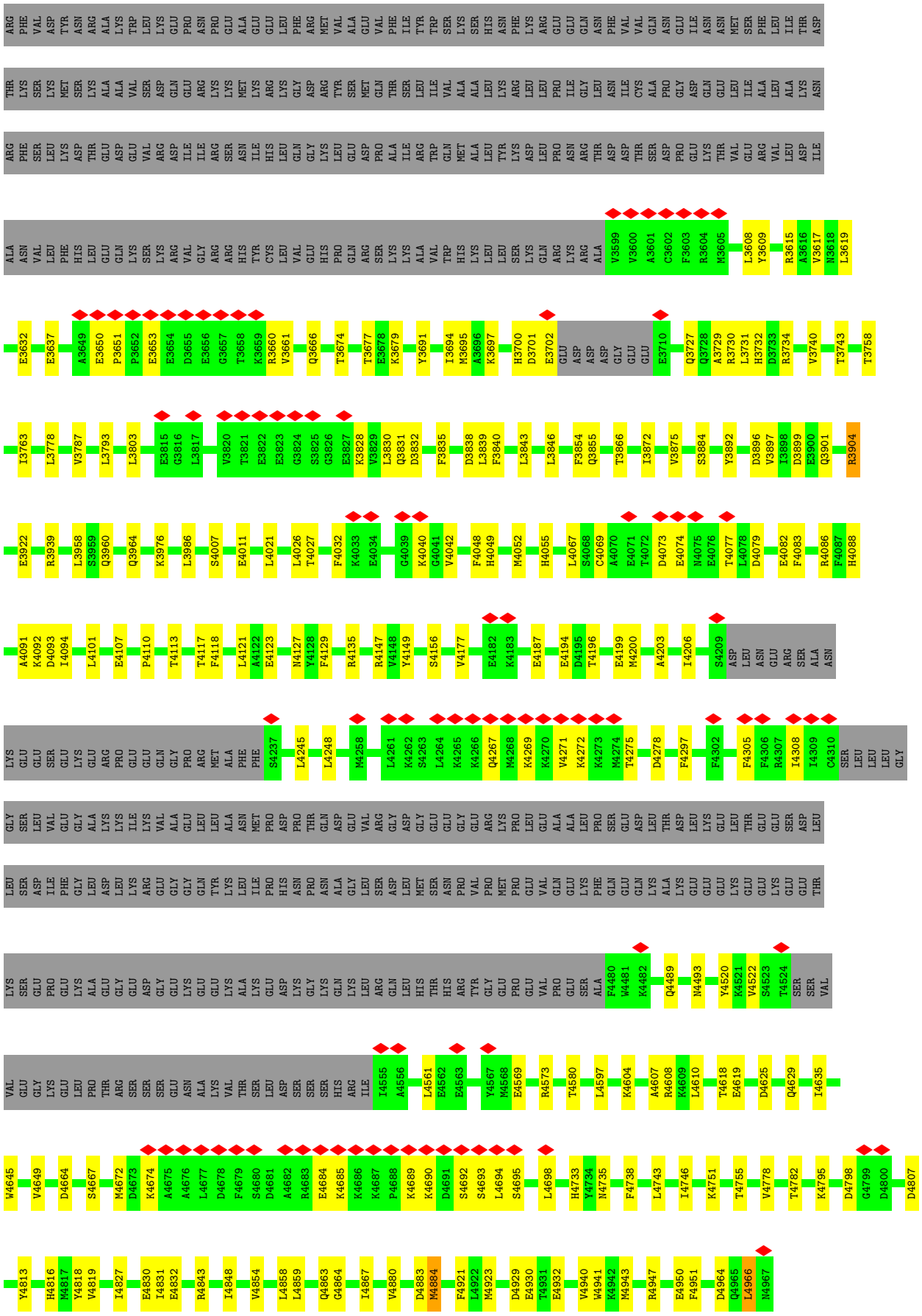
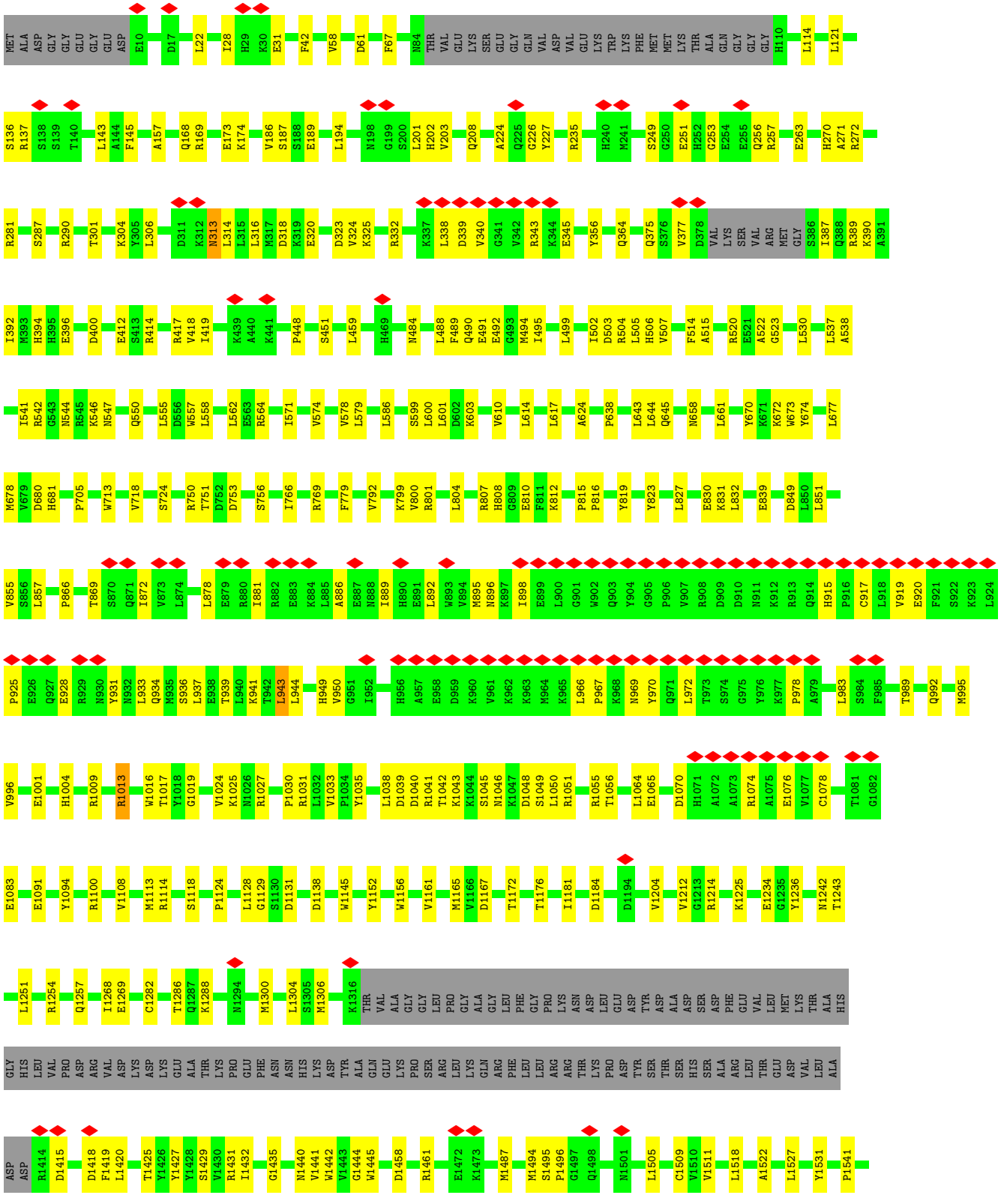
R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 H949 V950 G951 I952 H956 A957 E958 D959 K960 V961 K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 L983 S984 F985 T989 Q992 M995 V996 E1001
H1004 R1009 R1013 W1016 T1017 Y1018 G1019 V1024 K1025 N1026 R1027 P1030 R1031 L1032 V1033 P1034 Y1035 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 R1055 T1056 L1064 E1065 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 T1081 G1082 E1083 R1086
E1091 Y1094 R1100 V1108 M1113 R1114 S1118 P1124 L1128 G1129 S1130 D1131 D1138 W1145 Y1152 W1156 V1161 M1165 V1166 D1167 T1172 T1176 I1181 D1184 V1204 V1212 G1213 R1214 G1218 K1225 E1234 G1235 Y1236 E1237 P1238 N1242
T1243 L1251 S1252 K1253 R1254 Q1257 E1269 C1282 T1286 Q1287 K1288 N1294 L1304 S1305 M1306 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 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 LEU ASP VAL LEU ALA ASP
ASP R1414 D1415 D1418 F1419 T1425 Y1426 Y1427 Y1428 S1429 V1430 R1431 I1432 G1435 N1440 V1441 W1442 V1443 G1444 W1445 D1458 R1461 E1472 K1473 M1487 M1494 S1495 P1496 G1497 Q1498 L1505 C1509 V1510 V1511 L1518 A1522 L1527 Y1531 P1541 F1544 A1545 Q1546
N1551 E1556 R1559 V1563 L1566 L1570 L1586 V1594 L1595 E1613 R1614 W1617 L1618 L1630 E1635 N1636 R1637 E1649 L1650 L1667 L1685 I1689 E1690 G1696 Y1703 L1706 L1711 T1716 A1717 R1718 L1719 M1720 M1721 M1729 E1732 L1748
I1751 G1752 L1753 R1758 P1766 P1780 K1788 S1789 K1790 Q1793 M1794 L1795 T1796 E1797 H1805 A1806 R1807 D1808 F1816 F1825 I1830 M1831 G1832 I1833 I1842 L1843 Q1844 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS

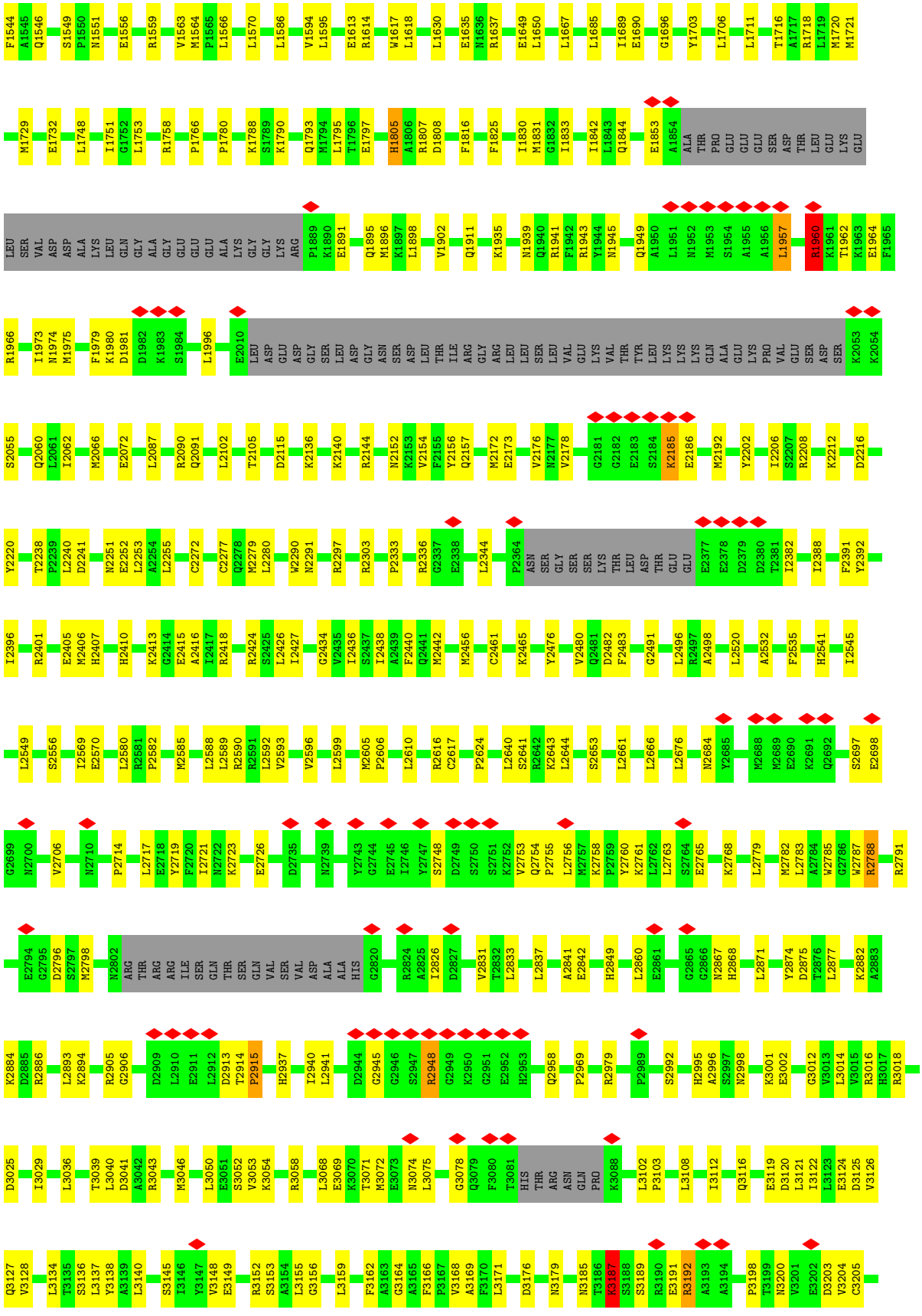


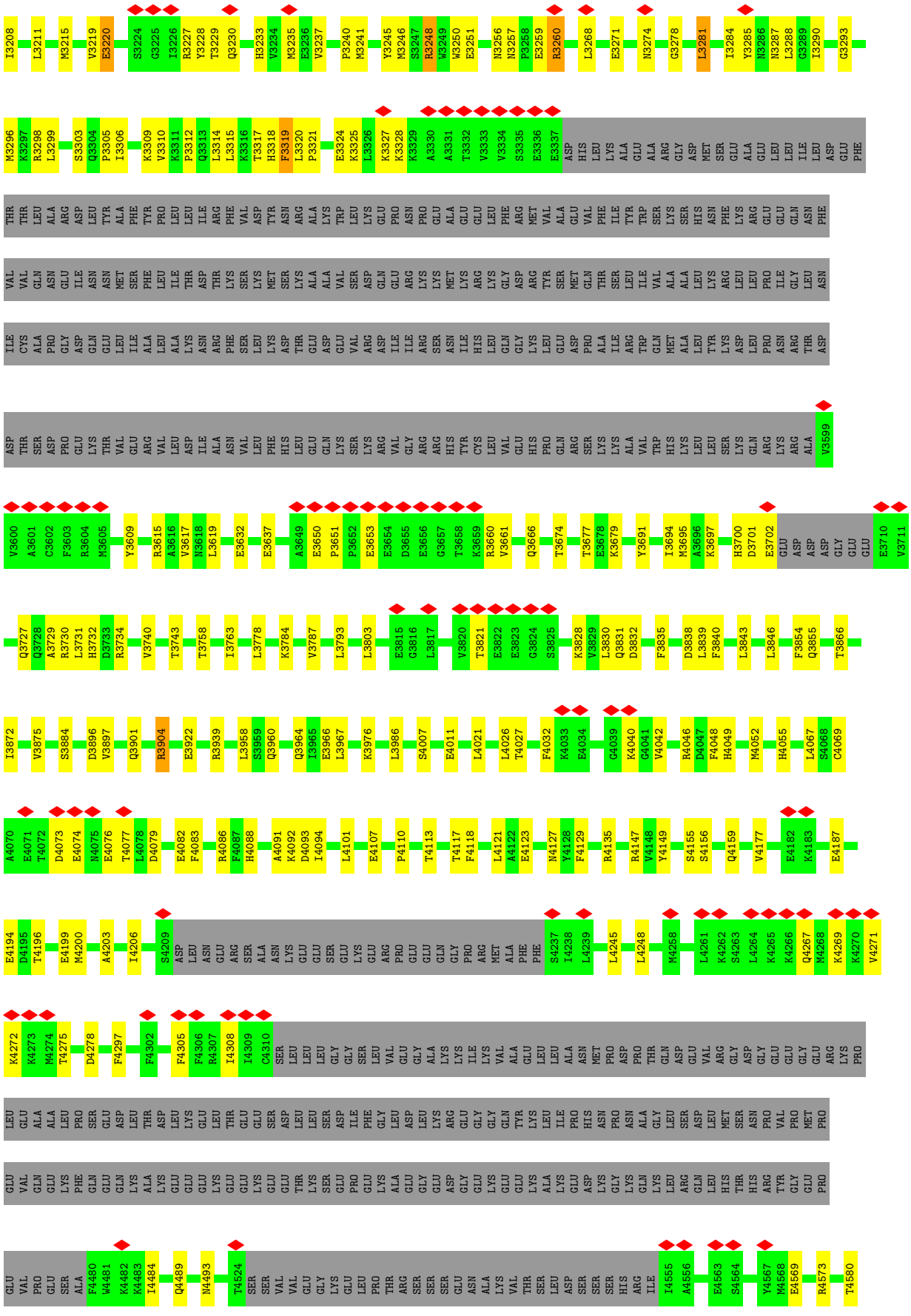


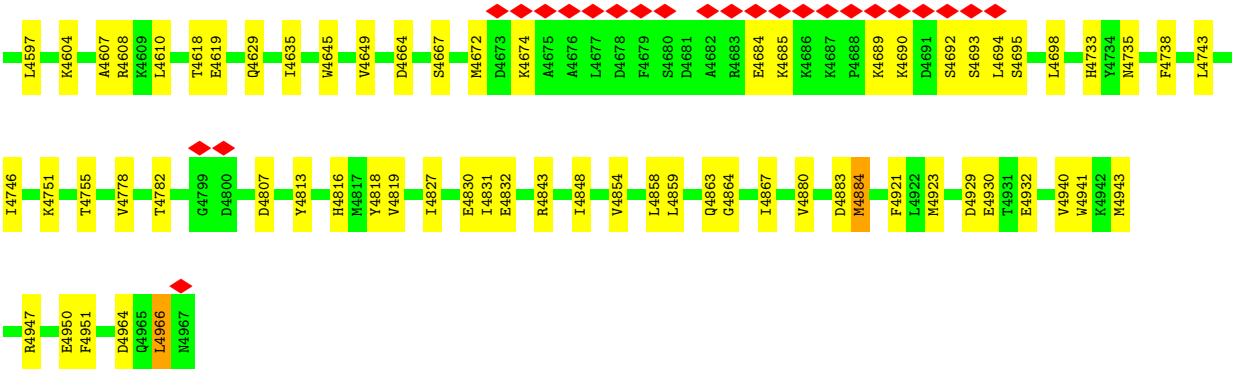
• Molecule 1: Ryanodine receptor 2

Chain D:









• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:

• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:

• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:

• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113172	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	1.040	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.036	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: KVR, ZN, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/34506	0.49	5/46608 (0.0%)
1	B	0.25	0/34506	0.49	5/46608 (0.0%)
1	C	0.25	0/34506	0.49	5/46608 (0.0%)
1	D	0.25	0/34506	0.49	5/46608 (0.0%)
2	E	0.29	0/834	0.55	0/1123
2	F	0.29	0/834	0.55	0/1123
2	G	0.29	0/834	0.55	0/1123
2	H	0.29	0/834	0.55	0/1123
All	All	0.26	0/141360	0.49	20/190924 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1957	LEU	CA-CB-CG	7.92	133.51	115.30
1	D	1957	LEU	CA-CB-CG	7.91	133.49	115.30
1	C	1957	LEU	CA-CB-CG	7.90	133.47	115.30
1	A	1957	LEU	CA-CB-CG	7.89	133.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1960	ARG	CG-CD-NE	-6.99	97.11	111.80
1	B	1960	ARG	CG-CD-NE	-6.99	97.12	111.80
1	D	1960	ARG	CG-CD-NE	-6.99	97.13	111.80
1	C	1960	ARG	CG-CD-NE	-6.99	97.13	111.80
1	B	1960	ARG	CA-CB-CG	6.86	128.50	113.40
1	A	1960	ARG	CA-CB-CG	6.86	128.50	113.40
1	D	1960	ARG	CA-CB-CG	6.86	128.49	113.40
1	C	1960	ARG	CA-CB-CG	6.84	128.46	113.40
1	A	3281	LEU	CA-CB-CG	6.49	130.23	115.30
1	C	3281	LEU	CA-CB-CG	6.48	130.19	115.30
1	D	3281	LEU	CA-CB-CG	6.48	130.19	115.30
1	B	3281	LEU	CA-CB-CG	6.47	130.19	115.30
1	B	943	LEU	CA-CB-CG	5.99	129.07	115.30
1	C	943	LEU	CA-CB-CG	5.99	129.07	115.30
1	A	943	LEU	CA-CB-CG	5.97	129.03	115.30
1	D	943	LEU	CA-CB-CG	5.97	129.03	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3187	LYS	Peptide
1	B	3187	LYS	Peptide
1	C	3187	LYS	Peptide
1	D	3187	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33766	0	33444	581	0
1	B	33766	0	33444	571	0
1	C	33766	0	33444	571	0
1	D	33766	0	33444	574	0
2	E	818	0	821	12	0
2	F	818	0	821	12	0
2	G	818	0	821	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	818	0	821	12	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	9	0
4	B	62	0	24	0	0
4	C	62	0	24	0	0
4	D	62	0	24	0	0
5	A	23	0	0	3	0
5	B	23	0	0	0	0
5	C	23	0	0	0	0
5	D	23	0	0	0	0
All	All	138680	0	137156	2298	0

