Full wwPDB EM Validation Report ⓘ

Nov 13, 2023 – 05:35 PM EST

PDB ID	:	8UXH
EMDB ID	:	EMD-42764
Title	:	Structure of PKA phosphorylated human RyR2-R420W in the primed state in the presence of calcium
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2023-11-09
Resolution	:	3.52 Å(reported)
Based on initial model	:	7UA5

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:

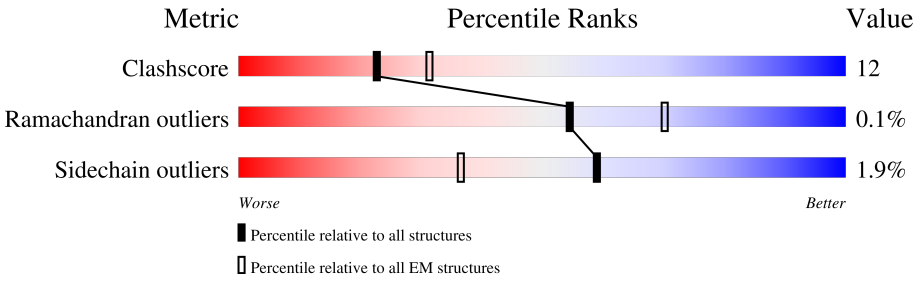
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.52 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	10% 57% 23% • 19%
1	B	4967	10% 57% 23% • 19%
1	C	4967	10% 57% 23% • 19%
1	D	4967	11% 57% 22% • 19%
2	E	108	77% 22% •
2	F	108	79% 20% •
2	G	108	78% 21% •
2	H	108	78% 21% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 131656 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	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0
1	B	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0
1	C	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0
1	D	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	TRP	ARG	variant	UNP Q92736
B	420	TRP	ARG	variant	UNP Q92736
C	420	TRP	ARG	variant	UNP Q92736
D	420	TRP	ARG	variant	UNP Q92736

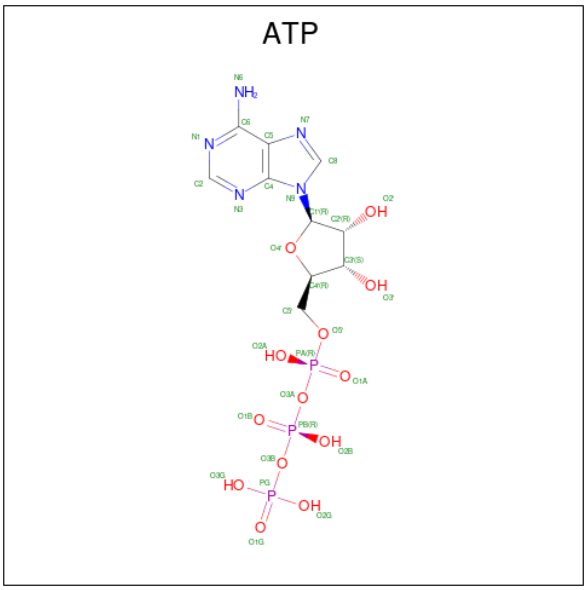
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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 31 10 5 13 3	0
4	A	1	Total C N O P 31 10 5 13 3	0
4	B	1	Total C N O P 31 10 5 13 3	0
4	B	1	Total C N O P 31 10 5 13 3	0
4	C	1	Total C N O P 31 10 5 13 3	0
4	C	1	Total C N O P 31 10 5 13 3	0
4	D	1	Total C N O P 31 10 5 13 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

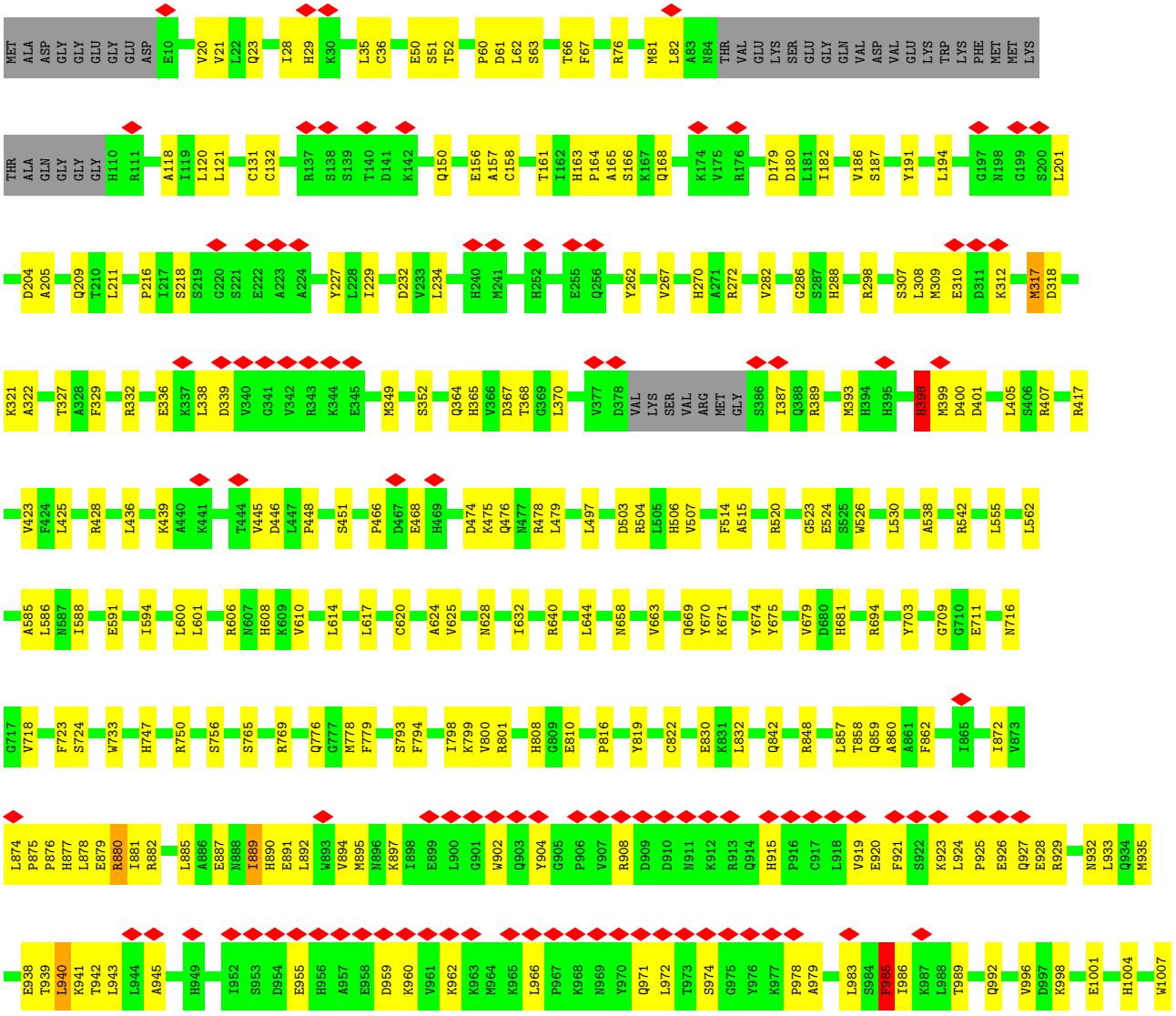
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

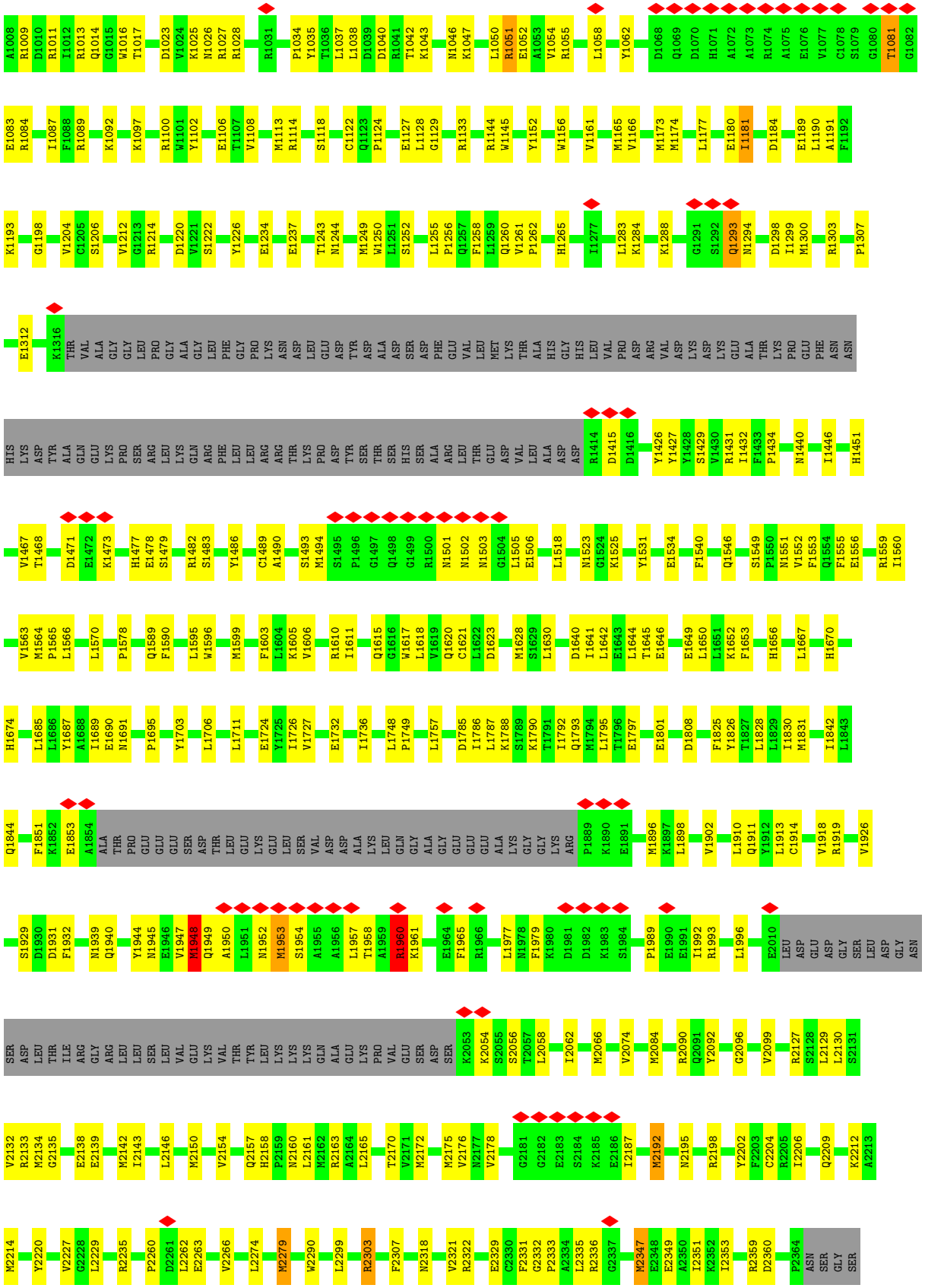
3 Residue-property plots (i)

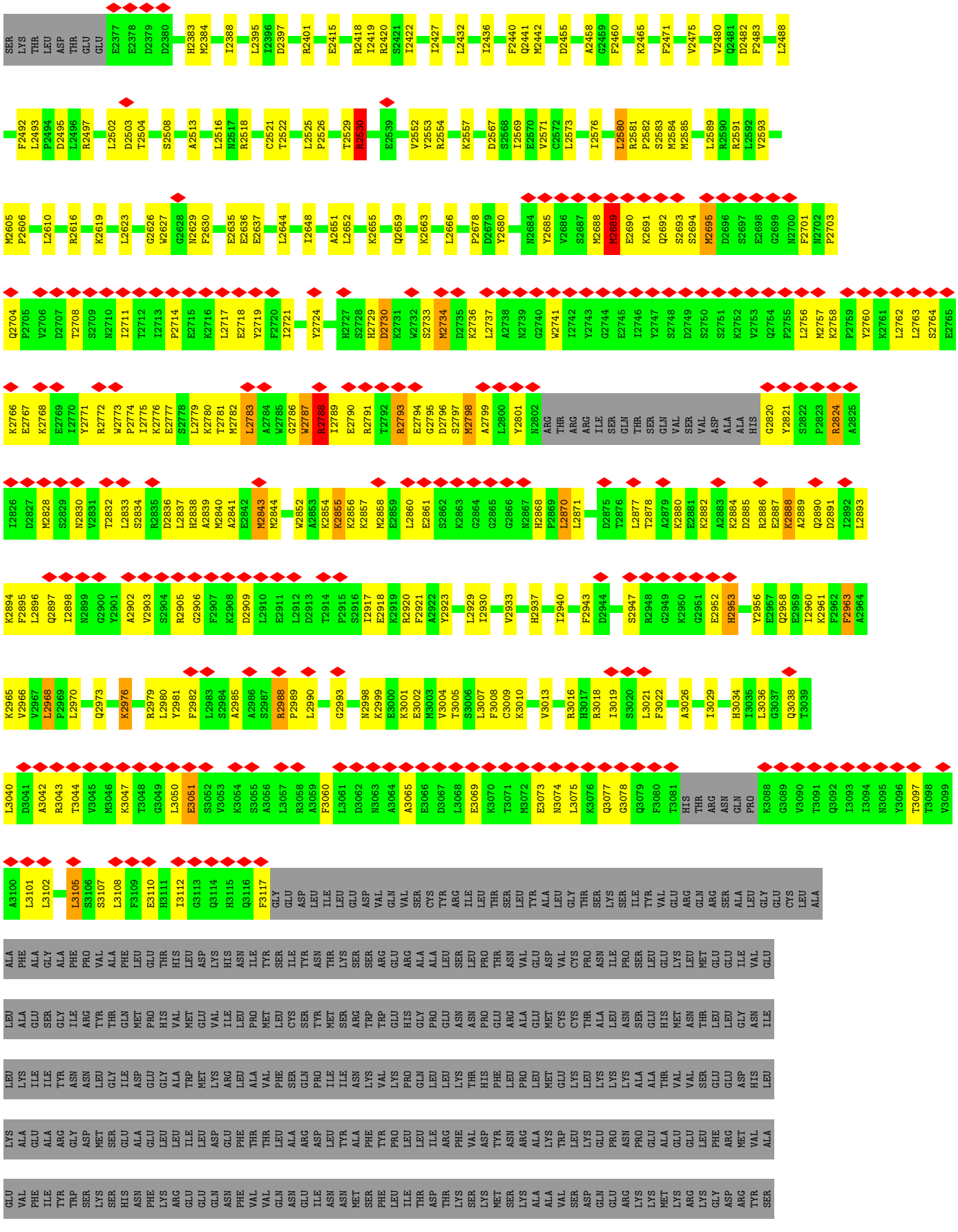
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

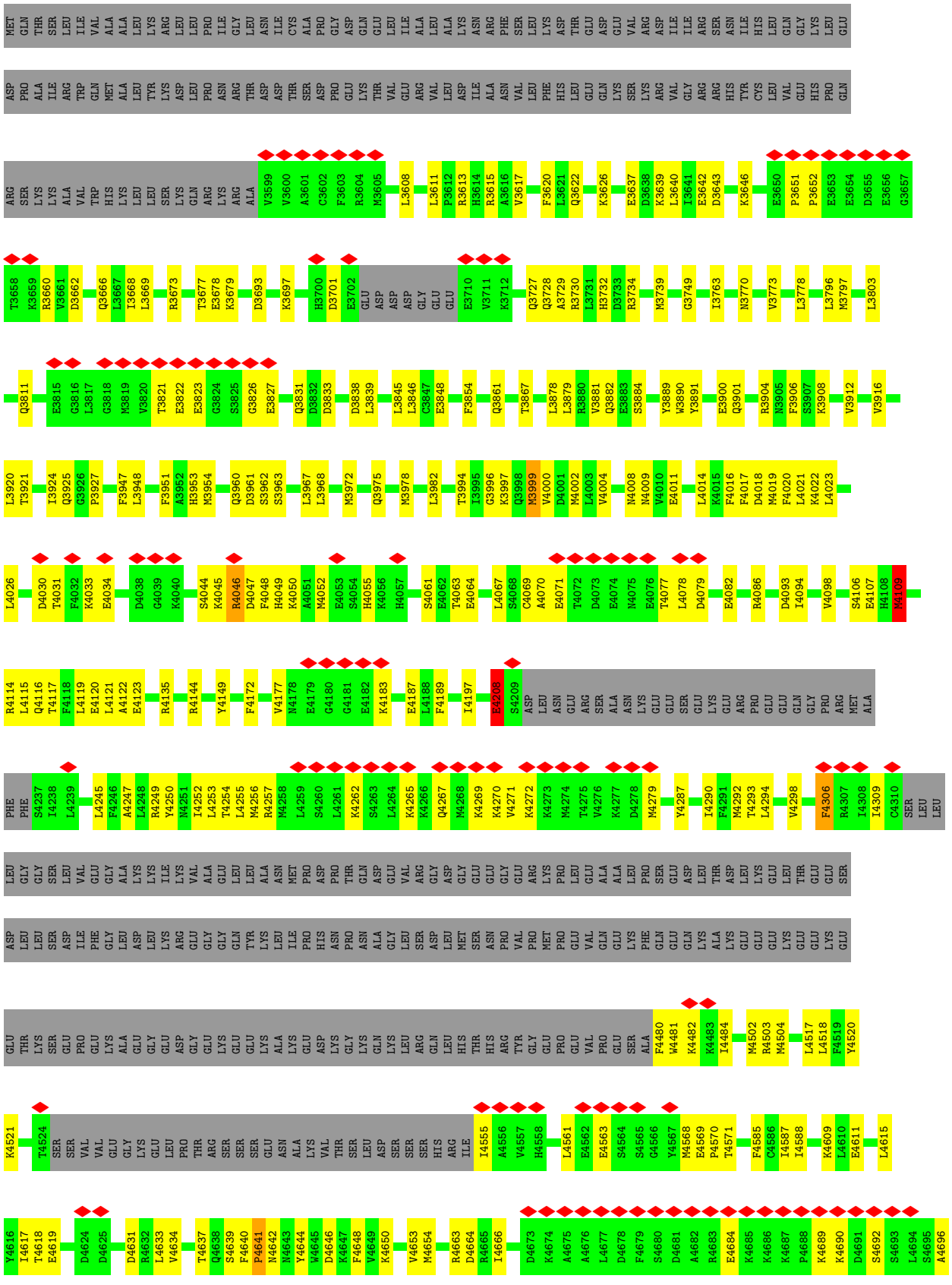
- Molecule 1: Ryanodine receptor 2

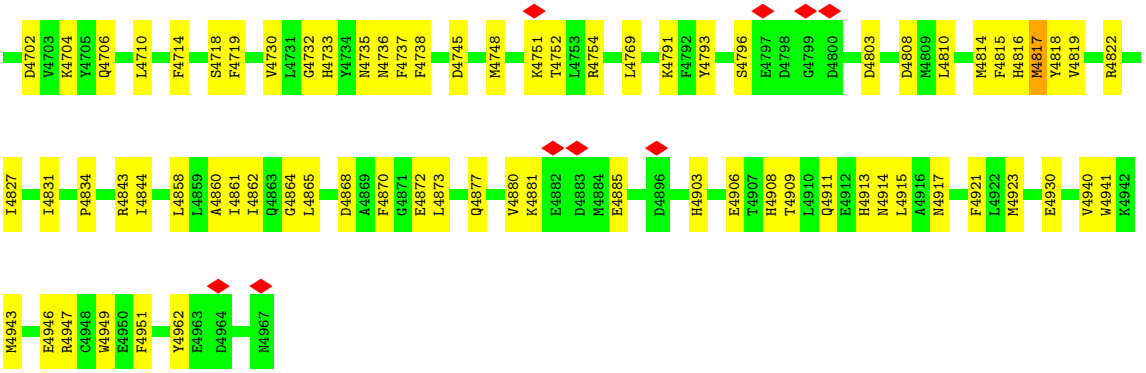
Chain A:





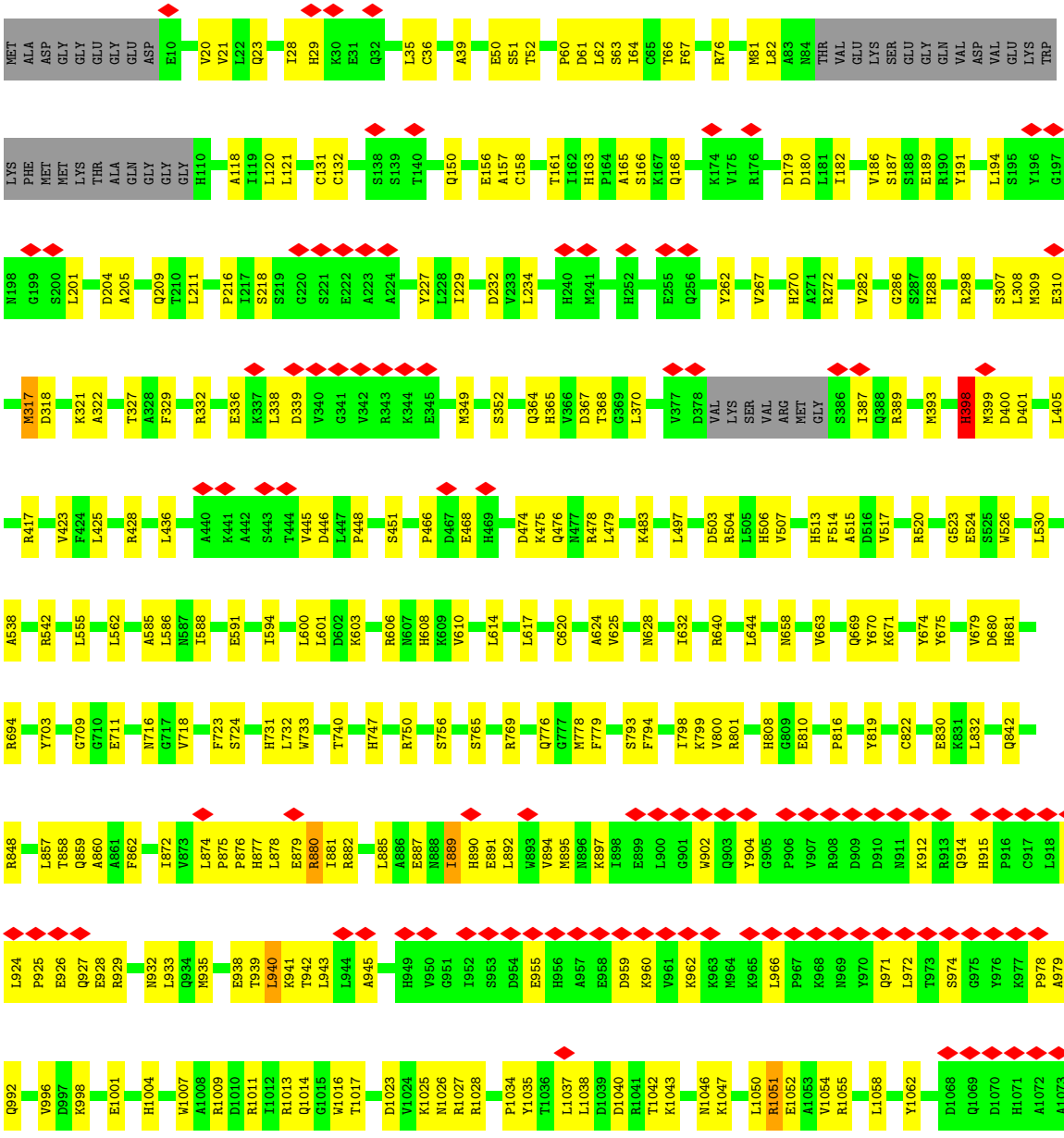

SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 H2383 M2384 I2388 L2395 I2396 D2397 R2401 E2415 R2418 I2419 R2420 S2421 I2422 I2427 L2432 I2436 F2440 Q2441 M2442 D2455 A2458 G2459 F2460 K2465 F2471 V2475 V2480 Q2481 D2482 F2483 L2488
F2492 L2493 P2494 D2495 L2496 R2497 L2502 D2503 T2504 S2508 A2513 L2516 N2517 R2518 C2521 T2522 L2525 P2526 T2529 R2530 E2539 V2552 Y2553 R2554 K2557 D2567 S2568 I2569 E2570 V2571 G2572 L2573 I2576 L2580 R2581 P2582 S2583 M2584 M2585 L2589 R2590 R2591 L2592 V2593
M2605 P2606 L2610 R2616 K2619 L2623 G2626 W2627 G2628 N2629 F2630 E2635 E2636 E2637 L2644 I2648 A2651 L2652 K2655 Q2659 K2663 L2666 P2678 D2679 Y2680 N2684 Y2685 V2686 S2687 M2688 M2689 E2690 K2691 Q2692 S2693 S2694 M2695 D2696 S2697 E2698 G2699 N2700 F2701 N2702 P2703
Q2704 P2705 V2706 D2707 T2708 S2709 N2710 I2711 T2712 I2713 P2714 E2715 K2716 L2717 E2718 Y2719 F2720 I2721 Y2724 H2727 S2728 H2729 D2730 K2731 W2732 S2733 M2734 D2735 K2736 L2737 A2738 N2739 G2740 W2741 I2742 Y2743 G2744 E2745 I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759 Y2760 K2761 L2762 L2763 S2764 E2765
K2766 E2767 K2768 E2769 I2770 Y2771 R2772 W2773 P2774 I2775 K2776 E2777 S2778 L2779 K2780 T2781 M2782 L2783 A2784 W2785 G2786 W2787 R2788 I2789 E2790 R2791 T2792 R2793 E2794 G2795 D2796 S2797 M2798 A2799 L2800 Y2801 N2802 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823 R2824 A2825
I2826 D2827 M2828 S2829 N2830 V2831 T2832 L2833 S2834 R2835 D2836 L2837 H2838 A2839 M2840 A2841 E2842 M2843 M2844 W2852 A2853 K2854 K2855 K2856 K2857 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870 L2871 D2875 T2876 L2877 T2878 A2879 K2880 E2881 K2882 A2883 K2884 D2885 R2886 E2887 K2888 A2889 Q2890 D2891 I2892 L2893
K2894 F2895 L2896 Q2897 I2898 N2899 G2900 Y2901 A2902 V2903 S2904 R2905 G2906 F2907 K2908 D2909 L2910 E2911 L2912 D2913 T2914 P2915 S2916 I2917 E2918 K2919 R2920 F2921 A2922 Y2923 L2929 I2930 V2933 H2937 I2940 F2943 D2944 S2947 R2948 G2949 K2950 G2951 E2952 H2953 Y2956 E2957 Q2958 E2959 I2960 K2961 F2962 F2963 A2964
K2965 V2966 Y2967 L2968 P2969 L2970 Q2973 K2976 R2979 L2980 Y2981 F2982 L2983 S2984 A2985 A2986 S2987 R2988 P2989 L2990 G2993 N2998 K2999 E3000 K3001 E3002 M3003 V3004 T3005 S3006 L3007 F3008 C3009 K3010 V3013 H3016 H3017 R3018 I3019 S3020 L3021 F3022 A3026 I3029 H3034 I3035 L3036 G3037 Q3038 T3039
L3040 D3041 A3042 R3043 T3044 V3045 M3046 K3047 T3048 G3049 L3050 E3051 S3052 V3053 K3064 S3055 A3056 L3057 R3058 A3059 F3060 L3061 D3062 N3063 A3064 A3065 E3066 D3067 L3068 E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 I3094 N3095 Y3096 T3097 T3098 V3099
A3100 L3101 L3102 L3105 S3106 S3107 L3108 F3109 E3110 H3111 I3112 G3113 Q3114 H3115 Q3116 F3117 GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE ILE PRO ASN LEU ASP VAL GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLU GLU ILE VAL GLU
ALA PHE ALA GLY ALA PHE PRO VAL ALA PHE LEU GLU THR HIS LEU ASP LYS HIS ASN ILE TYR SER ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU SER LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL GLU
LEU ALA GLU SER GLY ILE TYR ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL ILE LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU GLU ASN ASN PRO GLU ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU LEU GLU GLU ILE VAL GLY
LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LYS LEU LYS LYS LYS LYS SER ALA ALA THR HIS VAL VAL SER LEU LEU GLU GLU ASP HIS LEU
LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU LEU PHE ARG MET VAL ALA
GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER

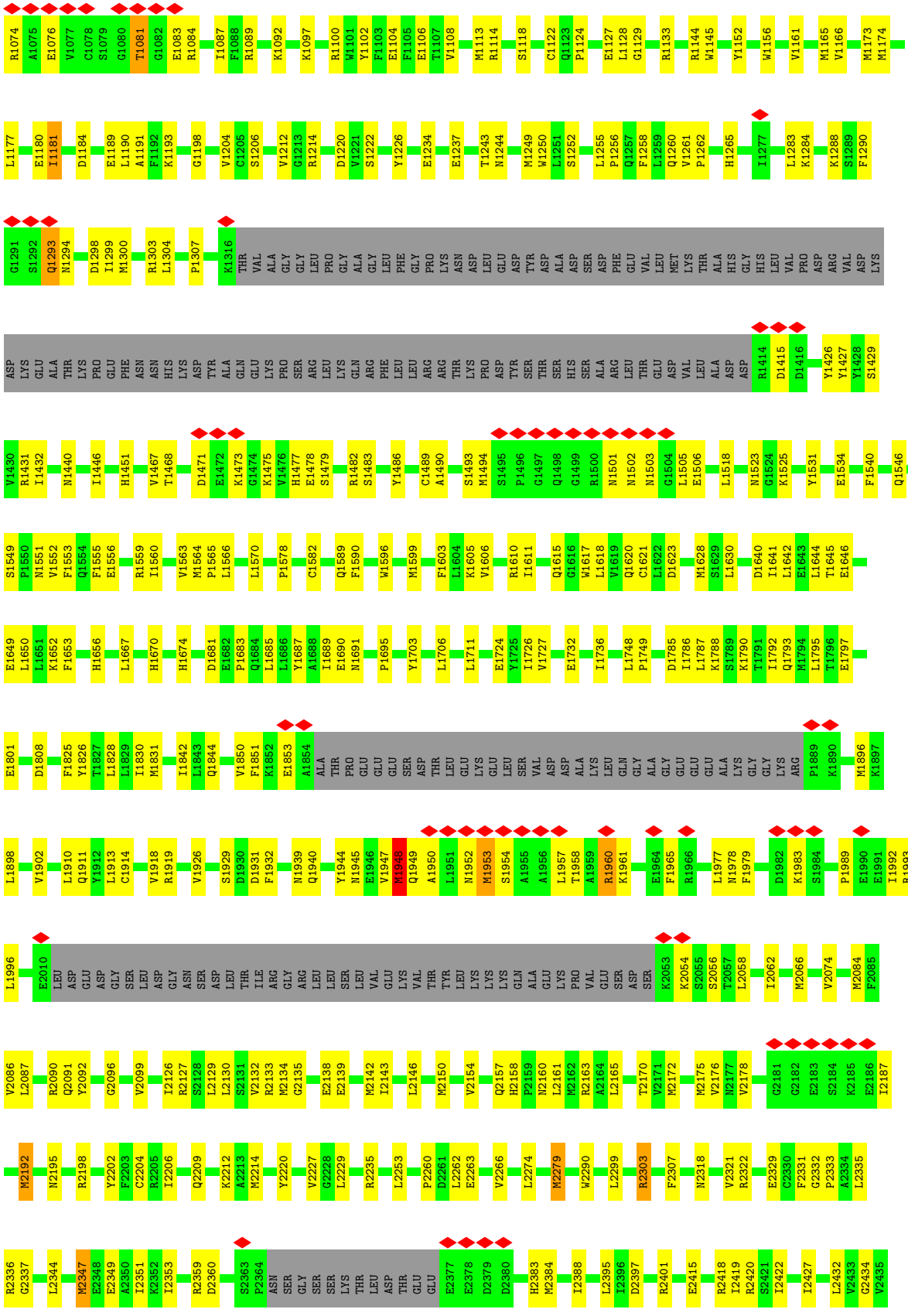


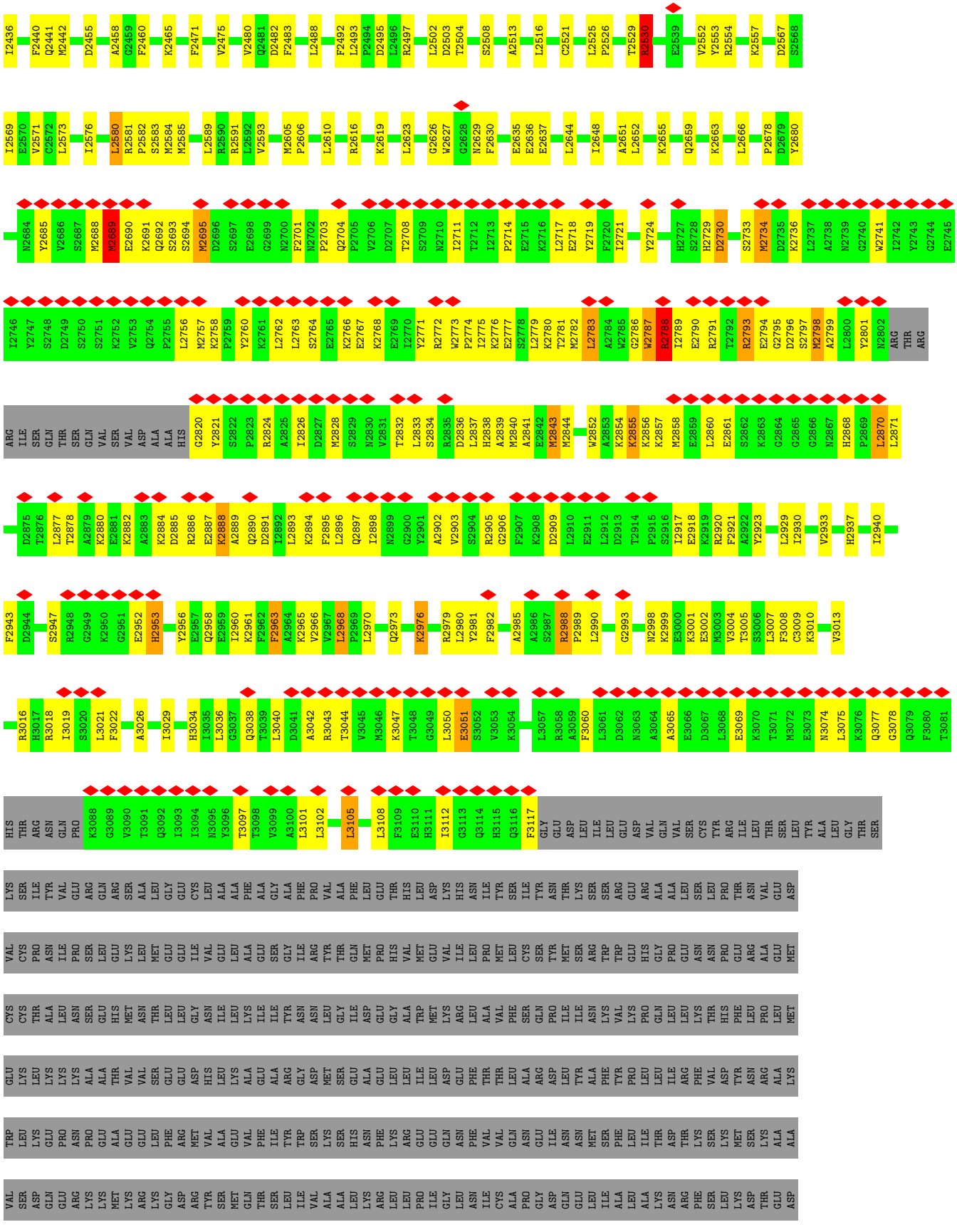


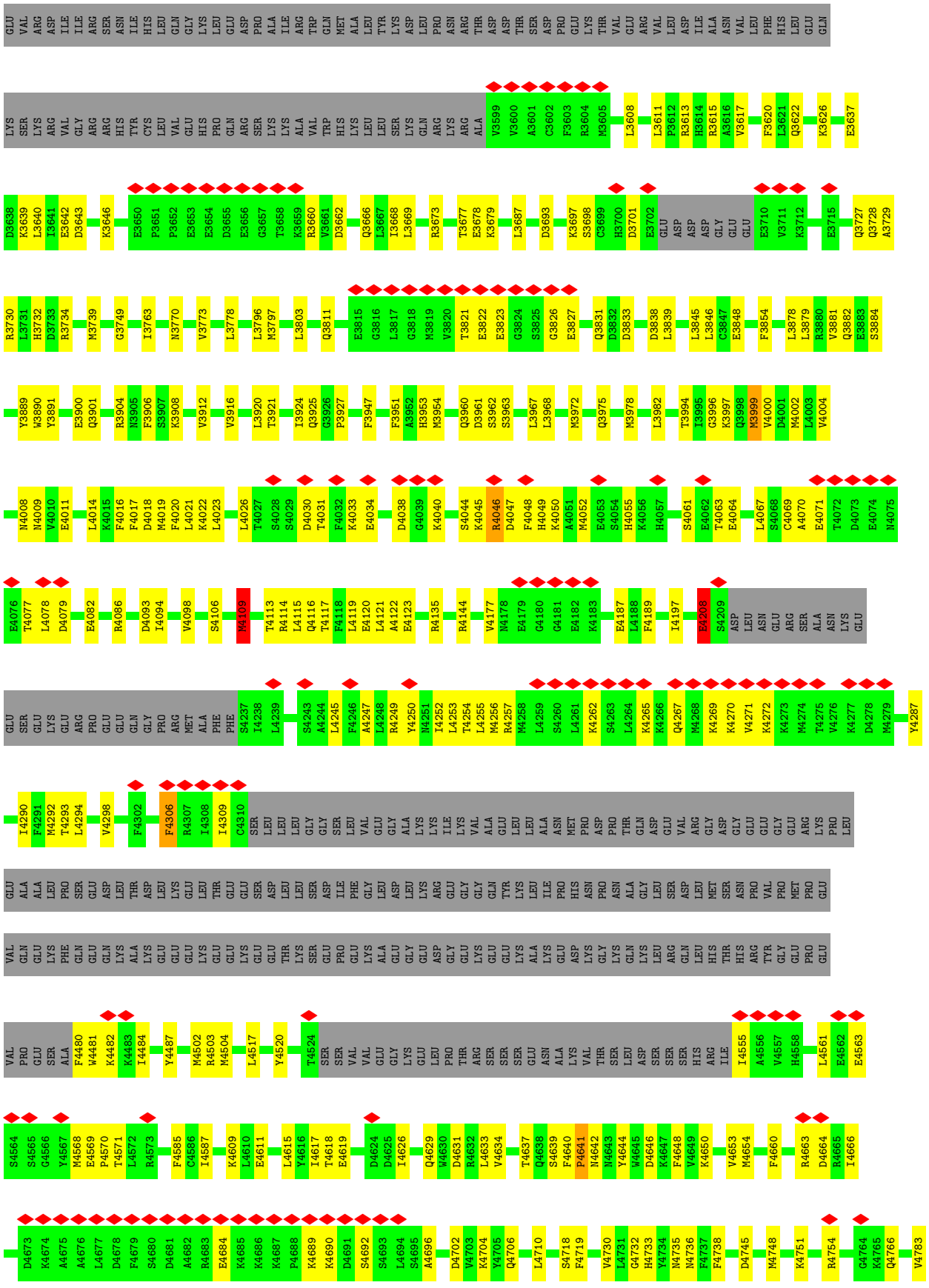
• Molecule 1: Ryanodine receptor 2

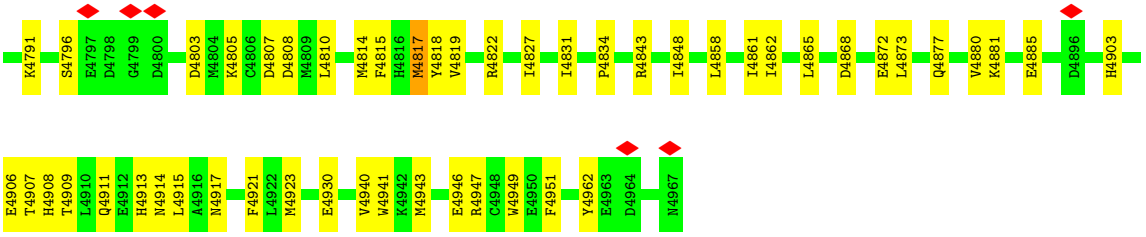
Chain B:




R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1084 I1087 F1088 R1089 K1092 K1097 R1100 W1101 Y1102 F1103 E1104 F1105 E1106 T1107 V1108 M1113 R1114 S1118 C1122 Q1123 P1124 E1127 L1128 G1129 R1133 R1144 W1145 Y1152 W1156 V1161 M1165 V1166 M1173 M1174
L1177 E1180 I1181 D1184 E1189 L1190 A1191 F1192 K1193 G1198 V1204 C1205 S1206 V1212 G1213 R1214 D1220 V1221 S1222 Y1226 E1234 E1237 T1243 N1244 M1249 W1250 L1251 S1252 L1255 P1256 Q1257 F1258 L1259 Q1260 V1261 P1262 H1265 I1277 L1283 K1284 K1288 S1289 F1290
G1291 S1292 Q1293 N1294 D1298 I1299 M1300 R1303 L1304 P1307 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS
ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LEU LYS GLN ARG ARG THR THR LYS PRO ASP ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1426 Y1427 Y1428 S1429
V1430 R1431 I1432 N1440 I1446 H1451 V1467 T1468 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 S1479 R1482 S1483 Y1486 C1489 A1490 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 E1506 L1518 N1523 G1524 K1525 Y1531 E1534 F1540 Q1546
S1549 P1550 N1551 V1552 F1553 Q1554 F1555 E1556 R1559 I1560 V1563 M1564 P1565 L1566 L1570 P1578 C1582 Q1589 F1590 W1596 M1599 F1603 L1604 K1605 V1606 R1610 I1611 Q1615 G1616 W1617 L1618 V1619 Q1620 C1621 L1622 D1623 M1628 S1629 L1630 D1640 I1641 L1642 E1643 L1644 T1645 E1646
E1649 L1650 L1651 K1652 F1653 H1656 L1667 H1670 H1674 D1681 E1682 P1683 Q1684 L1685 L1686 Y1687 A1688 I1689 E1690 N1691 P1695 Y1703 L1706 L1711 E1724 Y1725 I1726 V1727 E1732 I1736 L1748 P1749 D1785 I1786 L1787 K1788 S1789 K1790 T1791 I1792 Q1793 M1794 L1795 T1796 E1797
E1801 D1808 F1825 Y1826 T1827 L1828 L1829 I1830 M1831 I1842 L1843 Q1844 V1850 F1851 K1852 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 M1896 K1897
L1898 V1902 L1910 Q1911 Y1912 L1913 C1914 V1918 R1919 V1926 S1929 D1930 D1931 F1932 N1939 Q1940 Y1944 N1945 E1946 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 E1964 F1965 R1966 L1977 N1978 F1979 D1982 K1983 S1984 P1989 E1990 E1991 I1992 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 S2055 S2056 T2057 L2058 I2062 M2066 V2074 M2084 F2085
V2086 L2087 R2090 Q2091 Y2092 G2096 V2099 I2126 R2127 S2128 L2129 L2130 S2131 V2132 R2133 M2134 G2135 E2138 E2139 M2142 I2143 L2146 M2150 V2154 Q2157 H2158 P2159 N2160 L2161 M2162 R2163 A2164 L2165 T2170 V2171 M2172 M2175 V2176 N2177 V2178 G2181 G2182 E2183 S2184 K2185 E2186 I2187
M2192 N2195 R2198 Y2202 F2203 C2204 R2205 I2206 Q2209 K2212 A2213 M2214 Y2220 V2227 G2228 L2229 R2235 L2253 P2260 D2261 L2262 E2263 V2266 L2274 M2279 W2290 L2299 R2303 F2307 N2318 V2321 R2322 E2329 C2330 F2331 G2332 P2333 A2334 L2335
R2336 G2337 L2344 M2347 E2348 E2349 A2350 I2351 K2352 I2353 R2359 D2360 S2363 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 H2383 M2384 I2388 L2395 I2396 D2397 R2401 E2415 R2418 I2419 R2420 S2421 I2422 I2427 L2432 V2433 G2434 V2435

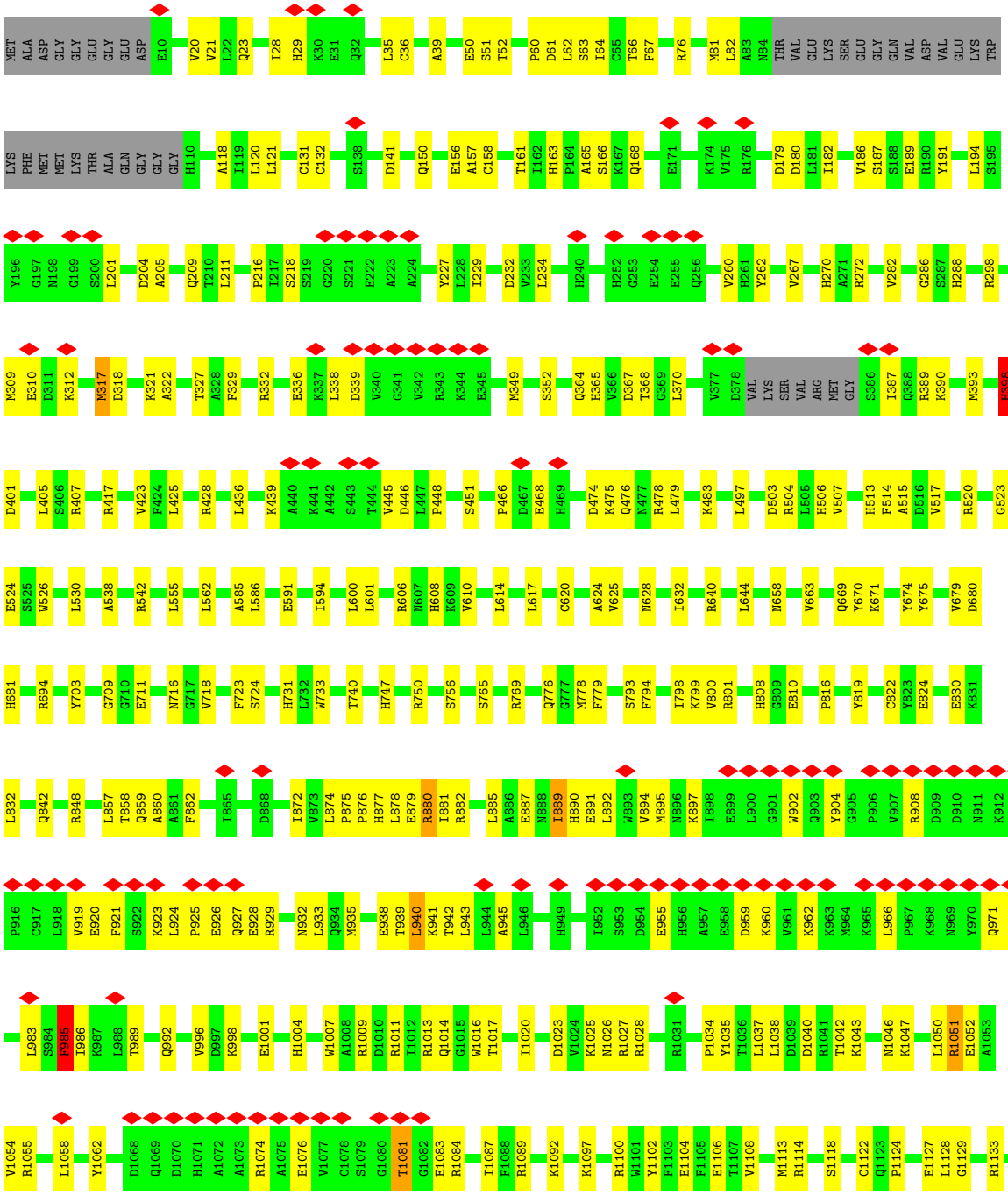

I2436 F2440 Q2441 M2442 D2455 A2458 G2459 F2460 K2465 F2471 V2475 V2480 Q2481 D2482 F2483 L2488 F2492 L2493 P2494 D2495 L2496 R2497 L2502 D2503 T2504 S2508 A2513 L2516 C2521 L2525 P2526 T2529 R2530 E2539 V2552 Y2553 R2554 K2557 D2567 S2568
I2569 E2570 V2571 C2572 L2573 I2576 L2580 R2581 P2582 S2583 M2584 M2585 L2589 R2590 R2591 L2592 V2593 M2605 P2606 L2610 R2616 K2619 L2623 G2626 W2627 G2628 N2629 F2630 E2635 E2636 E2637 L2644 I2648 A2651 L2652 K2655 Q2659 K2663 L2666 P2678 D2679 Y2680
W2684 Y2685 V2686 S2687 M2688 W2689 E2690 K2691 Q2692 S2693 S2694 M2695 D2696 S2697 E2698 G2699 N2700 F2701 N2702 P2703 Q2704 P2705 V2706 D2707 T2708 S2709 N2710 I2711 T2712 I2713 P2714 E2715 K2716 L2717 E2718 Y2719 F2720 I2721 Y2724 H2727 S2728 H2729 D2730 S2733 M2734 D2735 K2736 L2737 A2738 N2739 G2740 W2741 I2742 Y2743 G2744 E2745
I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759 Y2760 K2761 L2762 L2763 S2764 E2765 K2766 E2767 K2768 E2769 I2770 Y2771 R2772 W2773 P2774 I2775 K2776 E2777 S2778 L2779 K2780 T2781 M2782 L2783 A2784 W2785 G2786 W2787 R2788 I2789 E2790 R2791 T2792 R2793 E2794 G2795 D2796 S2797 M2798 A2799 L2800 Y2801 N2802 ARG THR ARG
ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823 R2824 A2825 I2826 D2827 M2828 S2829 N2830 V2831 T2832 L2833 S2834 R2835 D2836 L2837 H2838 A2839 M2840 A2841 E2842 M2843 M2844 W2852 A2853 K2854 K2855 K2856 K2857 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870 L2871
D2875 T2876 L2877 T2878 A2879 K2880 E2881 K2882 A2883 K2884 D2885 R2886 E2887 K2888 A2889 Q2890 D2891 I2892 L2893 K2894 F2895 L2896 Q2897 I2898 N2899 G2900 Y2901 A2902 V2903 S2904 R2905 G2906 F2907 K2908 D2909 L2910 E2911 L2912 D2913 T2914 P2915 S2916 I2917 E2918 K2919 R2920 F2921 A2922 Y2923 L2929 I2930 V2933 H2937 I2940
F2943 D2944 S2947 R2948 G2949 K2950 G2951 E2952 H2953 Y2956 E2957 Q2958 E2959 I2960 K2961 F2962 F2963 A2964 K2965 V2966 V2967 L2968 P2969 L2970 Q2973 K2976 R2979 L2980 Y2981 F2982 A2985 A2986 S2987 R2988 P2989 L2990 G2993 N2998 K2999 E3000 K3001 E3002 M3003 V3004 T3005 S3006 L3007 F3008 C3009 K3010 V3013
R3016 H3017 R3018 I3019 S3020 L3021 F3022 A3026 I3029 H3034 I3035 L3036 G3037 Q3038 T3039 L3040 D3041 A3042 R3043 T3044 V3045 M3046 K3047 T3048 G3049 L3050 E3051 S3052 V3053 K3054 L3057 R3058 A3059 F3060 L3061 D3062 N3063 A3064 A3065 E3066 D3067 L3068 E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 G3078 Q3079 F3080 T3081
HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 I3094 N3095 Y3096 T3097 T3098 V3099 A3100 L3101 L3102 L3105 L3108 F3109 E3110 H3111 I3112 G3113 Q3114 H3115 Q3116 F3117 GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER
LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PRO VAL ALA PHE LEU GLU THR HIS LEU ASP LYS HIS ASN ILE TYR SER ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU SER SER LEU PRO THR ASN VAL ASP
VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL GLU LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL ILE LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN PRO GLU ARG ALA GLU MET
CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA MET THR LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET
GLU LYS LEU LYS LYS ALA ALA THR VAL VAL SER GLU GLU ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU GLU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU LEU ILE ARG THR PHE VAL ASP TYR ASN ARG GLU ALA LYS
TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA
VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP

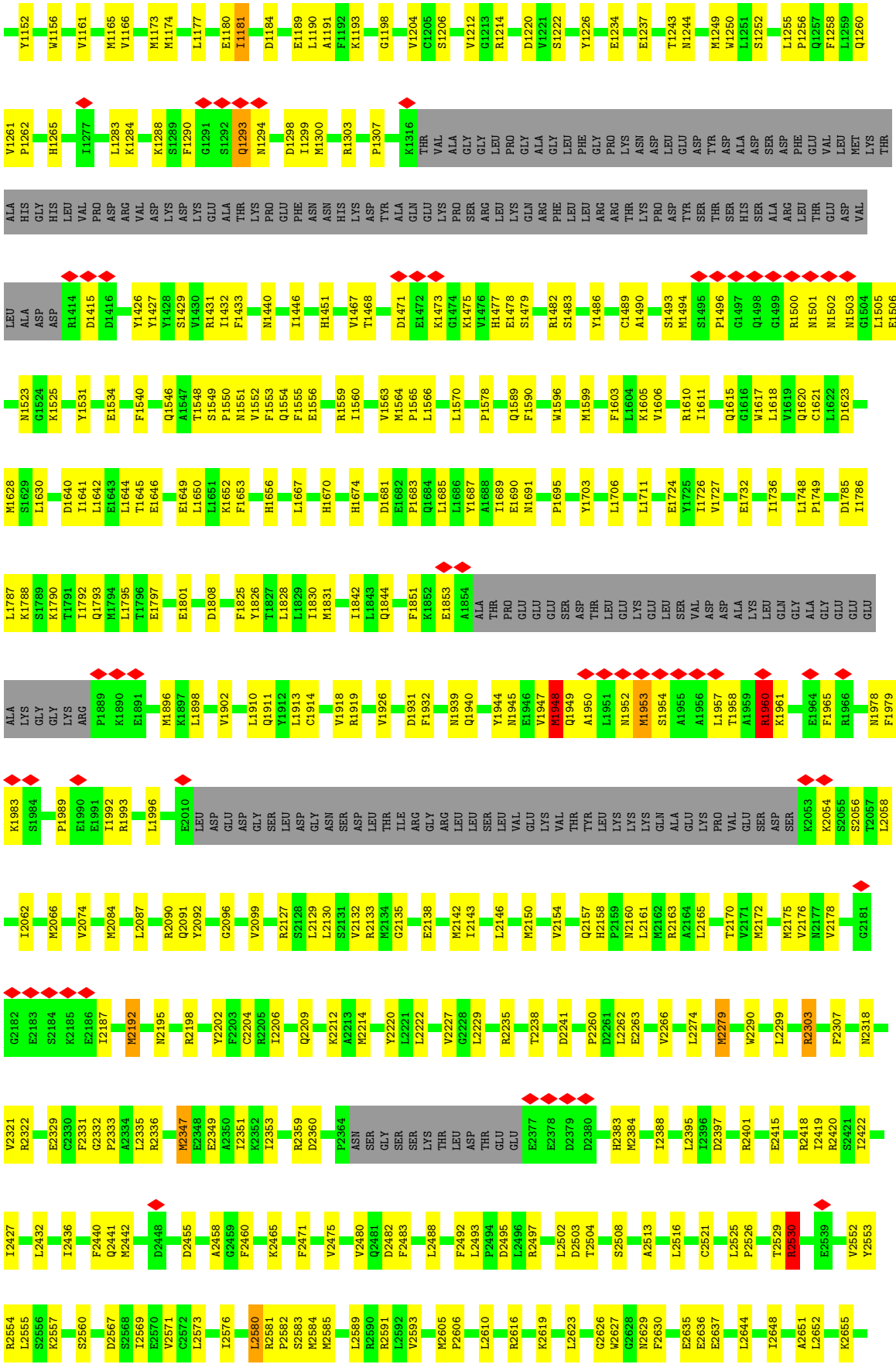


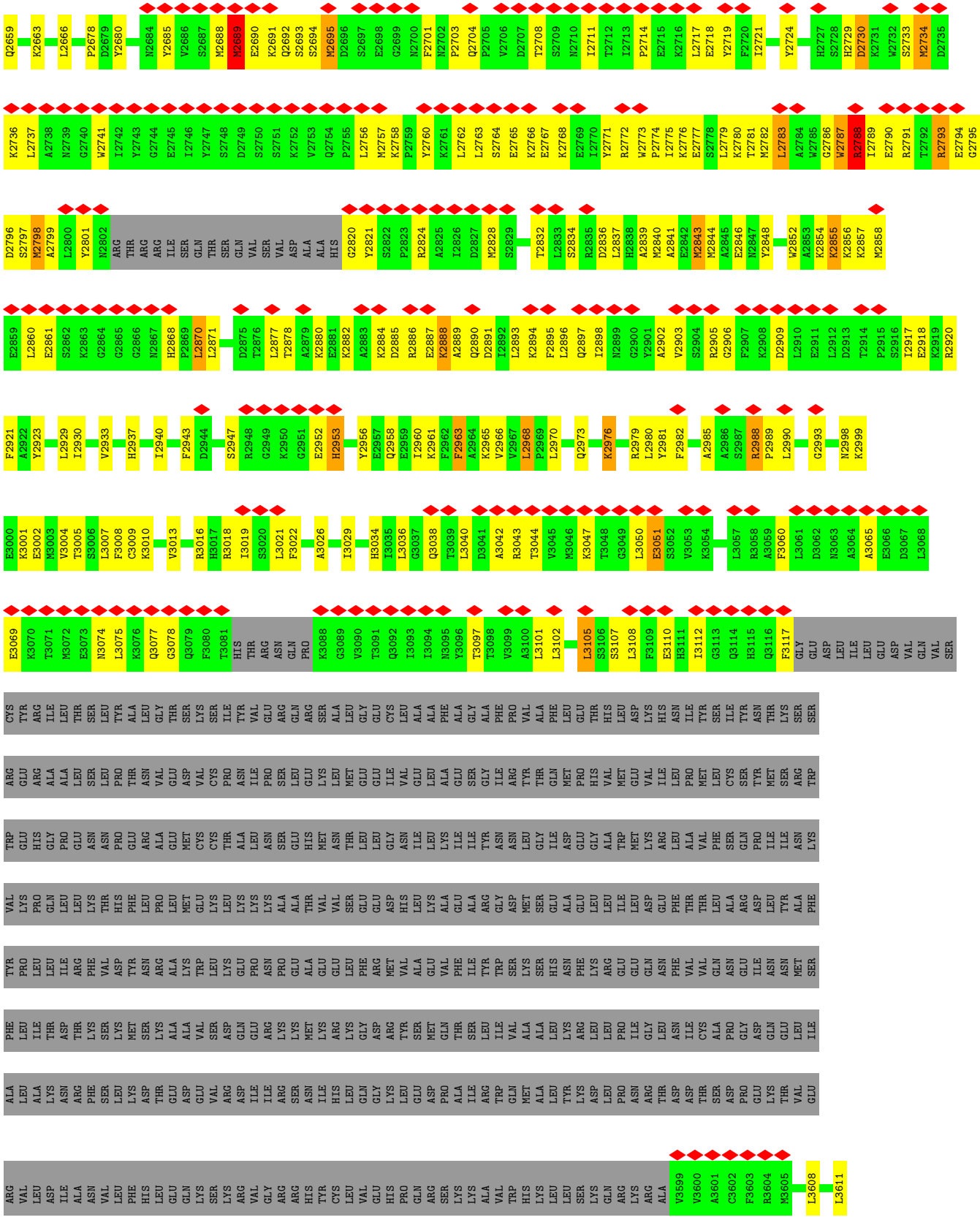


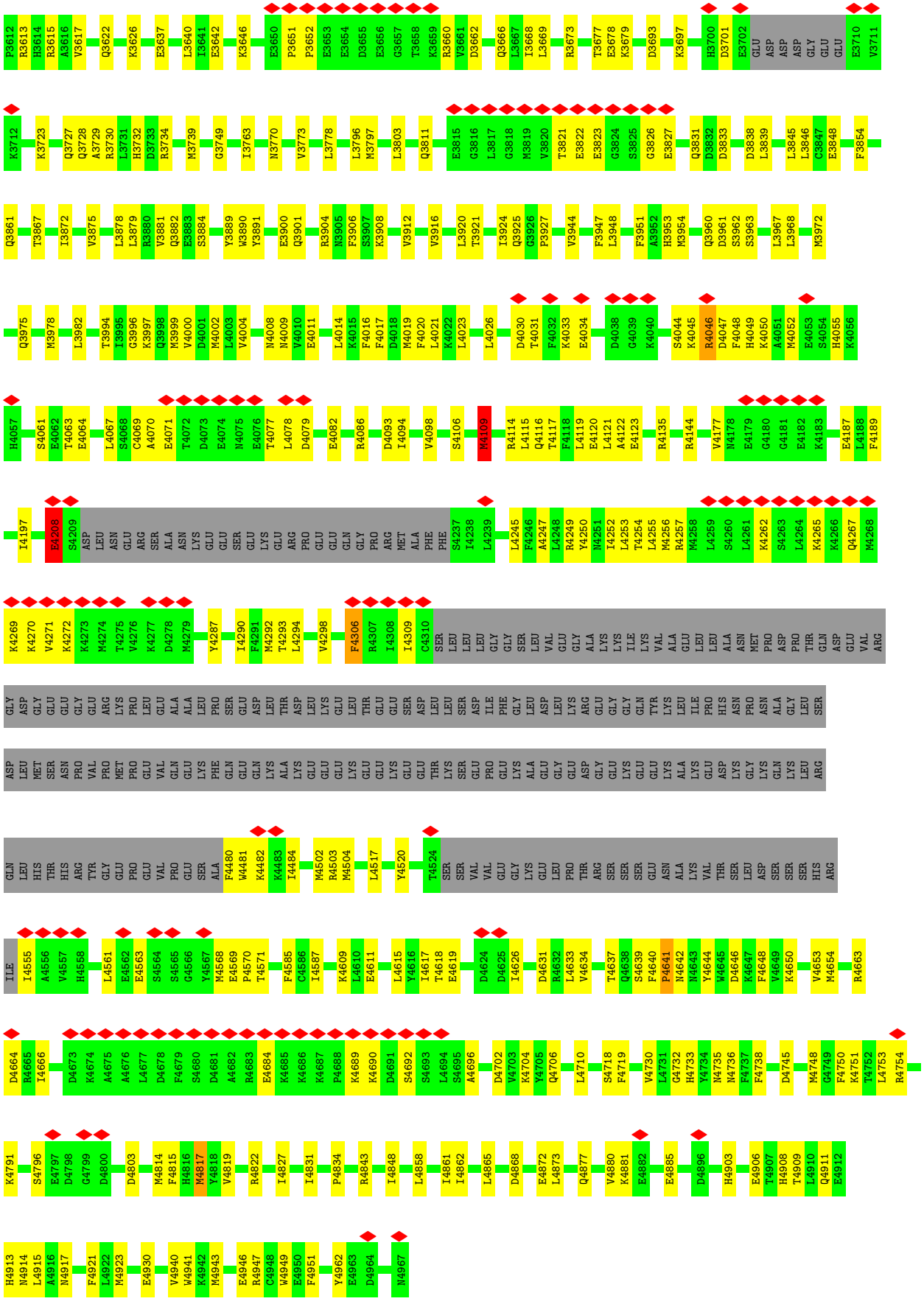
• Molecule 1: Ryanodine receptor 2

Chain C:



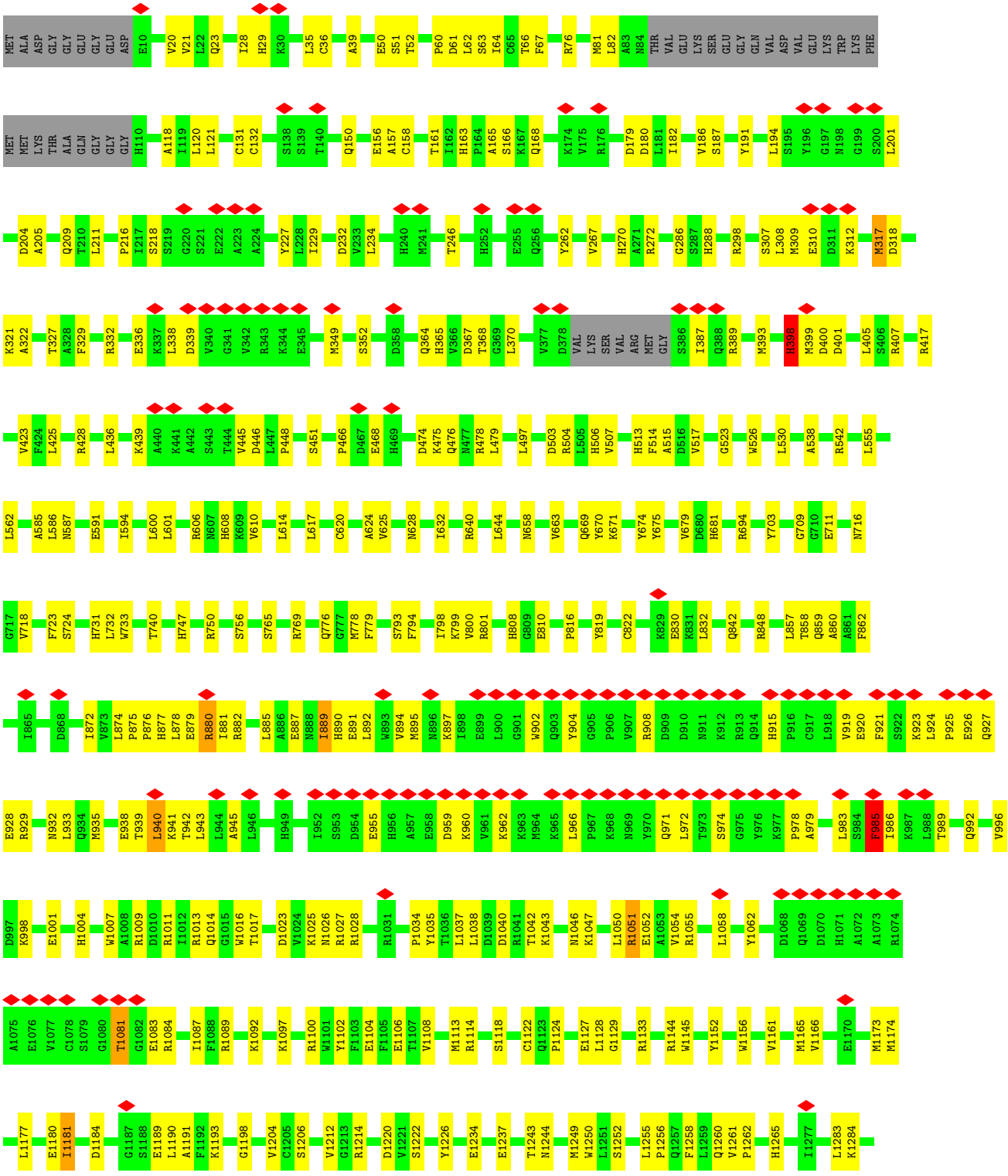

Y1152 W1156 V1161 M1165 V1166 M1173 M1174 L1177 E1180 I1181 D1184 E1189 L1190 A1191 F1192 K1193 G1198 V1204 C1205 S1206 V1212 G1213 R1214 D1220 V1221 S1222 Y1226 E1234 E1237 T1243 N1244 M1249 W1250 L1251 S1252 L1255 P1256 Q1257 F1258 L1259 Q1260
V1261 P1262 H1265 I1277 L1283 K1284 K1288 S1289 F1290 G1291 S1292 Q1293 N1294 D1298 I1299 M1300 R1303 P1307 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR
ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO GLU THR LEU GLU ASP
LEU ALA ASP ASP R1414 D1415 D1416 Y1426 Y1427 Y1428 S1429 V1430 R1431 I1432 F1433 N1440 I1446 H1451 V1467 T1468 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 S1479 R1482 S1483 Y1486 C1489 A1490 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 E1506 L1518
N1523 G1524 K1525 Y1531 E1534 F1540 Q1546 A1547 T1548 S1549 P1550 N1551 V1552 F1553 Q1554 F1555 E1556 R1559 I1560 V1563 M1564 P1565 L1566 L1570 P1578 Q1589 F1590 W1596 M1599 F1603 L1604 K1605 V1606 R1610 I1611 Q1615 G1616 W1617 L1618 V1619 Q1620 C1621 L1622 D1623
M1628 S1629 L1630 D1640 I1641 L1642 E1643 L1644 T1645 E1646 E1649 L1650 L1651 K1652 F1653 H1656 L1667 H1670 H1674 D1681 E1682 P1683 Q1684 L1685 L1686 Y1687 A1688 I1689 E1690 N1691 P1695 Y1703 L1706 L1711 E1724 Y1725 I1726 V1727 E1732 L1736 L1748 P1749 D1785 I1786
L1787 K1788 S1789 K1790 T1791 I1792 Q1793 M1794 L1795 T1796 E1797 E1801 D1808 F1825 Y1826 T1827 L1828 L1829 I1830 M1831 I1842 L1843 Q1844 F1851 K1852 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU
ALA LYS GLY GLY LYS ARG P1889 K1890 E1891 M1896 K1897 L1898 V1902 L1910 Q1911 Y1912 L1913 C1914 V1918 R1919 V1926 D1931 F1932 N1939 Q1940 Y1944 N1945 E1946 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 E1964 F1965 R1966 N1978 F1979 D1982
K1983 S1984 P1989 E1990 E1991 I1992 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 S2055 S2056 T2057 L2058
I2062 M2066 V2074 M2084 L2087 R2090 Q2091 Y2092 G2096 V2099 R2127 S2128 L2129 L2130 S2131 V2132 R2133 M2134 G2135 E2138 M2142 I2143 L2146 M2150 V2154 Q2157 H2158 P2159 N2160 L2161 M2162 R2163 A2164 L2165 T2170 V2171 M2172 M2175 V2176 N2177 V2178 G2181
G2182 E2183 S2184 K2185 E2186 I2187 M2192 N2195 R2198 Y2202 F2203 C2204 R2205 I2206 Q2209 K2212 A2213 M2214 Y2220 L2221 L2222 V2227 G2228 L2229 R2235 T2238 D2241 P2260 D2261 L2262 E2263 V2266 L2274 M2279 W2290 L2299 R2303 F2307 N2318
V2321 R2322 E2329 C2330 F2331 G2332 P2333 A2334 L2335 R2336 M2347 E2348 E2349 A2350 I2351 K2352 I2353 R2359 D2360 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 H2383 M2384 I2388 L2395 I2396 D2397 R2401 E2415 R2418 I2419 R2420 S2421 I2422
I2427 L2432 I2436 F2440 Q2441 M2442 D2448 D2455 A2458 G2459 F2460 K2465 F2471 V2475 V2480 Q2481 D2482 F2483 L2488 F2492 L2493 P2494 D2495 L2496 R2497 L2502 D2503 T2504 S2508 A2513 L2516 C2521 L2525 P2526 T2529 R2530 E2539 V2552 Y2553
R2554 L2555 S2556 K2557 S2560 D2567 S2568 I2569 E2570 V2571 C2572 L2573 I2576 L2580 R2581 P2582 S2583 M2584 M2585 L2589 R2590 R2591 L2592 V2593 M2605 P2606 L2610 R2616 K2619 L2623 G2626 W2627 G2628 N2629 F2630 E2635 E2636 E2637 L2644 I2648 A2651 L2652 K2655

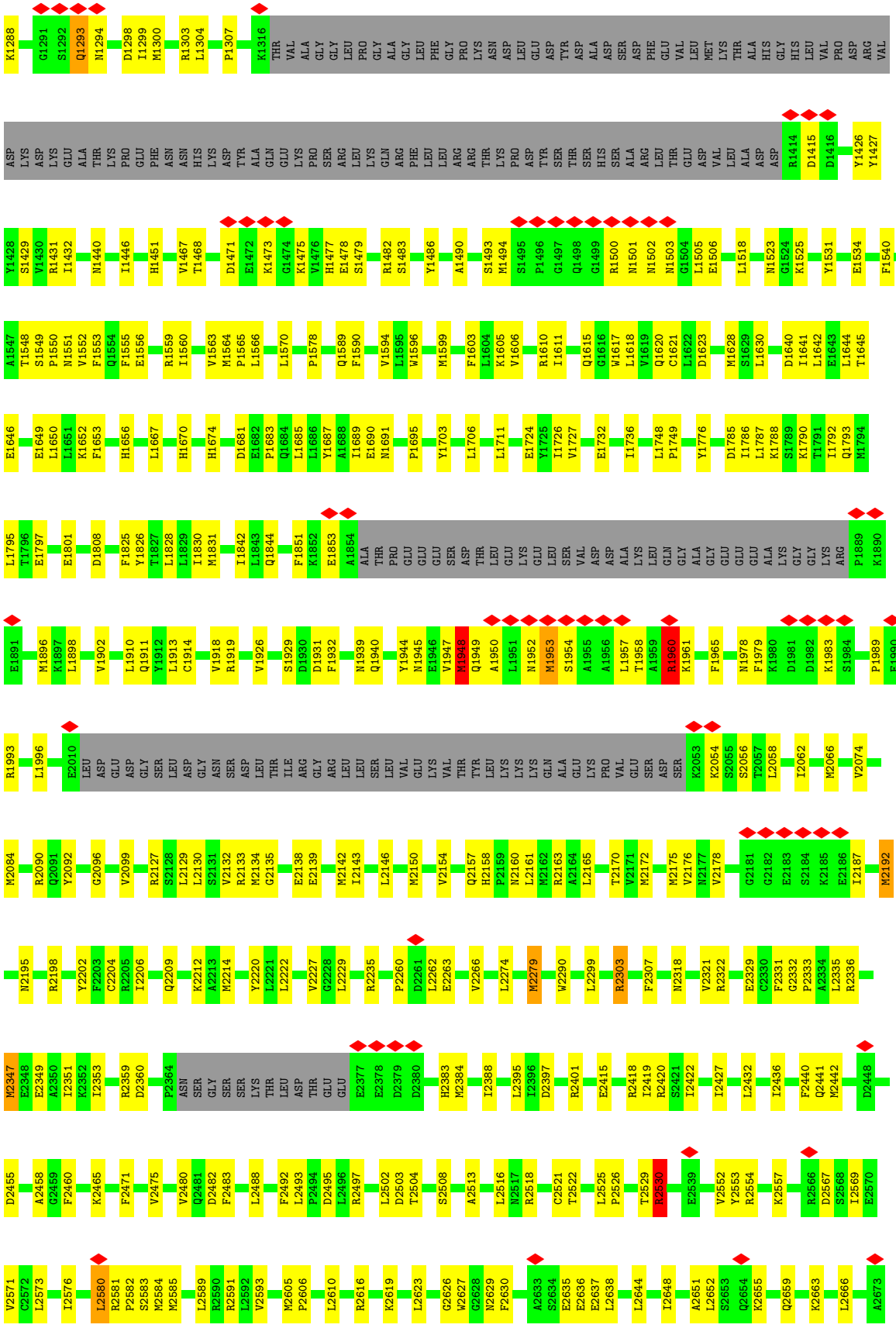

Q2659 K2663 L2666 P2678 D2679 Y2680 N2684 Y2685 V2686 S2687 M2688 M2689 E2690 K2691 Q2692 S2693 S2694 M2695 D2696 S2697 E2698 G2699 N2700 F2701 N2702 P2703 Q2704 P2705 V2706 D2707 T2708 S2709 N2710 I2711 T2712 I2713 P2714 E2715 K2716 L2717 E2718 Y2719 F2720 I2721 Y2724 H2727 S2728 H2729 D2730 K2731 W2732 S2733 M2734 D2735
K2736 L2737 A2738 N2739 G2740 W2741 I2742 Y2743 G2744 E2745 I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759 Y2760 K2761 L2762 L2763 S2764 E2765 K2766 E2767 K2768 E2769 I2770 Y2771 R2772 W2773 P2774 I2775 K2776 E2777 S2778 L2779 K2780 T2781 M2782 L2783 A2784 W2785 G2786 W2787 R2788 I2789 E2790 R2791 T2792 R2793 E2794 G2795
D2796 S2797 M2798 A2799 L2800 Y2801 N2802 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823 R2824 A2825 I2826 D2827 M2828 S2829 T2832 L2833 S2834 R2835 D2836 L2837 H2838 A2839 M2840 A2841 E2842 M2843 M2844 A2845 E2846 N2847 Y2848 W2852 A2853 K2854 K2855 K2856 K2857 M2858
E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870 L2871 D2875 T2876 L2877 T2878 A2879 K2880 E2881 K2882 A2883 K2884 D2885 R2886 E2887 K2888 A2889 Q2890 D2891 I2892 L2893 K2894 F2895 L2896 Q2897 I2898 N2899 G2900 Y2901 A2902 V2903 S2904 R2905 G2906 F2907 K2908 D2909 L2910 E2911 L2912 D2913 T2914 P2915 S2916 I2917 E2918 K2919 R2920
F2921 A2922 Y2923 L2929 I2930 V2933 H2937 I2940 F2943 D2944 S2947 R2948 G2949 K2950 G2951 E2952 H2953 Y2956 E2957 Q2958 E2959 I2960 K2961 F2962 F2963 A2964 K2965 V2966 V2967 L2968 P2969 L2970 Q2973 K2976 R2979 L2980 Y2981 F2982 A2985 A2986 S2987 R2988 P2989 L2990 G2993 N2998 K2999
E3000 K3001 E3002 M3003 V3004 T3005 S3006 L3007 F3008 C3009 K3010 V3013 R3016 H3017 R3018 I3019 S3020 L3021 F3022 A3026 I3029 H3034 I3035 L3036 G3037 Q3038 T3039 L3040 D3041 A3042 R3043 T3044 V3045 M3046 K3047 T3048 G3049 L3050 E3051 S3052 V3053 K3054 L3057 R3058 A3059 F3060 L3061 D3062 N3063 A3064 A3065 E3066 D3067 L3068
E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 I3094 N3095 Y3096 T3097 T3098 V3099 A3100 L3101 L3102 L3105 S3106 S3107 L3108 F3109 E3110 H3111 I3112 G3113 Q3114 H3115 Q3116 F3117 GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL SER
CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO VAL ALA PHE LEU GLU THR HIS LEU ASP LYS HIS ASN ILE TYR SER ILE TYR ASN THR LYS SER
ARG GLU ARG ALA ALA LEU SER LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU GLU LYS LEU MET GLU GLU ILE VAL GLU LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL ILE LEU PRO MET LEU CYS SER TYR MET LEU SER ARG TRP
TRP GLU HIS GLY PRO GLU ASN ASN PRO GLU ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS
VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS ALA ALA THR VAL VAL SER GLU GLU HIS GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU LEU ALA ARG ASP LEU TYR ALA PHE
TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLN ASN PHE VAL VAL GLN ASN ASN GLU ILE ASN ASN MET SER
PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE
ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA ALA LEU TYR LYS ASP LEU PRO ASN ARG THR ASP ASP THR SER ASP PRO GLU LYS THR VAL GLU
ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA V3599 V3600 A3601 C3602 F3603 R3604 M3605 L3608 L3611