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

All (2298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:TYR:HD2	4:A:5003:ATP:N6	0.96	1.44
1:A:931:TYR:CD2	4:A:5003:ATP:N6	1.86	1.41
4:A:5003:ATP:H5'1	5:A:5004:KVR:C19	1.97	0.95
1:C:3149:GLU:HA	1:C:3152:ARG:HG2	1.52	0.92
1:A:3149:GLU:HA	1:A:3152:ARG:HG2	1.52	0.91
1:B:3149:GLU:HA	1:B:3152:ARG:HG2	1.52	0.91
1:D:3149:GLU:HA	1:D:3152:ARG:HG2	1.52	0.90
1:A:931:TYR:HD2	4:A:5003:ATP:HN62	0.93	0.89
1:A:928:GLU:OE2	4:A:5003:ATP:C2	2.24	0.86
1:C:1957:LEU:O	1:C:1960:ARG:NH1	2.11	0.84
1:D:1960:ARG:H	1:D:1960:ARG:HD3	1.43	0.84
1:A:1960:ARG:HD3	1:A:1960:ARG:H	1.43	0.83
1:C:1960:ARG:HD3	1:C:1960:ARG:H	1.43	0.83
1:A:1957:LEU:O	1:A:1960:ARG:NH1	2.11	0.83
1:B:1960:ARG:H	1:B:1960:ARG:HD3	1.43	0.83
1:B:1957:LEU:O	1:B:1960:ARG:NH1	2.11	0.83
1:D:1957:LEU:O	1:D:1960:ARG:NH1	2.11	0.83
1:D:3314:LEU:O	1:D:3318:HIS:HB3	1.82	0.80
1:A:3189:SER:HA	1:A:3192:ARG:HG2	1.64	0.80
1:C:3314:LEU:O	1:C:3318:HIS:HB3	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3314:LEU:O	1:B:3318:HIS:HB3	1.82	0.80
1:D:3189:SER:HA	1:D:3192:ARG:HG2	1.64	0.79
1:B:3189:SER:HA	1:B:3192:ARG:HG2	1.64	0.79
1:B:3227:ARG:HE	1:B:3228:TYR:H	1.30	0.79
1:A:3227:ARG:HE	1:A:3228:TYR:H	1.30	0.79
1:A:3314:LEU:O	1:A:3318:HIS:HB3	1.82	0.79
1:D:3227:ARG:HE	1:D:3228:TYR:H	1.30	0.79
1:C:2592:LEU:HD22	1:C:2606:PRO:HB3	1.64	0.78
1:C:3189:SER:HA	1:C:3192:ARG:HG2	1.64	0.78
1:A:2592:LEU:HD22	1:A:2606:PRO:HB3	1.64	0.78
1:C:1957:LEU:HG	1:C:1960:ARG:HH12	1.49	0.78
1:B:2592:LEU:HD22	1:B:2606:PRO:HB3	1.64	0.78
1:D:1957:LEU:HG	1:D:1960:ARG:HH12	1.49	0.78
1:B:3281:LEU:HA	1:B:3284:ILE:HG12	1.66	0.78
1:C:3281:LEU:HA	1:C:3284:ILE:HG12	1.66	0.77
1:D:2592:LEU:HD22	1:D:2606:PRO:HB3	1.64	0.77
1:D:3281:LEU:HA	1:D:3284:ILE:HG12	1.66	0.77
1:B:1957:LEU:HG	1:B:1960:ARG:HH12	1.49	0.77
1:A:3281:LEU:HA	1:A:3284:ILE:HG12	1.66	0.77
1:C:3227:ARG:HE	1:C:3228:TYR:H	1.30	0.77
1:A:1957:LEU:HG	1:A:1960:ARG:HH12	1.49	0.76
1:C:4269:LYS:HA	1:C:4272:LYS:HE3	1.68	0.75
1:B:4269:LYS:HA	1:B:4272:LYS:HE3	1.68	0.75
1:A:4269:LYS:HA	1:A:4272:LYS:HE3	1.69	0.75
1:D:4269:LYS:HA	1:D:4272:LYS:HE3	1.68	0.74
2:F:91:VAL:HG23	2:F:92:ILE:HD12	1.70	0.73
1:A:2418:ARG:HD2	1:B:189:GLU:HG2	1.69	0.73
2:G:91:VAL:HG23	2:G:92:ILE:HD12	1.70	0.73
1:D:3227:ARG:HB3	1:D:3230:GLN:HG2	1.71	0.73
1:A:3828:LYS:O	1:A:3831:GLN:NE2	2.22	0.72
2:E:91:VAL:HG23	2:E:92:ILE:HD12	1.70	0.72
1:C:3227:ARG:HB3	1:C:3230:GLN:HG2	1.71	0.72
1:C:1795:LEU:HD23	1:C:1842:ILE:HD11	1.72	0.72
1:D:1795:LEU:HD23	1:D:1842:ILE:HD11	1.72	0.72
1:C:3828:LYS:O	1:C:3831:GLN:NE2	2.23	0.72
1:D:3828:LYS:O	1:D:3831:GLN:NE2	2.22	0.72
2:H:91:VAL:HG23	2:H:92:ILE:HD12	1.70	0.72
1:A:3227:ARG:HB3	1:A:3230:GLN:HG2	1.71	0.72
1:B:3828:LYS:O	1:B:3831:GLN:NE2	2.22	0.72
1:B:1795:LEU:HD23	1:B:1842:ILE:HD11	1.72	0.72
1:B:3227:ARG:HB3	1:B:3230:GLN:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1766:PRO:HG3	1:C:1780:PRO:HB3	1.72	0.71
1:D:1766:PRO:HG3	1:D:1780:PRO:HB3	1.72	0.71
1:A:1795:LEU:HD23	1:A:1842:ILE:HD11	1.72	0.71
1:D:3228:TYR:HB2	1:D:3287:ASN:HD21	1.56	0.71
1:A:1766:PRO:HG3	1:A:1780:PRO:HB3	1.72	0.71
1:A:3228:TYR:HB2	1:A:3287:ASN:HD21	1.56	0.71
1:C:2418:ARG:HD2	1:D:189:GLU:HG2	1.73	0.71
1:C:3228:TYR:HB2	1:C:3287:ASN:HD21	1.56	0.71
1:A:3119:GLU:OE2	1:A:3248:ARG:NH2	2.24	0.70
1:D:502:ILE:HG23	1:D:506:HIS:CE1	2.26	0.70
1:A:502:ILE:HG23	1:A:506:HIS:CE1	2.26	0.70
1:B:1766:PRO:HG3	1:B:1780:PRO:HB3	1.72	0.70
1:B:3119:GLU:OE2	1:B:3248:ARG:NH2	2.24	0.70
1:C:502:ILE:HG23	1:C:506:HIS:CE1	2.26	0.70
1:D:3119:GLU:OE2	1:D:3248:ARG:NH2	2.24	0.70
1:B:2418:ARG:HD2	1:C:189:GLU:HG2	1.73	0.70
1:B:502:ILE:HG23	1:B:506:HIS:CE1	2.26	0.69
1:B:3228:TYR:HB2	1:B:3287:ASN:HD21	1.56	0.69
1:C:3119:GLU:OE2	1:C:3248:ARG:NH2	2.24	0.69
1:D:3205:CYS:HB3	1:D:3208:ILE:HB	1.75	0.69
1:A:323:ASP:O	1:A:325:LYS:N	2.25	0.69
1:B:3205:CYS:HB3	1:B:3208:ILE:HB	1.75	0.69
1:C:939:THR:O	1:C:943:LEU:HD12	1.93	0.69
1:A:939:THR:O	1:A:943:LEU:HD12	1.93	0.69
1:C:2868:HIS:HB3	1:C:2871:LEU:HD23	1.74	0.69
1:D:644:LEU:HD13	1:D:1630:LEU:HD21	1.75	0.69
1:D:3200:ASN:HB3	1:D:3203:ASP:HB2	1.75	0.69
1:A:2868:HIS:HB3	1:A:2871:LEU:HD23	1.74	0.69
1:C:644:LEU:HD13	1:C:1630:LEU:HD21	1.75	0.69
1:C:3205:CYS:HB3	1:C:3208:ILE:HB	1.75	0.69
1:C:2684:ASN:ND2	1:C:2913:ASP:OD2	2.26	0.69
1:A:189:GLU:HG2	1:D:2418:ARG:HD2	1.74	0.69
1:A:644:LEU:HD13	1:A:1630:LEU:HD21	1.75	0.69
1:A:2684:ASN:ND2	1:A:2913:ASP:OD2	2.26	0.69
1:B:2684:ASN:ND2	1:B:2913:ASP:OD2	2.26	0.69
1:A:3200:ASN:HB3	1:A:3203:ASP:HB2	1.75	0.68
1:D:2868:HIS:HB3	1:D:2871:LEU:HD23	1.74	0.68
1:B:939:THR:O	1:B:943:LEU:HD12	1.93	0.68
1:B:3200:ASN:HB3	1:B:3203:ASP:HB2	1.75	0.68
1:A:3205:CYS:HB3	1:A:3208:ILE:HB	1.75	0.68
1:B:644:LEU:HD13	1:B:1630:LEU:HD21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2868:HIS:HB3	1:B:2871:LEU:HD23	1.74	0.68
1:C:2418:ARG:NH1	1:D:186:VAL:O	2.27	0.68
1:C:3832:ASP:HB3	1:C:3835:PHE:HB3	1.75	0.68
1:C:4782:THR:HG21	1:C:4813:TYR:HA	1.76	0.68
1:D:2684:ASN:ND2	1:D:2913:ASP:OD2	2.26	0.68
1:C:1129:GLY:HA3	1:C:1145:TRP:HB3	1.76	0.68
1:A:4782:THR:HG21	1:A:4813:TYR:HA	1.76	0.68
1:C:3200:ASN:HB3	1:C:3203:ASP:HB2	1.75	0.68
1:D:4782:THR:HG21	1:D:4813:TYR:HA	1.76	0.68
1:B:1129:GLY:HA3	1:B:1145:TRP:HB3	1.76	0.68
1:B:2173:GLU:HA	1:B:2176:VAL:HG22	1.76	0.68
1:B:3832:ASP:HB3	1:B:3835:PHE:HB3	1.75	0.68
1:B:4782:THR:HG21	1:B:4813:TYR:HA	1.76	0.67
1:D:939:THR:O	1:D:943:LEU:HD12	1.93	0.67
1:A:186:VAL:O	1:D:2418:ARG:NH1	2.28	0.67
1:B:3312:PRO:HA	1:B:3315:LEU:HD23	1.76	0.67
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	1.76	0.67
1:D:3832:ASP:HB3	1:D:3835:PHE:HB3	1.75	0.67
1:B:168:GLN:HG3	1:B:169:ARG:HD2	1.77	0.67
1:A:168:GLN:HG3	1:A:169:ARG:HD2	1.77	0.67
1:C:2405:GLU:OE1	1:C:2407:HIS:ND1	2.25	0.67
1:D:2173:GLU:HA	1:D:2176:VAL:HG22	1.75	0.67
1:D:323:ASP:O	1:D:325:LYS:N	2.25	0.67
1:A:889:ILE:HG21	1:A:936:SER:HB3	1.76	0.67
1:B:889:ILE:HG21	1:B:936:SER:HB3	1.76	0.67
1:A:1496:PRO:HA	1:D:2798:MET:HG2	1.77	0.66
1:D:1440:ASN:HB3	1:D:1546:GLN:HB3	1.78	0.66
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	1.76	0.66
1:A:2405:GLU:OE1	1:A:2407:HIS:ND1	2.25	0.66
1:C:1440:ASN:HB3	1:C:1546:GLN:HB3	1.78	0.66
1:C:2173:GLU:HA	1:C:2176:VAL:HG22	1.75	0.66
1:A:2860:LEU:HD11	1:A:2867:ASN:HA	1.78	0.66
1:A:1100:ARG:NH1	1:A:1234:GLU:O	2.29	0.66
1:C:892:LEU:HD11	1:C:1056:THR:HG21	1.78	0.66
1:A:2173:GLU:HA	1:A:2176:VAL:HG22	1.75	0.66
1:A:3312:PRO:HA	1:A:3315:LEU:HD23	1.76	0.66
1:B:2860:LEU:HD11	1:B:2867:ASN:HA	1.78	0.66
1:D:168:GLN:HG3	1:D:169:ARG:HD2	1.77	0.66
1:D:3312:PRO:HA	1:D:3315:LEU:HD23	1.77	0.66
1:C:168:GLN:HG3	1:C:169:ARG:HD2	1.77	0.66
1:C:989:THR:HB	1:C:992:GLN:OE1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1100:ARG:NH1	1:C:1234:GLU:O	2.29	0.66
1:A:3832:ASP:HB3	1:A:3835:PHE:HB3	1.75	0.66
1:C:889:ILE:HG21	1:C:936:SER:HB3	1.76	0.66
1:C:3312:PRO:HA	1:C:3315:LEU:HD23	1.76	0.66
1:D:892:LEU:HD11	1:D:1056:THR:HG21	1.78	0.66
1:A:972:LEU:HG	1:A:978:PRO:HG3	1.78	0.66
1:C:1685:LEU:HB3	1:C:1706:LEU:HD12	1.78	0.66
1:C:4689:LYS:NZ	1:C:4694:LEU:O	2.29	0.66
1:B:2418:ARG:NH1	1:C:186:VAL:O	2.29	0.66
1:B:4689:LYS:NZ	1:B:4694:LEU:O	2.29	0.66
1:A:2418:ARG:NH1	1:B:186:VAL:O	2.28	0.65
1:B:1685:LEU:HB3	1:B:1706:LEU:HD12	1.78	0.65
1:A:989:THR:HB	1:A:992:GLN:OE1	1.95	0.65
1:D:2726:GLU:OE2	1:D:2761:LYS:NZ	2.30	0.65
1:B:1048:ASP:HA	1:B:1051:ARG:HG2	1.79	0.65
1:B:1100:ARG:NH1	1:B:1234:GLU:O	2.29	0.65
1:C:323:ASP:O	1:C:325:LYS:N	2.25	0.65
1:D:989:THR:HB	1:D:992:GLN:OE1	1.95	0.65
1:A:4689:LYS:NZ	1:A:4694:LEU:O	2.29	0.65
1:B:989:THR:HB	1:B:992:GLN:OE1	1.95	0.65
1:B:972:LEU:HG	1:B:978:PRO:HG3	1.78	0.65
1:B:1440:ASN:HB3	1:B:1546:GLN:HB3	1.77	0.65
1:B:4123:GLU:OE2	1:B:4127:ASN:ND2	2.30	0.65
1:D:889:ILE:HG21	1:D:936:SER:HB3	1.76	0.65
1:D:1100:ARG:NH1	1:D:1234:GLU:O	2.29	0.65
1:D:1685:LEU:HB3	1:D:1706:LEU:HD12	1.78	0.65
1:D:4689:LYS:NZ	1:D:4694:LEU:O	2.29	0.65
1:A:1048:ASP:HA	1:A:1051:ARG:HG2	1.79	0.65
1:D:1048:ASP:HA	1:D:1051:ARG:HG2	1.79	0.65
1:A:892:LEU:HD11	1:A:1056:THR:HG21	1.78	0.65
1:A:4883:ASP:O	1:A:4884:MET:HG2	1.96	0.65
1:C:2726:GLU:OE2	1:C:2761:LYS:NZ	2.30	0.65
1:A:4123:GLU:OE2	1:A:4127:ASN:ND2	2.30	0.65
1:B:677:LEU:HD22	1:B:792:VAL:HG11	1.79	0.65
1:C:4883:ASP:O	1:C:4884:MET:HG2	1.97	0.65
1:A:1685:LEU:HB3	1:A:1706:LEU:HD12	1.78	0.65
1:A:1440:ASN:HB3	1:A:1546:GLN:HB3	1.78	0.64
1:B:4883:ASP:O	1:B:4884:MET:HG2	1.97	0.64
1:C:972:LEU:HG	1:C:978:PRO:HG3	1.78	0.64
1:D:4123:GLU:OE2	1:D:4127:ASN:ND2	2.30	0.64
1:B:323:ASP:O	1:B:325:LYS:N	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2726:GLU:OE2	1:A:2761:LYS:NZ	2.30	0.64
1:D:677:LEU:HD22	1:D:792:VAL:HG11	1.79	0.64
1:D:972:LEU:HG	1:D:978:PRO:HG3	1.78	0.64
1:D:2860:LEU:HD11	1:D:2867:ASN:HA	1.78	0.64
1:C:2860:LEU:HD11	1:C:2867:ASN:HA	1.78	0.64
1:B:892:LEU:HD11	1:B:1056:THR:HG21	1.78	0.64
1:C:1048:ASP:HA	1:C:1051:ARG:HG2	1.79	0.64
1:D:4883:ASP:O	1:D:4884:MET:HG2	1.97	0.64
1:A:677:LEU:HD22	1:A:792:VAL:HG11	1.79	0.64
1:A:1269:GLU:HB2	1:A:1288:LYS:HG3	1.80	0.64
1:D:1269:GLU:HB2	1:D:1288:LYS:HG3	1.80	0.64
2:F:78:THR:OG1	2:F:80:ASP:OD1	2.15	0.64
1:B:2726:GLU:OE2	1:B:2761:LYS:NZ	2.30	0.64
1:C:677:LEU:HD22	1:C:792:VAL:HG11	1.79	0.64
1:C:4123:GLU:OE2	1:C:4127:ASN:ND2	2.30	0.64
1:B:1269:GLU:HB2	1:B:1288:LYS:HG3	1.80	0.63
1:D:3846:LEU:HB3	1:D:3854:PHE:CE2	2.34	0.63
1:C:2748:SER:HB2	1:C:2753:VAL:HB	1.81	0.63
1:B:599:SER:OG	1:B:603:LYS:NZ	2.32	0.63
1:B:3149:GLU:HA	1:B:3152:ARG:CG	2.28	0.63
1:A:3846:LEU:HB3	1:A:3854:PHE:CE2	2.34	0.63
1:D:3148:VAL:HG12	1:D:3152:ARG:HD2	1.81	0.63
1:C:599:SER:OG	1:C:603:LYS:NZ	2.32	0.63
1:D:2748:SER:HB2	1:D:2753:VAL:HB	1.81	0.63
1:A:249:SER:H	1:A:272:ARG:HH21	1.47	0.63
1:A:599:SER:OG	1:A:603:LYS:NZ	2.32	0.63
1:B:2748:SER:HB2	1:B:2753:VAL:HB	1.81	0.63
1:D:2405:GLU:OE1	1:D:2407:HIS:ND1	2.25	0.63
1:B:3153:SER:O	1:B:3156:GLY:N	2.32	0.62
1:C:1269:GLU:HB2	1:C:1288:LYS:HG3	1.80	0.62
1:C:3148:VAL:HG12	1:C:3152:ARG:HD2	1.81	0.62
1:C:3153:SER:O	1:C:3156:GLY:N	2.32	0.62
1:C:3846:LEU:HB3	1:C:3854:PHE:CE2	2.34	0.62
1:D:1286:THR:HG23	1:D:1551:ASN:HA	1.81	0.62
1:D:3152:ARG:HH21	1:D:3237:VAL:HG21	1.65	0.62
1:D:3153:SER:O	1:D:3156:GLY:N	2.32	0.62
1:A:1962:THR:O	1:A:1966:ARG:HG2	1.99	0.62
2:G:78:THR:OG1	2:G:80:ASP:OD1	2.15	0.62
1:B:3148:VAL:HG12	1:B:3152:ARG:HD2	1.81	0.62
1:D:599:SER:OG	1:D:603:LYS:NZ	2.32	0.62
1:D:1541:PRO:HG2	1:D:1566:LEU:HD21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2996:ALA:O	1:D:3001:LYS:NZ	2.33	0.62
1:A:1541:PRO:HG2	1:A:1566:LEU:HD21	1.82	0.62
1:A:2748:SER:HB2	1:A:2753:VAL:HB	1.81	0.62
1:A:3149:GLU:HA	1:A:3152:ARG:CG	2.28	0.62
1:B:2405:GLU:OE1	1:B:2407:HIS:ND1	2.25	0.62
1:B:2653:SER:O	1:B:2958:GLN:NE2	2.33	0.62
1:C:1962:THR:O	1:C:1966:ARG:HG2	1.99	0.62
1:C:2996:ALA:O	1:C:3001:LYS:NZ	2.33	0.62
1:D:3697:LYS:HA	1:D:3700:HIS:CD2	2.35	0.62
1:A:3148:VAL:HG12	1:A:3152:ARG:HD2	1.81	0.62
1:B:249:SER:H	1:B:272:ARG:HH21	1.47	0.62
1:B:3846:LEU:HB3	1:B:3854:PHE:CE2	2.34	0.62
1:C:3697:LYS:HA	1:C:3700:HIS:CD2	2.34	0.62
1:A:281:ARG:NH2	1:A:287:SER:OG	2.33	0.62
1:A:3152:ARG:HH21	1:A:3237:VAL:HG21	1.65	0.62
1:A:3701:ASP:OD2	1:A:3727:GLN:NE2	2.33	0.62
1:C:3050:LEU:HB3	1:C:3053:VAL:HG23	1.82	0.62
1:D:1494:MET:O	1:D:1496:PRO:HD2	2.00	0.62
1:A:2996:ALA:O	1:A:3001:LYS:NZ	2.33	0.62
2:H:78:THR:OG1	2:H:80:ASP:OD1	2.15	0.62
1:B:2721:ILE:HD11	1:B:2779:LEU:HD12	1.82	0.62
1:B:2996:ALA:O	1:B:3001:LYS:NZ	2.33	0.62
1:B:3050:LEU:HB3	1:B:3053:VAL:HG23	1.82	0.62
1:C:3149:GLU:HA	1:C:3152:ARG:CG	2.28	0.62
1:D:249:SER:H	1:D:272:ARG:HH21	1.47	0.62
1:A:2721:ILE:HD11	1:A:2779:LEU:HD12	1.82	0.62
1:A:3153:SER:O	1:A:3156:GLY:N	2.32	0.62
1:C:2238:THR:HG22	1:C:2240:LEU:H	1.65	0.62
1:C:2721:ILE:HD11	1:C:2779:LEU:HD12	1.82	0.62
1:D:281:ARG:NH2	1:D:287:SER:OG	2.33	0.62
1:D:1962:THR:O	1:D:1966:ARG:HG2	1.99	0.62
1:A:1286:THR:HG23	1:A:1551:ASN:HA	1.81	0.61
1:A:1494:MET:O	1:A:1496:PRO:HD2	2.00	0.61
1:B:1494:MET:O	1:B:1496:PRO:HD2	2.00	0.61
1:B:2238:THR:HG22	1:B:2240:LEU:H	1.65	0.61
1:B:3701:ASP:OD2	1:B:3727:GLN:NE2	2.33	0.61
1:C:281:ARG:NH2	1:C:287:SER:OG	2.33	0.61
1:D:2721:ILE:HD11	1:D:2779:LEU:HD12	1.82	0.61
1:A:2653:SER:O	1:A:2958:GLN:NE2	2.33	0.61
1:A:4859:LEU:O	1:A:4863:GLN:HG2	2.01	0.61
1:B:4667:SER:OG	1:B:4672:MET:O	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2072:GLU:O	1:D:3660:ARG:NH1	2.33	0.61
1:D:4187:GLU:OE2	1:D:4947:ARG:NH2	2.33	0.61
1:A:3697:LYS:HA	1:A:3700:HIS:CD2	2.35	0.61
1:B:281:ARG:NH2	1:B:287:SER:OG	2.33	0.61
1:B:1286:THR:HG23	1:B:1551:ASN:HA	1.81	0.61
1:C:3701:ASP:OD2	1:C:3727:GLN:NE2	2.33	0.61
1:C:3152:ARG:HH21	1:C:3237:VAL:HG21	1.65	0.61
1:A:2072:GLU:O	1:A:3660:ARG:NH1	2.33	0.61
2:E:106:ASN:OD1	2:E:107:LEU:N	2.33	0.61
1:C:249:SER:H	1:C:272:ARG:HH21	1.47	0.61
1:C:1176:THR:HG22	1:C:1181:ILE:HA	1.83	0.61
1:D:3149:GLU:HA	1:D:3152:ARG:CG	2.27	0.61
1:A:4667:SER:OG	1:A:4672:MET:O	2.18	0.61
1:B:1962:THR:O	1:B:1966:ARG:HG2	1.99	0.61
1:B:2072:GLU:O	1:B:3660:ARG:NH1	2.33	0.61
1:B:3697:LYS:HA	1:B:3700:HIS:CD2	2.34	0.61
1:D:2653:SER:O	1:D:2958:GLN:NE2	2.33	0.61
2:G:106:ASN:OD1	2:G:107:LEU:N	2.33	0.61
1:B:1176:THR:HG22	1:B:1181:ILE:HA	1.83	0.61
1:C:1494:MET:O	1:C:1496:PRO:HD2	2.00	0.61
1:C:2072:GLU:O	1:C:3660:ARG:NH1	2.33	0.61
1:C:2653:SER:O	1:C:2958:GLN:NE2	2.33	0.61
1:D:4859:LEU:O	1:D:4863:GLN:HG2	2.01	0.61
2:E:78:THR:OG1	2:E:80:ASP:OD1	2.15	0.61
1:B:2788:ARG:HE	1:B:2906:GLY:HA3	1.66	0.61
1:B:4187:GLU:OE2	1:B:4947:ARG:NH2	2.33	0.61
1:D:1176:THR:HG22	1:D:1181:ILE:HA	1.83	0.61
1:D:2788:ARG:HE	1:D:2906:GLY:HA3	1.66	0.61
1:D:4667:SER:OG	1:D:4672:MET:O	2.18	0.61
1:B:3152:ARG:HH21	1:B:3237:VAL:HG21	1.65	0.61
1:D:3050:LEU:HB3	1:D:3053:VAL:HG23	1.82	0.61
1:B:1541:PRO:HG2	1:B:1566:LEU:HD21	1.82	0.61
1:C:1541:PRO:HG2	1:C:1566:LEU:HD21	1.82	0.61
1:C:4569:GLU:OE2	1:C:4573:ARG:NH1	2.34	0.61
1:C:4667:SER:OG	1:C:4672:MET:O	2.18	0.61
1:C:2788:ARG:HE	1:C:2906:GLY:HA3	1.66	0.60
1:C:3840:PHE:HA	1:C:3843:LEU:HD12	1.83	0.60
1:A:3050:LEU:HB3	1:A:3053:VAL:HG23	1.82	0.60
1:B:4569:GLU:OE2	1:B:4573:ARG:NH1	2.34	0.60
1:C:1286:THR:HG23	1:C:1551:ASN:HA	1.81	0.60
1:D:1418:ASP:OD1	1:D:1419:PHE:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:ASN:OD1	2:F:107:LEU:N	2.33	0.60
1:A:2238:THR:HG22	1:A:2240:LEU:H	1.65	0.60
1:B:3840:PHE:HA	1:B:3843:LEU:HD12	1.83	0.60
1:B:4859:LEU:O	1:B:4863:GLN:HG2	2.01	0.60
1:C:3192:ARG:HH11	1:C:3192:ARG:HG3	1.65	0.60
1:D:4569:GLU:OE2	1:D:4573:ARG:NH1	2.34	0.60
1:A:2212:LYS:NZ	1:A:2216:ASP:OD1	2.33	0.60
1:C:4489:GLN:NE2	1:C:4493:ASN:OD1	2.33	0.60
1:D:2238:THR:HG22	1:D:2240:LEU:H	1.65	0.60
1:D:3840:PHE:HA	1:D:3843:LEU:HD12	1.83	0.60
1:A:1418:ASP:OD1	1:A:1419:PHE:N	2.34	0.60
2:H:26:HIS:CD2	2:H:105:LEU:HD11	2.37	0.60
1:B:1685:LEU:O	1:B:1689:ILE:HG12	2.02	0.60
1:C:2798:MET:HG2	1:D:1496:PRO:HA	1.82	0.60
1:D:2697:SER:O	1:D:2698:GLU:HG3	2.02	0.60
1:D:3192:ARG:HG3	1:D:3192:ARG:HH11	1.65	0.60
1:A:1176:THR:HG22	1:A:1181:ILE:HA	1.83	0.60
1:A:1685:LEU:O	1:A:1689:ILE:HG12	2.02	0.60
1:D:1721:MET:HE2	1:D:1758:ARG:HA	1.84	0.60
1:A:4177:VAL:HG11	1:A:4880:VAL:HA	1.84	0.60
2:E:63:GLY:HA3	2:E:75:LEU:HD13	1.84	0.60
1:B:2798:MET:HG2	1:C:1496:PRO:HA	1.82	0.60
1:B:3192:ARG:HH11	1:B:3192:ARG:HG3	1.66	0.60
1:B:4832:GLU:O	1:B:4843:ARG:NH2	2.21	0.60
1:C:1685:LEU:O	1:C:1689:ILE:HG12	2.02	0.60
2:H:106:ASN:OD1	2:H:107:LEU:N	2.33	0.60
1:B:2697:SER:O	1:B:2698:GLU:HG3	2.02	0.60
1:A:1007:TRP:HE1	4:A:5003:ATP:PG	2.25	0.60
1:A:2697:SER:O	1:A:2698:GLU:HG3	2.02	0.60
1:C:2697:SER:O	1:C:2698:GLU:HG3	2.02	0.60
1:A:2798:MET:HG2	1:B:1496:PRO:HA	1.84	0.59
1:A:3192:ARG:HH11	1:A:3192:ARG:HG3	1.66	0.59
1:A:4569:GLU:OE2	1:A:4573:ARG:NH1	2.34	0.59
1:C:4859:LEU:O	1:C:4863:GLN:HG2	2.01	0.59
1:D:515:ALA:HB2	1:D:523:GLY:HA3	1.83	0.59
1:A:2580:LEU:O	1:A:2616:ARG:NH2	2.35	0.59
2:G:26:HIS:CD2	2:G:105:LEU:HD11	2.37	0.59
1:C:4832:GLU:O	1:C:4843:ARG:NH2	2.21	0.59
1:D:1685:LEU:O	1:D:1689:ILE:HG12	2.02	0.59
1:D:3701:ASP:OD2	1:D:3727:GLN:NE2	2.33	0.59
1:A:419:ILE:HG21	1:A:492:GLU:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4187:GLU:OE2	1:A:4947:ARG:NH2	2.33	0.59
2:F:26:HIS:CD2	2:F:105:LEU:HD11	2.37	0.59
1:C:3171:LEU:HD11	1:C:3241:MET:HE1	1.83	0.59
1:A:1721:MET:HE2	1:A:1758:ARG:HA	1.83	0.59
1:C:502:ILE:HG23	1:C:506:HIS:HE1	1.67	0.59
1:D:2590:ARG:NH2	1:D:2875:ASP:OD2	2.33	0.59
1:D:4177:VAL:HG11	1:D:4880:VAL:HA	1.84	0.59
1:B:541:ILE:HD11	1:B:574:VAL:HG13	1.84	0.59
1:C:1418:ASP:OD1	1:C:1419:PHE:N	2.34	0.59
1:C:1721:MET:HE2	1:C:1758:ARG:HA	1.85	0.59
1:A:2788:ARG:HE	1:A:2906:GLY:HA3	1.66	0.59
1:A:3840:PHE:HA	1:A:3843:LEU:HD12	1.83	0.59
1:B:3674:THR:O	1:B:3679:LYS:NZ	2.36	0.59
2:E:26:HIS:CD2	2:E:105:LEU:HD11	2.37	0.59
1:B:515:ALA:HB2	1:B:523:GLY:HA3	1.83	0.59
1:B:1418:ASP:OD1	1:B:1419:PHE:N	2.34	0.59
1:C:2590:ARG:NH2	1:C:2875:ASP:OD2	2.33	0.59
1:D:1013:ARG:HG2	1:D:1013:ARG:HH11	1.66	0.59
1:D:3695:MET:HB3	1:D:3731:LEU:HD11	1.85	0.59
1:A:1242:ASN:HB3	1:A:1807:ARG:HG3	1.85	0.59
1:B:1844:GLN:NE2	1:B:1853:GLU:OE1	2.35	0.59
1:B:4177:VAL:HG11	1:B:4880:VAL:HA	1.84	0.59
1:C:515:ALA:HB2	1:C:523:GLY:HA3	1.83	0.59
1:D:1844:GLN:NE2	1:D:1853:GLU:OE1	2.35	0.59
1:C:4187:GLU:OE2	1:C:4947:ARG:NH2	2.33	0.59
1:D:502:ILE:HG23	1:D:506:HIS:HE1	1.67	0.59
1:A:515:ALA:HB2	1:A:523:GLY:HA3	1.83	0.59
1:C:1242:ASN:HB3	1:C:1807:ARG:HG3	1.85	0.59
1:D:419:ILE:HG21	1:D:492:GLU:HG3	1.85	0.59
1:D:1242:ASN:HB3	1:D:1807:ARG:HG3	1.85	0.59
1:B:1721:MET:HE2	1:B:1758:ARG:HA	1.85	0.58
1:C:1844:GLN:NE2	1:C:1853:GLU:OE1	2.35	0.58
1:C:2580:LEU:O	1:C:2616:ARG:NH2	2.35	0.58
1:A:1013:ARG:HG2	1:A:1013:ARG:HH11	1.66	0.58
2:H:63:GLY:HA3	2:H:75:LEU:HD13	1.84	0.58
1:B:2580:LEU:O	1:B:2616:ARG:NH2	2.36	0.58
1:B:419:ILE:HG21	1:B:492:GLU:HG3	1.85	0.58
1:B:1013:ARG:HG2	1:B:1013:ARG:HH11	1.66	0.58
1:C:3695:MET:HB3	1:C:3731:LEU:HD11	1.85	0.58
1:A:1844:GLN:NE2	1:A:1853:GLU:OE1	2.35	0.58
2:F:63:GLY:HA3	2:F:75:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:63:GLY:HA3	2:G:75:LEU:HD13	1.84	0.58
1:B:502:ILE:HG23	1:B:506:HIS:HE1	1.67	0.58
1:C:541:ILE:HD11	1:C:574:VAL:HG13	1.85	0.58
1:A:502:ILE:HG23	1:A:506:HIS:HE1	1.67	0.58
1:A:983:LEU:O	1:A:1055:ARG:NH1	2.37	0.58
1:A:3674:THR:O	1:A:3679:LYS:NZ	2.36	0.58
1:C:4177:VAL:HG11	1:C:4880:VAL:HA	1.84	0.58
1:D:2580:LEU:O	1:D:2616:ARG:NH2	2.35	0.58
1:B:983:LEU:O	1:B:1055:ARG:NH1	2.37	0.58
1:D:681:HIS:HA	1:D:751:THR:HG22	1.85	0.58
1:C:681:HIS:HA	1:C:751:THR:HG22	1.85	0.58
1:C:2442:MET:HE1	1:C:2498:ALA:HB1	1.84	0.58
1:D:3674:THR:O	1:D:3679:LYS:NZ	2.36	0.58
1:A:541:ILE:HD11	1:A:574:VAL:HG13	1.84	0.58
1:C:983:LEU:O	1:C:1055:ARG:NH1	2.37	0.58
1:D:1957:LEU:CG	1:D:1960:ARG:HH12	2.17	0.58
1:D:983:LEU:O	1:D:1055:ARG:NH1	2.37	0.58
1:A:3695:MET:HB3	1:A:3731:LEU:HD11	1.85	0.58
1:B:249:SER:HB3	1:B:272:ARG:HE	1.69	0.58
1:D:3171:LEU:HD11	1:D:3241:MET:HE1	1.85	0.58
1:A:249:SER:HB3	1:A:272:ARG:HE	1.69	0.57
4:A:5003:ATP:H5'1	5:A:5004:KVR:C18	2.34	0.57
1:B:1242:ASN:HB3	1:B:1807:ARG:HG3	1.85	0.57
1:B:2212:LYS:NZ	1:B:2216:ASP:OD1	2.33	0.57
1:D:249:SER:HB3	1:D:272:ARG:HE	1.69	0.57
1:D:3259:GLU:O	1:D:3260:ARG:HD3	2.04	0.57
1:C:1013:ARG:HG2	1:C:1013:ARG:HH11	1.66	0.57
1:C:2212:LYS:NZ	1:C:2216:ASP:OD1	2.33	0.57
1:D:2333:PRO:HA	1:D:2336:ARG:HE	1.69	0.57
1:A:3171:LEU:HD11	1:A:3241:MET:HE1	1.86	0.57
1:B:3259:GLU:O	1:B:3260:ARG:HD3	2.04	0.57
1:C:332:ARG:NH1	1:C:364:GLN:OE1	2.35	0.57
1:C:2333:PRO:HA	1:C:2336:ARG:HE	1.70	0.57
1:A:3259:GLU:O	1:A:3260:ARG:HD3	2.04	0.57
1:B:681:HIS:HA	1:B:751:THR:HG22	1.85	0.57
1:B:3695:MET:HB3	1:B:3731:LEU:HD11	1.85	0.57
1:C:419:ILE:HG21	1:C:492:GLU:HG3	1.84	0.57
1:D:2706:VAL:HG21	1:D:2785:TRP:NE1	2.20	0.57
1:A:680:ASP:OD1	1:A:801:ARG:NH2	2.38	0.57
1:A:2176:VAL:HG12	1:A:2220:TYR:CE2	2.40	0.57
1:A:2706:VAL:HG21	1:A:2785:TRP:NE1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3259:GLU:O	1:C:3260:ARG:HD3	2.04	0.57
1:A:2333:PRO:HA	1:A:2336:ARG:HE	1.69	0.57
1:A:3043:ARG:NH2	1:A:3116:GLN:O	2.38	0.57
1:B:680:ASP:OD1	1:B:801:ARG:NH2	2.38	0.57
1:B:3043:ARG:NH2	1:B:3116:GLN:O	2.38	0.57
1:C:680:ASP:OD1	1:C:801:ARG:NH2	2.38	0.57
1:C:2995:HIS:HE2	1:D:1070:ASP:HB3	1.69	0.57
1:A:670:TYR:HD1	1:A:1017:THR:HG21	1.70	0.57
1:A:681:HIS:HA	1:A:751:THR:HG22	1.85	0.57
1:B:2590:ARG:NH2	1:B:2875:ASP:OD2	2.33	0.57
1:B:2979:ARG:HG3	1:B:3039:THR:HG22	1.87	0.57
1:B:3152:ARG:HH22	1:B:3233:HIS:HB2	1.69	0.57
1:C:249:SER:HB3	1:C:272:ARG:HE	1.69	0.57
1:B:1793:GLN:NE2	1:B:1797:GLU:OE2	2.38	0.57
1:D:541:ILE:HD11	1:D:574:VAL:HG13	1.84	0.57
1:D:1716:THR:O	1:D:1720:MET:HG3	2.05	0.57
1:D:3152:ARG:HH22	1:D:3233:HIS:HB2	1.69	0.57
1:A:1957:LEU:CG	1:A:1960:ARG:HH12	2.17	0.57
1:A:2833:LEU:HB3	1:A:2837:LEU:HB3	1.87	0.57
1:B:1957:LEU:CG	1:B:1960:ARG:HH12	2.17	0.57
1:B:2202:TYR:O	1:B:2206:ILE:HG12	2.05	0.57
1:C:1793:GLN:NE2	1:C:1797:GLU:OE2	2.38	0.57
1:A:1716:THR:O	1:A:1720:MET:HG3	2.05	0.56
1:B:601:LEU:HG	1:B:610:VAL:HG11	1.87	0.56
1:B:2833:LEU:HB3	1:B:2837:LEU:HB3	1.87	0.56
1:D:4489:GLN:NE2	1:D:4493:ASN:OD1	2.33	0.56
1:A:2590:ARG:NH2	1:A:2875:ASP:OD2	2.33	0.56
1:A:2979:ARG:HG3	1:A:3039:THR:HG22	1.87	0.56
1:A:3152:ARG:HH22	1:A:3233:HIS:HB2	1.69	0.56
1:B:1941:ARG:NH2	1:B:3609:TYR:O	2.38	0.56
1:B:2593:VAL:HG12	1:B:2644:LEU:HG	1.88	0.56
1:C:2593:VAL:HG12	1:C:2644:LEU:HG	1.87	0.56
1:C:3152:ARG:HH22	1:C:3233:HIS:HB2	1.69	0.56
1:D:3043:ARG:NH2	1:D:3116:GLN:O	2.38	0.56
1:B:2176:VAL:HG12	1:B:2220:TYR:CE2	2.40	0.56
1:C:866:PRO:HG3	1:C:1009:ARG:HD3	1.88	0.56
1:C:1716:THR:O	1:C:1720:MET:HG3	2.05	0.56
1:C:1941:ARG:NH2	1:C:3609:TYR:O	2.38	0.56
1:C:2176:VAL:HG12	1:C:2220:TYR:CE2	2.40	0.56
1:D:670:TYR:HD1	1:D:1017:THR:HG21	1.70	0.56
1:D:866:PRO:HG3	1:D:1009:ARG:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1793:GLN:NE2	1:D:1797:GLU:OE2	2.38	0.56
1:D:1941:ARG:NH2	1:D:3609:TYR:O	2.38	0.56
1:A:143:LEU:HD22	1:D:2426:LEU:HD23	1.88	0.56
1:B:304:LYS:HB2	1:B:316:LEU:HD23	1.87	0.56
1:B:2706:VAL:HG21	1:B:2785:TRP:NE1	2.20	0.56
1:B:3171:LEU:HD11	1:B:3241:MET:HE1	1.86	0.56
1:D:2176:VAL:HG12	1:D:2220:TYR:CE2	2.40	0.56
1:D:2589:LEU:O	1:D:2593:VAL:HG13	2.06	0.56
1:A:332:ARG:NH1	1:A:364:GLN:OE1	2.36	0.56
1:A:950:VAL:HG22	1:A:1064:LEU:HD13	1.88	0.56
1:A:4489:GLN:NE2	1:A:4493:ASN:OD1	2.33	0.56
2:F:90:GLY:HA2	1:B:638:PRO:HD3	1.86	0.56
1:C:2979:ARG:HG3	1:C:3039:THR:HG22	1.87	0.56
1:D:680:ASP:OD1	1:D:801:ARG:NH2	2.38	0.56
1:B:808:HIS:CG	1:B:832:LEU:HD23	2.41	0.56
1:B:3271:GLU:HA	1:B:3274:ASN:HD21	1.70	0.56
1:B:4489:GLN:NE2	1:B:4493:ASN:OD1	2.33	0.56
1:C:827:LEU:HB2	1:C:830:GLU:HB2	1.88	0.56
1:C:2202:TYR:O	1:C:2206:ILE:HG12	2.05	0.56
1:C:2277:CYS:SG	1:C:2280:LEU:HD23	2.46	0.56
1:C:2589:LEU:O	1:C:2593:VAL:HG13	2.06	0.56
1:C:3043:ARG:NH2	1:C:3116:GLN:O	2.38	0.56
1:D:2277:CYS:SG	1:D:2280:LEU:HD23	2.46	0.56
1:B:670:TYR:HD1	1:B:1017:THR:HG21	1.70	0.56
1:B:1716:THR:O	1:B:1720:MET:HG3	2.05	0.56
1:C:2706:VAL:HG21	1:C:2785:TRP:NE1	2.20	0.56
1:C:3661:VAL:HG23	1:C:3666:GLN:HG2	1.88	0.56
1:D:601:LEU:HG	1:D:610:VAL:HG11	1.87	0.56
1:D:2212:LYS:NZ	1:D:2216:ASP:OD1	2.33	0.56
1:D:2979:ARG:HG3	1:D:3039:THR:HG22	1.87	0.56
1:A:3278:GLY:HA2	1:A:3281:LEU:HD23	1.88	0.56
1:C:2779:LEU:HD23	1:C:2782:MET:HE3	1.87	0.56
1:D:2593:VAL:HG12	1:D:2644:LEU:HG	1.87	0.56
1:A:808:HIS:CG	1:A:832:LEU:HD23	2.41	0.56
1:A:866:PRO:HG3	1:A:1009:ARG:HD3	1.88	0.56
1:A:2593:VAL:HG12	1:A:2644:LEU:HG	1.88	0.56
1:B:3661:VAL:HG23	1:B:3666:GLN:HG2	1.87	0.56
1:C:601:LEU:HG	1:C:610:VAL:HG11	1.87	0.56
1:C:3271:GLU:HA	1:C:3274:ASN:HD21	1.70	0.56
1:C:4604:LYS:HD2	1:C:4608:ARG:HH21	1.71	0.56
1:D:304:LYS:HB2	1:D:316:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:808:HIS:CG	1:D:832:LEU:HD23	2.41	0.56
1:B:827:LEU:HB2	1:B:830:GLU:HB2	1.88	0.56
1:B:3134:LEU:HB2	1:B:3162:PHE:CE2	2.41	0.56
1:D:827:LEU:HB2	1:D:830:GLU:HB2	1.88	0.56
1:D:4832:GLU:O	1:D:4843:ARG:NH2	2.21	0.56
1:B:1974:ASN:OD1	1:B:1975:MET:N	2.39	0.55
1:B:2333:PRO:HA	1:B:2336:ARG:HE	1.69	0.55
1:C:304:LYS:HB2	1:C:316:LEU:HD23	1.87	0.55
1:C:950:VAL:HG22	1:C:1064:LEU:HD13	1.87	0.55
1:C:2833:LEU:HB3	1:C:2837:LEU:HB3	1.87	0.55
1:D:4604:LYS:HD2	1:D:4608:ARG:HH21	1.71	0.55
1:A:304:LYS:HB2	1:A:316:LEU:HD23	1.87	0.55
1:A:1511:VAL:HG22	1:A:1518:LEU:HG	1.89	0.55
1:A:1793:GLN:NE2	1:A:1797:GLU:OE2	2.38	0.55
1:B:332:ARG:NH1	1:B:364:GLN:OE1	2.35	0.55
1:B:3116:GLN:OE1	1:B:3116:GLN:N	2.40	0.55
1:B:4854:VAL:HA	1:B:4858:LEU:HD12	1.88	0.55
1:A:562:LEU:HB3	1:A:600:LEU:HD13	1.89	0.55
1:A:1941:ARG:NH2	1:A:3609:TYR:O	2.38	0.55
1:A:2202:TYR:O	1:A:2206:ILE:HG12	2.05	0.55
1:B:866:PRO:HG3	1:B:1009:ARG:HD3	1.88	0.55
1:B:2779:LEU:HD23	1:B:2782:MET:HE3	1.87	0.55
1:C:808:HIS:CG	1:C:832:LEU:HD23	2.41	0.55
1:C:1974:ASN:OD1	1:C:1975:MET:N	2.39	0.55
1:C:3278:GLY:HA2	1:C:3281:LEU:HD23	1.88	0.55
1:D:2202:TYR:O	1:D:2206:ILE:HG12	2.05	0.55
1:D:2833:LEU:HB3	1:D:2837:LEU:HB3	1.87	0.55
1:A:3134:LEU:HB2	1:A:3162:PHE:CE2	2.41	0.55
1:A:3271:GLU:HA	1:A:3274:ASN:ND2	2.22	0.55
1:B:950:VAL:HG22	1:B:1064:LEU:HD13	1.87	0.55
1:D:950:VAL:HG22	1:D:1064:LEU:HD13	1.87	0.55
1:D:1511:VAL:HG22	1:D:1518:LEU:HG	1.89	0.55
1:D:3271:GLU:HA	1:D:3274:ASN:ND2	2.22	0.55
1:A:1974:ASN:OD1	1:A:1975:MET:N	2.39	0.55
1:C:3674:THR:O	1:C:3679:LYS:NZ	2.36	0.55
1:D:3661:VAL:HG23	1:D:3666:GLN:HG2	1.87	0.55
1:A:506:HIS:HB3	1:A:564:ARG:NH1	2.22	0.55
1:A:601:LEU:HG	1:A:610:VAL:HG11	1.87	0.55
1:A:3074:ASN:OD1	1:A:3075:LEU:N	2.40	0.55
1:A:3271:GLU:HA	1:A:3274:ASN:HD21	1.70	0.55
1:B:2589:LEU:O	1:B:2593:VAL:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:670:TYR:HD1	1:C:1017:THR:HG21	1.70	0.55
1:C:4854:VAL:HA	1:C:4858:LEU:HD12	1.88	0.55
1:D:562:LEU:HB3	1:D:600:LEU:HD13	1.89	0.55
1:D:1257:GLN:HG3	1:D:1595:LEU:HD11	1.88	0.55
1:D:2442:MET:HE1	1:D:2498:ALA:HB1	1.89	0.55
1:A:827:LEU:HB2	1:A:830:GLU:HB2	1.88	0.55
1:A:1070:ASP:HB3	1:D:2995:HIS:HE2	1.71	0.55
1:B:4604:LYS:HD2	1:B:4608:ARG:HH21	1.71	0.55
1:C:562:LEU:HB3	1:C:600:LEU:HD13	1.89	0.55
1:C:3134:LEU:HB2	1:C:3162:PHE:CE2	2.41	0.55
1:D:1974:ASN:OD1	1:D:1975:MET:N	2.39	0.55
1:B:4580:THR:OG1	1:B:4733:HIS:NE2	2.26	0.55
1:C:1957:LEU:CG	1:C:1960:ARG:HH12	2.17	0.55
1:D:3134:LEU:HB2	1:D:3162:PHE:CE2	2.41	0.55
1:B:3074:ASN:OD1	1:B:3075:LEU:N	2.40	0.55
1:C:506:HIS:HB3	1:C:564:ARG:NH1	2.22	0.55
1:C:3838:ASP:OD1	1:C:3839:LEU:N	2.40	0.55
1:D:4854:VAL:HA	1:D:4858:LEU:HD12	1.88	0.55
1:A:2277:CYS:SG	1:A:2280:LEU:HD23	2.46	0.55
1:A:3116:GLN:OE1	1:A:3116:GLN:N	2.40	0.55
1:C:1511:VAL:HG22	1:C:1518:LEU:HG	1.89	0.55