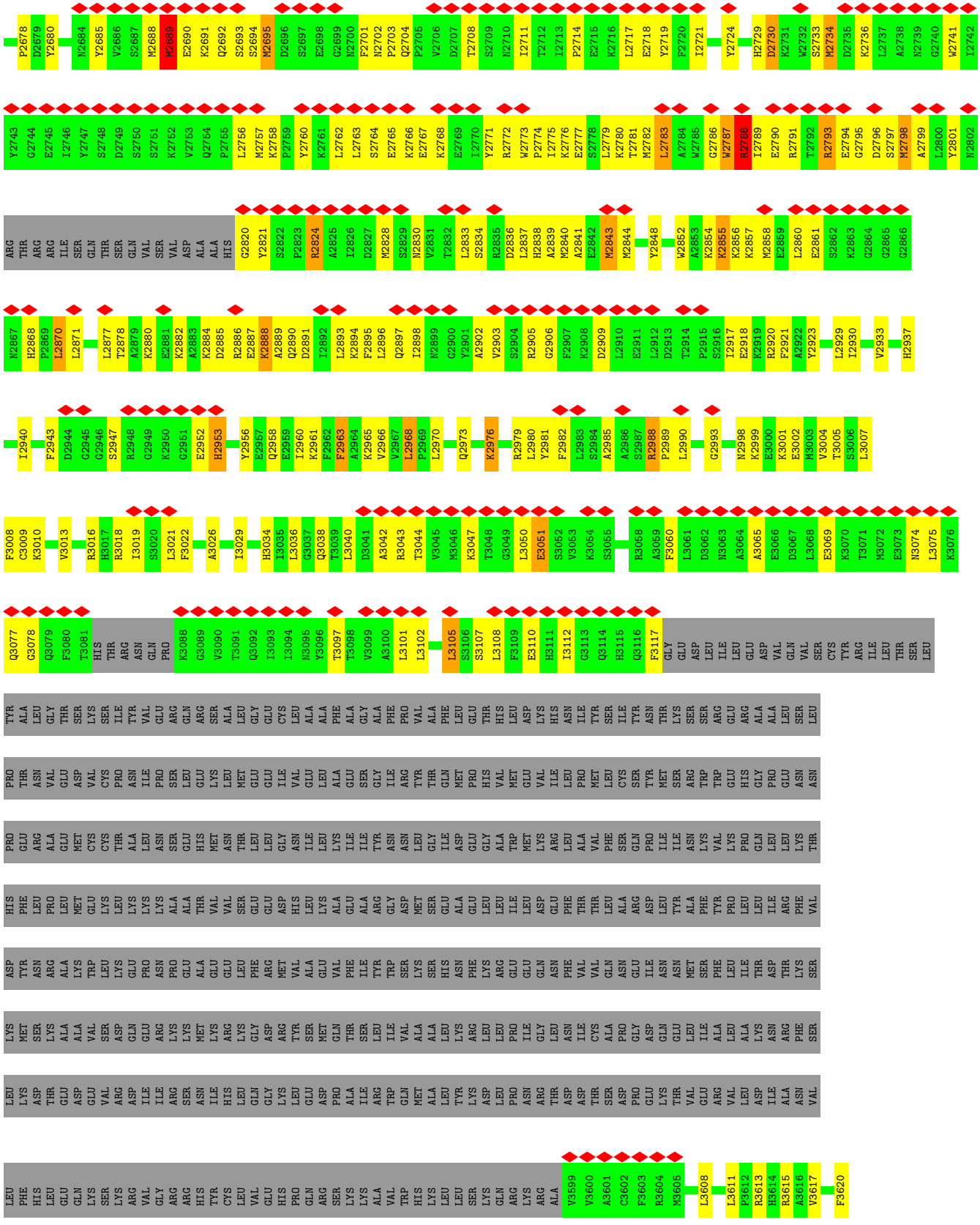


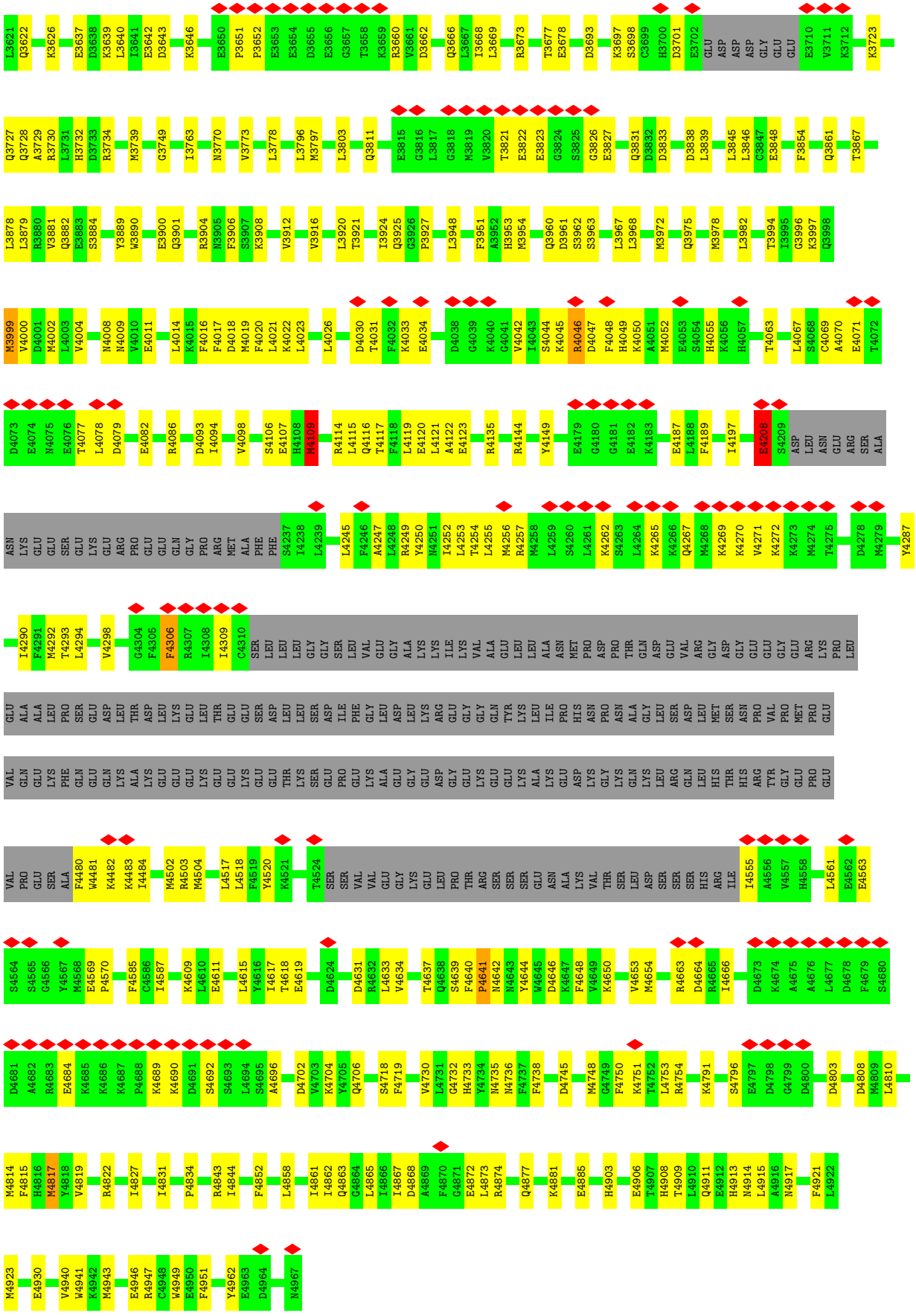
• Molecule 1: Ryanodine receptor 2

Chain D:



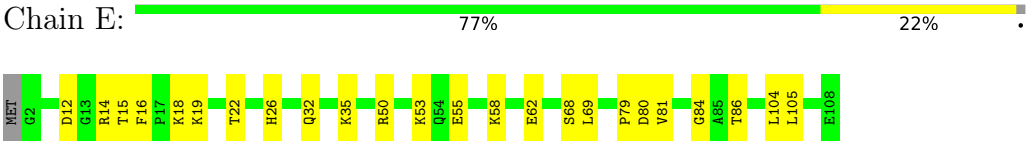



P2678 D2679 Y2680 N2684 Y2685 V2686 S2687 M2688 M2689 E2690 K2691 Q2692 S2693 S2694 M2695 D2696 S2697 E2698 G2699 N2700 F2701 N2702 P2703 Q2704 P2705 V2706 D2707 T2708 S2709 N2710 I2711 T2712 I2713 P2714 E2715 K2716 L2717 E2718 Y2719 F2720 I2721 Y2724 H2729 D2730 K2731 W2732 S2733 M2734 D2735 K2736 L2737 A2738 N2739 G2740 W2741 I2742
Y2743 G2744 E2745 I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759 Y2760 K2761 L2762 L2763 S2764 E2765 K2766 E2767 K2768 E2769 I2770 Y2771 R2772 W2773 P2774 I2775 K2776 E2777 S2778 L2779 K2780 T2781 M2782 L2783 A2784 W2785 G2786 W2787 R2788 I2789 E2790 R2791 T2792 R2793 E2794 G2795 D2796 S2797 M2798 A2799 L2800 Y2801 N2802
ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823 R2824 A2825 I2826 D2827 M2828 S2829 N2830 V2831 T2832 L2833 S2834 R2835 D2836 L2837 H2838 A2839 M2840 A2841 E2842 M2843 M2844 Y2848 W2852 A2853 K2854 K2855 K2856 K2857 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866
N2867 H2868 P2869 L2870 L2871 L2877 T2878 A2879 K2880 E2881 K2882 A2883 K2884 D2885 R2886 E2887 K2888 A2889 Q2890 D2891 I2892 L2893 K2894 F2895 L2896 Q2897 I2898 N2899 G2900 Y2901 A2902 V2903 S2904 R2905 G2906 F2907 K2908 D2909 L2910 E2911 L2912 D2913 T2914 P2915 S2916 I2917 E2918 K2919 R2920 F2921 A2922 Y2923 L2929 I2930 V2933 H2937
I2940 F2943 D2944 G2945 G2946 S2947 R2948 G2949 K2950 G2951 E2952 H2953 Y2956 E2957 Q2958 E2959 I2960 K2961 F2962 F2963 A2964 K2965 V2966 V2967 L2968 P2969 L2970 Q2973 K2976 R2979 L2980 Y2981 F2982 L2983 S2984 A2985 A2986 S2987 R2988 P2989 L2990 G2993 N2998 K2999 E3000 K3001 E3002 M3003 V3004 T3005 S3006 L3007
F3008 C3009 K3010 V3013 R3016 H3017 R3018 I3019 S3020 L3021 F3022 A3026 I3029 H3034 I3035 L3036 G3037 Q3038 T3039 L3040 D3041 A3042 R3043 T3044 V3045 M3046 K3047 T3048 G3049 L3050 E3051 S3052 V3053 K3054 S3055 R3058 A3059 F3060 L3061 D3062 N3063 A3064 A3065 E3066 D3067 L3068 E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076
Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 I3094 N3095 Y3096 T3097 T3098 V3099 A3100 L3101 L3102 L3105 S3106 S3107 L3108 F3109 E3110 H3111 I3112 G3113 Q3114 H3115 Q3116 F3117 GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU
TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO VAL ALA PHE LEU GLU THR HIS LEU ASP LYS HIS ASN ILE TYR SER ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU SER LEU
PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL GLU LEU ALA GLU GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL ILE LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN
PRO GLU ARG ALA GLU MET CYS CYS THR ALA LEU LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR
HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS LYS ALA ALA THR VAL VAL SER GLU GLU ASP HIS LEU LEU LYS ALA GLU GLY ASP MET SER GLU ALA GLU LEU LEU LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU LEU ILE ARG PHE VAL
ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER
LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER
LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP LEU ASN ALA VAL
LEU PHE HIS LEU GLU GLN LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ALA V3599 V3600 A3601 C3602 F3603 R3604 M3605 L3608 L3611 P3612 R3613 H3614 R3615 A3616 V3617 F3620



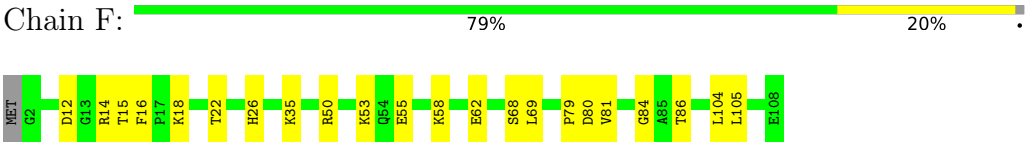
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



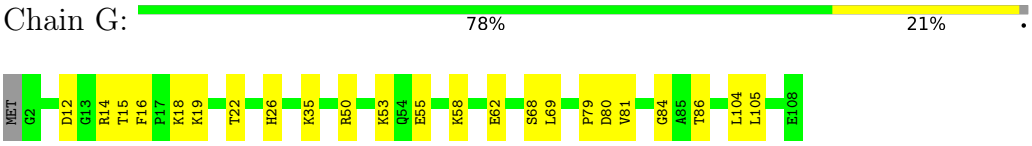
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