1:C:2765:GLU:HA	1:C:2768:LYS:HG2	1.89	0.55
1:D:506:HIS:HB3	1:D:564:ARG:NH1	2.22	0.55
1:D:3072:MET:HE3	1:D:3136:SER:HA	1.89	0.55
1:D:3271:GLU:HA	1:D:3274:ASN:HD21	1.70	0.55
1:D:3278:GLY:HA2	1:D:3281:LEU:HD23	1.88	0.55
1:A:3176:ASP:O	1:A:3185:ASN:ND2	2.31	0.54
1:A:3661:VAL:HG23	1:A:3666:GLN:HG2	1.87	0.54
1:B:506:HIS:HB3	1:B:564:ARG:NH1	2.22	0.54
1:B:2277:CYS:SG	1:B:2280:LEU:HD23	2.46	0.54
1:B:3072:MET:HE3	1:B:3136:SER:HA	1.89	0.54
1:B:3271:GLU:HA	1:B:3274:ASN:ND2	2.22	0.54
1:C:1257:GLN:HG3	1:C:1595:LEU:HD11	1.88	0.54
1:C:2426:LEU:HD23	1:D:143:LEU:HD22	1.88	0.54
1:C:3271:GLU:HA	1:C:3274:ASN:ND2	2.22	0.54
1:D:3116:GLN:OE1	1:D:3116:GLN:N	2.40	0.54
1:A:2765:GLU:HA	1:A:2768:LYS:HG2	1.89	0.54
1:A:3838:ASP:OD1	1:A:3839:LEU:N	2.40	0.54
1:C:3074:ASN:OD1	1:C:3075:LEU:N	2.40	0.54
1:D:1039:ASP:OD1	1:D:1042:THR:OG1	2.25	0.54
1:D:3074:ASN:OD1	1:D:3075:LEU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3838:ASP:OD1	1:D:3839:LEU:N	2.40	0.54
1:A:3729:ALA:HA	1:A:3732:HIS:CD2	2.43	0.54
1:A:4604:LYS:HD2	1:A:4608:ARG:HH21	1.71	0.54
1:A:4854:VAL:HA	1:A:4858:LEU:HD12	1.88	0.54
1:B:1511:VAL:HG22	1:B:1518:LEU:HG	1.89	0.54
1:B:3278:GLY:HA2	1:B:3281:LEU:HD23	1.88	0.54
1:C:3116:GLN:N	1:C:3116:GLN:OE1	2.40	0.54
1:D:3729:ALA:HA	1:D:3732:HIS:CD2	2.43	0.54
1:A:42:PHE:HZ	1:A:459:LEU:HG	1.73	0.54
1:A:1257:GLN:HG3	1:A:1595:LEU:HD11	1.88	0.54
1:A:2589:LEU:O	1:A:2593:VAL:HG13	2.06	0.54
1:A:3072:MET:HE3	1:A:3136:SER:HA	1.89	0.54
1:B:562:LEU:HB3	1:B:600:LEU:HD13	1.89	0.54
1:C:3729:ALA:HA	1:C:3732:HIS:CD2	2.43	0.54
1:A:2779:LEU:HD23	1:A:2782:MET:HE3	1.89	0.54
1:B:2833:LEU:HD22	1:B:2837:LEU:HD23	1.89	0.54
1:B:3838:ASP:OD1	1:B:3839:LEU:N	2.40	0.54
1:A:1024:VAL:HG23	1:A:1025:LYS:HD3	1.90	0.54
1:A:1031:ARG:NH2	1:A:1046:ASN:OD1	2.41	0.54
1:A:1898:LEU:HD13	1:A:1902:VAL:HG12	1.90	0.54
1:A:4580:THR:OG1	1:A:4733:HIS:NE2	2.26	0.54
1:B:42:PHE:HZ	1:B:459:LEU:HG	1.73	0.54
1:B:253:GLY:O	1:B:257:ARG:HG3	2.08	0.54
1:B:1024:VAL:HG23	1:B:1025:LYS:HD3	1.90	0.54
1:D:2833:LEU:HD22	1:D:2837:LEU:HD23	1.89	0.54
1:B:2593:VAL:HG11	1:B:2640:LEU:HD12	1.90	0.54
1:D:253:GLY:O	1:D:257:ARG:HG3	2.08	0.54
1:D:4107:GLU:OE2	1:D:4147:ARG:NH1	2.41	0.54
1:D:4580:THR:OG1	1:D:4733:HIS:NE2	2.26	0.54
1:A:1980:LYS:HZ1	1:A:3632:GLU:HG2	1.73	0.53
1:A:2833:LEU:HD22	1:A:2837:LEU:HD23	1.89	0.53
1:A:4618:THR:OG1	1:A:4619:GLU:OE1	2.26	0.53
1:D:1024:VAL:HG23	1:D:1025:LYS:HD3	1.90	0.53
1:D:4618:THR:OG1	1:D:4619:GLU:OE1	2.26	0.53
1:A:4107:GLU:OE2	1:A:4147:ARG:NH1	2.41	0.53
1:B:1124:PRO:HD2	1:B:1594:VAL:HG23	1.91	0.53
1:B:2995:HIS:HE2	1:C:1070:ASP:HB3	1.73	0.53
1:C:1124:PRO:HD2	1:C:1594:VAL:HG23	1.91	0.53
1:C:1980:LYS:HZ1	1:C:3632:GLU:HG2	1.74	0.53
1:D:1635:GLU:OE1	1:D:1637:ARG:NH1	2.41	0.53
1:D:2765:GLU:HA	1:D:2768:LYS:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:PRO:HD2	1:A:1594:VAL:HG23	1.91	0.53
1:A:4832:GLU:O	1:A:4843:ARG:NH2	2.21	0.53
1:C:4107:GLU:OE2	1:C:4147:ARG:NH1	2.41	0.53
1:A:2995:HIS:HE2	1:B:1070:ASP:HB3	1.74	0.53
1:C:919:VAL:HG22	1:C:920:GLU:H	1.74	0.53
1:C:2593:VAL:HG11	1:C:2640:LEU:HD12	1.90	0.53
1:C:2706:VAL:HG21	1:C:2785:TRP:HE1	1.74	0.53
1:D:1031:ARG:NH2	1:D:1046:ASN:OD1	2.41	0.53
1:B:1898:LEU:HD13	1:B:1902:VAL:HG12	1.90	0.53
1:B:3729:ALA:HA	1:B:3732:HIS:CD2	2.43	0.53
1:D:3803:LEU:HB2	1:D:3884:SER:HB2	1.91	0.53
1:A:3803:LEU:HB2	1:A:3884:SER:HB2	1.91	0.53
1:B:919:VAL:HG22	1:B:920:GLU:H	1.74	0.53
1:B:2706:VAL:HG21	1:B:2785:TRP:HE1	1.74	0.53
1:B:3074:ASN:O	1:B:3078:GLY:HA3	2.08	0.53
1:C:3074:ASN:O	1:C:3078:GLY:HA3	2.08	0.53
1:C:3803:LEU:HB2	1:C:3884:SER:HB2	1.91	0.53
1:D:42:PHE:HZ	1:D:459:LEU:HG	1.73	0.53
1:A:643:LEU:O	1:A:645:GLN:NE2	2.42	0.53
1:B:1257:GLN:HG3	1:B:1595:LEU:HD11	1.88	0.53
1:B:2426:LEU:HD23	1:C:143:LEU:HD22	1.90	0.53
1:B:3803:LEU:HB2	1:B:3884:SER:HB2	1.91	0.53
1:C:1024:VAL:HG23	1:C:1025:LYS:HD3	1.90	0.53
1:C:3072:MET:HE3	1:C:3136:SER:HA	1.91	0.53
1:C:4618:THR:OG1	1:C:4619:GLU:OE1	2.26	0.53
1:D:919:VAL:HG22	1:D:920:GLU:H	1.74	0.53
1:D:1980:LYS:HZ1	1:D:3632:GLU:HG2	1.74	0.53
1:A:2706:VAL:HG21	1:A:2785:TRP:HE1	1.74	0.53
1:A:3179:ASN:O	1:A:3185:ASN:ND2	2.42	0.53
1:B:643:LEU:O	1:B:645:GLN:NE2	2.42	0.53
1:D:3074:ASN:O	1:D:3078:GLY:HA3	2.08	0.53
1:A:3074:ASN:O	1:A:3078:GLY:HA3	2.08	0.53
1:B:1013:ARG:HG2	1:B:1013:ARG:NH1	2.24	0.53
1:B:4107:GLU:OE2	1:B:4147:ARG:NH1	2.41	0.53
1:D:332:ARG:NH1	1:D:364:GLN:OE1	2.36	0.53
1:A:4819:VAL:HG12	1:A:4830:GLU:HG3	1.90	0.53
1:B:2102:LEU:O	1:B:2105:THR:HG22	2.09	0.53
1:B:4819:VAL:HG12	1:B:4830:GLU:HG3	1.90	0.53
1:C:42:PHE:HZ	1:C:459:LEU:HG	1.73	0.53
1:C:2833:LEU:HD22	1:C:2837:LEU:HD23	1.89	0.53
1:D:1124:PRO:HD2	1:D:1594:VAL:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2706:VAL:HG21	1:D:2785:TRP:HE1	1.74	0.53
1:A:1891:GLU:HB3	1:A:1895:GLN:HG3	1.91	0.52
1:A:2593:VAL:HG11	1:A:2640:LEU:HD12	1.90	0.52
1:A:3700:HIS:CE1	1:A:3702:GLU:HG2	2.44	0.52
1:B:3176:ASP:O	1:B:3185:ASN:ND2	2.31	0.52
1:B:4618:THR:OG1	1:B:4619:GLU:OE1	2.26	0.52
1:C:520:ARG:O	1:C:523:GLY:N	2.43	0.52
1:C:3677:THR:HB	1:C:3679:LYS:HZ2	1.74	0.52
1:D:3317:THR:H	1:D:3320:LEU:HD23	1.75	0.52
1:D:3700:HIS:CE1	1:D:3702:GLU:HG2	2.44	0.52
1:D:4607:ALA:HB1	1:D:4649:VAL:HG21	1.91	0.52
1:A:253:GLY:O	1:A:257:ARG:HG3	2.08	0.52
1:C:1031:ARG:NH2	1:C:1046:ASN:OD1	2.41	0.52
1:D:643:LEU:O	1:D:645:GLN:NE2	2.42	0.52
1:D:1891:GLU:HB3	1:D:1895:GLN:HG3	1.92	0.52
1:D:1898:LEU:HD13	1:D:1902:VAL:HG12	1.90	0.52
1:D:2717:LEU:O	1:D:2721:ILE:HG12	2.10	0.52
1:A:919:VAL:HG22	1:A:920:GLU:H	1.74	0.52
1:A:4607:ALA:HB1	1:A:4649:VAL:HG21	1.91	0.52
1:C:1039:ASP:OD1	1:C:1042:THR:OG1	2.25	0.52
1:A:202:HIS:HD2	1:A:203:VAL:N	2.08	0.52
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.75	0.52
1:B:3166:PHE:CE1	1:B:3168:VAL:HB	2.45	0.52
1:C:253:GLY:O	1:C:257:ARG:HG3	2.08	0.52
1:C:643:LEU:O	1:C:645:GLN:NE2	2.42	0.52
1:C:1891:GLU:HB3	1:C:1895:GLN:HG3	1.91	0.52
1:C:2717:LEU:O	1:C:2721:ILE:HG12	2.10	0.52
1:A:3317:THR:H	1:A:3320:LEU:HD23	1.75	0.52
1:A:4011:GLU:HG2	1:A:4121:LEU:HD22	1.92	0.52
1:B:520:ARG:O	1:B:523:GLY:N	2.42	0.52
1:B:1980:LYS:HZ1	1:B:3632:GLU:HG2	1.73	0.52
1:B:2241:ASP:OD2	1:B:2297:ARG:NH2	2.38	0.52
1:B:2717:LEU:O	1:B:2721:ILE:HG12	2.10	0.52
1:B:3740:VAL:HG13	1:B:3758:THR:HG22	1.92	0.52
1:C:1013:ARG:HG2	1:C:1013:ARG:NH1	2.24	0.52
1:C:1635:GLU:OE1	1:C:1637:ARG:NH1	2.41	0.52
1:C:1898:LEU:HD13	1:C:1902:VAL:HG12	1.90	0.52
1:C:3317:THR:H	1:C:3320:LEU:HD23	1.75	0.52
1:C:4011:GLU:HG2	1:C:4121:LEU:HD22	1.92	0.52
1:D:2593:VAL:HG11	1:D:2640:LEU:HD12	1.90	0.52
1:A:3166:PHE:CE1	1:A:3168:VAL:HB	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:PHE:CE2	1:B:522:ALA:HB1	2.45	0.52
1:B:1031:ARG:NH2	1:B:1046:ASN:OD1	2.41	0.52
1:B:3700:HIS:CE1	1:B:3702:GLU:HG2	2.44	0.52
1:C:202:HIS:HD2	1:C:203:VAL:N	2.08	0.52
1:C:514:PHE:CE2	1:C:522:ALA:HB1	2.45	0.52
1:C:4827:ILE:O	1:C:4831:ILE:HG12	2.10	0.52
1:D:520:ARG:O	1:D:523:GLY:N	2.43	0.52
1:D:4011:GLU:HG2	1:D:4121:LEU:HD22	1.92	0.52
1:A:514:PHE:CE2	1:A:522:ALA:HB1	2.45	0.52
1:A:3740:VAL:HG13	1:A:3758:THR:HG22	1.92	0.52
1:B:2765:GLU:HA	1:B:2768:LYS:HG2	1.89	0.52
1:C:2102:LEU:O	1:C:2105:THR:HG22	2.09	0.52
1:D:1114:ARG:NH1	1:D:1128:LEU:O	2.43	0.52
1:D:2102:LEU:O	1:D:2105:THR:HG22	2.09	0.52
1:B:1039:ASP:OD1	1:B:1042:THR:OG1	2.25	0.52
1:B:4011:GLU:HG2	1:B:4121:LEU:HD22	1.92	0.52
1:C:313:ASN:HD21	1:C:390:LYS:NZ	2.07	0.52
1:A:313:ASN:HD21	1:A:390:LYS:NZ	2.07	0.52
1:A:520:ARG:O	1:A:523:GLY:N	2.42	0.52
1:A:1013:ARG:HG2	1:A:1013:ARG:NH1	2.24	0.52
1:A:1635:GLU:OE1	1:A:1637:ARG:NH1	2.41	0.52
1:A:2102:LEU:O	1:A:2105:THR:HG22	2.09	0.52
1:A:3215:MET:O	1:A:3219:VAL:HG23	2.10	0.52
1:B:202:HIS:HD2	1:B:203:VAL:N	2.08	0.52
1:B:313:ASN:HD21	1:B:390:LYS:NZ	2.07	0.52
1:B:2442:MET:HE1	1:B:2498:ALA:HB1	1.91	0.52
1:C:3166:PHE:CE1	1:C:3168:VAL:HB	2.45	0.52
1:C:3700:HIS:CE1	1:C:3702:GLU:HG2	2.44	0.52
1:C:4819:VAL:HG12	1:C:4830:GLU:HG3	1.91	0.52
1:D:235:ARG:NH2	1:D:412:GLU:OE2	2.25	0.52
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.75	0.52
1:A:2717:LEU:O	1:A:2721:ILE:HG12	2.09	0.52
1:B:1091:GLU:HB3	1:B:1094:TYR:HD2	1.75	0.52
1:B:3043:ARG:NE	1:B:3120:ASP:OD2	2.43	0.52
1:A:1114:ARG:NH1	1:A:1128:LEU:O	2.43	0.51
1:B:1891:GLU:HB3	1:B:1895:GLN:HG3	1.92	0.51
1:C:67:PHE:HB3	1:C:121:LEU:HD22	1.91	0.51
1:C:4607:ALA:HB1	1:C:4649:VAL:HG21	1.91	0.51
1:D:202:HIS:HD2	1:D:203:VAL:N	2.08	0.51
1:D:3166:PHE:CE1	1:D:3168:VAL:HB	2.45	0.51
1:A:1825:PHE:CE1	1:A:1842:ILE:HG12	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3215:MET:O	1:B:3219:VAL:HG23	2.10	0.51
1:B:4778:VAL:O	1:B:4782:THR:HG23	2.10	0.51
1:C:1004:HIS:NE2	1:C:1033:VAL:O	2.42	0.51
1:D:849:ASP:OD1	1:D:1214:ARG:NE	2.43	0.51
1:D:3215:MET:O	1:D:3219:VAL:HG23	2.10	0.51
1:D:4819:VAL:HG12	1:D:4830:GLU:HG3	1.90	0.51
1:D:4827:ILE:O	1:D:4831:ILE:HG12	2.10	0.51
1:B:2914:THR:N	1:B:2915:PRO:HD2	2.26	0.51
1:B:3179:ASN:O	1:B:3185:ASN:ND2	2.42	0.51
1:C:1091:GLU:HB3	1:C:1094:TYR:HD2	1.75	0.51
1:C:1304:LEU:HB3	1:C:1586:LEU:HD11	1.92	0.51
1:C:3740:VAL:HG13	1:C:3758:THR:HG22	1.92	0.51
1:C:4695:SER:HA	1:C:4698:LEU:HD12	1.93	0.51
1:D:67:PHE:HB3	1:D:121:LEU:HD22	1.91	0.51
1:D:1013:ARG:HG2	1:D:1013:ARG:NH1	2.24	0.51
1:A:67:PHE:HB3	1:A:121:LEU:HD22	1.91	0.51
1:A:4827:ILE:O	1:A:4831:ILE:HG12	2.10	0.51
1:D:4778:VAL:O	1:D:4782:THR:HG23	2.10	0.51
1:B:1304:LEU:HB3	1:B:1586:LEU:HD11	1.92	0.51
1:B:3317:THR:H	1:B:3320:LEU:HD23	1.75	0.51
1:B:4827:ILE:O	1:B:4831:ILE:HG12	2.10	0.51
1:D:313:ASN:HD21	1:D:390:LYS:NZ	2.07	0.51
1:D:1825:PHE:CE1	1:D:1842:ILE:HG12	2.46	0.51
1:D:3740:VAL:HG13	1:D:3758:THR:HG22	1.92	0.51
1:B:678:MET:SD	1:B:812:LYS:NZ	2.84	0.51
1:A:2426:LEU:HD23	1:B:143:LEU:HD22	1.91	0.51
1:B:4695:SER:HA	1:B:4698:LEU:HD12	1.93	0.51
1:C:1825:PHE:CE1	1:C:1842:ILE:HG12	2.46	0.51
1:D:4695:SER:HA	1:D:4698:LEU:HD12	1.93	0.51
1:A:2442:MET:HE1	1:A:2498:ALA:HB1	1.93	0.51
1:A:4778:VAL:O	1:A:4782:THR:HG23	2.10	0.51
1:B:3976:LYS:HB2	1:B:4094:ILE:HG12	1.93	0.51
1:A:235:ARG:NH2	1:A:412:GLU:OE2	2.25	0.51
1:B:235:ARG:NH2	1:B:412:GLU:OE2	2.25	0.51
1:B:969:ASN:OD1	1:B:970:TYR:N	2.44	0.51
1:B:1825:PHE:CE1	1:B:1842:ILE:HG12	2.46	0.51
1:C:801:ARG:HA	1:C:1617:TRP:O	2.11	0.51
1:C:969:ASN:OD1	1:C:970:TYR:N	2.44	0.51
1:D:514:PHE:CE2	1:D:522:ALA:HB1	2.45	0.51
1:A:1304:LEU:HB3	1:A:1586:LEU:HD11	1.92	0.51
1:A:1435:GLY:HA2	1:D:2831:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1161:VAL:HG21	1:C:1225:LYS:HD2	1.93	0.51
1:C:3976:LYS:HB2	1:C:4094:ILE:HG12	1.93	0.51
1:D:2937:HIS:HA	1:D:3014:LEU:HD21	1.93	0.51
1:A:1039:ASP:OD1	1:A:1042:THR:OG1	2.25	0.50
1:B:67:PHE:HB3	1:B:121:LEU:HD22	1.91	0.50
1:B:1635:GLU:OE1	1:B:1637:ARG:NH1	2.41	0.50
1:B:3250:TRP:CZ3	1:B:3309:LYS:HB3	2.46	0.50
1:B:4607:ALA:HB1	1:B:4649:VAL:HG21	1.91	0.50
1:C:3215:MET:O	1:C:3219:VAL:HG23	2.10	0.50
1:D:713:TRP:HZ2	1:D:1251:LEU:HD21	1.76	0.50
1:A:3901:GLN:OE1	1:A:3904:ARG:NH2	2.45	0.50
1:B:2599:LEU:HB3	1:B:2661:LEU:HD21	1.94	0.50
1:B:4831:ILE:HB	1:B:4843:ARG:HH22	1.76	0.50
1:C:3043:ARG:NE	1:C:3120:ASP:OD2	2.43	0.50
1:C:3250:TRP:CZ3	1:C:3309:LYS:HB3	2.46	0.50
1:A:4831:ILE:HB	1:A:4843:ARG:HH22	1.77	0.50
1:B:801:ARG:HA	1:B:1617:TRP:O	2.11	0.50
1:B:2937:HIS:HA	1:B:3014:LEU:HD21	1.93	0.50
1:C:849:ASP:OD1	1:C:1214:ARG:NE	2.43	0.50
1:D:801:ARG:HA	1:D:1617:TRP:O	2.11	0.50
1:D:1304:LEU:HB3	1:D:1586:LEU:HD11	1.92	0.50
1:A:1431:ARG:HA	1:A:1505:LEU:O	2.12	0.50
1:C:713:TRP:HZ2	1:C:1251:LEU:HD21	1.76	0.50
1:C:1431:ARG:HA	1:C:1505:LEU:O	2.12	0.50
1:C:2937:HIS:HA	1:C:3014:LEU:HD21	1.93	0.50
1:C:3179:ASN:O	1:C:3185:ASN:ND2	2.42	0.50
1:C:3901:GLN:OE1	1:C:3904:ARG:NH2	2.45	0.50
1:D:925:PRO:HB2	1:D:928:GLU:HB3	1.94	0.50
1:D:1718:ARG:NH1	1:D:1758:ARG:HD3	2.27	0.50
1:D:4042:VAL:HB	1:D:4077:THR:HB	1.93	0.50
1:A:849:ASP:OD1	1:A:1214:ARG:NE	2.43	0.50
1:A:992:GLN:HA	1:A:995:MET:HE2	1.94	0.50
1:A:2914:THR:N	1:A:2915:PRO:HD2	2.26	0.50
1:B:925:PRO:HB2	1:B:928:GLU:HB3	1.94	0.50
1:C:1074:ARG:NH2	1:C:1076:GLU:OE1	2.43	0.50
1:D:1161:VAL:HG21	1:D:1225:LYS:HD2	1.93	0.50
1:D:3793:LEU:HD21	1:D:3843:LEU:HD21	1.94	0.50
1:D:4048:PHE:CE2	1:D:4052:MET:HE3	2.46	0.50
1:A:3250:TRP:CZ3	1:A:3309:LYS:HB3	2.46	0.50
1:B:713:TRP:HZ2	1:B:1251:LEU:HD21	1.77	0.50
1:B:3793:LEU:HD21	1:B:3843:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3901:GLN:OE1	1:B:3904:ARG:NH2	2.45	0.50
1:C:677:LEU:HD11	1:C:800:VAL:HB	1.94	0.50
1:C:3176:ASP:O	1:C:3185:ASN:ND2	2.31	0.50
1:C:4580:THR:OG1	1:C:4733:HIS:NE2	2.26	0.50
1:C:4831:ILE:HB	1:C:4843:ARG:HH22	1.76	0.50
1:D:1074:ARG:NH2	1:D:1076:GLU:OE1	2.43	0.50
1:D:1083:GLU:OE1	1:D:1254:ARG:NH1	2.45	0.50
1:D:1429:SER:OG	1:D:1556:GLU:HB2	2.12	0.50
1:A:678:MET:SD	1:A:812:LYS:NZ	2.84	0.50
1:A:1718:ARG:NH1	1:A:1758:ARG:HD3	2.27	0.50
1:A:2599:LEU:HB3	1:A:2661:LEU:HD21	1.94	0.50
1:A:4199:GLU:HG2	1:A:4597:LEU:HD13	1.94	0.50
1:A:4695:SER:HA	1:A:4698:LEU:HD12	1.93	0.50
1:B:1431:ARG:HA	1:B:1505:LEU:O	2.12	0.50
1:B:1718:ARG:NH1	1:B:1758:ARG:HD3	2.27	0.50
1:B:2442:MET:CE	1:B:2498:ALA:HB1	2.42	0.50
1:C:925:PRO:HB2	1:C:928:GLU:HB3	1.94	0.50
1:A:1083:GLU:OE1	1:A:1254:ARG:NH1	2.45	0.50
1:A:2874:TYR:CZ	1:A:2882:LYS:HD2	2.47	0.50
1:B:674:TYR:OH	1:B:676:GLU:OE2	2.26	0.50
1:C:810:GLU:HG2	1:C:1614:ARG:HA	1.94	0.50
1:C:1718:ARG:NH1	1:C:1758:ARG:HD3	2.27	0.50
1:C:2914:THR:N	1:C:2915:PRO:HD2	2.26	0.50
1:C:4118:PHE:HA	1:C:4121:LEU:HD12	1.94	0.50
1:D:3901:GLN:OE1	1:D:3904:ARG:NH2	2.45	0.50
1:A:387:ILE:HG22	1:A:389:ARG:HG3	1.94	0.50
1:B:1004:HIS:NE2	1:B:1033:VAL:O	2.42	0.50
1:B:1415:ASP:OD2	1:B:1559:ARG:NH2	2.43	0.50
1:C:235:ARG:NH2	1:C:412:GLU:OE2	2.25	0.50
1:C:992:GLN:HA	1:C:995:MET:HE2	1.94	0.50
1:C:1083:GLU:OE1	1:C:1254:ARG:NH1	2.45	0.50
1:D:3179:ASN:O	1:D:3185:ASN:ND2	2.42	0.50
1:A:713:TRP:HZ2	1:A:1251:LEU:HD21	1.76	0.49
1:A:925:PRO:HB2	1:A:928:GLU:HB3	1.94	0.49
1:A:3303:SER:O	1:A:3306:ILE:HG22	2.12	0.49
1:A:4929:ASP:HB3	1:A:4932:GLU:HG2	1.94	0.49
1:B:4042:VAL:HB	1:B:4077:THR:HB	1.93	0.49
1:C:2599:LEU:HB3	1:C:2661:LEU:HD21	1.94	0.49
1:A:969:ASN:OD1	1:A:970:TYR:N	2.44	0.49
1:A:2937:HIS:HA	1:A:3014:LEU:HD21	1.93	0.49
1:B:1429:SER:OG	1:B:1556:GLU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2480:VAL:HG23	1:B:2483:PHE:HB3	1.94	0.49
1:C:1114:ARG:NH1	1:C:1128:LEU:O	2.43	0.49
1:C:2279:MET:SD	1:C:2280:LEU:HD22	2.52	0.49
1:C:3325:LYS:HA	1:C:3328:LYS:HG2	1.94	0.49
1:C:4778:VAL:O	1:C:4782:THR:HG23	2.11	0.49
1:D:992:GLN:HA	1:D:995:MET:HE2	1.94	0.49
1:D:2279:MET:SD	1:D:2280:LEU:HD22	2.52	0.49
1:D:3176:ASP:O	1:D:3185:ASN:ND2	2.31	0.49
1:D:3250:TRP:CZ3	1:D:3309:LYS:HB3	2.46	0.49
1:D:4199:GLU:HG2	1:D:4597:LEU:HD13	1.94	0.49
1:A:1981:ASP:N	1:A:1981:ASP:OD1	2.45	0.49
1:B:2556:SER:HB3	1:B:2569:ILE:HG21	1.93	0.49
1:B:4118:PHE:HA	1:B:4121:LEU:HD12	1.94	0.49
1:C:1167:ASP:HB3	1:C:1172:THR:HG22	1.94	0.49
1:D:3976:LYS:HB2	1:D:4094:ILE:HG12	1.93	0.49
1:A:2279:MET:SD	1:A:2280:LEU:HD22	2.52	0.49
1:B:677:LEU:HD11	1:B:800:VAL:HB	1.94	0.49
1:D:387:ILE:HG22	1:D:389:ARG:HG3	1.94	0.49
1:D:969:ASN:OD1	1:D:970:TYR:N	2.44	0.49
1:D:1981:ASP:N	1:D:1981:ASP:OD1	2.45	0.49
1:D:4831:ILE:HB	1:D:4843:ARG:HH22	1.76	0.49
1:A:801:ARG:HA	1:A:1617:TRP:O	2.11	0.49
1:A:1074:ARG:NH2	1:A:1076:GLU:OE1	2.43	0.49
1:A:2442:MET:CE	1:A:2498:ALA:HB1	2.42	0.49
1:A:2556:SER:HB3	1:A:2569:ILE:HG21	1.93	0.49
1:A:4049:HIS:ND1	1:A:4067:LEU:HD11	2.28	0.49
1:B:1161:VAL:HG21	1:B:1225:LYS:HD2	1.93	0.49
1:B:2279:MET:SD	1:B:2280:LEU:HD22	2.52	0.49
1:C:1429:SER:OG	1:C:1556:GLU:HB2	2.12	0.49
1:D:2914:THR:N	1:D:2915:PRO:HD2	2.26	0.49
1:A:3976:LYS:HB2	1:A:4094:ILE:HG12	1.93	0.49
1:B:558:LEU:HG	1:B:571:ILE:HG23	1.95	0.49
1:B:810:GLU:HG2	1:B:1614:ARG:HA	1.94	0.49
1:B:849:ASP:OD1	1:B:1214:ARG:NE	2.43	0.49
1:B:2406:MET:O	1:B:2410:HIS:ND1	2.46	0.49
1:B:2496:LEU:HD23	1:B:2520:LEU:HD13	1.95	0.49
1:B:3152:ARG:HH12	1:B:3233:HIS:HB3	1.78	0.49
1:C:2157:GLN:O	1:C:3615:ARG:NH2	2.46	0.49
1:C:2556:SER:HB3	1:C:2569:ILE:HG21	1.93	0.49
1:C:4049:HIS:ND1	1:C:4067:LEU:HD11	2.28	0.49
1:C:4818:TYR:HA	1:D:4848:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2480:VAL:HG23	1:D:2483:PHE:HB3	1.95	0.49
1:D:2556:SER:HB3	1:D:2569:ILE:HG21	1.93	0.49
1:D:3235:MET:O	1:D:3299:LEU:HD12	2.13	0.49
1:A:1118:SER:HB3	1:A:1204:VAL:HG11	1.94	0.49
1:A:1429:SER:OG	1:A:1556:GLU:HB2	2.12	0.49
1:A:2480:VAL:HG23	1:A:2483:PHE:HB3	1.94	0.49
1:B:4275:THR:HG22	1:B:4278:ASP:H	1.78	0.49
1:C:387:ILE:HG22	1:C:389:ARG:HG3	1.94	0.49
1:C:1114:ARG:HG2	1:C:1138:ASP:HB2	1.95	0.49
1:C:2874:TYR:CZ	1:C:2882:LYS:HD2	2.47	0.49
1:C:3793:LEU:HD21	1:C:3843:LEU:HD21	1.94	0.49
1:C:4042:VAL:HB	1:C:4077:THR:HB	1.93	0.49
1:D:2157:GLN:O	1:D:3615:ARG:NH2	2.46	0.49
1:D:2442:MET:CE	1:D:2498:ALA:HB1	2.42	0.49
1:D:2599:LEU:HB3	1:D:2661:LEU:HD21	1.94	0.49
1:D:4049:HIS:ND1	1:D:4067:LEU:HD11	2.28	0.49
1:A:1689:ILE:HG23	1:A:1703:TYR:CZ	2.48	0.49
1:A:2157:GLN:O	1:A:3615:ARG:NH2	2.46	0.49
1:A:4118:PHE:HA	1:A:4121:LEU:HD12	1.94	0.49
1:B:1083:GLU:OE1	1:B:1254:ARG:NH1	2.45	0.49
1:B:1167:ASP:HB3	1:B:1172:THR:HG22	1.94	0.49
1:B:3227:ARG:HG3	1:B:3229:THR:H	1.78	0.49
1:B:3303:SER:O	1:B:3306:ILE:HG22	2.12	0.49
1:B:4049:HIS:ND1	1:B:4067:LEU:HD11	2.28	0.49
1:C:490:GLN:HG2	1:C:495:ILE:HD13	1.95	0.49
1:C:756:SER:OG	1:C:769:ARG:HB2	2.13	0.49
1:C:886:ALA:HB1	1:C:933:LEU:HD11	1.95	0.49
1:C:2442:MET:CE	1:C:2498:ALA:HB1	2.42	0.49
1:C:3303:SER:O	1:C:3306:ILE:HG22	2.12	0.49
1:C:4199:GLU:HG2	1:C:4597:LEU:HD13	1.94	0.49
1:D:810:GLU:HG2	1:D:1614:ARG:HA	1.94	0.49
1:D:2874:TYR:CZ	1:D:2882:LYS:HD2	2.47	0.49
1:D:3152:ARG:HH12	1:D:3233:HIS:HB3	1.78	0.49
1:D:3303:SER:O	1:D:3306:ILE:HG22	2.12	0.49
1:A:1161:VAL:HG21	1:A:1225:LYS:HD2	1.93	0.49
1:A:4042:VAL:HB	1:A:4077:THR:HB	1.93	0.49
1:A:4275:THR:HG22	1:A:4278:ASP:H	1.78	0.49
1:B:1689:ILE:HG23	1:B:1703:TYR:CZ	2.48	0.49
1:C:558:LEU:HG	1:C:571:ILE:HG23	1.95	0.49
1:D:1118:SER:HB3	1:D:1204:VAL:HG11	1.94	0.49
1:D:4943:MET:HE2	1:D:4951:PHE:HD1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:SER:OG	1:A:769:ARG:HB2	2.13	0.49
1:A:886:ALA:HB1	1:A:933:LEU:HD11	1.95	0.49
1:A:3325:LYS:HA	1:A:3328:LYS:HG2	1.94	0.49
1:A:3793:LEU:HD21	1:A:3843:LEU:HD21	1.94	0.49
1:B:387:ILE:HG22	1:B:389:ARG:HG3	1.94	0.49
1:B:799:LYS:HG2	1:B:1618:LEU:HD11	1.95	0.49
1:C:1689:ILE:HG23	1:C:1703:TYR:CZ	2.48	0.49
1:C:2406:MET:O	1:C:2410:HIS:ND1	2.46	0.49
1:C:2496:LEU:HD23	1:C:2520:LEU:HD13	1.95	0.49
1:D:677:LEU:HD11	1:D:800:VAL:HB	1.94	0.49
1:D:799:LYS:HG2	1:D:1618:LEU:HD11	1.95	0.49
1:D:1167:ASP:HB3	1:D:1172:THR:HG22	1.94	0.49
1:D:2406:MET:O	1:D:2410:HIS:ND1	2.46	0.49
1:D:4118:PHE:HA	1:D:4121:LEU:HD12	1.94	0.49
1:A:558:LEU:HG	1:A:571:ILE:HG23	1.95	0.48
1:A:677:LEU:HD11	1:A:800:VAL:HB	1.94	0.48
1:A:799:LYS:HG2	1:A:1618:LEU:HD11	1.95	0.48
1:A:3227:ARG:HG3	1:A:3229:THR:H	1.78	0.48
1:B:28:ILE:O	1:B:31:GLU:HG3	2.13	0.48
1:B:756:SER:OG	1:B:769:ARG:HB2	2.13	0.48
1:B:1114:ARG:HG2	1:B:1138:ASP:HB2	1.95	0.48
1:B:3325:LYS:HA	1:B:3328:LYS:HG2	1.94	0.48
1:B:4199:GLU:HG2	1:B:4597:LEU:HD13	1.94	0.48
1:C:3235:MET:O	1:C:3299:LEU:HD12	2.13	0.48
1:D:226:GLY:HA2	1:D:356:TYR:HD2	1.78	0.48
1:D:756:SER:OG	1:D:769:ARG:HB2	2.13	0.48
1:D:1114:ARG:HG2	1:D:1138:ASP:HB2	1.95	0.48
1:D:4929:ASP:HB3	1:D:4932:GLU:HG2	1.94	0.48
1:A:2406:MET:O	1:A:2410:HIS:ND1	2.46	0.48
1:A:4831:ILE:HD12	1:A:4843:ARG:NH1	2.28	0.48
1:B:490:GLN:HG2	1:B:495:ILE:HD13	1.95	0.48
1:B:3025:ASP:O	1:B:3029:ILE:HD12	2.13	0.48
1:B:4831:ILE:HD12	1:B:4843:ARG:NH1	2.28	0.48
1:C:1981:ASP:OD1	1:C:1981:ASP:N	2.45	0.48
1:C:4048:PHE:CE2	1:C:4052:MET:HE3	2.48	0.48
1:D:28:ILE:O	1:D:31:GLU:HG3	2.13	0.48
1:D:1415:ASP:OD2	1:D:1559:ARG:NH2	2.43	0.48
1:D:1431:ARG:HA	1:D:1505:LEU:O	2.12	0.48
1:D:4831:ILE:HD12	1:D:4843:ARG:NH1	2.28	0.48
1:B:2549:LEU:HD13	1:B:2588:LEU:HD22	1.95	0.48
1:C:1945:ASN:O	1:C:1949:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3025:ASP:O	1:D:3029:ILE:HD12	2.14	0.48
1:A:338:LEU:HG	1:A:340:VAL:HG13	1.96	0.48
1:A:1167:ASP:HB3	1:A:1172:THR:HG22	1.94	0.48
1:A:1945:ASN:O	1:A:1949:GLN:HG2	2.13	0.48
1:A:2588:LEU:O	1:A:2592:LEU:HG	2.14	0.48
1:A:3068:LEU:O	1:A:3071:THR:OG1	2.28	0.48
1:A:3310:VAL:HG21	1:A:3314:LEU:HD23	1.95	0.48
1:B:1243:THR:HG22	1:B:1808:ASP:HB2	1.96	0.48
1:B:2874:TYR:CZ	1:B:2882:LYS:HD2	2.47	0.48
1:B:3855:GLN:NE2	1:B:3922:GLU:O	2.46	0.48
1:C:28:ILE:O	1:C:31:GLU:HG3	2.13	0.48
1:C:799:LYS:HG2	1:C:1618:LEU:HD11	1.95	0.48
1:C:1108:VAL:HB	1:C:1212:VAL:HB	1.96	0.48
1:C:2482:ASP:OD1	1:C:2483:PHE:N	2.47	0.48
1:D:2588:LEU:O	1:D:2592:LEU:HG	2.14	0.48
1:D:3325:LYS:HA	1:D:3328:LYS:HG2	1.94	0.48
1:A:28:ILE:O	1:A:31:GLU:HG3	2.13	0.48
1:A:1004:HIS:NE2	1:A:1033:VAL:O	2.42	0.48
1:A:1243:THR:HG22	1:A:1808:ASP:HB2	1.96	0.48
1:A:3677:THR:HB	1:A:3679:LYS:HZ2	1.78	0.48
1:C:226:GLY:HA2	1:C:356:TYR:HD2	1.78	0.48
1:C:4831:ILE:HD12	1:C:4843:ARG:NH1	2.28	0.48
1:A:1415:ASP:OD2	1:A:1559:ARG:NH2	2.43	0.48
1:A:2719:TYR:CZ	1:A:2723:LYS:HD2	2.49	0.48
1:B:61:ASP:OD2	1:B:417:ARG:NH2	2.42	0.48
1:B:506:HIS:HB3	1:B:564:ARG:HH12	1.79	0.48
1:B:886:ALA:HB1	1:B:933:LEU:HD11	1.95	0.48
1:B:3310:VAL:HG21	1:B:3314:LEU:HD23	1.95	0.48
1:B:4943:MET:HE2	1:B:4951:PHE:HD1	1.78	0.48
1:C:658:ASN:ND2	1:C:831:LYS:O	2.34	0.48
1:C:1243:THR:HG22	1:C:1808:ASP:HB2	1.96	0.48
1:D:579:LEU:HD22	1:D:586:LEU:HD23	1.96	0.48
1:D:1945:ASN:O	1:D:1949:GLN:HG2	2.13	0.48
1:D:2788:ARG:NE	1:D:2906:GLY:HA3	2.28	0.48
1:A:194:LEU:HD11	1:A:201:LEU:HB3	1.96	0.48
1:A:810:GLU:HG2	1:A:1614:ARG:HA	1.94	0.48
1:A:3235:MET:O	1:A:3299:LEU:HD12	2.13	0.48
1:A:3855:GLN:NE2	1:A:3922:GLU:O	2.46	0.48
1:B:579:LEU:HD22	1:B:586:LEU:HD23	1.96	0.48
1:B:1108:VAL:HB	1:B:1212:VAL:HB	1.96	0.48
1:C:678:MET:SD	1:C:812:LYS:NZ	2.84	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2480:VAL:HG23	1:C:2483:PHE:HB3	1.94	0.48
1:C:2719:TYR:CZ	1:C:2723:LYS:HD2	2.49	0.48
1:C:3939:ARG:HH12	1:D:173:GLU:HG2	1.77	0.48
1:C:4275:THR:HG22	1:C:4278:ASP:H	1.78	0.48
1:D:558:LEU:HG	1:D:571:ILE:HG23	1.95	0.48
1:D:1689:ILE:HG23	1:D:1703:TYR:CZ	2.48	0.48
1:D:2779:LEU:HD23	1:D:2782:MET:HE3	1.94	0.48
1:D:3855:GLN:NE2	1:D:3922:GLU:O	2.46	0.48
1:D:4275:THR:HG22	1:D:4278:ASP:H	1.78	0.48
1:A:2549:LEU:HD13	1:A:2588:LEU:HD22	1.95	0.48
1:A:4156:SER:HB3	1:A:4923:MET:HE1	1.96	0.48
2:G:90:GLY:HA2	1:C:638:PRO:HD3	1.96	0.48
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.96	0.48
1:B:271:ALA:HB2	1:B:488:LEU:HD12	1.96	0.48
1:B:489:PHE:CD2	1:B:494:MET:HG3	2.49	0.48
1:B:1074:ARG:NH2	1:B:1076:GLU:OE1	2.43	0.48
1:B:2062:ILE:O	1:B:2066:MET:HG2	2.14	0.48
1:B:2157:GLN:O	1:B:3615:ARG:NH2	2.46	0.48
1:C:489:PHE:CD2	1:C:494:MET:HG3	2.49	0.48
1:C:1016:TRP:CD2	1:C:1027:ARG:HG2	2.49	0.48
1:C:3152:ARG:HH12	1:C:3233:HIS:HB3	1.78	0.48
1:C:3939:ARG:NH1	1:D:173:GLU:HG2	2.29	0.48
1:C:4929:ASP:HB3	1:C:4932:GLU:HG2	1.94	0.48
1:D:1016:TRP:CD2	1:D:1027:ARG:HG2	2.49	0.48
1:D:1243:THR:HG22	1:D:1808:ASP:HB2	1.96	0.48
1:D:1896:MET:HB2	1:D:1896:MET:HE3	1.69	0.48
1:D:3043:ARG:NE	1:D:3120:ASP:OD2	2.43	0.48
1:A:271:ALA:HB2	1:A:488:LEU:HD12	1.96	0.48
1:A:490:GLN:HG2	1:A:495:ILE:HD13	1.95	0.48
1:A:1114:ARG:HG2	1:A:1138:ASP:HB2	1.95	0.48
1:A:3939:ARG:HH12	1:B:173:GLU:HG2	1.79	0.48
1:C:3068:LEU:O	1:C:3071:THR:OG1	2.28	0.48
1:D:2756:LEU:O	1:D:2758:LYS:HG2	2.14	0.48
1:A:281:ARG:NH1	1:A:345:GLU:OE2	2.44	0.48
1:B:1118:SER:HB3	1:B:1204:VAL:HG11	1.94	0.48
1:B:2588:LEU:O	1:B:2592:LEU:HG	2.14	0.48
1:A:579:LEU:HD22	1:A:586:LEU:HD23	1.96	0.47
1:A:2756:LEU:O	1:A:2758:LYS:HG2	2.14	0.47
1:A:3152:ARG:HH12	1:A:3233:HIS:HB3	1.78	0.47
1:A:4079:ASP:O	1:A:4082:GLU:HG3	2.14	0.47
1:B:194:LEU:HD11	1:B:201:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1945:ASN:O	1:B:1949:GLN:HG2	2.13	0.47
1:C:579:LEU:HD22	1:C:586:LEU:HD23	1.96	0.47
1:C:1118:SER:HB3	1:C:1204:VAL:HG11	1.94	0.47
1:C:1718:ARG:HD2	1:C:1830:ILE:O	2.14	0.47
1:C:2290:TRP:CZ2	1:C:2388:ILE:HG12	2.49	0.47
1:C:2588:LEU:O	1:C:2592:LEU:HG	2.14	0.47
1:D:506:HIS:HB3	1:D:564:ARG:HH12	1.79	0.47
1:D:624:ALA:HB2	1:D:1667:LEU:HD12	1.96	0.47
1:D:1431:ARG:NH1	1:D:1556:GLU:OE2	2.47	0.47
1:D:2062:ILE:O	1:D:2066:MET:HG2	2.14	0.47
1:D:2290:TRP:CZ2	1:D:2388:ILE:HG12	2.49	0.47
1:D:2496:LEU:HD23	1:D:2520:LEU:HD13	1.95	0.47
1:D:4079:ASP:O	1:D:4082:GLU:HG3	2.14	0.47
1:A:226:GLY:HA2	1:A:356:TYR:HD2	1.78	0.47
1:A:3102:LEU:HB2	1:A:3103:PRO:HD3	1.96	0.47
1:B:624:ALA:HB2	1:B:1667:LEU:HD12	1.96	0.47
1:B:1114:ARG:NH1	1:B:1128:LEU:O	2.43	0.47
1:B:1431:ARG:NH1	1:B:1556:GLU:OE2	2.47	0.47
1:B:2719:TYR:CZ	1:B:2723:LYS:HD2	2.49	0.47
1:B:3137:LEU:HB3	1:B:3159:LEU:HD12	1.96	0.47
1:B:4079:ASP:O	1:B:4082:GLU:HG3	2.14	0.47
1:C:281:ARG:NH1	1:C:345:GLU:OE2	2.44	0.47
1:C:2937:HIS:O	1:C:2941:LEU:HG	2.14	0.47
1:C:3025:ASP:O	1:C:3029:ILE:HD12	2.13	0.47
1:D:886:ALA:HB1	1:D:933:LEU:HD11	1.95	0.47
1:D:2753:VAL:O	1:D:2753:VAL:HG12	2.14	0.47
1:D:3122:ILE:HG22	1:D:3127:GLN:HG3	1.97	0.47
1:A:537:LEU:O	1:A:541:ILE:HG12	2.15	0.47
1:A:2482:ASP:OD1	1:A:2483:PHE:N	2.47	0.47
1:A:2496:LEU:HD23	1:A:2520:LEU:HD13	1.95	0.47
1:A:4818:TYR:HA	1:B:4848:ILE:HD11	1.95	0.47
1:A:4943:MET:HE1	1:A:4951:PHE:HD1	1.79	0.47
2:E:24:VAL:HG22	2:E:48:LYS:HG2	1.96	0.47
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.96	0.47
1:B:226:GLY:HA2	1:B:356:TYR:HD2	1.78	0.47
1:B:1718:ARG:HD2	1:B:1830:ILE:O	2.14	0.47
1:B:4929:ASP:HB3	1:B:4932:GLU:HG2	1.94	0.47
1:C:506:HIS:HB3	1:C:564:ARG:HH12	1.79	0.47
1:C:1431:ARG:NH1	1:C:1556:GLU:OE2	2.47	0.47
1:C:4079:ASP:O	1:C:4082:GLU:HG3	2.14	0.47
1:C:4684:GLU:HG2	1:C:4685:LYS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:LEU:HG	1:D:340:VAL:HG13	1.96	0.47
1:D:489:PHE:CD2	1:D:494:MET:HG3	2.49	0.47
1:D:678:MET:SD	1:D:812:LYS:NZ	2.84	0.47
1:D:1718:ARG:HD2	1:D:1830:ILE:O	2.14	0.47
1:D:4156:SER:HB3	1:D:4923:MET:HE1	1.96	0.47
1:A:2062:ILE:O	1:A:2066:MET:HG2	2.14	0.47
1:A:2290:TRP:CZ2	1:A:2388:ILE:HG12	2.49	0.47
1:B:1016:TRP:CD2	1:B:1027:ARG:HG2	2.49	0.47
1:B:3235:MET:O	1:B:3299:LEU:HD12	2.13	0.47
1:D:490:GLN:HG2	1:D:495:ILE:HD13	1.95	0.47
1:D:1004:HIS:NE2	1:D:1033:VAL:O	2.42	0.47
1:D:2482:ASP:OD1	1:D:2483:PHE:N	2.47	0.47
1:D:3124:GLU:HG2	1:D:3125:ASP:H	1.80	0.47
1:D:3227:ARG:HG3	1:D:3229:THR:H	1.78	0.47
1:A:61:ASP:OD2	1:A:417:ARG:NH2	2.42	0.47
1:A:304:LYS:NZ	1:A:318:ASP:OD1	2.45	0.47
1:A:489:PHE:CD2	1:A:494:MET:HG3	2.49	0.47
1:A:2241:ASP:OD2	1:A:2297:ARG:NH2	2.38	0.47
1:A:2753:VAL:HG12	1:A:2753:VAL:O	2.14	0.47
1:A:2842:GLU:OE2	1:A:2886:ARG:NE	2.48	0.47
1:A:3025:ASP:O	1:A:3029:ILE:HD12	2.14	0.47
1:B:338:LEU:HG	1:B:340:VAL:HG13	1.96	0.47
1:C:2062:ILE:O	1:C:2066:MET:HG2	2.14	0.47
1:C:2549:LEU:HD13	1:C:2588:LEU:HD22	1.96	0.47
1:C:2788:ARG:NE	1:C:2906:GLY:HA3	2.28	0.47
1:D:2241:ASP:OD2	1:D:2297:ARG:NH2	2.38	0.47
1:D:2719:TYR:CZ	1:D:2723:LYS:HD2	2.49	0.47
1:A:674:TYR:OH	1:A:676:GLU:OE2	2.26	0.47
1:A:3043:ARG:NE	1:A:3120:ASP:OD2	2.43	0.47
2:H:90:GLY:HA2	1:D:638:PRO:HD3	1.95	0.47
1:B:2756:LEU:O	1:B:2758:LYS:HG2	2.14	0.47
1:B:3691:TYR:O	1:B:3695:MET:HG3	2.14	0.47
1:B:4684:GLU:HG2	1:B:4685:LYS:H	1.79	0.47
1:C:2841:ALA:HB2	1:C:2893:LEU:HD12	1.96	0.47
1:C:3227:ARG:HG3	1:C:3229:THR:H	1.78	0.47
1:D:766:ILE:HB	1:D:779:PHE:HB2	1.97	0.47
1:D:2842:GLU:OE2	1:D:2886:ARG:NE	2.48	0.47
1:A:934:GLN:HA	1:A:937:LEU:HG	1.95	0.47
1:A:1016:TRP:CD2	1:A:1027:ARG:HG2	2.49	0.47
1:A:1431:ARG:NH1	1:A:1556:GLU:OE2	2.47	0.47
1:A:4092:LYS:HA	1:A:4129:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:51:ILE:HD12	2:F:61:GLU:OE1	2.14	0.47
1:B:281:ARG:NH1	1:B:345:GLU:OE2	2.44	0.47
1:B:537:LEU:O	1:B:541:ILE:HG12	2.15	0.47
1:B:934:GLN:HA	1:B:937:LEU:HG	1.95	0.47
1:B:2156:TYR:HE1	1:B:2202:TYR:HE2	1.63	0.47
1:B:2413:LYS:HZ2	1:B:2416:ALA:N	2.13	0.47
1:B:2841:ALA:HB2	1:B:2893:LEU:HD12	1.97	0.47
1:B:2842:GLU:OE2	1:B:2886:ARG:NE	2.48	0.47
1:B:2945:GLY:O	1:B:2948:ARG:NH1	2.48	0.47
1:B:3046:MET:HA	1:B:3054:LYS:HE2	1.97	0.47
1:C:271:ALA:HB2	1:C:488:LEU:HD12	1.96	0.47
1:C:624:ALA:HB2	1:C:1667:LEU:HD12	1.96	0.47
1:C:934:GLN:HA	1:C:937:LEU:HG	1.95	0.47
1:C:1019:GLY:O	1:C:1030:PRO:HA	2.14	0.47
1:C:2756:LEU:O	1:C:2758:LYS:HG2	2.14	0.47
1:C:3122:ILE:HG22	1:C:3127:GLN:HG3	1.97	0.47
1:C:3124:GLU:HG2	1:C:3125:ASP:H	1.79	0.47
1:C:3691:TYR:O	1:C:3695:MET:HG3	2.14	0.47
1:C:4867:ILE:HG12	1:D:4864:GLY:HA2	1.97	0.47
1:D:61:ASP:OD2	1:D:417:ARG:NH2	2.42	0.47
1:D:934:GLN:HA	1:D:937:LEU:HG	1.95	0.47
1:D:2549:LEU:HD13	1:D:2588:LEU:HD22	1.96	0.47
1:D:2937:HIS:O	1:D:2941:LEU:HG	2.14	0.47
1:D:2945:GLY:O	1:D:2948:ARG:NH1	2.48	0.47
1:D:3102:LEU:HB2	1:D:3103:PRO:HD3	1.97	0.47
1:D:3310:VAL:HG21	1:D:3314:LEU:HD23	1.95	0.47
1:A:506:HIS:HB3	1:A:564:ARG:HH12	1.79	0.47
1:A:1019:GLY:O	1:A:1030:PRO:HA	2.14	0.47
1:A:1108:VAL:HB	1:A:1212:VAL:HB	1.96	0.47
1:A:1718:ARG:HD2	1:A:1830:ILE:O	2.14	0.47
1:A:2788:ARG:NE	1:A:2906:GLY:HA3	2.28	0.47
1:A:2945:GLY:O	1:A:2948:ARG:NH1	2.48	0.47
1:B:1019:GLY:O	1:B:1030:PRO:HA	2.14	0.47
1:B:2937:HIS:O	1:B:2941:LEU:HG	2.14	0.47
1:B:3285:TYR:HA	1:B:3288:LEU:HD23	1.97	0.47
1:C:338:LEU:HG	1:C:340:VAL:HG13	1.96	0.47
1:C:2241:ASP:OD2	1:C:2297:ARG:NH2	2.38	0.47
1:C:3046:MET:HA	1:C:3054:LYS:HE2	1.97	0.47
1:C:3278:GLY:HA2	1:C:3281:LEU:CD2	2.44	0.47
1:A:3278:GLY:HA2	1:A:3281:LEU:CD2	2.44	0.47
1:A:3691:TYR:O	1:A:3695:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2290:TRP:CZ2	1:B:2388:ILE:HG12	2.49	0.47
1:B:3122:ILE:HG22	1:B:3127:GLN:HG3	1.97	0.47
1:B:4048:PHE:CE2	1:B:4052:MET:HE3	2.50	0.47
1:B:4690:LYS:O	1:B:4693:SER:OG	2.33	0.47
1:C:304:LYS:NZ	1:C:318:ASP:OD1	2.45	0.47
1:C:2842:GLU:OE2	1:C:2886:ARG:NE	2.48	0.47
1:C:3855:GLN:NE2	1:C:3922:GLU:O	2.46	0.47
1:C:3872:ILE:HA	1:C:3875:VAL:HG12	1.97	0.47
1:C:4196:THR:O	1:C:4200:MET:HG3	2.15	0.47
1:A:878:LEU:HA	1:A:881:ILE:HG22	1.97	0.47
1:A:1929:SER:HG	1:A:3620:PHE:HD2	1.63	0.47
1:A:2156:TYR:HE1	1:A:2202:TYR:HE2	1.63	0.47
1:B:2753:VAL:O	1:B:2753:VAL:HG12	2.14	0.47
1:C:2753:VAL:O	1:C:2753:VAL:HG12	2.14	0.47
1:C:3310:VAL:HG21	1:C:3314:LEU:HD23	1.95	0.47
1:C:4943:MET:HE2	1:C:4951:PHE:HD1	1.80	0.47
1:D:537:LEU:O	1:D:541:ILE:HG12	2.15	0.47
1:D:1019:GLY:O	1:D:1030:PRO:HA	2.14	0.47
1:D:1108:VAL:HB	1:D:1212:VAL:HB	1.96	0.47
1:D:3958:LEU:HD22	1:D:3964:GLN:HG3	1.97	0.47
1:A:766:ILE:HB	1:A:779:PHE:HB2	1.97	0.46
1:A:2937:HIS:O	1:A:2941:LEU:HG	2.14	0.46
1:A:4684:GLU:HG2	1:A:4685:LYS:H	1.79	0.46
2:F:24:VAL:HG22	2:F:48:LYS:HG2	1.96	0.46
2:H:51:ILE:HD12	2:H:61:GLU:OE1	2.14	0.46
1:B:766:ILE:HB	1:B:779:PHE:HB2	1.97	0.46
1:B:878:LEU:HA	1:B:881:ILE:HG22	1.97	0.46
1:B:992:GLN:HA	1:B:995:MET:HE2	1.96	0.46
1:B:3102:LEU:HB2	1:B:3103:PRO:HD3	1.97	0.46
1:B:3227:ARG:HH12	1:B:3290:ILE:HG21	1.81	0.46
1:B:4092:LYS:HA	1:B:4129:PHE:CZ	2.50	0.46
1:C:3285:TYR:HA	1:C:3288:LEU:HD23	1.97	0.46
1:D:136:SER:HB2	1:D:145:PHE:HA	1.97	0.46
1:D:2413:LYS:HZ2	1:D:2415:GLU:HB3	1.78	0.46
1:D:3046:MET:HA	1:D:3054:LYS:HE2	1.97	0.46
1:D:3137:LEU:HB3	1:D:3159:LEU:HD12	1.96	0.46
1:D:3778:LEU:HD13	1:D:3854:PHE:HD1	1.81	0.46
1:D:4684:GLU:HG2	1:D:4685:LYS:H	1.79	0.46
1:A:1690:GLU:HG3	1:A:1790:LYS:HD2	1.97	0.46
1:A:3046:MET:HA	1:A:3054:LYS:HE2	1.97	0.46
1:A:3227:ARG:HH12	1:A:3290:ILE:HG21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:51:ILE:HD12	2:E:61:GLU:OE1	2.14	0.46
1:B:137:ARG:HD3	1:B:202:HIS:HE1	1.80	0.46
1:B:3778:LEU:HD13	1:B:3854:PHE:HD1	1.81	0.46
1:D:137:ARG:HD3	1:D:202:HIS:HE1	1.80	0.46
1:D:271:ALA:HB2	1:D:488:LEU:HD12	1.96	0.46
1:D:281:ARG:NH1	1:D:345:GLU:OE2	2.44	0.46
1:D:3285:TYR:HA	1:D:3288:LEU:HD23	1.97	0.46
1:C:194:LEU:HD11	1:C:201:LEU:HB3	1.96	0.46
1:C:2178:VAL:HG21	1:C:2192:MET:CE	2.45	0.46
1:C:2945:GLY:O	1:C:2948:ARG:NH1	2.48	0.46
1:C:4156:SER:HB3	1:C:4923:MET:HE1	1.95	0.46
1:D:194:LEU:HD11	1:D:201:LEU:HB3	1.96	0.46
1:D:304:LYS:NZ	1:D:318:ASP:OD1	2.45	0.46
1:D:3691:TYR:O	1:D:3695:MET:HG3	2.14	0.46
1:A:3251:GLU:O	1:A:3257:ASN:ND2	2.48	0.46
1:A:4048:PHE:CE2	1:A:4052:MET:HE3	2.50	0.46
1:A:4196:THR:O	1:A:4200:MET:HG3	2.15	0.46
2:G:51:ILE:HD12	2:G:61:GLU:OE1	2.14	0.46
1:B:136:SER:HB2	1:B:145:PHE:HA	1.97	0.46
1:B:3124:GLU:HG2	1:B:3125:ASP:H	1.80	0.46
1:B:3278:GLY:HA2	1:B:3281:LEU:CD2	2.44	0.46
1:C:137:ARG:HD3	1:C:202:HIS:HE1	1.80	0.46
1:C:3137:LEU:HB3	1:C:3159:LEU:HD12	1.96	0.46
1:C:3778:LEU:HD13	1:C:3854:PHE:HD1	1.80	0.46
1:C:3958:LEU:HD22	1:C:3964:GLN:HG3	1.98	0.46
1:A:2178:VAL:HG21	1:A:2192:MET:CE	2.45	0.46
1:B:3872:ILE:HA	1:B:3875:VAL:HG12	1.97	0.46
1:C:3152:ARG:HH21	1:C:3237:VAL:CG2	2.28	0.46
1:D:658:ASN:ND2	1:D:831:LYS:O	2.34	0.46
1:D:949:HIS:CE1	1:D:1065:GLU:HB3	2.50	0.46
1:A:3108:LEU:O	1:A:3112:ILE:HG12	2.16	0.46
1:A:3939:ARG:NH1	1:B:173:GLU:HG2	2.31	0.46
1:B:2788:ARG:NE	1:B:2906:GLY:HA3	2.28	0.46
1:B:4196:THR:O	1:B:4200:MET:HG3	2.15	0.46
1:C:537:LEU:O	1:C:541:ILE:HG12	2.15	0.46
1:C:4092:LYS:HA	1:C:4129:PHE:CZ	2.50	0.46
1:D:3278:GLY:HA2	1:D:3281:LEU:CD2	2.44	0.46
1:A:1518:LEU:HB2	1:A:1531:TYR:HB2	1.97	0.46
1:A:2841:ALA:HB2	1:A:2893:LEU:HD12	1.97	0.46
1:A:3137:LEU:HB3	1:A:3159:LEU:HD12	1.96	0.46
1:A:3285:TYR:HA	1:A:3288:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3778:LEU:HD13	1:A:3854:PHE:HD1	1.80	0.46
1:B:555:LEU:HD21	1:B:578:VAL:HG11	1.98	0.46
1:B:2413:LYS:HD2	1:B:2416:ALA:H	1.81	0.46
1:B:3152:ARG:HH21	1:B:3237:VAL:CG2	2.28	0.46
1:B:3939:ARG:HH12	1:C:173:GLU:HG2	1.80	0.46
1:C:878:LEU:HA	1:C:881:ILE:HG22	1.97	0.46
1:C:3108:LEU:O	1:C:3112:ILE:HG12	2.16	0.46
1:D:2136:LYS:HD3	1:D:2136:LYS:HA	1.76	0.46
1:D:2178:VAL:HG21	1:D:2192:MET:CE	2.45	0.46
1:A:624:ALA:HB2	1:A:1667:LEU:HD12	1.96	0.46
1:A:2937:HIS:O	1:A:2940:ILE:HG22	2.16	0.46
1:A:3122:ILE:HG22	1:A:3127:GLN:HG3	1.97	0.46
1:A:3872:ILE:HA	1:A:3875:VAL:HG12	1.97	0.46
1:A:4867:ILE:HG12	1:B:4864:GLY:HA2	1.97	0.46
2:H:88:HIS:HD2	2:H:89:PRO:HD2	1.80	0.46
1:B:1690:GLU:HG3	1:B:1790:LYS:HD2	1.97	0.46
1:B:3939:ARG:NH1	1:C:173:GLU:HG2	2.31	0.46
1:B:3958:LEU:HD22	1:B:3964:GLN:HG3	1.98	0.46
1:C:503:ASP:O	1:C:507:VAL:HG13	2.16	0.46
1:C:2156:TYR:HE1	1:C:2202:TYR:HE2	1.63	0.46
1:D:3227:ARG:HH12	1:D:3290:ILE:HG21	1.81	0.46
1:D:3872:ILE:HA	1:D:3875:VAL:HG12	1.97	0.46
1:D:4092:LYS:HA	1:D:4129:PHE:CZ	2.50	0.46
1:A:2754:GLN:N	1:A:2755:PRO:HD2	2.31	0.46
1:B:2178:VAL:HG21	1:B:2192:MET:CE	2.45	0.46
1:C:555:LEU:HD21	1:C:578:VAL:HG11	1.98	0.46
1:C:2754:GLN:N	1:C:2755:PRO:HD2	2.31	0.46
1:C:3102:LEU:HB2	1:C:3103:PRO:HD3	1.96	0.46
1:A:2413:LYS:HD2	1:A:2416:ALA:H	1.81	0.46
2:E:88:HIS:HD2	2:E:89:PRO:HD2	1.80	0.46
2:H:88:HIS:CD2	2:H:89:PRO:HD2	2.51	0.46
1:B:448:PRO:HB2	1:B:451:SER:HB2	1.98	0.46
1:B:2754:GLN:N	1:B:2755:PRO:HD2	2.31	0.46
1:B:2937:HIS:O	1:B:2940:ILE:HG22	2.16	0.46
1:B:4091:ALA:C	1:B:4093:ASP:H	2.20	0.46
1:C:136:SER:HB2	1:C:145:PHE:HA	1.97	0.46
1:C:3227:ARG:HH12	1:C:3290:ILE:HG21	1.81	0.46
1:D:448:PRO:HB2	1:D:451:SER:HB2	1.98	0.46
1:D:1788:LYS:NZ	1:D:1833:ILE:O	2.48	0.46
1:D:2841:ALA:HB2	1:D:2893:LEU:HD12	1.97	0.46
1:D:2937:HIS:O	1:D:2940:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3152:ARG:HH21	1:D:3237:VAL:CG2	2.28	0.46
1:D:4196:THR:O	1:D:4200:MET:HG3	2.15	0.46
1:A:3293:GLY:H	1:A:3296:MET:HE1	1.81	0.45
1:A:3784:LYS:HA	1:A:3784:LYS:HD3	1.79	0.45
1:B:4964:ASP:OD1	1:B:4964:ASP:N	2.49	0.45
1:C:766:ILE:HB	1:C:779:PHE:HB2	1.97	0.45
1:D:2754:GLN:N	1:D:2755:PRO:HD2	2.31	0.45
1:A:173:GLU:HG2	1:D:3939:ARG:HH12	1.80	0.45
1:A:503:ASP:O	1:A:507:VAL:HG13	2.16	0.45
1:A:2252:GLU:HG2	1:A:2253:LEU:N	2.32	0.45
1:A:3958:LEU:HD22	1:A:3964:GLN:HG3	1.98	0.45
2:E:88:HIS:CD2	2:E:89:PRO:HD2	2.51	0.45
1:B:949:HIS:CE1	1:B:1065:GLU:HB3	2.50	0.45
1:B:3108:LEU:O	1:B:3112:ILE:HG12	2.16	0.45
1:C:949:HIS:CE1	1:C:1065:GLU:HB3	2.50	0.45
1:C:2252:GLU:HG2	1:C:2253:LEU:N	2.32	0.45
1:D:1518:LEU:HB2	1:D:1531:TYR:HB2	1.98	0.45
1:D:4690:LYS:HE3	1:D:4692:SER:HB2	1.98	0.45
1:A:949:HIS:CE1	1:A:1065:GLU:HB3	2.50	0.45
1:A:3124:GLU:HG2	1:A:3125:ASP:H	1.80	0.45
1:A:3325:LYS:HD3	1:A:3328:LYS:HD3	1.97	0.45
2:G:88:HIS:HD2	2:G:89:PRO:HD2	1.80	0.45
1:B:306:LEU:HD11	1:B:314:LEU:HD22	1.99	0.45
1:B:503:ASP:O	1:B:507:VAL:HG13	2.16	0.45
1:B:505:LEU:HD13	1:B:530:LEU:HG	1.98	0.45
1:C:1001:GLU:OE1	1:C:1035:TYR:HB3	2.17	0.45
1:C:2937:HIS:O	1:C:2940:ILE:HG22	2.16	0.45
1:C:4091:ALA:C	1:C:4093:ASP:H	2.20	0.45
1:D:2156:TYR:HE1	1:D:2202:TYR:HE2	1.63	0.45
1:D:2413:LYS:HD2	1:D:2416:ALA:H	1.81	0.45
1:A:3986:LEU:HD12	1:A:4101:LEU:HD12	1.99	0.45
1:A:4690:LYS:O	1:A:4693:SER:OG	2.33	0.45
2:F:88:HIS:CD2	2:F:89:PRO:HD2	2.51	0.45
1:B:1518:LEU:HB2	1:B:1531:TYR:HB2	1.97	0.45
1:C:1415:ASP:OD2	1:C:1559:ARG:NH2	2.43	0.45
1:C:1690:GLU:HG3	1:C:1790:LYS:HD2	1.97	0.45
1:A:3152:ARG:HH21	1:A:3237:VAL:CG2	2.28	0.45
1:A:3164:GLY:O	1:A:3248:ARG:HG3	2.17	0.45
2:H:12:ASP:OD1	2:H:13:GLY:N	2.50	0.45
1:B:3986:LEU:HD12	1:B:4101:LEU:HD12	1.99	0.45
1:B:4156:SER:HB3	1:B:4923:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1518:LEU:HB2	1:C:1531:TYR:HB2	1.97	0.45
1:C:4690:LYS:HE3	1:C:4692:SER:HB2	1.99	0.45
1:C:4964:ASP:N	1:C:4964:ASP:OD1	2.49	0.45
1:D:1911:GLN:OE1	1:D:2090:ARG:NH1	2.37	0.45
1:A:555:LEU:HD21	1:A:578:VAL:HG11	1.98	0.45
1:A:2136:LYS:HD3	1:A:2136:LYS:HA	1.76	0.45
1:A:2413:LYS:HZ2	1:A:2415:GLU:HB3	1.82	0.45
1:B:270:HIS:CD2	1:B:491:GLU:HG3	2.52	0.45
1:B:1425:THR:HG22	1:B:1563:VAL:HG13	1.98	0.45
1:B:3325:LYS:HD3	1:B:3328:LYS:HD3	1.97	0.45
1:C:61:ASP:OD2	1:C:417:ARG:NH2	2.42	0.45
1:D:1690:GLU:HG3	1:D:1790:LYS:HD2	1.97	0.45
1:D:1732:GLU:HB3	1:D:1753:LEU:HD21	1.99	0.45
1:D:2570:GLU:HG2	1:D:2605:MET:HG3	1.99	0.45
1:D:3325:LYS:HD3	1:D:3328:LYS:HD3	1.97	0.45
1:A:136:SER:HB2	1:A:145:PHE:HA	1.97	0.45
1:A:137:ARG:HD3	1:A:202:HIS:HE1	1.80	0.45
1:A:504:ARG:O	1:A:507:VAL:HG22	2.17	0.45
1:A:892:LEU:HA	1:A:895:MET:HG2	1.99	0.45
1:A:4110:PRO:HG3	1:A:4966:LEU:HD12	1.99	0.45
1:B:1732:GLU:HB3	1:B:1753:LEU:HD21	1.99	0.45
1:B:3012:GLY:O	1:B:3016:ARG:HG3	2.17	0.45
1:B:3653:GLU:OE1	1:B:3660:ARG:NH2	2.50	0.45
1:C:2570:GLU:HG2	1:C:2605:MET:HG3	1.99	0.45
1:C:4690:LYS:O	1:C:4693:SER:OG	2.33	0.45
1:D:504:ARG:O	1:D:507:VAL:HG22	2.17	0.45
1:D:3108:LEU:O	1:D:3112:ILE:HG12	2.16	0.45
1:D:3164:GLY:O	1:D:3248:ARG:HG3	2.17	0.45
1:D:4305:PHE:HA	1:D:4308:ILE:HG12	1.99	0.45
1:A:1445:TRP:HE1	1:A:1509:CYS:HB3	1.82	0.45
1:A:3012:GLY:O	1:A:3016:ARG:HG3	2.17	0.45
1:B:400:ASP:N	1:B:400:ASP:OD1	2.50	0.45
1:B:2570:GLU:HG2	1:B:2605:MET:HG3	1.99	0.45
1:B:3164:GLY:O	1:B:3248:ARG:HG3	2.17	0.45
1:D:270:HIS:CD2	1:D:491:GLU:HG3	2.52	0.45
1:D:555:LEU:HD21	1:D:578:VAL:HG11	1.98	0.45
1:D:878:LEU:HA	1:D:881:ILE:HG22	1.97	0.45
1:D:1001:GLU:OE1	1:D:1035:TYR:HB3	2.17	0.45
1:D:1268:ILE:HD11	1:D:1300:MET:HE2	1.98	0.45
1:D:2252:GLU:HG2	1:D:2253:LEU:N	2.31	0.45
1:D:4091:ALA:C	1:D:4093:ASP:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LEU:HD13	1:A:530:LEU:HG	1.98	0.45
1:A:4245:LEU:HD21	1:B:4629:GLN:HB3	1.99	0.45
1:B:892:LEU:HA	1:B:895:MET:HG2	1.99	0.45
1:B:1788:LYS:NZ	1:B:1833:ILE:O	2.48	0.45
1:B:1929:SER:HG	1:B:3620:PHE:HD2	1.63	0.45
1:B:2831:VAL:HG22	1:C:1435:GLY:HA2	1.99	0.45
1:C:2154:VAL:HA	1:C:2157:GLN:HG2	1.99	0.45
1:C:3892:TYR:OH	1:C:3899:ASP:OD1	2.25	0.45
1:C:4305:PHE:HA	1:C:4308:ILE:HG12	1.99	0.45
1:C:4943:MET:HE2	1:C:4951:PHE:H	1.82	0.45
1:D:3653:GLU:OE1	1:D:3660:ARG:NH2	2.50	0.45
1:A:1415:ASP:N	1:A:1415:ASP:OD1	2.50	0.45
1:A:2154:VAL:HA	1:A:2157:GLN:HG2	1.99	0.45
1:A:2344:LEU:HD22	1:A:2434:GLY:HA3	1.99	0.45
1:A:2570:GLU:HG2	1:A:2605:MET:HG3	1.99	0.45
1:A:3321:PRO:HA	1:A:3324:GLU:HG3	1.99	0.45
2:G:12:ASP:OD1	2:G:13:GLY:N	2.50	0.45
1:B:304:LYS:NZ	1:B:318:ASP:OD1	2.45	0.45
1:B:2344:LEU:HD22	1:B:2434:GLY:HA3	1.99	0.45
1:B:2482:ASP:OD1	1:B:2483:PHE:N	2.47	0.45
1:C:306:LEU:HD11	1:C:314:LEU:HD22	1.98	0.45
1:C:705:PRO:HG3	1:C:857:LEU:HB2	1.99	0.45
1:C:892:LEU:HA	1:C:895:MET:HG2	1.99	0.45
1:C:1131:ASP:N	1:C:1131:ASP:OD1	2.50	0.45
1:C:1960:ARG:HD3	1:C:1960:ARG:N	2.23	0.45
1:C:3012:GLY:O	1:C:3016:ARG:HG3	2.17	0.45
1:C:3653:GLU:OE1	1:C:3660:ARG:NH2	2.50	0.45
1:D:202:HIS:CD2	1:D:203:VAL:N	2.85	0.45
1:D:503:ASP:O	1:D:507:VAL:HG13	2.16	0.45
1:D:1445:TRP:HE1	1:D:1509:CYS:HB3	1.82	0.45
1:D:2087:LEU:O	1:D:2091:GLN:HG2	2.17	0.45
1:D:2344:LEU:HD22	1:D:2434:GLY:HA3	1.99	0.45
1:A:202:HIS:CD2	1:A:203:VAL:N	2.85	0.44
1:A:375:GLN:HG3	1:A:377:VAL:HG12	1.99	0.44
1:A:448:PRO:HB2	1:A:451:SER:HB2	1.98	0.44
1:A:1960:ARG:HD3	1:A:1960:ARG:N	2.23	0.44
1:A:3653:GLU:OE1	1:A:3660:ARG:NH2	2.50	0.44
2:F:12:ASP:OD1	2:F:13:GLY:N	2.50	0.44
2:F:88:HIS:HD2	2:F:89:PRO:HD2	1.80	0.44
1:B:504:ARG:O	1:B:507:VAL:HG22	2.17	0.44
1:B:1001:GLU:OE1	1:B:1035:TYR:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1445:TRP:HE1	1:B:1509:CYS:HB3	1.82	0.44
1:B:1981:ASP:OD1	1:B:1981:ASP:N	2.45	0.44
1:B:2252:GLU:HG2	1:B:2253:LEU:N	2.31	0.44
1:B:3219:VAL:HG12	1:B:3220:GLU:OE1	2.17	0.44
1:C:400:ASP:OD1	1:C:400:ASP:N	2.50	0.44
1:C:4110:PRO:HG3	1:C:4966:LEU:HD12	1.99	0.44
1:D:2436:ILE:HG22	1:D:2491:GLY:HA3	1.98	0.44
1:D:3012:GLY:O	1:D:3016:ARG:HG3	2.17	0.44
1:D:3986:LEU:HD12	1:D:4101:LEU:HD12	1.99	0.44
1:A:750:ARG:HG2	1:A:753:ASP:OD2	2.17	0.44
1:A:1001:GLU:OE1	1:A:1035:TYR:HB3	2.17	0.44
1:A:1100:ARG:HB3	1:A:1236:TYR:CD1	2.53	0.44
1:A:3198:PRO:CG	1:A:3204:VAL:HA	2.47	0.44
2:G:88:HIS:CD2	2:G:89:PRO:HD2	2.51	0.44
1:B:705:PRO:HG3	1:B:857:LEU:HB2	1.99	0.44
1:B:1113:MET:HB2	1:B:1156:TRP:HZ2	1.82	0.44
1:B:3124:GLU:CG	1:B:3125:ASP:H	2.31	0.44
1:C:505:LEU:HD13	1:C:530:LEU:HG	1.98	0.44
1:C:750:ARG:HG2	1:C:753:ASP:OD2	2.17	0.44
1:C:1415:ASP:OD1	1:C:1415:ASP:N	2.50	0.44
1:D:400:ASP:OD1	1:D:400:ASP:N	2.50	0.44
1:D:1425:THR:HG22	1:D:1563:VAL:HG13	1.98	0.44
1:A:1425:THR:HG22	1:A:1563:VAL:HG13	1.98	0.44
1:A:3124:GLU:CG	1:A:3125:ASP:H	2.31	0.44
1:A:4091:ALA:C	1:A:4093:ASP:H	2.20	0.44
1:B:2154:VAL:HA	1:B:2157:GLN:HG2	1.99	0.44
1:B:4818:TYR:HA	1:C:4848:ILE:HD11	1.98	0.44
1:C:504:ARG:O	1:C:507:VAL:HG22	2.17	0.44
1:C:1896:MET:HB2	1:C:1896:MET:HE3	1.70	0.44
1:C:3050:LEU:HG	1:C:3052:SER:H	1.83	0.44
1:C:3325:LYS:HD3	1:C:3328:LYS:HD3	1.97	0.44
1:D:1960:ARG:HD3	1:D:1960:ARG:N	2.23	0.44
1:D:3124:GLU:CG	1:D:3125:ASP:H	2.31	0.44
1:D:4690:LYS:O	1:D:4693:SER:OG	2.33	0.44
1:A:173:GLU:HG2	1:D:3939:ARG:NH1	2.32	0.44
1:A:915:HIS:NE2	1:A:917:CYS:HB2	2.32	0.44
1:B:1038:LEU:HB3	1:B:1043:LYS:HE2	1.99	0.44
1:B:1696:GLY:HA3	1:B:1816:PHE:CD2	2.53	0.44
1:B:2436:ILE:HG22	1:B:2491:GLY:HA3	1.98	0.44
1:B:3140:LEU:HD12	1:B:3155:LEU:HD11	2.00	0.44
1:C:1113:MET:HB2	1:C:1156:TRP:HZ2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4522:VAL:HG12	1:D:4807:ASP:O	2.18	0.44
1:D:313:ASN:ND2	1:D:392:ILE:HG22	2.33	0.44
1:D:4610:LEU:HD11	1:D:4635:ILE:HG22	2.00	0.44
1:A:270:HIS:CD2	1:A:491:GLU:HG3	2.52	0.44
1:A:306:LEU:HD11	1:A:314:LEU:HD22	1.98	0.44
1:A:2087:LEU:O	1:A:2091:GLN:HG2	2.17	0.44
1:A:3219:VAL:HG12	1:A:3220:GLU:OE1	2.18	0.44
1:B:4110:PRO:HG3	1:B:4966:LEU:HD12	1.99	0.44
1:C:1973:ILE:HG13	1:C:3619:LEU:HB3	2.00	0.44
1:C:2344:LEU:HD22	1:C:2434:GLY:HA3	1.99	0.44
1:C:2413:LYS:HD2	1:C:2416:ALA:H	1.81	0.44
1:C:3219:VAL:HG12	1:C:3220:GLU:OE1	2.18	0.44
1:C:3321:PRO:HA	1:C:3324:GLU:HG3	1.99	0.44
1:D:253:GLY:HA3	1:D:256:GLN:NE2	2.33	0.44
1:D:1100:ARG:HB3	1:D:1236:TYR:CD1	2.53	0.44
1:D:2185:LYS:HD2	1:D:2186:GLU:O	2.18	0.44
1:D:3650:GLU:HB2	1:D:3651:PRO:HD3	2.00	0.44
1:A:658:ASN:ND2	1:A:831:LYS:O	2.34	0.44
1:A:996:VAL:HG13	1:A:1050:LEU:CD1	2.48	0.44
1:A:1031:ARG:HG3	1:A:1038:LEU:HD11	2.00	0.44
1:A:1911:GLN:OE1	1:A:2090:ARG:NH1	2.37	0.44
1:A:2436:ILE:HG22	1:A:2491:GLY:HA3	1.98	0.44
1:A:4027:THR:HA	1:A:4032:PHE:CD2	2.53	0.44
1:A:4203:ALA:HA	1:A:4206:ILE:HG12	2.00	0.44
1:A:4305:PHE:HA	1:A:4308:ILE:HG12	1.99	0.44
1:A:4964:ASP:N	1:A:4964:ASP:OD1	2.49	0.44
1:B:1031:ARG:HG3	1:B:1038:LEU:HD11	2.00	0.44
1:B:3187:LYS:O	1:B:3191:GLU:HB2	2.18	0.44
1:B:4690:LYS:HE3	1:B:4692:SER:HB2	1.98	0.44
1:C:58:VAL:HG22	1:C:320:GLU:HA	2.00	0.44
1:C:1425:THR:HG22	1:C:1563:VAL:HG13	1.98	0.44
1:C:2087:LEU:O	1:C:2091:GLN:HG2	2.17	0.44
1:C:3164:GLY:O	1:C:3248:ARG:HG3	2.17	0.44
1:D:1038:LEU:HB3	1:D:1043:LYS:HE2	1.99	0.44
1:D:4110:PRO:HG3	1:D:4966:LEU:HD12	1.99	0.44
1:A:1988:CYS:O	1:A:1993:ARG:NE	2.44	0.44
1:A:4848:ILE:HD11	1:D:4818:TYR:HA	2.00	0.44
1:B:375:GLN:HG3	1:B:377:VAL:HG12	1.99	0.44
1:B:750:ARG:HG2	1:B:753:ASP:OD2	2.17	0.44
1:B:3050:LEU:HG	1:B:3052:SER:H	1.83	0.44
1:B:4305:PHE:HA	1:B:4308:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:HIS:CD2	1:C:491:GLU:HG3	2.52	0.44
1:C:2436:ILE:HG22	1:C:2491:GLY:HA3	1.98	0.44
1:C:3069:GLU:O	1:C:3072:MET:HB2	2.18	0.44
1:C:3251:GLU:O	1:C:3257:ASN:ND2	2.48	0.44
1:C:4021:LEU:HD23	1:C:4088:HIS:CD2	2.53	0.44
1:C:4203:ALA:HA	1:C:4206:ILE:HG12	2.00	0.44
1:D:996:VAL:HG13	1:D:1050:LEU:CD1	2.48	0.44
1:D:2624:PRO:HD2	1:D:2992:SER:HB2	2.00	0.44
1:D:3198:PRO:CG	1:D:3204:VAL:HA	2.47	0.44
1:D:3312:PRO:O	1:D:3315:LEU:HB2	2.18	0.44
1:A:804:LEU:O	1:A:823:TYR:HD1	2.01	0.44
1:A:1732:GLU:HB3	1:A:1753:LEU:HD21	1.99	0.44
1:A:3140:LEU:HD12	1:A:3155:LEU:HD11	2.00	0.44
1:A:4026:LEU:HD12	1:A:4055:HIS:CG	2.53	0.44
1:A:4690:LYS:HE3	1:A:4692:SER:HB2	1.99	0.44
2:E:12:ASP:OD1	2:E:13:GLY:N	2.50	0.44
2:H:50:ARG:NH1	2:H:53:LYS:HG3	2.33	0.44
1:B:1131:ASP:OD1	1:B:1131:ASP:N	2.50	0.44
1:B:1415:ASP:N	1:B:1415:ASP:OD1	2.50	0.44
1:B:3198:PRO:CG	1:B:3204:VAL:HA	2.47	0.44
1:C:804:LEU:O	1:C:823:TYR:HD1	2.01	0.44
1:C:869:THR:O	1:C:872:ILE:HG12	2.18	0.44
1:C:996:VAL:HG13	1:C:1050:LEU:CD1	2.48	0.44
1:C:1414:ARG:NE	1:C:1415:ASP:OD1	2.50	0.44
1:C:2185:LYS:HD2	1:C:2186:GLU:O	2.18	0.44
1:C:4610:LEU:HD11	1:C:4635:ILE:HG22	2.00	0.44
1:D:58:VAL:HG22	1:D:320:GLU:HA	2.00	0.44
1:D:306:LEU:HD11	1:D:314:LEU:HD22	1.99	0.44
1:D:892:LEU:HA	1:D:895:MET:HG2	1.99	0.44
1:D:1040:ASP:OD1	1:D:1041:ARG:N	2.51	0.44
1:D:1131:ASP:OD1	1:D:1131:ASP:N	2.50	0.44
1:D:1549:SER:OG	1:D:1551:ASN:O	2.33	0.44
1:D:1979:PHE:CZ	1:D:1996:LEU:HD23	2.53	0.44
1:D:2115:ASP:HB2	1:D:2152:ASN:OD1	2.18	0.44
1:D:2172:MET:O	1:D:2176:VAL:HG13	2.18	0.44
1:A:1896:MET:HB2	1:A:1896:MET:HE3	1.70	0.44
1:A:1979:PHE:CZ	1:A:1996:LEU:HD23	2.53	0.44
1:A:3050:LEU:HG	1:A:3052:SER:H	1.83	0.44
1:A:3312:PRO:O	1:A:3315:LEU:HB2	2.18	0.44
1:A:4921:PHE:HE2	1:A:4940:VAL:HG11	1.83	0.44
2:E:50:ARG:NH1	2:E:53:LYS:HG3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:HG22	1:B:320:GLU:HA	2.00	0.44
1:B:1979:PHE:CZ	1:B:1996:LEU:HD23	2.53	0.44
1:B:2590:ARG:O	1:B:2593:VAL:HG22	2.18	0.44
1:B:2624:PRO:HD2	1:B:2992:SER:HB2	2.00	0.44
1:B:2760:TYR:HA	1:B:2763:LEU:HD23	2.00	0.44
1:B:3319:PHE:N	1:B:3319:PHE:CD1	2.86	0.44
1:B:4203:ALA:HA	1:B:4206:ILE:HG12	2.00	0.44
1:C:202:HIS:CD2	1:C:203:VAL:N	2.85	0.44
1:C:375:GLN:HG3	1:C:377:VAL:HG12	1.99	0.44
1:C:931:TYR:HA	1:C:934:GLN:HG3	2.00	0.44
1:C:1445:TRP:HE1	1:C:1509:CYS:HB3	1.82	0.44
1:D:505:LEU:HD13	1:D:530:LEU:HG	1.98	0.44
1:D:895:MET:HA	1:D:898:ILE:HG22	1.99	0.44
1:D:915:HIS:NE2	1:D:917:CYS:HB2	2.32	0.44
1:D:4021:LEU:HD23	1:D:4088:HIS:CD2	2.53	0.44
1:D:4026:LEU:HD12	1:D:4055:HIS:CG	2.53	0.44
1:D:4203:ALA:HA	1:D:4206:ILE:HG12	2.00	0.44
1:D:4248:LEU:HG	1:D:4297:PHE:CE1	2.53	0.44
1:A:1040:ASP:OD1	1:A:1041:ARG:N	2.51	0.43
1:A:3137:LEU:HD13	1:A:3159:LEU:HA	2.00	0.43
1:B:2172:MET:O	1:B:2176:VAL:HG13	2.18	0.43
1:B:4027:THR:HA	1:B:4032:PHE:CD2	2.53	0.43
1:B:4921:PHE:HE2	1:B:4940:VAL:HG11	1.83	0.43
1:C:249:SER:N	1:C:272:ARG:HH21	2.15	0.43
1:C:313:ASN:ND2	1:C:392:ILE:HG22	2.33	0.43
1:C:448:PRO:HB2	1:C:451:SER:HB2	1.98	0.43
1:C:1038:LEU:HB3	1:C:1043:LYS:HE2	1.99	0.43
1:C:1911:GLN:OE1	1:C:2090:ARG:NH1	2.37	0.43
1:C:2172:MET:O	1:C:2176:VAL:HG13	2.18	0.43
1:C:2277:CYS:HB3	1:C:2280:LEU:HB2	2.00	0.43
1:C:2413:LYS:HZ2	1:C:2416:ALA:N	2.15	0.43
1:D:375:GLN:HG3	1:D:377:VAL:HG12	1.99	0.43
1:D:750:ARG:HG2	1:D:753:ASP:OD2	2.17	0.43
1:D:931:TYR:HA	1:D:934:GLN:HG3	2.00	0.43
1:D:3137:LEU:HD13	1:D:3159:LEU:HA	2.00	0.43
1:D:3319:PHE:CD1	1:D:3319:PHE:N	2.86	0.43
1:D:4921:PHE:HE2	1:D:4940:VAL:HG11	1.83	0.43
1:A:1038:LEU:HB3	1:A:1043:LYS:HE2	1.99	0.43
1:A:1113:MET:HB2	1:A:1156:TRP:HZ2	1.82	0.43
1:A:2277:CYS:HB3	1:A:2280:LEU:HB2	2.00	0.43
1:A:3069:GLU:O	1:A:3072:MET:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3187:LYS:O	1:A:3191:GLU:HB2	2.18	0.43
1:B:313:ASN:ND2	1:B:392:ILE:HG22	2.33	0.43
1:B:996:VAL:HG13	1:B:1050:LEU:CD1	2.48	0.43
1:B:3246:MET:HA	1:B:3268:LEU:HD13	2.01	0.43
1:B:3803:LEU:HD23	1:B:3830:LEU:HB2	2.00	0.43
1:B:4026:LEU:HD12	1:B:4055:HIS:CG	2.53	0.43
1:C:895:MET:HA	1:C:898:ILE:HG22	1.99	0.43
1:C:915:HIS:NE2	1:C:917:CYS:HB2	2.32	0.43
1:C:2590:ARG:O	1:C:2593:VAL:HG22	2.18	0.43
1:C:2624:PRO:HD2	1:C:2992:SER:HB2	2.00	0.43
1:C:3187:LYS:O	1:C:3191:GLU:HB2	2.18	0.43
1:C:3198:PRO:CG	1:C:3204:VAL:HA	2.47	0.43
1:C:3803:LEU:HD23	1:C:3830:LEU:HB2	2.00	0.43
1:C:3986:LEU:HD12	1:C:4101:LEU:HD12	1.99	0.43
1:C:4027:THR:HA	1:C:4032:PHE:CD2	2.53	0.43
1:D:2154:VAL:HA	1:D:2157:GLN:HG2	1.99	0.43
1:D:2427:ILE:O	1:D:2476:TYR:OH	2.29	0.43
1:D:4027:THR:HA	1:D:4032:PHE:CD2	2.53	0.43
1:A:58:VAL:HG22	1:A:320:GLU:HA	2.00	0.43
1:A:253:GLY:HA3	1:A:256:GLN:NE2	2.33	0.43
1:A:313:ASN:ND2	1:A:392:ILE:HG22	2.33	0.43
1:A:400:ASP:OD1	1:A:400:ASP:N	2.50	0.43
1:A:2624:PRO:HD2	1:A:2992:SER:HB2	2.00	0.43
1:A:3237:VAL:C	1:A:3240:PRO:HD2	2.38	0.43
1:A:3650:GLU:HB2	1:A:3651:PRO:HD3	2.00	0.43
1:A:4248:LEU:HG	1:A:4297:PHE:CE1	2.53	0.43
1:B:253:GLY:HA3	1:B:256:GLN:NE2	2.33	0.43
1:B:915:HIS:NE2	1:B:917:CYS:HB2	2.32	0.43
1:B:3321:PRO:HA	1:B:3324:GLU:HG3	1.99	0.43
1:B:3730:ARG:O	1:B:3734:ARG:NH1	2.50	0.43
1:C:3246:MET:HA	1:C:3268:LEU:HD13	2.01	0.43
1:D:1113:MET:HB2	1:D:1156:TRP:HZ2	1.82	0.43
1:D:2760:TYR:HA	1:D:2763:LEU:HD23	2.00	0.43
1:D:3050:LEU:HG	1:D:3052:SER:H	1.83	0.43
1:D:3069:GLU:O	1:D:3072:MET:HB2	2.18	0.43
1:D:3237:VAL:C	1:D:3240:PRO:HD2	2.38	0.43
1:A:2115:ASP:HB2	1:A:2152:ASN:OD1	2.18	0.43
1:A:2590:ARG:O	1:A:2593:VAL:HG22	2.18	0.43
1:A:4021:LEU:HD23	1:A:4088:HIS:CD2	2.53	0.43
1:A:4943:MET:HE1	1:A:4951:PHE:H	1.83	0.43
1:B:804:LEU:O	1:B:823:TYR:HD1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:807:ARG:O	1:B:1613:GLU:HA	2.18	0.43
1:B:895:MET:HA	1:B:898:ILE:HG22	1.99	0.43
1:B:1040:ASP:OD1	1:B:1041:ARG:N	2.51	0.43
1:B:2087:LEU:O	1:B:2091:GLN:HG2	2.17	0.43
1:B:2596:VAL:HG22	1:B:2606:PRO:HB2	2.00	0.43
1:B:3036:LEU:HD23	1:B:3036:LEU:HA	1.90	0.43
1:B:3069:GLU:O	1:B:3072:MET:HB2	2.18	0.43
1:B:3312:PRO:O	1:B:3315:LEU:HB2	2.18	0.43
1:C:394:HIS:NE2	1:C:396:GLU:HG3	2.33	0.43
1:C:1729:MET:HE1	1:C:3617:VAL:HG21	1.99	0.43
1:C:2760:TYR:HA	1:C:2763:LEU:HD23	2.00	0.43
1:C:3137:LEU:HD13	1:C:3159:LEU:HA	2.00	0.43
1:C:3293:GLY:H	1:C:3296:MET:HE1	1.82	0.43
1:C:3319:PHE:N	1:C:3319:PHE:CD1	2.86	0.43
1:C:3650:GLU:HB2	1:C:3651:PRO:HD3	2.00	0.43
1:C:4245:LEU:HD21	1:D:4629:GLN:HB3	1.99	0.43
1:D:157:ALA:HA	1:D:187:SER:HB3	2.00	0.43
1:D:249:SER:N	1:D:272:ARG:HH21	2.15	0.43
1:D:804:LEU:O	1:D:823:TYR:HD1	2.01	0.43
1:A:157:ALA:HA	1:A:187:SER:HB3	2.00	0.43
1:A:249:SER:N	1:A:272:ARG:HH21	2.15	0.43
1:A:869:THR:O	1:A:872:ILE:HG12	2.18	0.43
1:A:3169:ALA:HB1	1:A:3245:TYR:OH	2.19	0.43
1:A:4206:ILE:HA	1:A:4493:ASN:ND2	2.34	0.43
1:B:271:ALA:O	1:B:301:THR:OG1	2.36	0.43
1:B:394:HIS:NE2	1:B:396:GLU:HG3	2.34	0.43
1:B:4610:LEU:HD11	1:B:4635:ILE:HG22	2.00	0.43
1:C:807:ARG:O	1:C:1613:GLU:HA	2.18	0.43
1:C:1040:ASP:OD1	1:C:1041:ARG:N	2.51	0.43
1:C:1979:PHE:CZ	1:C:1996:LEU:HD23	2.53	0.43
1:D:290:ARG:HH11	1:D:343:ARG:HH11	1.67	0.43
1:D:674:TYR:CD2	1:D:815:PRO:HB3	2.54	0.43
1:D:1696:GLY:HA3	1:D:1816:PHE:CD2	2.53	0.43
1:D:3169:ALA:HB1	1:D:3245:TYR:OH	2.19	0.43
1:D:3187:LYS:O	1:D:3191:GLU:HB2	2.18	0.43
1:D:3219:VAL:HG12	1:D:3220:GLU:OE1	2.18	0.43
1:A:674:TYR:CD2	1:A:815:PRO:HB3	2.54	0.43
1:A:895:MET:HA	1:A:898:ILE:HG22	1.99	0.43
1:A:1696:GLY:HA3	1:A:1816:PHE:CD2	2.53	0.43
1:A:2303:ARG:HG2	1:A:2401:ARG:HD2	2.00	0.43
2:G:50:ARG:NH1	2:G:53:LYS:HG3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ALA:HA	1:B:187:SER:HB3	2.00	0.43
1:B:869:THR:O	1:B:872:ILE:HG12	2.18	0.43
1:B:1100:ARG:HB3	1:B:1236:TYR:CD1	2.53	0.43
1:B:2115:ASP:HB2	1:B:2152:ASN:OD1	2.18	0.43
1:B:2277:CYS:HB3	1:B:2280:LEU:HB2	2.00	0.43
1:B:4206:ILE:HA	1:B:4493:ASN:ND2	2.34	0.43
1:C:253:GLY:HA3	1:C:256:GLN:NE2	2.33	0.43
1:C:2115:ASP:HB2	1:C:2152:ASN:OD1	2.18	0.43
1:C:4248:LEU:HG	1:C:4297:PHE:CE1	2.53	0.43
1:C:4271:VAL:HG23	1:C:4275:THR:HB	2.01	0.43
1:D:2277:CYS:HB3	1:D:2280:LEU:HB2	2.00	0.43
1:D:2590:ARG:O	1:D:2593:VAL:HG22	2.18	0.43
1:D:2596:VAL:HG22	1:D:2606:PRO:HB2	2.00	0.43
1:D:3140:LEU:HD12	1:D:3155:LEU:HD11	2.00	0.43
1:D:3321:PRO:HA	1:D:3324:GLU:HG3	1.99	0.43
1:D:3730:ARG:O	1:D:3734:ARG:NH1	2.50	0.43
1:D:4271:VAL:HG23	1:D:4275:THR:HB	2.01	0.43
1:D:4782:THR:HG22	1:D:4816:HIS:ND1	2.34	0.43
1:A:1973:ILE:HG13	1:A:3619:LEU:HB3	2.00	0.43
1:A:2185:LYS:HD2	1:A:2186:GLU:O	2.18	0.43
1:A:3121:LEU:HD23	1:A:3126:VAL:HG11	2.01	0.43
1:B:202:HIS:CD2	1:B:203:VAL:N	2.85	0.43
1:B:1549:SER:OG	1:B:1551:ASN:O	2.33	0.43
1:B:2185:LYS:HD2	1:B:2186:GLU:O	2.18	0.43
1:B:3237:VAL:C	1:B:3240:PRO:HD2	2.38	0.43
1:B:3305:PRO:O	1:B:3309:LYS:HG2	2.19	0.43
1:B:4021:LEU:HD23	1:B:4088:HIS:CD2	2.53	0.43
1:C:1100:ARG:HB3	1:C:1236:TYR:CD1	2.53	0.43
1:C:2596:VAL:HG22	1:C:2606:PRO:HB2	2.00	0.43
1:C:3124:GLU:CG	1:C:3125:ASP:H	2.31	0.43
1:C:3169:ALA:HB1	1:C:3245:TYR:OH	2.19	0.43
1:C:3305:PRO:O	1:C:3309:LYS:HG2	2.19	0.43
1:C:4026:LEU:HD12	1:C:4055:HIS:CG	2.53	0.43
1:D:251:GLU:HG3	1:D:256:GLN:HG3	2.01	0.43
1:D:4194:GLU:HG2	1:D:4645:TRP:HZ3	1.83	0.43
1:A:1045:SER:HA	1:A:1048:ASP:OD2	2.19	0.43
1:A:1131:ASP:N	1:A:1131:ASP:OD1	2.50	0.43
1:B:3637:GLU:HG2	1:B:3694:ILE:HA	2.01	0.43
1:C:538:ALA:O	1:C:542:ARG:HB2	2.19	0.43
1:C:1696:GLY:HA3	1:C:1816:PHE:CD2	2.53	0.43
1:D:224:ALA:HB3	1:D:227:TYR:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:HIS:NE2	1:D:396:GLU:HG3	2.33	0.43
1:D:1282:CYS:SG	1:D:1556:GLU:HG2	2.59	0.43
1:D:3246:MET:HA	1:D:3268:LEU:HD13	2.00	0.43
1:D:4943:MET:HE2	1:D:4951:PHE:H	1.84	0.43
1:A:394:HIS:NE2	1:A:396:GLU:HG3	2.33	0.43
1:A:538:ALA:O	1:A:542:ARG:HB2	2.19	0.43
1:A:807:ARG:O	1:A:1613:GLU:HA	2.18	0.43
1:B:224:ALA:HB3	1:B:227:TYR:HD2	1.84	0.43
1:B:1045:SER:HA	1:B:1048:ASP:OD2	2.19	0.43
1:B:1165:MET:HB3	1:B:1236:TYR:CE1	2.54	0.43
1:B:3137:LEU:HD13	1:B:3159:LEU:HA	2.00	0.43
1:B:3169:ALA:HB1	1:B:3245:TYR:OH	2.18	0.43
1:B:3251:GLU:O	1:B:3257:ASN:ND2	2.48	0.43
1:C:271:ALA:O	1:C:301:THR:OG1	2.36	0.43
1:C:1031:ARG:HG3	1:C:1038:LEU:HD11	2.00	0.43
1:C:1282:CYS:SG	1:C:1556:GLU:HG2	2.59	0.43
1:C:3237:VAL:C	1:C:3240:PRO:HD2	2.38	0.43
1:C:4194:GLU:HG2	1:C:4645:TRP:HZ3	1.83	0.43
1:D:271:ALA:O	1:D:301:THR:OG1	2.36	0.43
1:D:869:THR:O	1:D:872:ILE:HG12	2.18	0.43
1:A:705:PRO:HG3	1:A:857:LEU:HB2	1.99	0.43
1:A:1282:CYS:SG	1:A:1556:GLU:HG2	2.59	0.43
1:A:1501:ASN:HB3	1:D:2826:ILE:HD13	2.01	0.43
1:A:3803:LEU:HD23	1:A:3830:LEU:HB2	2.00	0.43
1:B:1432:ILE:HG12	1:B:1441:VAL:HG11	2.01	0.43
1:B:1943:ARG:NH2	1:B:1964:GLU:OE2	2.48	0.43
1:B:2849:HIS:CE1	1:B:2877:LEU:HD11	2.54	0.43
1:B:4271:VAL:HG23	1:B:4275:THR:HB	2.01	0.43
1:B:4867:ILE:HG12	1:C:4864:GLY:HA2	2.01	0.43
1:B:4943:MET:HE1	1:B:4950:GLU:HB3	2.01	0.43
1:C:224:ALA:HB3	1:C:227:TYR:HD2	1.84	0.43
1:C:2791:ARG:HE	1:C:2796:ASP:HB3	1.84	0.43
1:C:3140:LEU:HD12	1:C:3155:LEU:HD11	2.00	0.43
1:D:672:LYS:HB3	1:D:819:TYR:CD2	2.54	0.43
1:D:1045:SER:HA	1:D:1048:ASP:OD2	2.19	0.43
1:D:1442:TRP:HB2	1:D:1544:PHE:HB2	2.01	0.43
1:D:2849:HIS:CE1	1:D:2877:LEU:HD11	2.54	0.43
1:A:290:ARG:HH11	1:A:343:ARG:HH11	1.67	0.42
1:A:4782:THR:HG22	1:A:4816:HIS:ND1	2.34	0.42
1:A:4831:ILE:HD12	1:A:4843:ARG:HH12	1.84	0.42
1:B:1973:ILE:HG13	1:B:3619:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3121:LEU:HD23	1:B:3126:VAL:HG11	2.01	0.42
1:B:3125:ASP:HA	1:B:3128:VAL:HG12	2.01	0.42
1:B:4248:LEU:HG	1:B:4297:PHE:CE1	2.53	0.42
1:C:1649:GLU:HG2	1:C:1650:LEU:N	2.34	0.42
1:C:1732:GLU:HB3	1:C:1753:LEU:HD21	1.99	0.42
1:C:3324:GLU:OE2	1:C:3325:LYS:HE3	2.19	0.42
1:C:4206:ILE:HA	1:C:4493:ASN:ND2	2.34	0.42
1:D:705:PRO:HG3	1:D:857:LEU:HB2	1.99	0.42
1:D:1415:ASP:OD1	1:D:1415:ASP:N	2.50	0.42
1:A:224:ALA:HB3	1:A:227:TYR:HD2	1.84	0.42
1:A:1432:ILE:HG12	1:A:1441:VAL:HG11	2.01	0.42
1:A:2172:MET:O	1:A:2176:VAL:HG13	2.18	0.42
1:A:2596:VAL:HG22	1:A:2606:PRO:HB2	1.99	0.42
1:A:3730:ARG:O	1:A:3734:ARG:NH1	2.50	0.42
1:A:4083:PHE:O	1:A:4086:ARG:HG2	2.19	0.42
1:A:4267:GLN:O	1:A:4271:VAL:HG12	2.19	0.42
1:A:4610:LEU:HD11	1:A:4635:ILE:HG22	2.00	0.42
1:A:4943:MET:HE3	1:A:4950:GLU:HB3	2.01	0.42
1:B:1282:CYS:SG	1:B:1556:GLU:HG2	2.59	0.42
1:B:2251:ASN:O	1:B:2255:LEU:HG	2.19	0.42
1:C:290:ARG:HH11	1:C:343:ARG:HH11	1.67	0.42
1:C:672:LYS:HB3	1:C:819:TYR:CD2	2.54	0.42
1:C:966:LEU:HD23	1:C:967:PRO:O	2.20	0.42
1:C:1165:MET:HB3	1:C:1236:TYR:CE1	2.54	0.42
1:C:3730:ARG:O	1:C:3734:ARG:NH1	2.50	0.42
1:D:2303:ARG:HG2	1:D:2401:ARG:HD2	2.01	0.42
1:D:3068:LEU:O	1:D:3071:THR:OG1	2.28	0.42
1:D:3803:LEU:HD23	1:D:3830:LEU:HB2	2.01	0.42
1:D:4943:MET:HE1	1:D:4950:GLU:HB3	2.01	0.42
1:A:931:TYR:HA	1:A:934:GLN:HG3	2.00	0.42
1:A:2760:TYR:HA	1:A:2763:LEU:HD23	2.00	0.42
1:A:2914:THR:O	1:A:2915:PRO:C	2.58	0.42
2:F:50:ARG:NH1	2:F:53:LYS:HG3	2.33	0.42
1:B:931:TYR:HA	1:B:934:GLN:HG3	2.00	0.42
1:B:1748:LEU:O	1:B:1751:ILE:HG12	2.19	0.42
1:B:4782:THR:HG22	1:B:4816:HIS:ND1	2.34	0.42
1:C:674:TYR:CE1	1:C:756:SER:HB2	2.54	0.42
1:C:983:LEU:HD23	1:C:983:LEU:H	1.84	0.42
1:C:1038:LEU:HD23	1:C:1043:LYS:HB3	2.02	0.42
1:C:3315:LEU:HD13	1:C:3319:PHE:CD2	2.55	0.42
1:C:4743:LEU:O	1:C:4746:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4930:GLU:OE1	1:C:4941:TRP:NE1	2.52	0.42
1:D:966:LEU:HD23	1:D:967:PRO:O	2.20	0.42
1:D:983:LEU:HD23	1:D:983:LEU:H	1.84	0.42
1:D:1973:ILE:HG13	1:D:3619:LEU:HB3	2.00	0.42
1:D:2140:LYS:HG2	1:D:2144:ARG:HH21	1.84	0.42
1:D:2791:ARG:HE	1:D:2796:ASP:HB3	1.84	0.42
1:D:3305:PRO:O	1:D:3309:LYS:HG2	2.19	0.42
1:A:966:LEU:HD23	1:A:967:PRO:O	2.20	0.42
1:A:1748:LEU:O	1:A:1751:ILE:HG12	2.19	0.42
1:A:1894:LEU:HD23	1:A:1894:LEU:HA	1.88	0.42
1:A:2427:ILE:O	1:A:2476:TYR:OH	2.29	0.42
1:A:3305:PRO:O	1:A:3309:LYS:HG2	2.19	0.42
1:A:3315:LEU:HD13	1:A:3319:PHE:CD2	2.55	0.42
1:A:3637:GLU:HG2	1:A:3694:ILE:HA	2.01	0.42
1:A:4007:SER:HA	1:A:4118:PHE:HZ	1.84	0.42
1:A:4930:GLU:OE1	1:A:4941:TRP:NE1	2.52	0.42
1:B:3324:GLU:OE2	1:B:3325:LYS:HE3	2.19	0.42
1:B:4194:GLU:HG2	1:B:4645:TRP:HZ3	1.83	0.42
1:B:4743:LEU:O	1:B:4746:ILE:HG12	2.19	0.42
1:C:2585:MET:O	1:C:2589:LEU:HG	2.20	0.42
1:C:4782:THR:HG22	1:C:4816:HIS:ND1	2.34	0.42
1:D:1957:LEU:HG	1:D:1960:ARG:NH1	2.27	0.42
1:D:2424:ARG:HE	1:D:2424:ARG:HB2	1.54	0.42
1:D:4083:PHE:O	1:D:4086:ARG:HG2	2.19	0.42
1:A:2440:PHE:CZ	1:A:2465:LYS:HD3	2.55	0.42
1:A:4271:VAL:HG23	1:A:4275:THR:HB	2.01	0.42
1:B:208:GLN:OE1	1:B:208:GLN:N	2.53	0.42
1:B:251:GLU:HG3	1:B:256:GLN:HG3	2.01	0.42
1:B:538:ALA:O	1:B:542:ARG:HB2	2.19	0.42
1:B:1306:MET:HB2	1:B:1570:LEU:HD22	2.02	0.42
1:B:1522:ALA:HB2	1:B:1527:LEU:HD21	2.02	0.42
1:C:674:TYR:CD2	1:C:815:PRO:HB3	2.54	0.42
1:C:896:ASN:HD21	1:C:1049:SER:CB	2.33	0.42
1:C:3121:LEU:HD23	1:C:3126:VAL:HG11	2.01	0.42
1:D:1031:ARG:HG3	1:D:1038:LEU:HD11	2.00	0.42
1:D:4267:GLN:O	1:D:4271:VAL:HG12	2.19	0.42
1:A:1165:MET:HB3	1:A:1236:TYR:CE1	2.54	0.42
1:A:1442:TRP:HB2	1:A:1544:PHE:HB2	2.01	0.42
1:A:1649:GLU:HG2	1:A:1650:LEU:N	2.34	0.42
1:A:2666:LEU:HD21	1:A:2969:PRO:HB2	2.02	0.42
1:A:3319:PHE:CD1	1:A:3319:PHE:N	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:LEU:HD23	1:B:967:PRO:O	2.20	0.42
1:B:1911:GLN:OE1	1:B:2090:ARG:NH1	2.37	0.42
1:B:3650:GLU:HB2	1:B:3651:PRO:HD3	2.00	0.42
1:C:966:LEU:HA	1:C:967:PRO:HD3	1.93	0.42
1:C:2178:VAL:HG21	1:C:2192:MET:HE2	2.02	0.42
1:C:2641:SER:HB2	1:C:2676:LEU:HD21	2.01	0.42
1:C:3312:PRO:O	1:C:3315:LEU:HB2	2.18	0.42
1:C:4921:PHE:HE2	1:C:4940:VAL:HG11	1.83	0.42
1:D:338:LEU:HD12	1:D:338:LEU:HA	1.91	0.42
1:D:674:TYR:CE1	1:D:756:SER:HB2	2.54	0.42
1:D:807:ARG:O	1:D:1613:GLU:HA	2.18	0.42
1:D:1748:LEU:O	1:D:1751:ILE:HG12	2.19	0.42
1:D:2251:ASN:O	1:D:2255:LEU:HG	2.19	0.42
1:D:3315:LEU:HD13	1:D:3319:PHE:CD2	2.55	0.42
1:D:4206:ILE:HA	1:D:4493:ASN:ND2	2.34	0.42
1:D:4743:LEU:O	1:D:4746:ILE:HG12	2.19	0.42
1:A:896:ASN:HD21	1:A:1049:SER:CB	2.33	0.42
1:A:2791:ARG:HE	1:A:2796:ASP:HB3	1.84	0.42
1:A:3125:ASP:HA	1:A:3128:VAL:HG12	2.01	0.42
1:A:3246:MET:HA	1:A:3268:LEU:HD13	2.01	0.42
1:A:4135:ARG:HG2	1:A:4149:TYR:CD1	2.55	0.42
1:B:1649:GLU:HG2	1:B:1650:LEU:N	2.34	0.42
1:B:2585:MET:O	1:B:2589:LEU:HG	2.20	0.42
1:B:2914:THR:O	1:B:2915:PRO:C	2.58	0.42
1:B:3068:LEU:O	1:B:3071:THR:OG1	2.28	0.42
1:B:3315:LEU:HD13	1:B:3319:PHE:CD2	2.55	0.42
1:B:4267:GLN:O	1:B:4271:VAL:HG12	2.19	0.42
1:B:4930:GLU:OE1	1:B:4941:TRP:NE1	2.52	0.42
1:C:208:GLN:OE1	1:C:208:GLN:N	2.53	0.42
1:C:4083:PHE:O	1:C:4086:ARG:HG2	2.19	0.42
1:D:1943:ARG:NH2	1:D:1964:GLU:OE2	2.48	0.42
1:D:2585:MET:O	1:D:2589:LEU:HG	2.20	0.42
1:D:4735:ASN:HB3	1:D:4738:PHE:CD2	2.55	0.42
1:A:638:PRO:HD3	2:E:90:GLY:HA2	2.01	0.42
1:A:1306:MET:HB2	1:A:1570:LEU:HD22	2.02	0.42
1:A:2849:HIS:CE1	1:A:2877:LEU:HD11	2.54	0.42
1:A:3324:GLU:OE2	1:A:3325:LYS:HE3	2.19	0.42
4:A:5003:ATP:H5'1	5:A:5004:KVR:C20	2.49	0.42
1:B:249:SER:N	1:B:272:ARG:HH21	2.15	0.42
1:B:896:ASN:HD21	1:B:1049:SER:CB	2.33	0.42
1:B:1458:ASP:OD1	1:B:1461:ARG:NE	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2136:LYS:HD3	1:B:2136:LYS:HA	1.77	0.42
1:B:2440:PHE:CZ	1:B:2465:LYS:HD3	2.55	0.42
1:B:4943:MET:HE2	1:B:4951:PHE:H	1.84	0.42
1:C:157:ALA:HA	1:C:187:SER:HB3	2.00	0.42
1:C:411:GLU:OE2	1:C:485:ARG:NE	2.35	0.42
1:C:546:LYS:O	1:C:550:GLN:HG2	2.20	0.42
1:C:1432:ILE:HG12	1:C:1441:VAL:HG11	2.01	0.42
1:C:2640:LEU:HA	1:C:2643:LYS:HZ3	1.85	0.42
1:D:414:ARG:O	1:D:418:VAL:HG23	2.20	0.42
1:D:941:LYS:HA	1:D:944:LEU:HG	2.01	0.42
1:D:1649:GLU:HG2	1:D:1650:LEU:N	2.35	0.42
1:D:1711:LEU:HB3	1:D:1831:MET:SD	2.60	0.42
1:D:4930:GLU:OE1	1:D:4941:TRP:NE1	2.52	0.42
1:A:414:ARG:O	1:A:418:VAL:HG23	2.20	0.42
1:A:546:LYS:O	1:A:550:GLN:HG2	2.20	0.42
1:A:672:LYS:HB3	1:A:819:TYR:CD2	2.54	0.42
1:A:816:PRO:HB2	1:A:819:TYR:CD1	2.55	0.42
1:A:1414:ARG:NE	1:A:1415:ASP:OD1	2.50	0.42
1:A:1788:LYS:NZ	1:A:1833:ILE:O	2.48	0.42
1:A:2641:SER:HB2	1:A:2676:LEU:HD21	2.01	0.42
1:A:4073:ASP:OD1	1:A:4074:GLU:N	2.53	0.42
1:A:4194:GLU:HG2	1:A:4645:TRP:HZ3	1.83	0.42
1:B:290:ARG:HH11	1:B:343:ARG:HH11	1.67	0.42
1:B:672:LYS:HB3	1:B:819:TYR:CD2	2.54	0.42
1:B:674:TYR:CD2	1:B:815:PRO:HB3	2.54	0.42
1:B:674:TYR:CE1	1:B:756:SER:HB2	2.54	0.42
1:B:983:LEU:HD23	1:B:983:LEU:H	1.84	0.42
1:B:1442:TRP:HB2	1:B:1544:PHE:HB2	2.01	0.42
1:B:1711:LEU:HB3	1:B:1831:MET:SD	2.60	0.42
1:B:1988:CYS:O	1:B:1993:ARG:NE	2.44	0.42
1:B:2140:LYS:HG2	1:B:2144:ARG:HH21	1.84	0.42
1:B:4735:ASN:HB3	1:B:4738:PHE:CD2	2.55	0.42
1:C:941:LYS:HA	1:C:944:LEU:HG	2.01	0.42
1:C:1152:TYR:HD1	1:C:1184:ASP:HB3	1.84	0.42
1:C:2140:LYS:HG2	1:C:2144:ARG:HH21	1.84	0.42
1:C:2222:LEU:HD23	1:C:2222:LEU:HA	1.89	0.42
1:C:2303:ARG:HG2	1:C:2401:ARG:HD2	2.00	0.42
1:C:2440:PHE:CZ	1:C:2465:LYS:HD3	2.55	0.42
1:C:2914:THR:O	1:C:2915:PRO:C	2.58	0.42
1:D:332:ARG:HH22	1:D:339:ASP:H	1.68	0.42
1:D:1420:LEU:HG	1:D:1564:MET:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1427:TYR:HB2	1:D:1563:VAL:HG11	2.01	0.42
1:D:2532:ALA:HA	1:D:2535:PHE:HD2	1.84	0.42
1:D:3324:GLU:OE2	1:D:3325:LYS:HE3	2.19	0.42
1:A:332:ARG:HH22	1:A:339:ASP:H	1.68	0.42
1:A:674:TYR:CE1	1:A:756:SER:HB2	2.54	0.42
1:A:2178:VAL:HG21	1:A:2192:MET:HE2	2.02	0.42
1:A:4735:ASN:HB3	1:A:4738:PHE:CD2	2.55	0.42
1:B:546:LYS:O	1:B:550:GLN:HG2	2.20	0.42
1:B:2666:LEU:HD21	1:B:2969:PRO:HB2	2.02	0.42
1:C:1458:ASP:OD1	1:C:1461:ARG:NE	2.45	0.42
1:C:1522:ALA:HB2	1:C:1527:LEU:HD21	2.02	0.42
1:C:1711:LEU:HB3	1:C:1831:MET:SD	2.60	0.42
1:C:2251:ASN:O	1:C:2255:LEU:HG	2.19	0.42
1:C:2596:VAL:HG21	1:C:2610:LEU:HD11	2.02	0.42
1:C:2849:HIS:CE1	1:C:2877:LEU:HD11	2.54	0.42
1:C:3138:TYR:CG	1:C:3208:ILE:HG12	2.55	0.42
1:C:4040:LYS:HG3	1:C:4042:VAL:HG13	2.02	0.42
1:C:4267:GLN:O	1:C:4271:VAL:HG12	2.19	0.42
1:C:4943:MET:HE1	1:C:4950:GLU:HB3	2.02	0.42
1:D:538:ALA:O	1:D:542:ARG:HB2	2.19	0.42
1:D:661:LEU:HD22	1:D:673:TRP:CE2	2.55	0.42
1:D:1165:MET:HB3	1:D:1236:TYR:CE1	2.54	0.42
1:D:1432:ILE:HG12	1:D:1441:VAL:HG11	2.01	0.42
1:D:2582:PRO:HG3	1:D:2617:CYS:SG	2.60	0.42
1:D:2666:LEU:HD21	1:D:2969:PRO:HB2	2.02	0.42
1:D:3121:LEU:HD23	1:D:3126:VAL:HG11	2.01	0.42
1:D:3251:GLU:HA	1:D:3256:ASN:HD22	1.85	0.42
1:D:3677:THR:HB	1:D:3679:LYS:HZ2	1.85	0.42
1:D:4073:ASP:OD1	1:D:4074:GLU:N	2.53	0.42
1:A:1268:ILE:HD11	1:A:1300:MET:HE2	2.02	0.41
1:A:2251:ASN:O	1:A:2255:LEU:HG	2.19	0.41
1:A:2532:ALA:HA	1:A:2535:PHE:HD2	1.84	0.41
1:B:816:PRO:HB2	1:B:819:TYR:CD1	2.55	0.41
1:B:1038:LEU:HD23	1:B:1043:LYS:HB3	2.02	0.41
1:B:1218:GLY:HA3	1:B:1238:PRO:HB3	2.02	0.41
1:B:2791:ARG:HE	1:B:2796:ASP:HB3	1.84	0.41
1:B:4007:SER:HA	1:B:4118:PHE:HZ	1.85	0.41
1:B:4073:ASP:OD1	1:B:4074:GLU:N	2.53	0.41
1:B:4083:PHE:O	1:B:4086:ARG:HG2	2.19	0.41
1:B:4135:ARG:HG2	1:B:4149:TYR:CD1	2.55	0.41
1:C:332:ARG:HH22	1:C:339:ASP:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1943:ARG:NH2	1:C:1964:GLU:OE2	2.48	0.41
1:C:3637:GLU:HG2	1:C:3694:ILE:HA	2.01	0.41
1:C:4735:ASN:HB3	1:C:4738:PHE:CD2	2.55	0.41
1:D:208:GLN:N	1:D:208:GLN:OE1	2.53	0.41
1:D:263:GLU:OE1	1:D:272:ARG:NH1	2.47	0.41
1:D:614:LEU:HA	1:D:617:LEU:HD12	2.02	0.41
1:D:896:ASN:HD21	1:D:1049:SER:CB	2.33	0.41
1:D:1805:HIS:ND1	1:D:1805:HIS:N	2.68	0.41
1:D:2914:THR:O	1:D:2915:PRO:C	2.58	0.41
1:D:4831:ILE:HD12	1:D:4843:ARG:HH12	1.84	0.41
1:A:544:ASN:HB3	1:A:547:ASN:HB2	2.03	0.41
1:A:1935:LYS:HE2	1:A:1935:LYS:HB3	1.90	0.41
1:A:2585:MET:O	1:A:2589:LEU:HG	2.20	0.41
1:B:2596:VAL:HG21	1:B:2610:LEU:HD11	2.02	0.41
1:C:251:GLU:HG3	1:C:256:GLN:HG3	2.01	0.41
1:C:816:PRO:HB2	1:C:819:TYR:CD1	2.55	0.41
1:C:1427:TYR:HB2	1:C:1563:VAL:HG11	2.01	0.41
1:C:2272:CYS:HB3	1:C:2291:ASN:HB3	2.02	0.41
1:C:3251:GLU:HA	1:C:3256:ASN:HD22	1.85	0.41
1:D:3138:TYR:CG	1:D:3208:ILE:HG12	2.55	0.41
1:D:4664:ASP:HA	1:D:4674:LYS:HD3	2.02	0.41
1:A:941:LYS:HA	1:A:944:LEU:HG	2.01	0.41
1:A:983:LEU:HD23	1:A:983:LEU:H	1.84	0.41
1:A:1522:ALA:HB2	1:A:1527:LEU:HD21	2.02	0.41
1:A:2541:HIS:O	1:A:2545:ILE:HG12	2.20	0.41
1:A:4743:LEU:O	1:A:4746:ILE:HG12	2.19	0.41
1:B:332:ARG:HH22	1:B:339:ASP:H	1.68	0.41
1:B:1152:TYR:HD1	1:B:1184:ASP:HB3	1.84	0.41
1:B:3787:VAL:HG11	1:B:3866:THR:HB	2.02	0.41
1:C:1748:LEU:O	1:C:1751:ILE:HG12	2.19	0.41
1:C:2135:GLY:H	1:C:2138:GLU:HB2	1.86	0.41
1:C:2582:PRO:HG3	1:C:2617:CYS:SG	2.60	0.41
1:C:3125:ASP:HA	1:C:3128:VAL:HG12	2.02	0.41
1:C:3277:LEU:HA	1:C:3280:ILE:HD12	2.02	0.41
1:C:4073:ASP:OD1	1:C:4074:GLU:N	2.53	0.41
1:C:4664:ASP:HA	1:C:4674:LYS:HD3	2.03	0.41
1:C:4751:LYS:O	1:C:4755:THR:HG23	2.21	0.41
1:D:2440:PHE:CZ	1:D:2465:LYS:HD3	2.55	0.41
1:D:2714:PRO:HD3	1:D:2783:LEU:HD11	2.03	0.41
1:D:2833:LEU:HD21	1:D:2894:LYS:HG3	2.03	0.41
1:A:614:LEU:HA	1:A:617:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1711:LEU:HB3	1:A:1831:MET:SD	2.60	0.41
1:A:4629:GLN:HB3	1:D:4245:LEU:HD21	2.02	0.41
1:B:2303:ARG:HG2	1:B:2401:ARG:HD2	2.00	0.41
1:B:2641:SER:HB2	1:B:2676:LEU:HD21	2.01	0.41
1:B:2833:LEU:HD21	1:B:2894:LYS:HG3	2.03	0.41
1:B:3293:GLY:H	1:B:3296:MET:HE1	1.85	0.41
1:B:4831:ILE:HD12	1:B:4843:ARG:HH12	1.84	0.41
1:C:315:LEU:HD12	1:C:315:LEU:HA	1.93	0.41
1:C:674:TYR:OH	1:C:676:GLU:OE2	2.26	0.41
1:C:1442:TRP:HB2	1:C:1544:PHE:HB2	2.01	0.41
1:C:2948:ARG:HD3	1:C:2948:ARG:H	1.86	0.41
1:C:4831:ILE:HD12	1:C:4843:ARG:HH12	1.84	0.41
1:D:1038:LEU:HD23	1:D:1043:LYS:HB3	2.02	0.41
1:D:2948:ARG:H	1:D:2948:ARG:HD3	1.86	0.41
1:D:3145:SER:O	1:D:3148:VAL:N	2.51	0.41
1:D:3637:GLU:HG2	1:D:3694:ILE:HA	2.01	0.41
1:D:3743:THR:HB	1:D:3758:THR:HG21	2.02	0.41
1:D:3784:LYS:HA	1:D:3784:LYS:HD3	1.79	0.41
1:D:4040:LYS:HG3	1:D:4042:VAL:HG13	2.02	0.41
1:D:4751:LYS:O	1:D:4755:THR:HG23	2.21	0.41
1:A:42:PHE:CZ	1:A:459:LEU:HG	2.55	0.41
1:A:251:GLU:HG3	1:A:256:GLN:HG3	2.01	0.41
1:A:1152:TYR:HD1	1:A:1184:ASP:HB3	1.85	0.41
1:A:1199:ASP:OD1	1:A:1199:ASP:N	2.50	0.41
1:A:2596:VAL:HG21	1:A:2610:LEU:HD11	2.02	0.41
1:B:1444:GLY:HA3	1:B:1487:MET:HG2	2.02	0.41
1:B:2741:TRP:O	1:B:2757:MET:HE3	2.21	0.41
1:B:3896:ASP:OD1	1:B:3897:VAL:N	2.54	0.41
1:C:661:LEU:HD22	1:C:673:TRP:CE2	2.55	0.41
1:C:2532:ALA:HA	1:C:2535:PHE:HD2	1.84	0.41
1:C:4135:ARG:HG2	1:C:4149:TYR:CD1	2.55	0.41
1:D:925:PRO:HB2	1:D:928:GLU:CB	2.51	0.41
1:D:1306:MET:HB2	1:D:1570:LEU:HD22	2.02	0.41
1:D:1935:LYS:HB3	1:D:1935:LYS:HE2	1.90	0.41
1:D:2641:SER:HB2	1:D:2676:LEU:HD21	2.01	0.41
1:A:661:LEU:HD22	1:A:673:TRP:CE2	2.55	0.41
1:A:1444:GLY:HA3	1:A:1487:MET:HG2	2.02	0.41
1:A:3124:GLU:HG2	1:A:3125:ASP:N	2.36	0.41
1:A:3743:THR:HB	1:A:3758:THR:HG21	2.02	0.41
1:A:3763:ILE:HD11	1:A:3838:ASP:O	2.21	0.41
1:B:42:PHE:CZ	1:B:459:LEU:HG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1086:ARG:HG3	1:B:1252:SER:OG	2.21	0.41
1:B:2532:ALA:HA	1:B:2535:PHE:HD2	1.84	0.41
1:B:3124:GLU:HG2	1:B:3125:ASP:N	2.36	0.41
1:B:3138:TYR:CG	1:B:3208:ILE:HG12	2.55	0.41
1:B:4245:LEU:HD21	1:C:4629:GLN:HB3	2.01	0.41
1:C:2392:TYR:O	1:C:2396:ILE:HG12	2.21	0.41
1:C:3960:GLN:HA	1:C:4069:CYS:HA	2.03	0.41
1:D:499:LEU:HD22	1:D:557:TRP:CZ3	2.56	0.41
1:D:3125:ASP:HA	1:D:3128:VAL:HG12	2.02	0.41
1:A:1218:GLY:HA3	1:A:1238:PRO:HB3	2.03	0.41
1:A:2140:LYS:HG2	1:A:2144:ARG:HH21	1.84	0.41
1:A:2714:PRO:HD3	1:A:2783:LEU:HD11	2.03	0.41
1:A:2833:LEU:HD21	1:A:2894:LYS:HG3	2.03	0.41
1:A:4046:ARG:HH12	1:A:4076:GLU:HG2	1.86	0.41
1:A:4522:VAL:HG12	1:B:4807:ASP:O	2.20	0.41
1:B:941:LYS:HA	1:B:944:LEU:HG	2.01	0.41
1:B:2135:GLY:H	1:B:2138:GLU:HB2	1.86	0.41
1:B:2787:TRP:CD1	1:B:2905:ARG:HA	2.56	0.41
1:B:4664:ASP:HA	1:B:4674:LYS:HD3	2.03	0.41
1:B:4751:LYS:O	1:B:4755:THR:HG23	2.21	0.41
1:C:1045:SER:HA	1:C:1048:ASP:OD2	2.19	0.41
1:D:816:PRO:HB2	1:D:819:TYR:CD1	2.55	0.41
1:D:3054:LYS:O	1:D:3058:ARG:HG3	2.21	0.41
1:D:4135:ARG:HG2	1:D:4149:TYR:CD1	2.55	0.41
1:A:208:GLN:N	1:A:208:GLN:OE1	2.53	0.41
1:A:925:PRO:HB2	1:A:928:GLU:CB	2.51	0.41
1:A:3054:LYS:O	1:A:3058:ARG:HG3	2.21	0.41
1:B:414:ARG:O	1:B:418:VAL:HG23	2.20	0.41
1:B:661:LEU:HD22	1:B:673:TRP:CE2	2.55	0.41
1:B:4040:LYS:HG3	1:B:4042:VAL:HG13	2.02	0.41
1:C:1937:GLN:NE2	1:C:3608:LEU:O	2.54	0.41
1:C:2831:VAL:HG22	1:D:1435:GLY:HA2	2.03	0.41
1:C:3896:ASP:OD1	1:C:3897:VAL:N	2.54	0.41
1:D:22:LEU:HD23	1:D:22:LEU:HA	1.95	0.41
1:D:2596:VAL:HG21	1:D:2610:LEU:HD11	2.02	0.41
1:A:499:LEU:HD22	1:A:557:TRP:CZ3	2.56	0.41
1:A:677:LEU:HD12	1:A:801:ARG:O	2.21	0.41
1:A:839:GLU:HB3	1:A:851:LEU:HD12	2.03	0.41
1:A:1086:ARG:HG3	1:A:1252:SER:OG	2.21	0.41
1:A:1427:TYR:HB2	1:A:1563:VAL:HG11	2.01	0.41
1:A:1697:LEU:HD23	1:A:1697:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2280:LEU:HD11	1:A:2382:ILE:HG13	2.02	0.41
1:A:2434:GLY:O	1:A:2438:ILE:HG13	2.20	0.41
1:A:2582:PRO:HG3	1:A:2617:CYS:SG	2.60	0.41
1:A:3178:HIS:CD2	1:A:3263:MET:HA	2.56	0.41
1:A:3277:LEU:HA	1:A:3280:ILE:HD12	2.02	0.41
1:A:3787:VAL:HG11	1:A:3866:THR:HB	2.02	0.41
1:B:544:ASN:HB3	1:B:547:ASN:HB2	2.03	0.41
1:B:658:ASN:ND2	1:B:831:LYS:O	2.34	0.41
1:B:872:ILE:HD12	1:B:941:LYS:NZ	2.36	0.41
1:B:941:LYS:O	1:B:944:LEU:HG	2.21	0.41
1:B:1805:HIS:ND1	1:B:1805:HIS:N	2.68	0.41
1:B:2178:VAL:HG21	1:B:2192:MET:HE2	2.03	0.41
1:B:2290:TRP:HZ3	1:B:2391:PHE:CD1	2.39	0.41
1:B:2392:TYR:O	1:B:2396:ILE:HG12	2.21	0.41
1:B:2434:GLY:O	1:B:2438:ILE:HG13	2.20	0.41
1:B:2582:PRO:HG3	1:B:2617:CYS:SG	2.60	0.41
1:B:2640:LEU:HA	1:B:2643:LYS:HZ3	1.86	0.41
1:B:4046:ARG:HH12	1:B:4076:GLU:HG2	1.86	0.41
1:B:4721:TYR:OH	1:B:4745:ASP:OD1	2.32	0.41
1:C:414:ARG:O	1:C:418:VAL:HG23	2.20	0.41
1:C:484:ASN:O	1:C:488:LEU:HD23	2.21	0.41
1:C:499:LEU:HD22	1:C:557:TRP:CZ3	2.56	0.41
1:C:872:ILE:HD12	1:C:941:LYS:NZ	2.36	0.41
1:C:1086:ARG:HG3	1:C:1252:SER:OG	2.21	0.41
1:C:1218:GLY:HA3	1:C:1238:PRO:HB3	2.02	0.41
1:C:1306:MET:HB2	1:C:1570:LEU:HD22	2.02	0.41
1:C:1444:GLY:HA3	1:C:1487:MET:HG2	2.02	0.41
1:C:1788:LYS:NZ	1:C:1833:ILE:O	2.48	0.41
1:C:2666:LEU:HD21	1:C:2969:PRO:HB2	2.02	0.41
1:C:2833:LEU:HD21	1:C:2894:LYS:HG3	2.03	0.41
1:C:2913:ASP:C	1:C:2915:PRO:HD2	2.42	0.41
1:C:3787:VAL:HG11	1:C:3866:THR:HB	2.02	0.41
1:D:114:LEU:HD11	1:D:174:LYS:HG2	2.03	0.41
1:D:546:LYS:O	1:D:550:GLN:HG2	2.20	0.41
1:D:1444:GLY:HA3	1:D:1487:MET:HG2	2.02	0.41
1:D:1458:ASP:OD1	1:D:1461:ARG:NE	2.45	0.41
1:D:2272:CYS:HB3	1:D:2291:ASN:HB3	2.02	0.41
1:D:2280:LEU:HD11	1:D:2382:ILE:HG13	2.02	0.41
1:D:2541:HIS:O	1:D:2545:ILE:HG12	2.20	0.41
1:D:2913:ASP:C	1:D:2915:PRO:HD2	2.42	0.41
1:D:3036:LEU:O	1:D:3040:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3251:GLU:O	1:D:3257:ASN:ND2	2.48	0.41
1:D:3960:GLN:HA	1:D:4069:CYS:HA	2.03	0.41
1:D:4007:SER:HA	1:D:4118:PHE:HZ	1.85	0.41
1:D:4046:ARG:HH12	1:D:4076:GLU:HG2	1.86	0.41
1:A:762:SER:OG	1:A:763:ALA:N	2.54	0.41
1:A:1038:LEU:HD23	1:A:1043:LYS:HB3	2.02	0.41
1:A:1805:HIS:ND1	1:A:1805:HIS:N	2.68	0.41
1:A:2135:GLY:H	1:A:2138:GLU:HB2	1.86	0.41
1:A:2640:LEU:HA	1:A:2643:LYS:HZ3	1.86	0.41
1:A:4040:LYS:HG3	1:A:4042:VAL:HG13	2.02	0.41
1:A:4664:ASP:HA	1:A:4674:LYS:HD3	2.03	0.41
1:B:1121:GLY:O	1:B:1123:GLN:NE2	2.53	0.41
1:B:2272:CYS:HB3	1:B:2291:ASN:HB3	2.02	0.41
1:B:3763:ILE:HD11	1:B:3838:ASP:O	2.21	0.41
1:B:4522:VAL:HG12	1:C:4807:ASP:O	2.21	0.41
1:C:2714:PRO:HD3	1:C:2783:LEU:HD11	2.03	0.41
1:C:2998:ASN:O	1:C:3002:GLU:HG3	2.21	0.41
1:C:3124:GLU:HG2	1:C:3125:ASP:N	2.36	0.41
1:C:3192:ARG:N	1:C:3192:ARG:HD3	2.36	0.41
1:C:4113:THR:O	1:C:4117:THR:HG23	2.21	0.41
1:D:544:ASN:HB3	1:D:547:ASN:HB2	2.03	0.41
1:D:2392:TYR:O	1:D:2396:ILE:HG12	2.21	0.41
1:D:3787:VAL:HG11	1:D:3866:THR:HB	2.02	0.41
1:A:315:LEU:HD12	1:A:315:LEU:HA	1.93	0.40
1:A:1458:ASP:OD1	1:A:1461:ARG:NE	2.46	0.40
1:A:2272:CYS:HB3	1:A:2291:ASN:HB3	2.02	0.40
1:A:2290:TRP:HZ3	1:A:2391:PHE:CD1	2.39	0.40
1:A:3138:TYR:CG	1:A:3208:ILE:HG12	2.55	0.40
1:A:3192:ARG:HD3	1:A:3192:ARG:N	2.36	0.40
1:A:3896:ASP:OD1	1:A:3897:VAL:N	2.54	0.40
1:B:2280:LEU:HD11	1:B:2382:ILE:HG13	2.02	0.40
1:B:3178:HIS:CD2	1:B:3263:MET:HA	2.56	0.40
1:C:925:PRO:HB2	1:C:928:GLU:CB	2.51	0.40
1:C:2208:ARG:NH2	1:C:2252:GLU:OE1	2.55	0.40
1:C:2265:VAL:HG21	1:C:2301:PHE:CE2	2.56	0.40
1:C:2541:HIS:O	1:C:2545:ILE:HG12	2.20	0.40
1:C:3743:THR:HB	1:C:3758:THR:HG21	2.02	0.40
1:C:4007:SER:HA	1:C:4118:PHE:HZ	1.85	0.40
1:C:4625:ASP:OD1	1:C:4625:ASP:N	2.46	0.40
1:D:202:HIS:HD2	1:D:203:VAL:H	1.68	0.40
1:D:484:ASN:O	1:D:488:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1152:TYR:HD1	1:D:1184:ASP:HB3	1.84	0.40
1:D:1729:MET:HE1	1:D:3617:VAL:HG21	2.02	0.40
1:D:3124:GLU:HG2	1:D:3125:ASP:N	2.36	0.40
1:D:3821:THR:HG23	1:D:3821:THR:O	2.21	0.40
1:D:4964:ASP:OD1	1:D:4964:ASP:N	2.49	0.40
1:A:3171:LEU:HB3	1:A:3211:LEU:HB2	2.03	0.40
1:A:3211:LEU:O	1:A:3215:MET:HG2	2.21	0.40
1:A:4155:SER:O	1:A:4159:GLN:HG2	2.22	0.40
1:A:4751:LYS:O	1:A:4755:THR:HG23	2.21	0.40
1:B:22:LEU:HD23	1:B:22:LEU:HA	1.95	0.40
1:B:677:LEU:HD12	1:B:801:ARG:O	2.21	0.40
1:B:1310:CYS:HA	1:B:1513:ALA:HB1	2.03	0.40
1:B:1427:TYR:HB2	1:B:1563:VAL:HG11	2.01	0.40
1:B:2714:PRO:HD3	1:B:2783:LEU:HD11	2.03	0.40
1:B:2724:TYR:OH	1:B:2891:ASP:OD2	2.35	0.40
1:B:3036:LEU:O	1:B:3040:LEU:HG	2.21	0.40
1:B:3171:LEU:HB3	1:B:3211:LEU:HB2	2.03	0.40
1:B:3192:ARG:HD3	1:B:3192:ARG:H	1.87	0.40
1:B:3211:LEU:O	1:B:3215:MET:HG2	2.21	0.40
1:B:3277:LEU:HA	1:B:3280:ILE:HD12	2.02	0.40
1:B:3960:GLN:HA	1:B:4069:CYS:HA	2.03	0.40
1:B:4520:TYR:HE1	1:B:4561:LEU:HG	1.86	0.40
1:C:514:PHE:HD2	1:C:526:TRP:HB2	1.87	0.40
1:C:2290:TRP:HZ3	1:C:2391:PHE:CD1	2.39	0.40
1:C:2787:TRP:CD1	1:C:2905:ARG:HA	2.56	0.40
1:D:2055:SER:HB3	1:D:2060:GLN:HB2	2.03	0.40
1:D:2333:PRO:O	1:D:2336:ARG:HG2	2.21	0.40
1:D:2434:GLY:O	1:D:2438:ILE:HG13	2.20	0.40
1:D:3001:LYS:HD2	1:D:3041:ASP:HB3	2.03	0.40
1:A:114:LEU:HD11	1:A:174:LYS:HG2	2.03	0.40
1:A:2392:TYR:O	1:A:2396:ILE:HG12	2.21	0.40
1:A:2497:ARG:HG2	1:A:2551:THR:HG21	2.04	0.40
1:A:2948:ARG:H	1:A:2948:ARG:HD3	1.86	0.40
1:A:4864:GLY:HA2	1:D:4867:ILE:HG12	2.02	0.40
4:A:5003:ATP:O3G	4:A:5003:ATP:H3'	2.21	0.40
1:B:484:ASN:O	1:B:488:LEU:HD23	2.21	0.40
1:B:2333:PRO:O	1:B:2336:ARG:HG2	2.21	0.40
1:C:227:TYR:HA	1:C:354:ILE:O	2.21	0.40
1:C:614:LEU:HA	1:C:617:LEU:HD12	2.02	0.40
1:C:677:LEU:HD12	1:C:801:ARG:O	2.21	0.40
1:C:718:VAL:HG13	1:C:724:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2280:LEU:HD11	1:C:2382:ILE:HG13	2.02	0.40
1:C:2434:GLY:O	1:C:2438:ILE:HG13	2.20	0.40
1:C:3036:LEU:O	1:C:3040:LEU:HG	2.21	0.40
1:C:3171:LEU:HB3	1:C:3211:LEU:HB2	2.03	0.40
1:C:3192:ARG:HH11	1:C:3192:ARG:CG	2.34	0.40
1:C:4520:TYR:HE1	1:C:4561:LEU:HG	1.86	0.40
1:C:4795:LYS:HA	1:C:4795:LYS:HD2	1.91	0.40
1:C:4798:ASP:N	1:C:4798:ASP:OD1	2.55	0.40
1:D:718:VAL:HG13	1:D:724:SER:HB2	2.03	0.40
1:D:839:GLU:HB3	1:D:851:LEU:HD12	2.03	0.40
1:D:2208:ARG:NH2	1:D:2252:GLU:OE1	2.54	0.40
1:D:2998:ASN:O	1:D:3002:GLU:HG3	2.21	0.40
1:D:3763:ILE:HD11	1:D:3838:ASP:O	2.21	0.40
1:D:3966:GLU:HG2	1:D:3967:LEU:N	2.37	0.40
1:D:4484:ILE:H	1:D:4484:ILE:HD12	1.87	0.40
1:A:679:VAL:HG22	1:A:800:VAL:HG12	2.04	0.40
1:A:838:ARG:HA	1:A:838:ARG:HD3	1.87	0.40
1:A:2055:SER:HB3	1:A:2060:GLN:HB2	2.04	0.40
1:A:2265:VAL:HG21	1:A:2301:PHE:CE2	2.56	0.40
1:A:2333:PRO:O	1:A:2336:ARG:HG2	2.21	0.40
1:A:2787:TRP:CD1	1:A:2905:ARG:HA	2.56	0.40
1:A:4484:ILE:HD12	1:A:4484:ILE:H	1.87	0.40
1:B:114:LEU:HD11	1:B:174:LYS:HG2	2.03	0.40
1:B:614:LEU:HA	1:B:617:LEU:HD12	2.02	0.40
1:B:1729:MET:HE1	1:B:3617:VAL:HG21	2.02	0.40
1:B:2070:ALA:O	1:B:3666:GLN:NE2	2.55	0.40
1:B:2541:HIS:O	1:B:2545:ILE:HG12	2.20	0.40
1:B:3821:THR:O	1:B:3821:THR:HG23	2.21	0.40
1:B:4484:ILE:HD12	1:B:4484:ILE:H	1.86	0.40
1:C:3763:ILE:HD11	1:C:3838:ASP:O	2.20	0.40
1:D:815:PRO:HA	1:D:816:PRO:HD3	1.97	0.40
1:D:1522:ALA:HB2	1:D:1527:LEU:HD21	2.02	0.40
1:D:2290:TRP:HZ3	1:D:2391:PHE:CD1	2.39	0.40
1:D:2456:MET:HB3	1:D:2461:CYS:SG	2.62	0.40
1:D:3293:GLY:H	1:D:3296:MET:HE1	1.87	0.40
1:D:3896:ASP:OD1	1:D:3897:VAL:N	2.54	0.40
1:D:4155:SER:O	1:D:4159:GLN:HG2	2.22	0.40
1:A:137:ARG:HD3	1:A:202:HIS:CE1	2.56	0.40
1:A:484:ASN:O	1:A:488:LEU:HD23	2.21	0.40
1:A:2070:ALA:O	1:A:3666:GLN:NE2	2.55	0.40
1:A:2322:ARG:O	1:A:2326:ARG:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2413:LYS:HZ2	1:A:2416:ALA:N	2.20	0.40
1:A:3848:GLU:HA	1:A:3922:GLU:OE2	2.22	0.40
1:A:3966:GLU:HG2	1:A:3967:LEU:N	2.37	0.40
1:A:4798:ASP:OD1	1:A:4798:ASP:N	2.55	0.40
1:B:499:LEU:HD22	1:B:557:TRP:CZ3	2.56	0.40
1:B:762:SER:OG	1:B:763:ALA:N	2.54	0.40
1:B:1937:GLN:NE2	1:B:3608:LEU:O	2.54	0.40
1:B:2244:ALA:O	1:B:2248:MET:HB2	2.21	0.40
1:B:2265:VAL:HG21	1:B:2301:PHE:CE2	2.56	0.40
1:B:2913:ASP:C	1:B:2915:PRO:HD2	2.42	0.40
1:B:2948:ARG:HD3	1:B:2948:ARG:H	1.86	0.40
1:B:3743:THR:HB	1:B:3758:THR:HG21	2.02	0.40
1:B:3784:LYS:HA	1:B:3784:LYS:HD3	1.79	0.40
1:C:718:VAL:HG23	1:C:793:SER:HB3	2.04	0.40
1:C:762:SER:OG	1:C:763:ALA:N	2.54	0.40
1:C:1805:HIS:ND1	1:C:1805:HIS:N	2.68	0.40
1:C:2244:ALA:O	1:C:2248:MET:HB2	2.21	0.40
1:D:677:LEU:HD12	1:D:801:ARG:O	2.21	0.40
1:D:855:VAL:HG23	1:D:1078:CYS:HB2	2.04	0.40
1:D:2640:LEU:HA	1:D:2643:LYS:HZ3	1.86	0.40
1:D:2787:TRP:CD1	1:D:2905:ARG:HA	2.56	0.40
1:D:3211:LEU:O	1:D:3215:MET:HG2	2.21	0.40
1:D:4113:THR:O	1:D:4117:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	4198/4967 (84%)	4053 (96%)	140 (3%)	5 (0%)	51 85
1	B	4198/4967 (84%)	4053 (96%)	140 (3%)	5 (0%)	51 85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	4198/4967 (84%)	4053 (96%)	140 (3%)	5 (0%)	51 85
1	D	4198/4967 (84%)	4053 (96%)	140 (3%)	5 (0%)	51 85
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100 100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100 100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100 100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100 100
All	All	17212/20300 (85%)	16620 (97%)	572 (3%)	20 (0%)	54 85

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1495	SER
1	A	2915	PRO
1	A	4884	MET
1	B	1495	SER
1	B	2915	PRO
1	B	4884	MET
1	C	1495	SER
1	C	2915	PRO
1	C	4884	MET
1	D	1495	SER
1	D	2915	PRO
1	D	4884	MET
1	A	324	VAL
1	B	324	VAL
1	C	324	VAL
1	D	324	VAL
1	A	313	ASN
1	B	313	ASN
1	C	313	ASN
1	D	313	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3708/4358 (85%)	3689 (100%)	19 (0%)	88 96
1	B	3708/4358 (85%)	3689 (100%)	19 (0%)	88 96
1	C	3708/4358 (85%)	3689 (100%)	19 (0%)	88 96
1	D	3708/4358 (85%)	3689 (100%)	19 (0%)	88 96
2	E	88/89 (99%)	86 (98%)	2 (2%)	50 80
2	F	88/89 (99%)	86 (98%)	2 (2%)	50 80
2	G	88/89 (99%)	86 (98%)	2 (2%)	50 80
2	H	88/89 (99%)	86 (98%)	2 (2%)	50 80
All	All	15184/17788 (85%)	15100 (99%)	84 (1%)	86 95

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1013	ARG
1	A	1805	HIS
1	A	1939	ASN
1	A	1960	ARG
1	A	2185	LYS
1	A	2788	ARG
1	A	2884	LYS
1	A	2948	ARG
1	A	3018	ARG
1	A	3187	LYS
1	A	3192	ARG
1	A	3220	GLU
1	A	3248	ARG
1	A	3260	ARG
1	A	3298	ARG
1	A	3319	PHE
1	A	3327	LYS
1	A	3904	ARG
1	A	4966	LEU
2	E	19	LYS
2	E	54	GLN
2	F	19	LYS
2	F	54	GLN
2	G	19	LYS
2	G	54	GLN
2	H	19	LYS
2	H	54	GLN

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Mol	Chain	Res	Type
1	B	1013	ARG
1	B	1805	HIS
1	B	1939	ASN
1	B	1960	ARG
1	B	2185	LYS
1	B	2788	ARG
1	B	2884	LYS
1	B	2948	ARG
1	B	3018	ARG
1	B	3187	LYS
1	B	3192	ARG
1	B	3220	GLU
1	B	3248	ARG
1	B	3260	ARG
1	B	3298	ARG
1	B	3319	PHE
1	B	3327	LYS
1	B	3904	ARG
1	B	4966	LEU
1	C	1013	ARG
1	C	1805	HIS
1	C	1939	ASN
1	C	1960	ARG
1	C	2185	LYS
1	C	2788	ARG
1	C	2884	LYS
1	C	2948	ARG
1	C	3018	ARG
1	C	3187	LYS
1	C	3192	ARG
1	C	3220	GLU
1	C	3248	ARG
1	C	3260	ARG
1	C	3298	ARG
1	C	3319	PHE
1	C	3327	LYS
1	C	3904	ARG
1	C	4966	LEU
1	D	1013	ARG
1	D	1805	HIS
1	D	1939	ASN
1	D	1960	ARG

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Mol	Chain	Res	Type
1	D	2185	LYS
1	D	2788	ARG
1	D	2884	LYS
1	D	2948	ARG
1	D	3018	ARG
1	D	3187	LYS
1	D	3192	ARG
1	D	3220	GLU
1	D	3248	ARG
1	D	3260	ARG
1	D	3298	ARG
1	D	3319	PHE
1	D	3327	LYS
1	D	3904	ARG
1	D	4966	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	HIS
1	A	313	ASN
1	A	3256	ASN
1	B	202	HIS
1	B	313	ASN
1	B	1939	ASN
1	B	3256	ASN
1	C	150	GLN
1	C	202	HIS
1	C	313	ASN
1	D	202	HIS
1	D	313	ASN
1	D	3274	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	D	5003	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
5	KVR	D	5004	1	24,25,25	1.62	3 (12%)	32,34,34	2.08	5 (15%)
4	ATP	B	5003	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
4	ATP	A	5003	-	26,33,33	0.89	1 (3%)	31,52,52	1.54	6 (19%)
5	KVR	A	5004	1	24,25,25	0.50	0	32,34,34	0.97	2 (6%)
4	ATP	C	5002	-	26,33,33	0.60	0	31,52,52	0.82	2 (6%)
4	ATP	C	5003	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
4	ATP	D	5002	-	26,33,33	0.60	0	31,52,52	0.81	2 (6%)
5	KVR	C	5004	1	24,25,25	1.60	3 (12%)	32,34,34	2.08	5 (15%)
4	ATP	B	5002	-	26,33,33	0.59	0	31,52,52	0.81	2 (6%)
5	KVR	B	5004	1	24,25,25	1.60	3 (12%)	32,34,34	2.08	5 (15%)
4	ATP	A	5002	-	26,33,33	0.60	0	31,52,52	0.82	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	D	5003	-	-	6/18/38/38	0/3/3/3
5	KVR	D	5004	1	-	6/10/20/20	0/2/3/3
4	ATP	B	5003	-	-	6/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	KVR	A	5004	1	-	8/10/20/20	0/2/3/3
4	ATP	C	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	C	5003	-	-	6/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	9/18/38/38	0/3/3/3
5	KVR	C	5004	1	-	6/10/20/20	0/2/3/3
4	ATP	B	5002	-	-	8/18/38/38	0/3/3/3
5	KVR	B	5004	1	-	6/10/20/20	0/2/3/3
4	ATP	A	5002	-	-	8/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5004	KVR	C06-S09	6.06	1.83	1.77
5	D	5004	KVR	C06-S09	6.06	1.83	1.77
5	C	5004	KVR	C06-S09	6.03	1.83	1.77
5	D	5004	KVR	C13-N12	-2.64	1.45	1.47
5	B	5004	KVR	C13-N12	-2.53	1.45	1.47
5	C	5004	KVR	C13-N12	-2.53	1.45	1.47
5	D	5004	KVR	C13-C05	2.37	1.55	1.51
5	B	5004	KVR	C13-C05	2.30	1.54	1.51
5	C	5004	KVR	C13-C05	2.30	1.54	1.51
4	A	5003	ATP	C5-C4	2.26	1.46	1.40

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	5004	KVR	C10-S09-C06	8.54	114.81	102.71
5	B	5004	KVR	C10-S09-C06	8.52	114.78	102.71
5	D	5004	KVR	C10-S09-C06	8.51	114.77	102.71
5	C	5004	KVR	C14-N12-C11	4.48	118.32	111.06
5	B	5004	KVR	C14-N12-C11	4.47	118.30	111.06
5	D	5004	KVR	C14-N12-C11	4.47	118.30	111.06
4	A	5003	ATP	PA-O3A-PB	-3.86	119.59	132.83
4	A	5003	ATP	N3-C2-N1	-3.23	123.63	128.68
4	A	5003	ATP	C3'-C2'-C1'	3.20	105.80	100.98
5	D	5004	KVR	C05-C13-N12	-3.19	106.64	114.05
5	B	5004	KVR	C05-C13-N12	-3.19	106.64	114.05
5	C	5004	KVR	C05-C13-N12	-3.19	106.64	114.05
5	A	5004	KVR	C11-C10-S09	-3.19	110.22	114.22
4	A	5003	ATP	PB-O3B-PG	-2.97	122.64	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	5004	KVR	C14-N12-C13	2.91	117.23	112.89
5	B	5004	KVR	C14-N12-C13	2.91	117.22	112.89
5	C	5004	KVR	C14-N12-C13	2.88	117.18	112.89
4	A	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	C	5002	ATP	C5-C6-N6	2.29	123.83	120.35
4	D	5003	ATP	C5-C6-N6	2.28	123.82	120.35
4	D	5002	ATP	C5-C6-N6	2.27	123.80	120.35
4	C	5003	ATP	C5-C6-N6	2.26	123.79	120.35
4	B	5002	ATP	C5-C6-N6	2.25	123.77	120.35
5	A	5004	KVR	C14-N12-C11	2.17	114.57	111.06
4	A	5003	ATP	C4-C5-N7	-2.11	107.20	109.40
5	D	5004	KVR	O23-C21-C18	2.06	120.19	114.85
4	B	5003	ATP	PB-O3B-PG	2.06	139.89	132.83
4	C	5002	ATP	PB-O3B-PG	2.06	139.88	132.83
4	A	5002	ATP	PB-O3B-PG	2.05	139.88	132.83
5	B	5004	KVR	O23-C21-C18	2.05	120.17	114.85
4	B	5002	ATP	PB-O3B-PG	2.05	139.86	132.83
4	D	5002	ATP	PB-O3B-PG	2.05	139.85	132.83
4	D	5003	ATP	PB-O3B-PG	2.04	139.82	132.83
4	C	5003	ATP	PB-O3B-PG	2.04	139.82	132.83
5	C	5004	KVR	O23-C21-C18	2.03	120.12	114.85
4	A	5003	ATP	O3G-PG-O2G	2.02	115.37	107.64

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O3A
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	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	C3'-C4'-C5'-O5'
4	B	5002	ATP	C5'-O5'-PA-O1A
4	B	5002	ATP	C5'-O5'-PA-O3A
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	B	5003	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	B	5003	ATP	C5'-O5'-PA-O3A
4	C	5002	ATP	C5'-O5'-PA-O1A
4	C	5002	ATP	C5'-O5'-PA-O3A
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	C	5003	ATP	C5'-O5'-PA-O2A
4	C	5003	ATP	C5'-O5'-PA-O3A
4	D	5002	ATP	C5'-O5'-PA-O1A
4	D	5002	ATP	C5'-O5'-PA-O3A
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	D	5003	ATP	C5'-O5'-PA-O2A
4	D	5003	ATP	C5'-O5'-PA-O3A
5	A	5004	KVR	C15-C14-N12-C11
5	A	5004	KVR	C15-C14-N12-C13
5	A	5004	KVR	C17-C18-C21-O23
5	A	5004	KVR	C19-C18-C21-O23
5	B	5004	KVR	C17-C18-C21-O23
5	B	5004	KVR	C19-C18-C21-O22
5	B	5004	KVR	C19-C18-C21-O23
5	C	5004	KVR	C17-C18-C21-O23
5	C	5004	KVR	C19-C18-C21-O22
5	C	5004	KVR	C19-C18-C21-O23
5	D	5004	KVR	C17-C18-C21-O23
5	D	5004	KVR	C19-C18-C21-O22
5	D	5004	KVR	C19-C18-C21-O23
5	A	5004	KVR	C17-C18-C21-O22
5	A	5004	KVR	C19-C18-C21-O22
5	B	5004	KVR	C17-C18-C21-O22
5	C	5004	KVR	C17-C18-C21-O22
5	D	5004	KVR	C17-C18-C21-O22
5	A	5004	KVR	C08-C03-O02-C01
5	A	5004	KVR	C04-C03-O02-C01
5	B	5004	KVR	C04-C03-O02-C01
5	B	5004	KVR	C08-C03-O02-C01
5	C	5004	KVR	C04-C03-O02-C01
5	C	5004	KVR	C08-C03-O02-C01
5	D	5004	KVR	C04-C03-O02-C01
5	D	5004	KVR	C08-C03-O02-C01
4	A	5003	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	B	5003	ATP	C3'-C4'-C5'-O5'
4	C	5003	ATP	C3'-C4'-C5'-O5'
4	D	5003	ATP	C3'-C4'-C5'-O5'
4	B	5003	ATP	O4'-C4'-C5'-O5'
4	C	5003	ATP	O4'-C4'-C5'-O5'
4	D	5003	ATP	O4'-C4'-C5'-O5'
4	B	5003	ATP	C4'-C5'-O5'-PA
4	C	5003	ATP	C4'-C5'-O5'-PA
4	D	5003	ATP	C4'-C5'-O5'-PA
4	A	5002	ATP	PB-O3B-PG-O1G
4	B	5002	ATP	PB-O3B-PG-O1G
4	C	5002	ATP	PB-O3B-PG-O1G
4	D	5002	ATP	PB-O3B-PG-O1G
4	A	5002	ATP	C5'-O5'-PA-O2A
4	B	5002	ATP	C5'-O5'-PA-O2A
4	C	5002	ATP	C5'-O5'-PA-O2A
4	D	5002	ATP	C5'-O5'-PA-O2A
4	A	5002	ATP	PA-O3A-PB-O1B
4	B	5002	ATP	PA-O3A-PB-O1B
4	C	5002	ATP	PA-O3A-PB-O1B
4	D	5002	ATP	PA-O3A-PB-O1B
4	D	5002	ATP	PB-O3B-PG-O3G
4	A	5002	ATP	PA-O3A-PB-O3B
4	B	5002	ATP	PA-O3A-PB-O3B
4	C	5002	ATP	PA-O3A-PB-O3B
4	D	5002	ATP	PA-O3A-PB-O3B

There are no ring outliers.

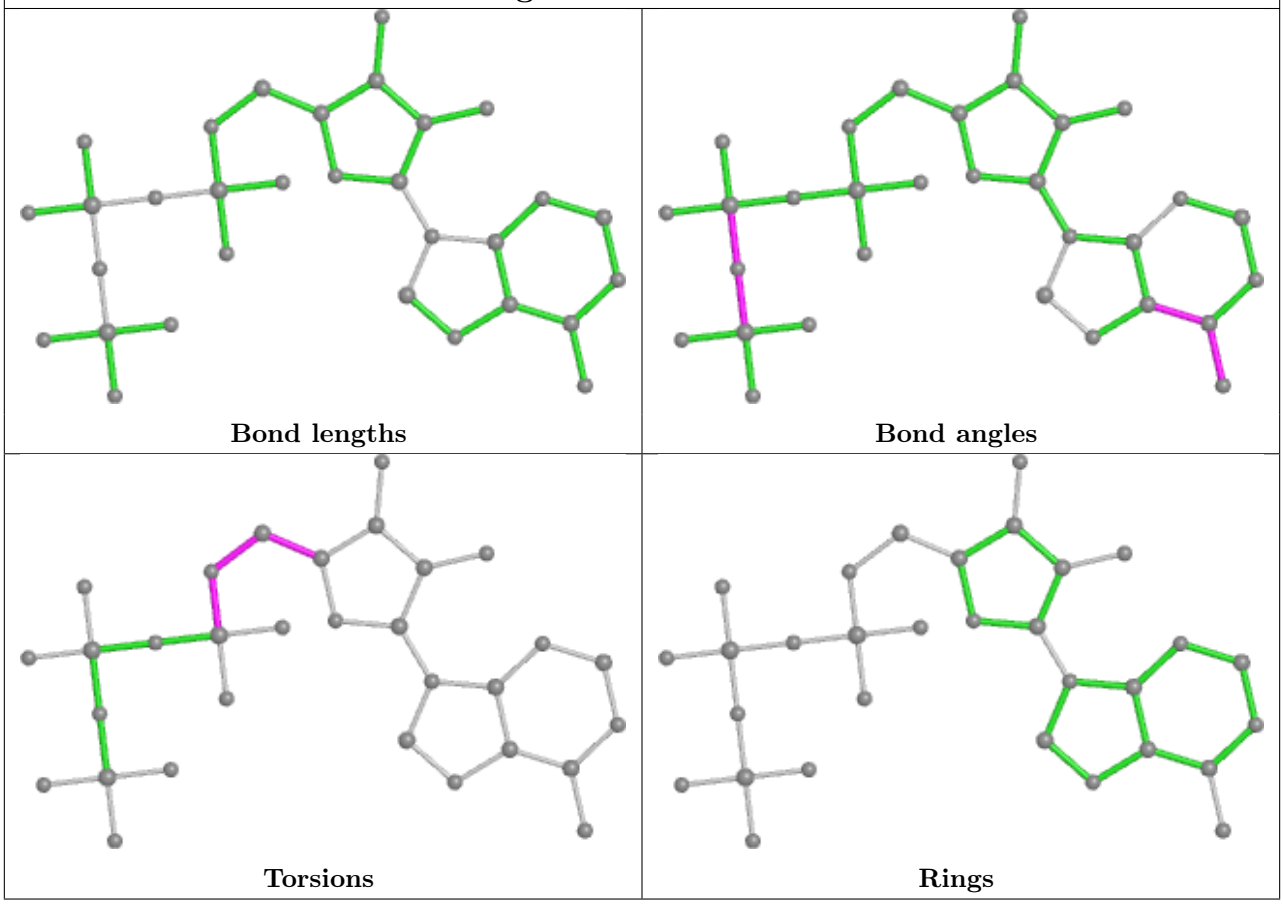
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5003	ATP	9	0
5	A	5004	KVR	3	0

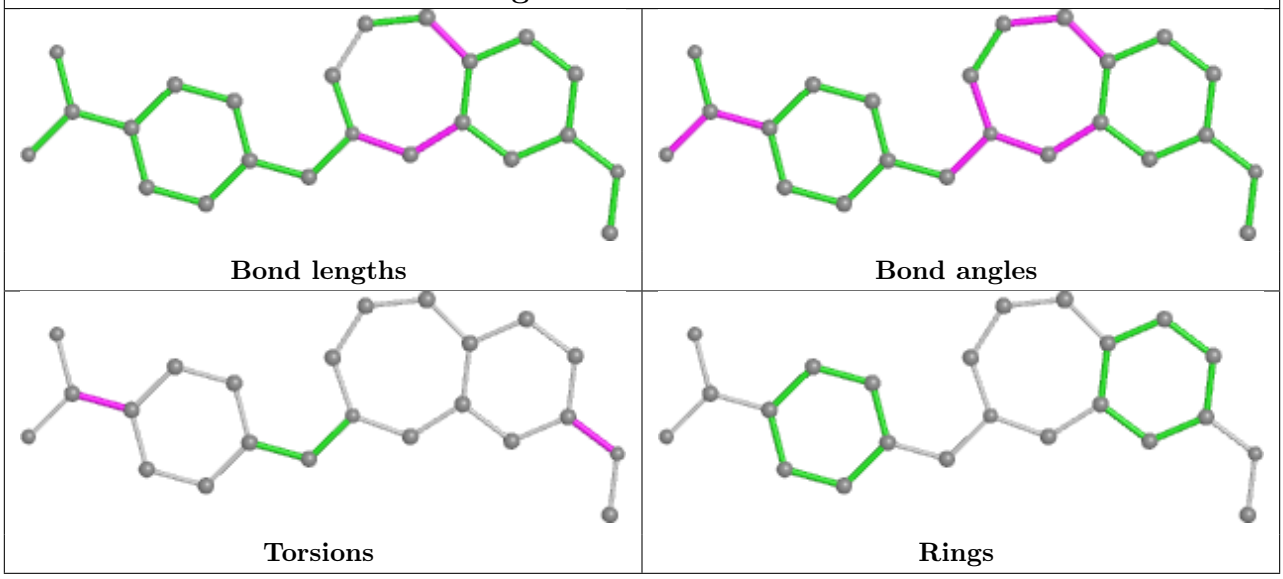
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

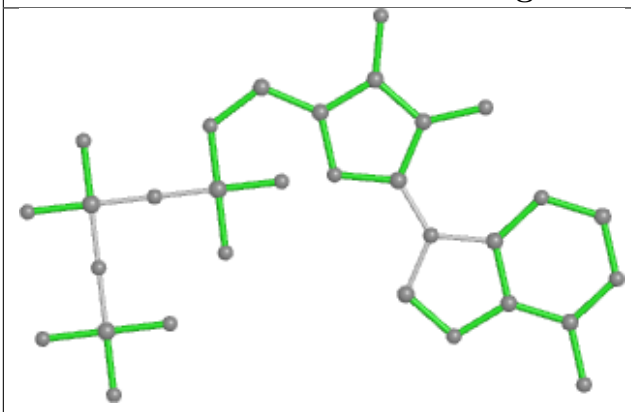
Ligand ATP D 5003



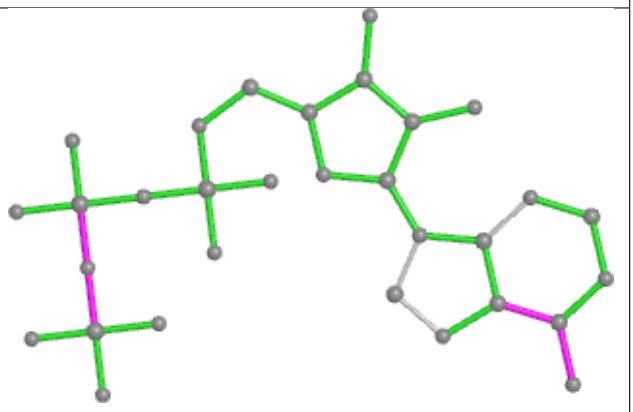
Ligand KVR D 5004



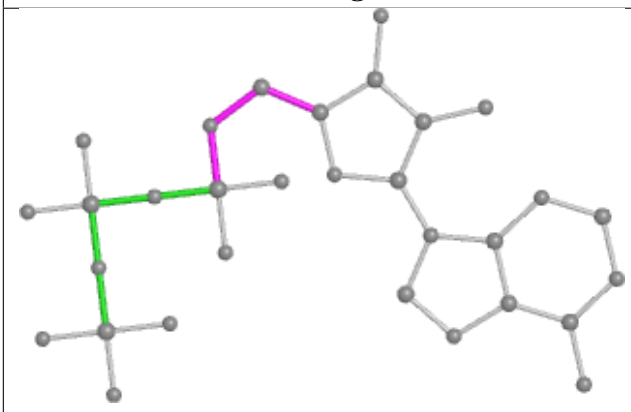
Ligand ATP B 5003



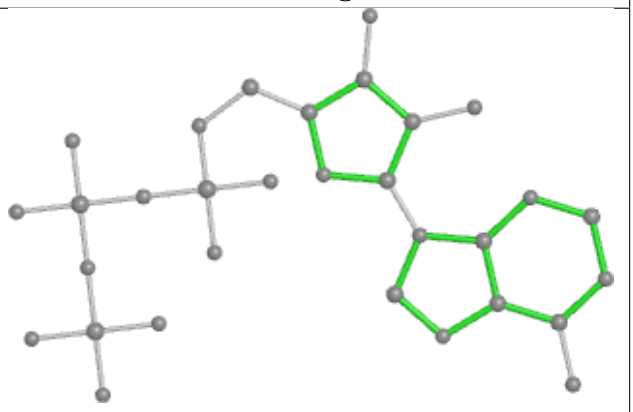
Bond lengths



Bond angles

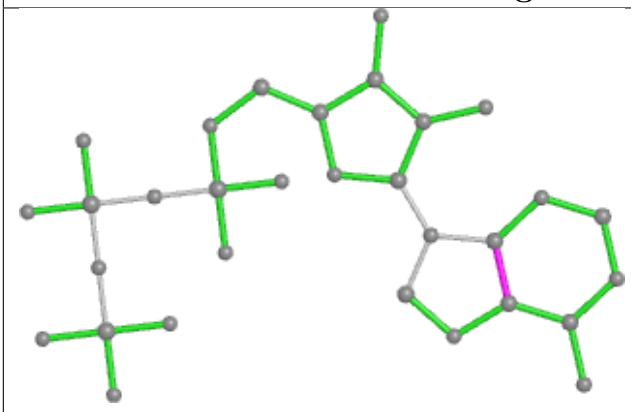


Torsions

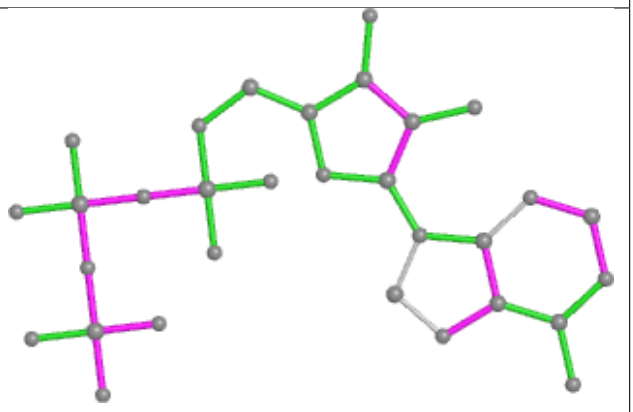


Rings

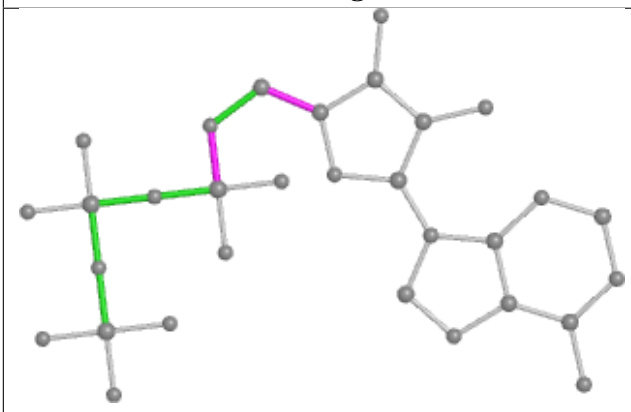
Ligand ATP A 5003



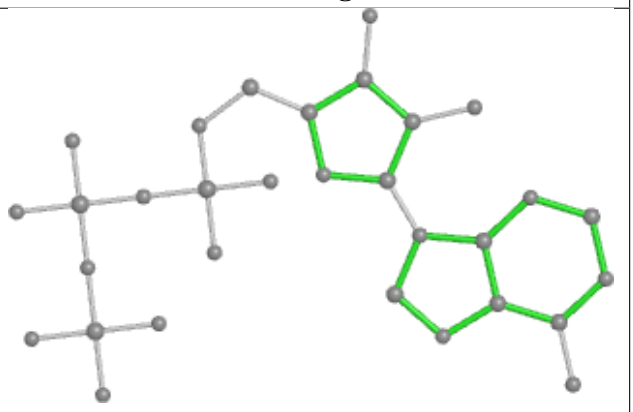
Bond lengths



Bond angles

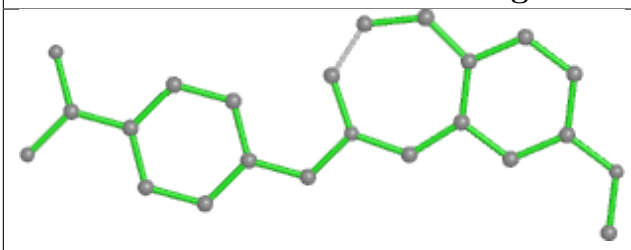


Torsions

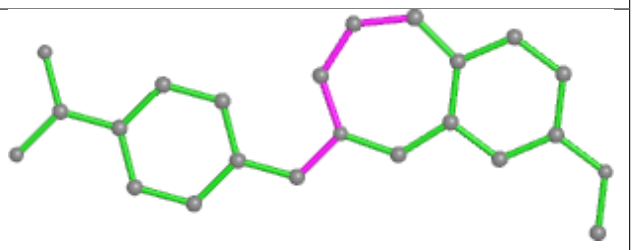


Rings

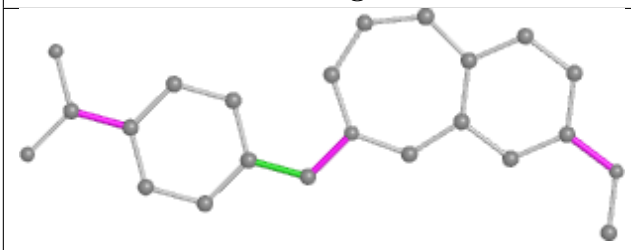
Ligand KVR A 5004



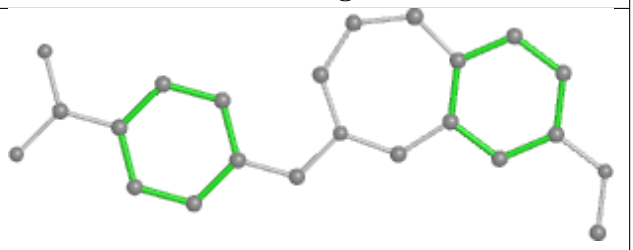
Bond lengths



Bond angles

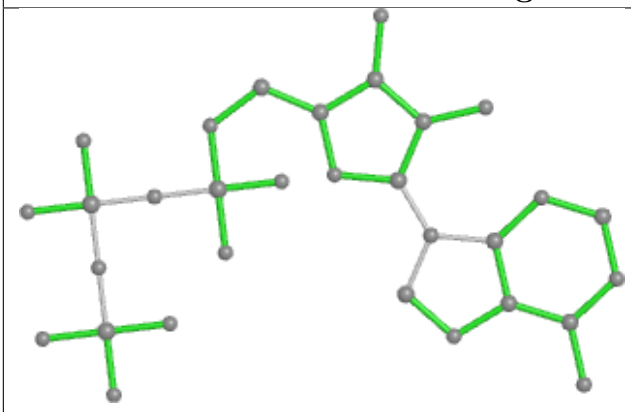


Torsions

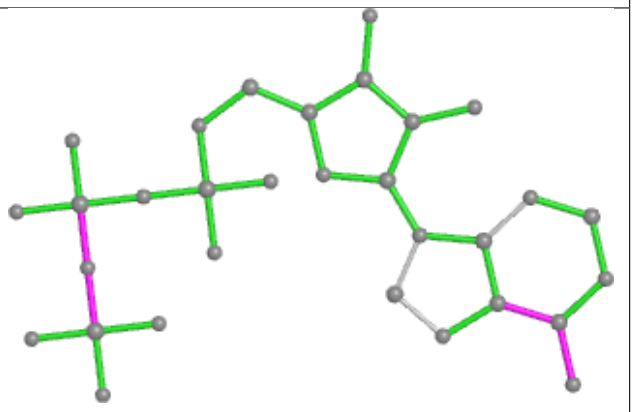


Rings

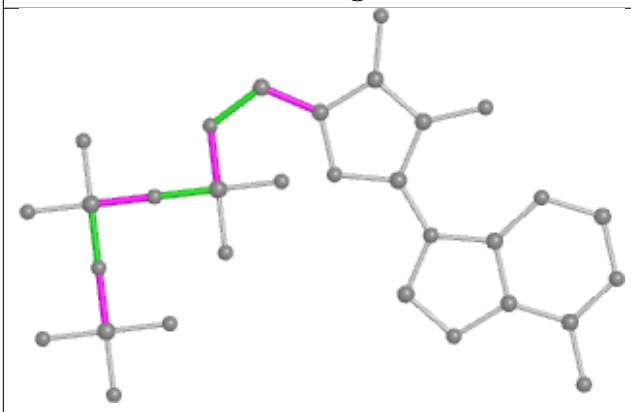
Ligand ATP C 5002



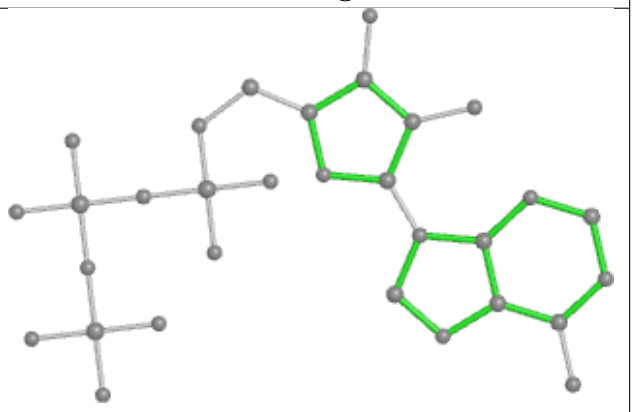
Bond lengths



Bond angles

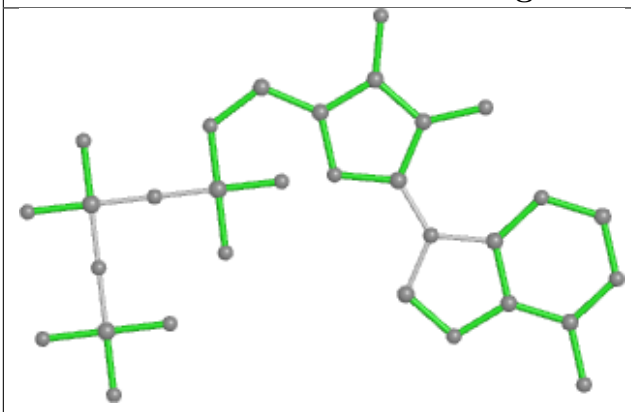


Torsions

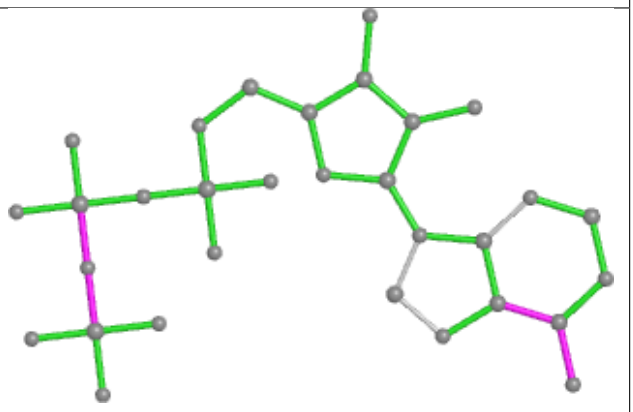


Rings

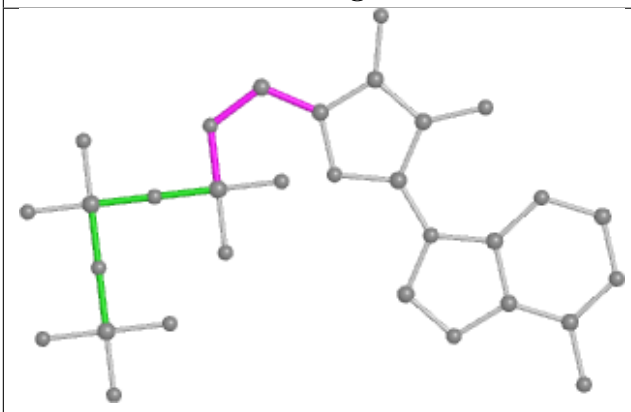
Ligand ATP C 5003



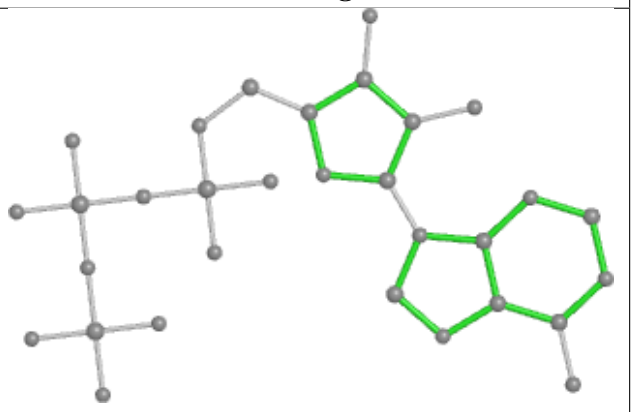
Bond lengths



Bond angles

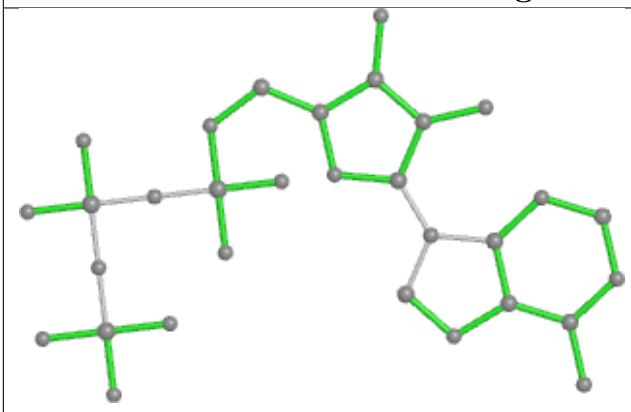


Torsions

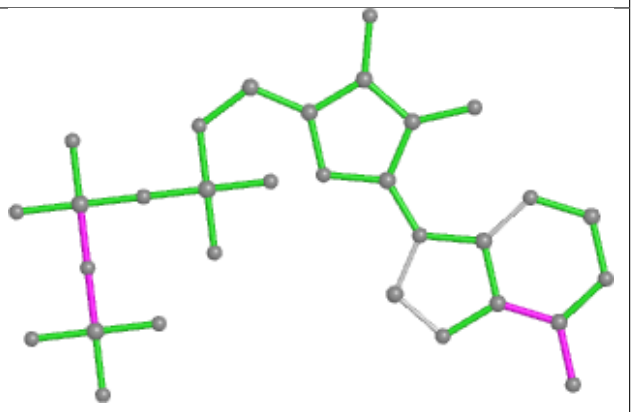


Rings

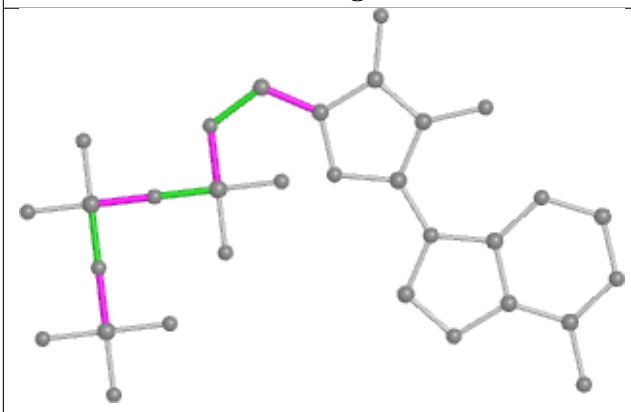
Ligand ATP D 5002



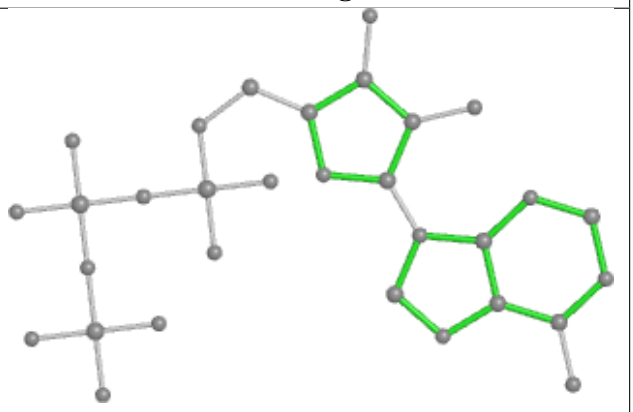
Bond lengths



Bond angles

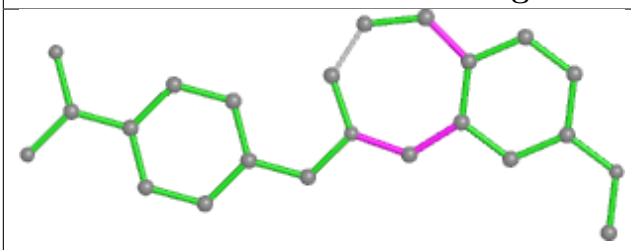


Torsions

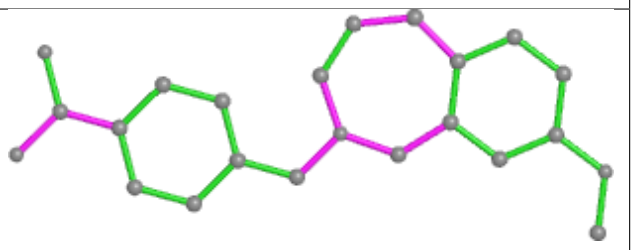


Rings

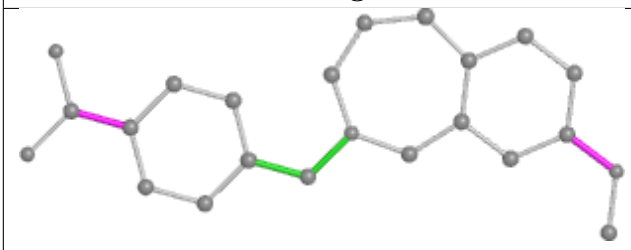
Ligand KVR C 5004



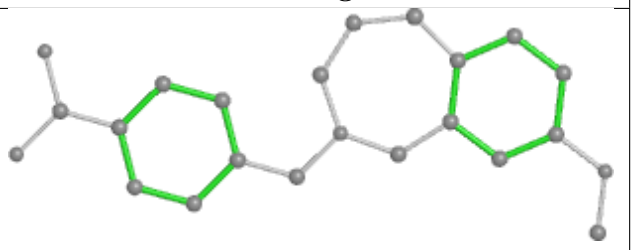
Bond lengths



Bond angles

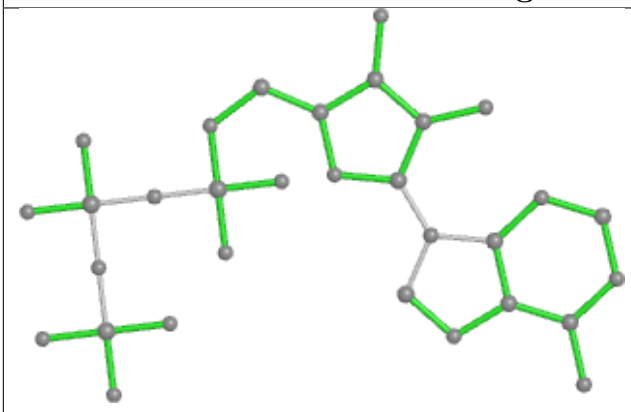


Torsions

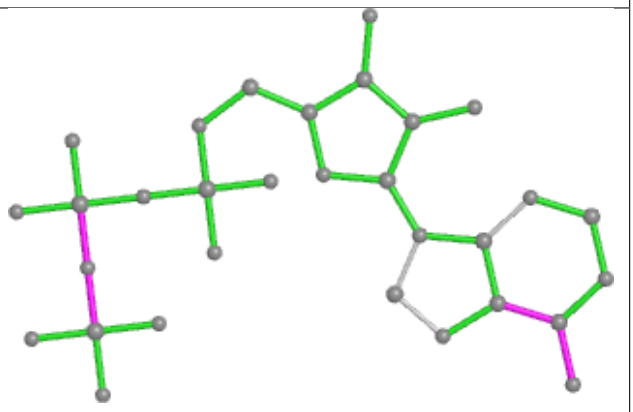


Rings

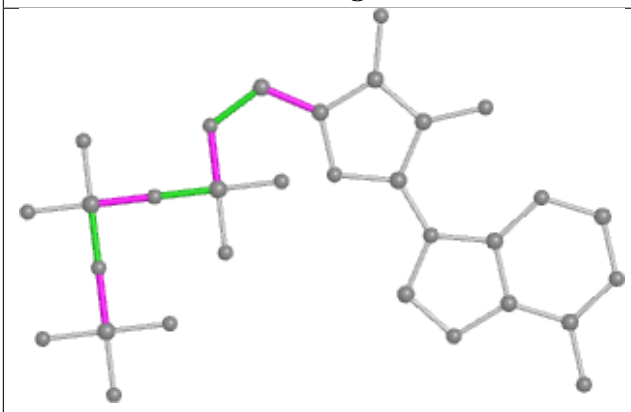
Ligand ATP B 5002



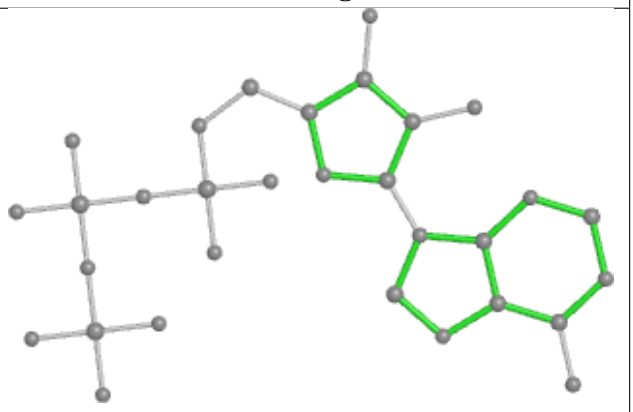
Bond lengths



Bond angles

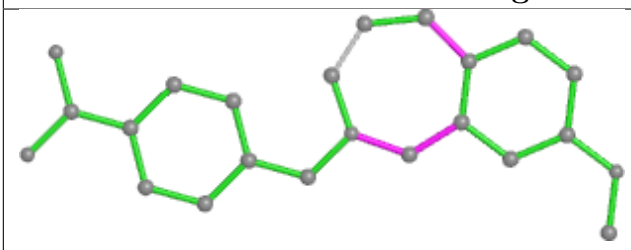


Torsions

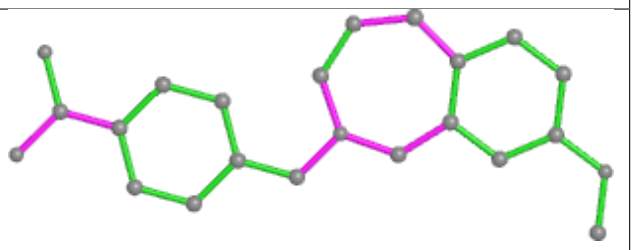


Rings

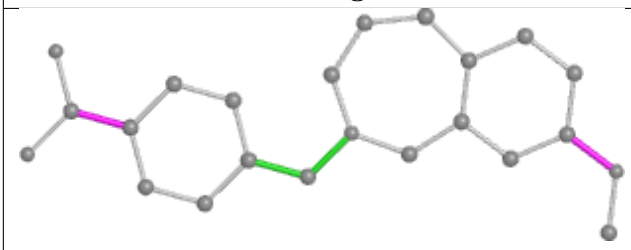
Ligand KVR B 5004



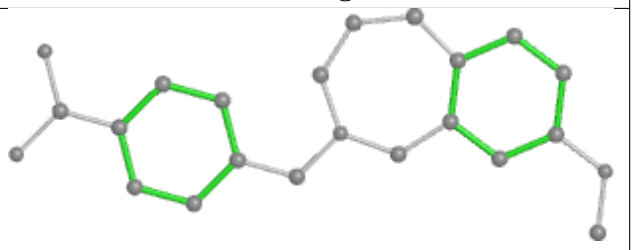
Bond lengths



Bond angles

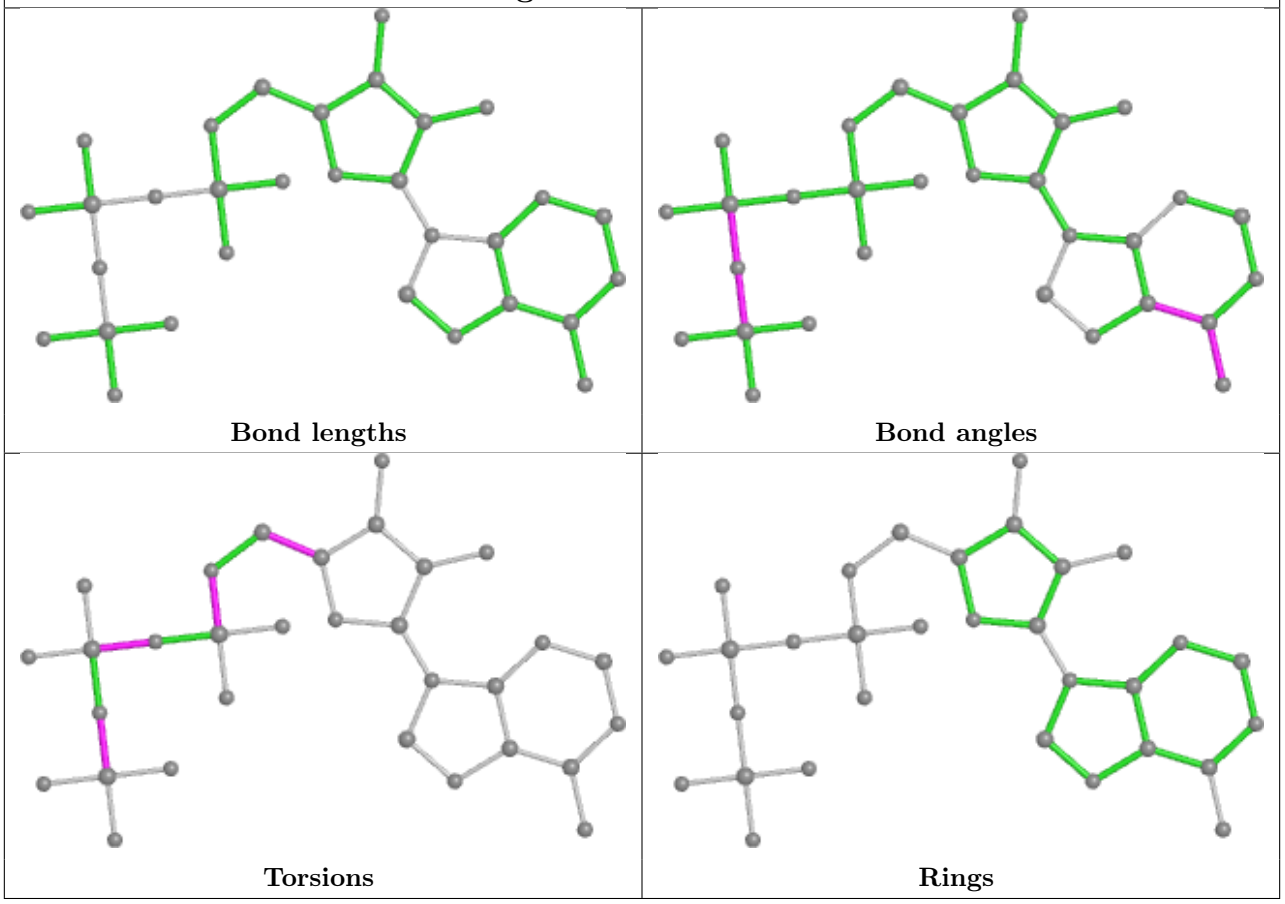


Torsions



Rings

Ligand ATP A 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.

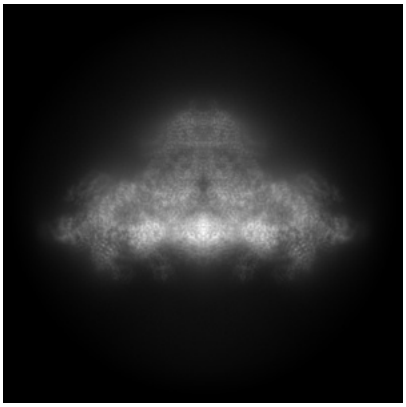
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26412. These allow visual inspection of the internal detail of the map and identification of artifacts.

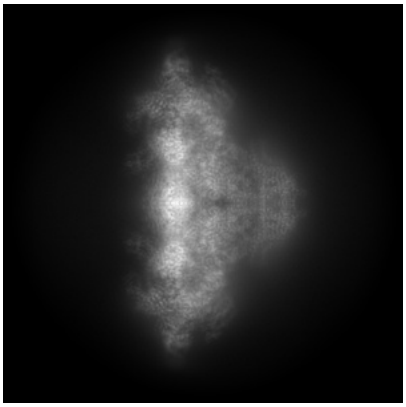
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

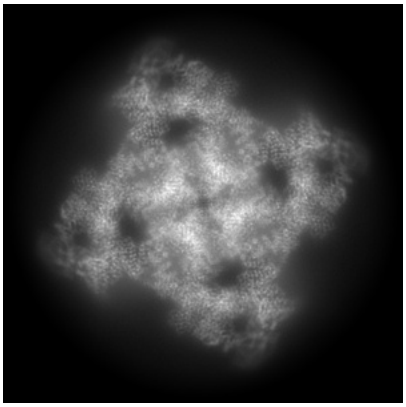
6.1.1 Primary map



X



Y

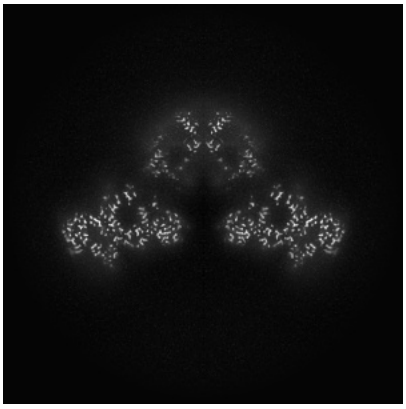


Z

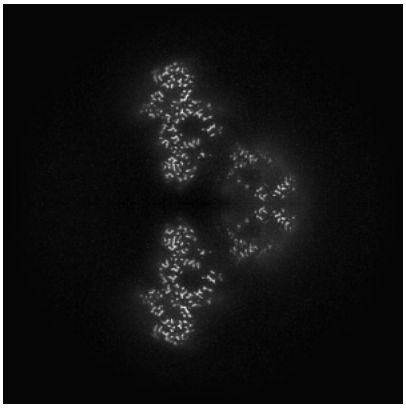
The images above show the map projected in three orthogonal directions.

6.2 Central slices

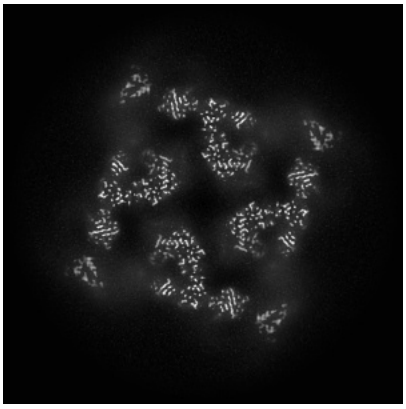
6.2.1 Primary map



X Index: 256



Y Index: 256

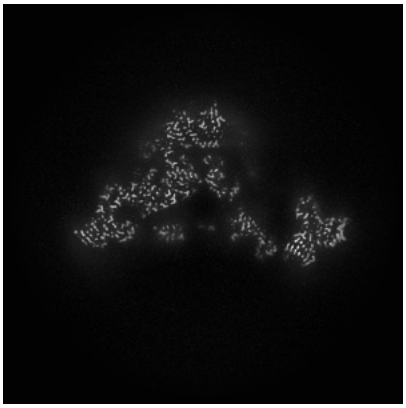


Z Index: 256

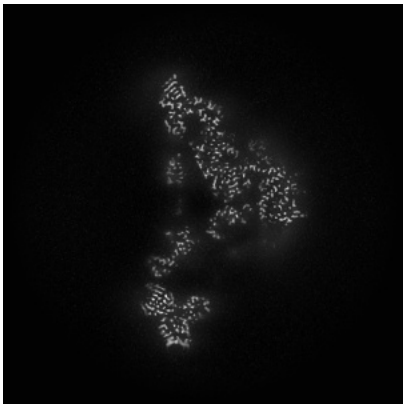
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

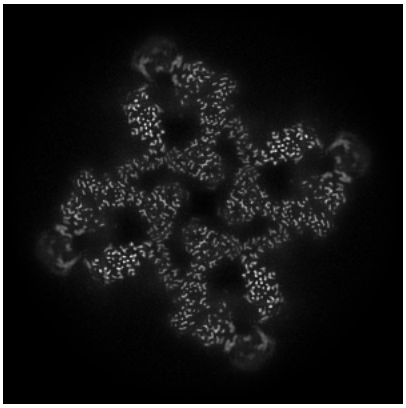
6.3.1 Primary map



X Index: 237



Y Index: 238

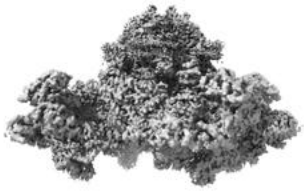


Z Index: 223

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.

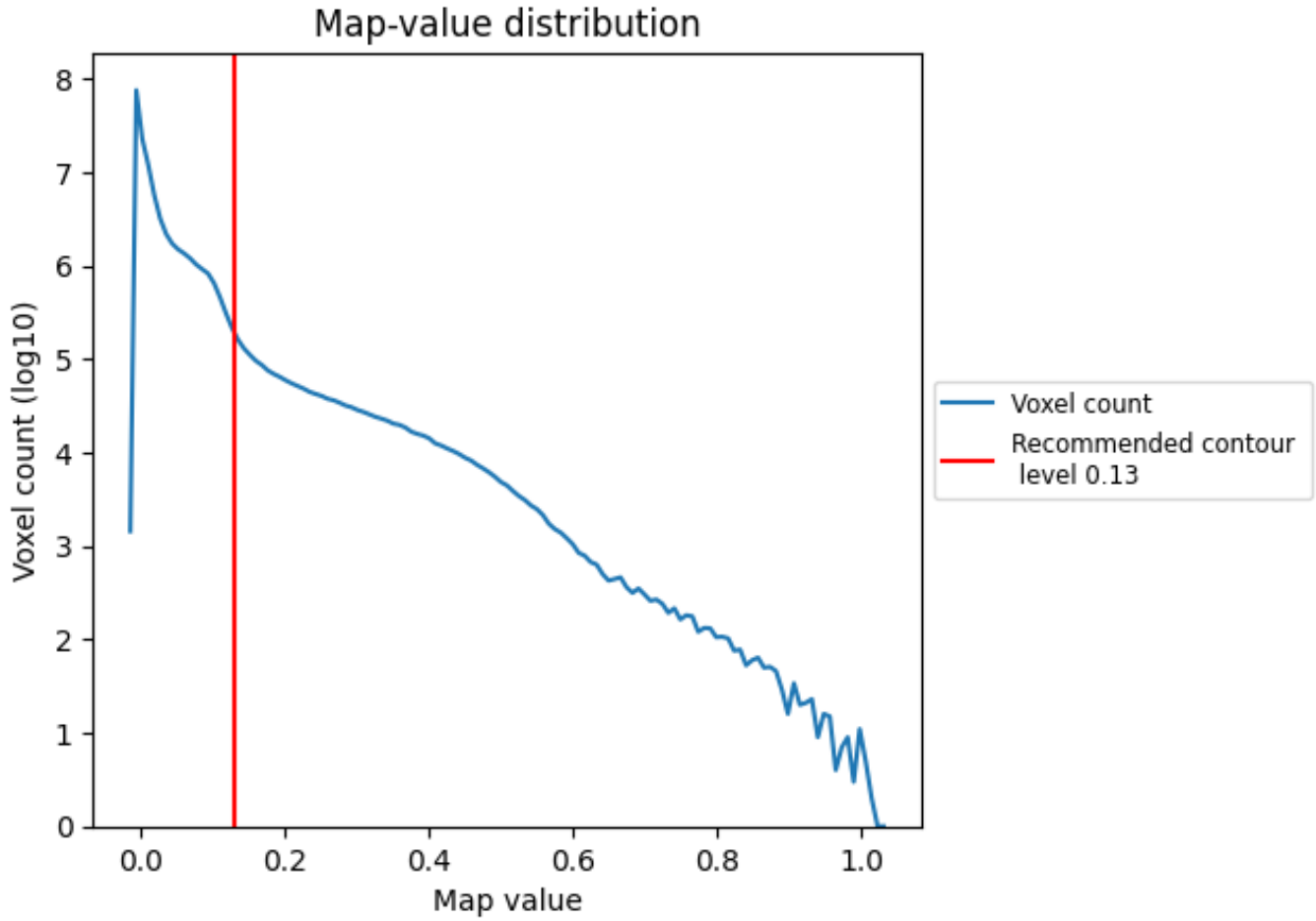
6.5 Mask visualisation (i)

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

7 Map analysis

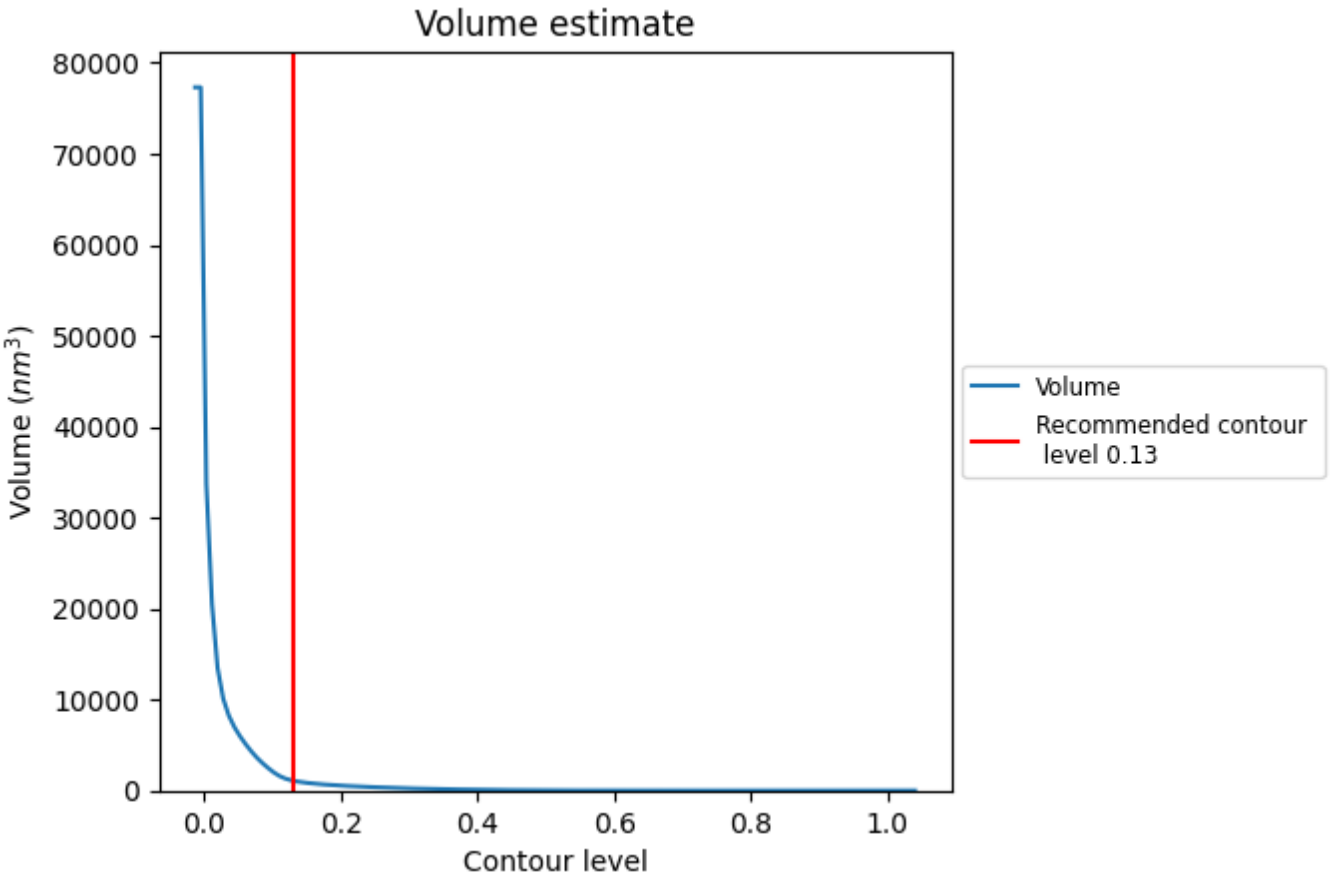
This section contains the results of statistical analysis of the map.

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.

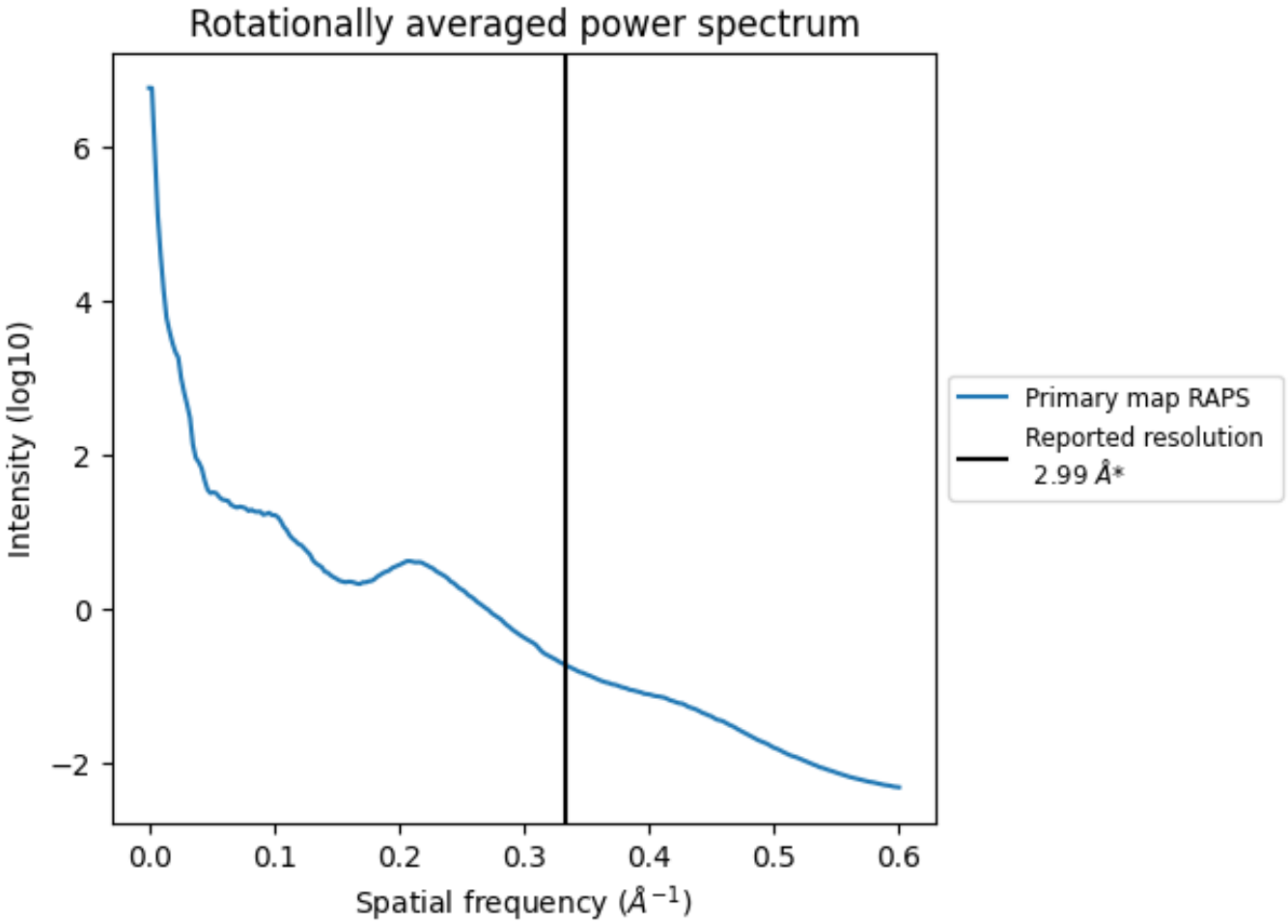
7.2 Volume estimate



The volume at the recommended contour level is 1081 nm^3; this corresponds to an approximate mass of 977 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 0.334 Å^{-1}

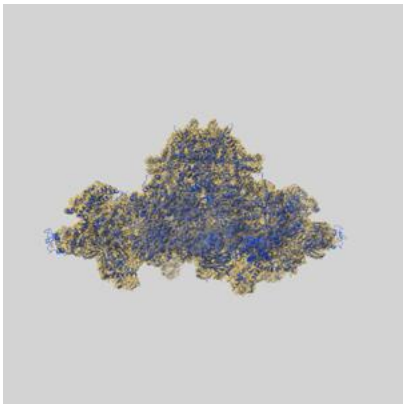
8 Fourier-Shell correlation

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

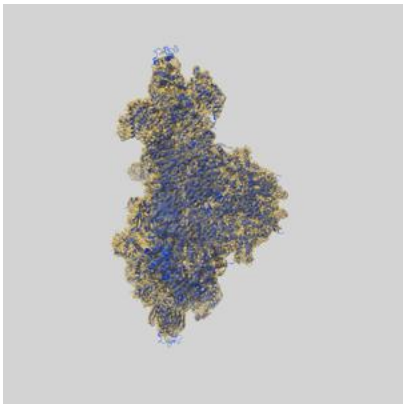
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26412 and PDB model 7UA1. Per-residue inclusion information can be found in section 3 on page 7.

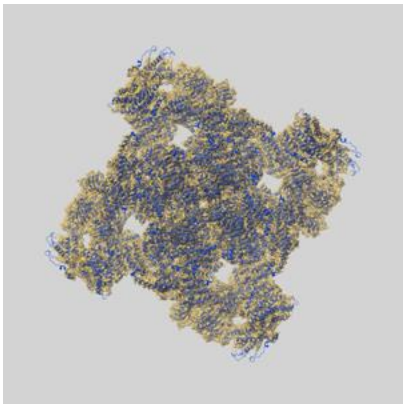
9.1 Map-model overlay



X



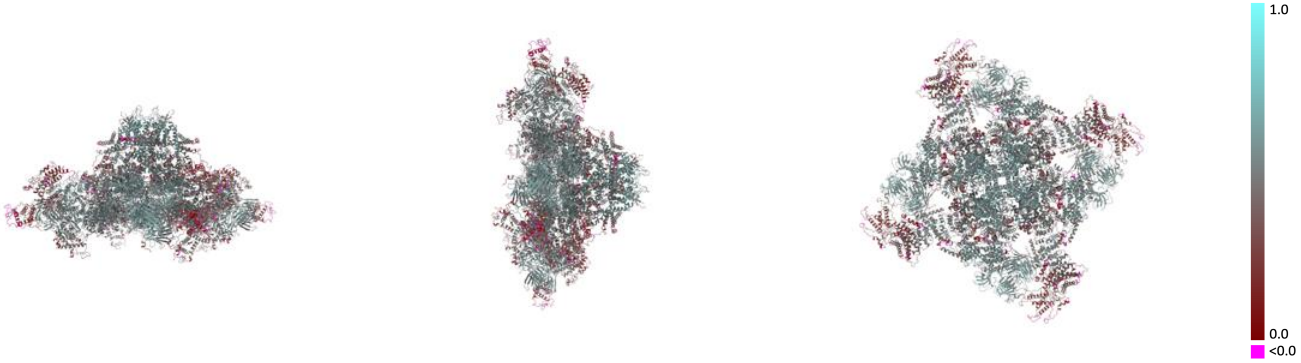
Y



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.

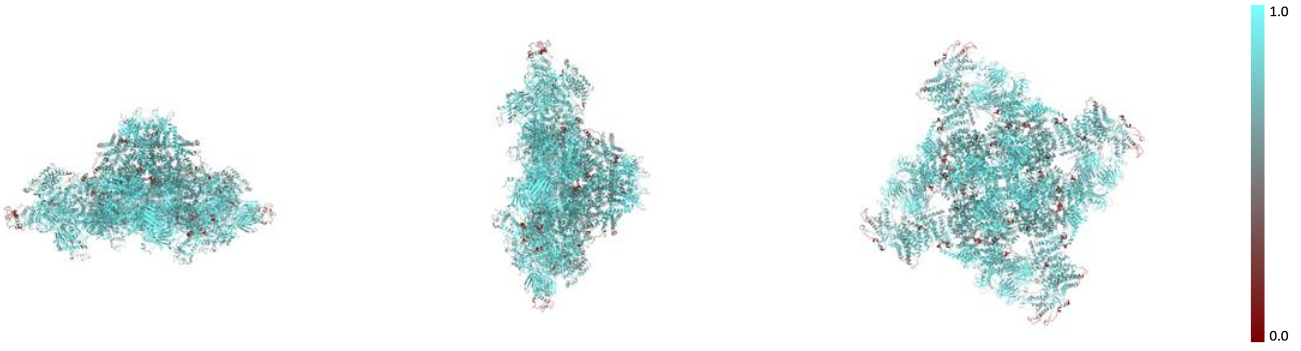
9.2 Q-score mapped to coordinate model



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.

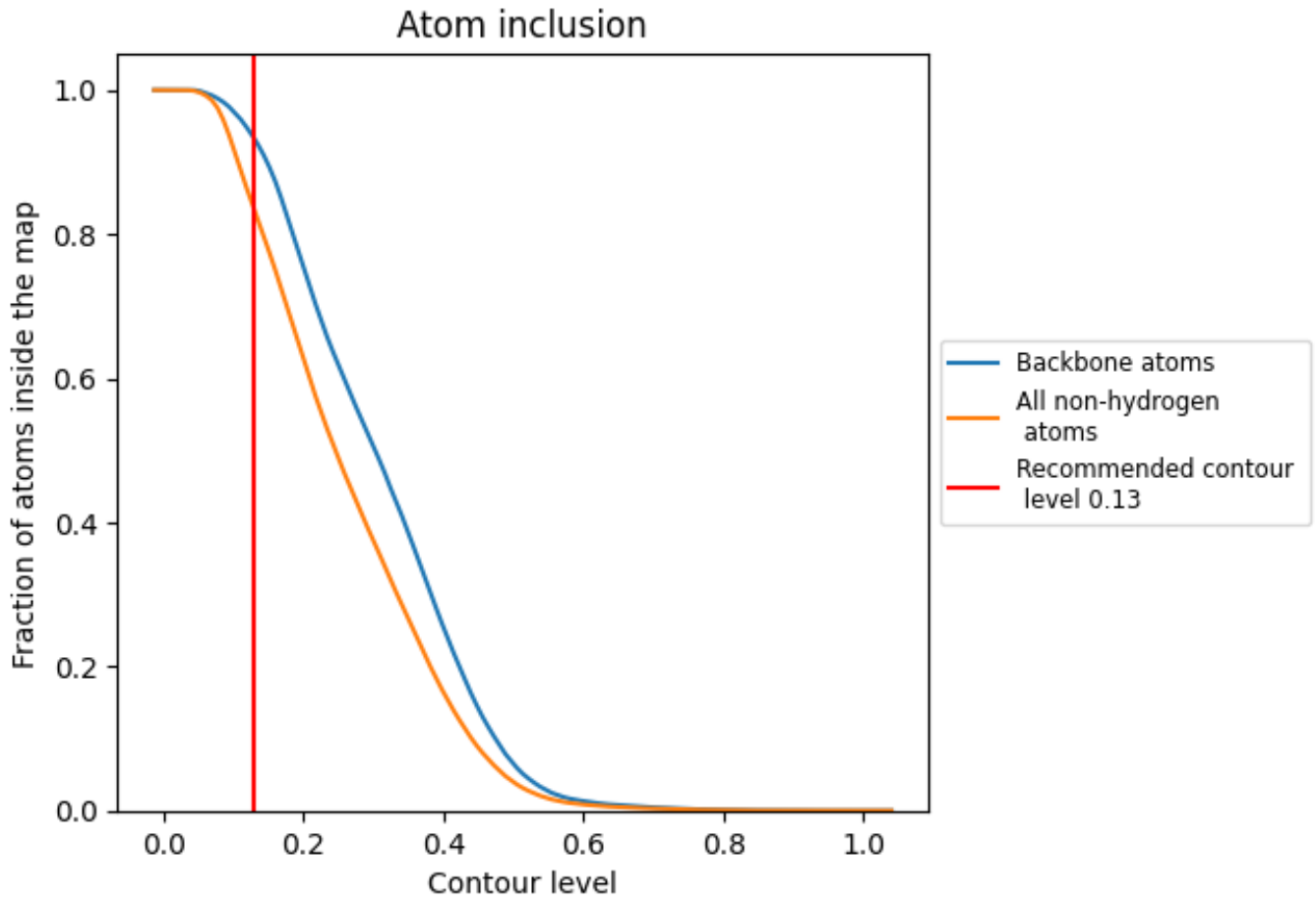
9.3 Atom inclusion mapped to coordinate model



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, 93% of all backbone atoms, 83% 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	0.8323	0.4650
A	0.8308	0.4660
B	0.8278	0.4580
C	0.8300	0.4630
D	0.8312	0.4660
E	0.9305	0.5600
F	0.9243	0.5540
G	0.9280	0.5570
H	0.9330	0.5720