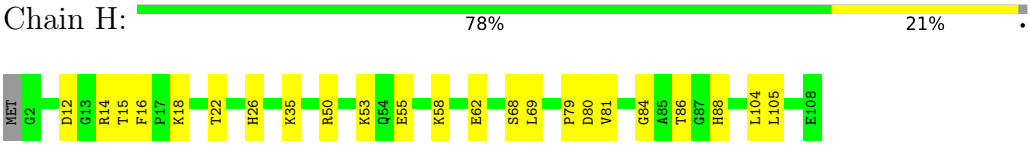
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

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	55886	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)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.564	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	431.36, 431.36, 431.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8425, 0.8425, 0.8425	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.27	1/32738 (0.0%)	0.55	17/44213 (0.0%)
1	B	0.27	1/32738 (0.0%)	0.55	17/44213 (0.0%)
1	C	0.27	1/32738 (0.0%)	0.54	17/44213 (0.0%)
1	D	0.27	1/32738 (0.0%)	0.55	17/44213 (0.0%)
2	E	0.27	0/834	0.53	0/1123
2	F	0.27	0/834	0.53	0/1123
2	G	0.27	0/834	0.53	0/1123
2	H	0.27	0/834	0.53	0/1123
All	All	0.27	4/134288 (0.0%)	0.54	68/181344 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2787	TRP	CB-CG	-6.00	1.39	1.50
1	D	2787	TRP	CB-CG	-6.00	1.39	1.50
1	A	2787	TRP	CB-CG	-5.99	1.39	1.50
1	C	2787	TRP	CB-CG	-5.98	1.39	1.50

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2279	MET	CB-CG-SD	10.74	144.62	112.40
1	C	2279	MET	CB-CG-SD	10.74	144.61	112.40
1	B	2279	MET	CB-CG-SD	10.73	144.60	112.40
1	D	2279	MET	CB-CG-SD	10.73	144.58	112.40
1	D	2279	MET	CA-CB-CG	10.43	131.03	113.30
1	B	2279	MET	CA-CB-CG	10.42	131.02	113.30
1	C	2279	MET	CA-CB-CG	10.42	131.01	113.30
1	A	2279	MET	CA-CB-CG	10.41	131.00	113.30
1	D	4208	GLU	CA-CB-CG	7.96	130.91	113.40
1	C	4208	GLU	CA-CB-CG	7.95	130.89	113.40
1	A	4208	GLU	CA-CB-CG	7.94	130.87	113.40
1	B	4208	GLU	CA-CB-CG	7.93	130.86	113.40
1	C	2788	ARG	CB-CG-CD	7.83	131.96	111.60
1	B	2788	ARG	CB-CG-CD	7.82	131.92	111.60
1	A	2788	ARG	CB-CG-CD	7.80	131.89	111.60
1	D	2788	ARG	CB-CG-CD	7.79	131.87	111.60
1	C	2689	MET	CA-CB-CG	7.59	126.21	113.30
1	B	2689	MET	CA-CB-CG	7.59	126.20	113.30
1	D	2689	MET	CA-CB-CG	7.59	126.20	113.30
1	A	2689	MET	CA-CB-CG	7.57	126.17	113.30
1	D	4109	MET	CA-CB-CG	7.00	125.19	113.30
1	C	4109	MET	CA-CB-CG	6.97	125.15	113.30
1	B	4109	MET	CA-CB-CG	6.96	125.14	113.30
1	A	4109	MET	CA-CB-CG	6.96	125.14	113.30
1	D	940	LEU	CA-CB-CG	6.82	130.99	115.30
1	C	940	LEU	CA-CB-CG	6.82	130.97	115.30
1	A	940	LEU	CA-CB-CG	6.79	130.92	115.30
1	B	940	LEU	CA-CB-CG	6.79	130.92	115.30
1	D	2783	LEU	CA-CB-CG	6.45	130.14	115.30
1	A	2783	LEU	CA-CB-CG	6.45	130.14	115.30
1	C	2783	LEU	CA-CB-CG	6.45	130.14	115.30
1	B	2783	LEU	CA-CB-CG	6.42	130.06	115.30
1	C	1948	MET	CB-CG-SD	6.32	131.36	112.40
1	B	1948	MET	CB-CG-SD	6.31	131.33	112.40
1	D	1948	MET	CB-CG-SD	6.31	131.32	112.40
1	A	1948	MET	CB-CG-SD	6.30	131.31	112.40
1	D	2530	ARG	CB-CG-CD	6.28	127.93	111.60
1	B	2530	ARG	CB-CG-CD	6.28	127.93	111.60
1	C	2530	ARG	CB-CG-CD	6.28	127.92	111.60
1	A	2530	ARG	CB-CG-CD	6.26	127.88	111.60
1	B	1051	ARG	CB-CG-CD	-5.89	96.28	111.60
1	D	1051	ARG	CB-CG-CD	-5.88	96.32	111.60
1	C	1051	ARG	CB-CG-CD	-5.87	96.33	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1051	ARG	CB-CG-CD	-5.87	96.34	111.60
1	D	2788	ARG	CG-CD-NE	5.85	124.08	111.80
1	A	2788	ARG	CG-CD-NE	5.83	124.05	111.80
1	C	2788	ARG	CG-CD-NE	5.83	124.04	111.80
1	B	2788	ARG	CG-CD-NE	5.83	124.03	111.80
1	A	985	PHE	CB-CG-CD2	5.81	124.86	120.80
1	B	985	PHE	CB-CG-CD2	5.77	124.84	120.80
1	C	985	PHE	CB-CG-CD2	5.76	124.83	120.80
1	D	985	PHE	CB-CG-CD2	5.75	124.83	120.80
1	D	2788	ARG	CA-CB-CG	-5.54	101.21	113.40
1	A	2788	ARG	CA-CB-CG	-5.54	101.21	113.40
1	B	2788	ARG	CA-CB-CG	-5.53	101.24	113.40
1	C	2788	ARG	CA-CB-CG	-5.52	101.25	113.40
1	D	399	MET	CA-CB-CG	5.50	122.66	113.30
1	A	399	MET	CA-CB-CG	5.49	122.64	113.30
1	A	1960	ARG	CA-CB-CG	-5.49	101.32	113.40
1	D	1960	ARG	CA-CB-CG	-5.48	101.34	113.40
1	C	399	MET	CA-CB-CG	5.48	122.61	113.30
1	B	399	MET	CA-CB-CG	5.47	122.60	113.30
1	B	1960	ARG	CA-CB-CG	-5.47	101.36	113.40
1	C	1960	ARG	CA-CB-CG	-5.47	101.37	113.40
1	C	985	PHE	CB-CG-CD1	-5.30	117.09	120.80
1	D	985	PHE	CB-CG-CD1	-5.28	117.10	120.80
1	A	985	PHE	CB-CG-CD1	-5.25	117.12	120.80
1	B	985	PHE	CB-CG-CD1	-5.25	117.12	120.80

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2530	ARG	Sidechain
1	A	2788	ARG	Sidechain
1	A	398	HIS	Peptide
1	B	2530	ARG	Sidechain
1	B	2788	ARG	Sidechain
1	B	398	HIS	Peptide
1	C	2530	ARG	Sidechain
1	C	2788	ARG	Sidechain
1	C	398	HIS	Peptide
1	D	2530	ARG	Sidechain
1	D	2788	ARG	Sidechain
1	D	398	HIS	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	32032	0	31689	830	0
1	B	32032	0	31689	827	0
1	C	32032	0	31689	812	0
1	D	32032	0	31689	815	0
2	E	818	0	821	14	0
2	F	818	0	821	12	0
2	G	818	0	821	13	0
2	H	818	0	821	13	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	0	0
4	B	62	0	24	0	0
4	C	62	0	24	0	0
4	D	62	0	24	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	131656	0	130136	3262	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (3262) 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:4279:MET:HE2	1:B:4487:TYR:HD1	1.30	0.93
1:D:2857:LYS:HE3	1:D:2871:LEU:HD23	1.52	0.92
1:A:2857:LYS:HE3	1:A:2871:LEU:HD23	1.52	0.92
1:C:2857:LYS:HE3	1:C:2871:LEU:HD23	1.52	0.91
1:B:2857:LYS:HE3	1:B:2871:LEU:HD23	1.52	0.90
1:A:4844:ILE:HD13	1:D:4814:MET:CE	2.04	0.86
1:D:4834:PRO:HB3	1:D:4843:ARG:HD3	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4834:PRO:HB3	1:A:4843:ARG:HD3	1.59	0.83
1:B:2130:LEU:HD11	1:B:2170:THR:HG23	1.61	0.83
1:B:986:ILE:HD11	1:B:1055:ARG:HD3	1.59	0.83
1:D:986:ILE:HD11	1:D:1055:ARG:HD3	1.59	0.83
1:C:4834:PRO:HB3	1:C:4843:ARG:HD3	1.59	0.83
1:B:4834:PRO:HB3	1:B:4843:ARG:HD3	1.59	0.82
1:A:875:PRO:HD2	1:A:878:LEU:HD13	1.62	0.82
1:B:875:PRO:HD2	1:B:878:LEU:HD13	1.62	0.82
1:A:2130:LEU:HD11	1:A:2170:THR:HG23	1.61	0.82
1:C:2130:LEU:HD11	1:C:2170:THR:HG23	1.61	0.82
1:C:4641:PRO:HB3	1:C:4644:TYR:HB3	1.61	0.82
1:A:986:ILE:HD11	1:A:1055:ARG:HD3	1.59	0.82
1:B:4641:PRO:HB3	1:B:4644:TYR:HB3	1.61	0.82
1:C:986:ILE:HD11	1:C:1055:ARG:HD3	1.59	0.82
1:D:875:PRO:HD2	1:D:878:LEU:HD13	1.62	0.81
1:D:2130:LEU:HD11	1:D:2170:THR:HG23	1.61	0.81
1:D:4641:PRO:HB3	1:D:4644:TYR:HB3	1.61	0.81
1:B:476:GLN:NE2	1:B:3678:GLU:OE1	2.14	0.81
1:C:875:PRO:HD2	1:C:878:LEU:HD13	1.61	0.81
1:D:476:GLN:NE2	1:D:3678:GLU:OE1	2.14	0.81
1:A:476:GLN:NE2	1:A:3678:GLU:OE1	2.14	0.81
1:B:2882:LYS:O	1:B:2886:ARG:HG3	1.81	0.81
1:C:476:GLN:NE2	1:C:3678:GLU:OE1	2.14	0.81
1:A:4641:PRO:HB3	1:A:4644:TYR:HB3	1.61	0.80
1:A:2882:LYS:O	1:A:2886:ARG:HG3	1.81	0.80
1:C:4814:MET:HE1	1:D:4844:ILE:HD13	1.62	0.80
1:B:3951:PHE:HB3	1:B:3975:GLN:HE21	1.46	0.80
1:C:3951:PHE:HB3	1:C:3975:GLN:HE21	1.46	0.80
1:D:2882:LYS:O	1:D:2886:ARG:HG3	1.81	0.80
1:C:2882:LYS:O	1:C:2886:ARG:HG3	1.81	0.79
1:A:4831:ILE:HG13	1:A:4843:ARG:HH21	1.47	0.79
1:B:4831:ILE:HG13	1:B:4843:ARG:HH21	1.47	0.79
1:A:3951:PHE:HB3	1:A:3975:GLN:HE21	1.46	0.78
1:D:3951:PHE:HB3	1:D:3975:GLN:HE21	1.46	0.78
1:A:4844:ILE:HD13	1:D:4814:MET:HE1	1.63	0.78
1:C:2465:LYS:NZ	1:C:2495:ASP:OD2	2.17	0.78
1:D:23:GLN:NE2	1:D:36:CYS:SG	2.57	0.78
1:A:23:GLN:NE2	1:A:36:CYS:SG	2.57	0.78
1:C:4044:SER:HA	1:C:4077:THR:HG22	1.66	0.78
1:B:23:GLN:NE2	1:B:36:CYS:SG	2.57	0.78
1:C:23:GLN:NE2	1:C:36:CYS:SG	2.57	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4831:ILE:HG13	1:D:4843:ARG:HH21	1.47	0.78
1:B:4044:SER:HA	1:B:4077:THR:HG22	1.66	0.77
1:C:4831:ILE:HG13	1:C:4843:ARG:HH21	1.48	0.77
1:C:2760:TYR:OH	1:C:2772:ARG:NH1	2.18	0.77
1:D:4044:SER:HA	1:D:4077:THR:HG22	1.66	0.77
1:B:2465:LYS:NZ	1:B:2495:ASP:OD2	2.17	0.77
1:D:4637:THR:HG22	1:D:4704:LYS:HG3	1.66	0.77
1:C:4637:THR:HG22	1:C:4704:LYS:HG3	1.66	0.77
1:A:4044:SER:HA	1:A:4077:THR:HG22	1.66	0.76
1:D:4640:PHE:CG	1:D:4641:PRO:HD2	2.20	0.76
1:D:996:VAL:HG21	1:D:1051:ARG:HB3	1.67	0.76
1:A:4637:THR:HG22	1:A:4704:LYS:HG3	1.66	0.76
1:A:4640:PHE:CG	1:A:4641:PRO:HD2	2.20	0.76
1:A:4737:PHE:HD2	1:B:4783:VAL:HG13	1.51	0.76
1:C:996:VAL:HG21	1:C:1051:ARG:HB3	1.68	0.76
1:A:3051:GLU:OE1	1:A:3051:GLU:N	2.14	0.76
1:D:2465:LYS:NZ	1:D:2495:ASP:OD2	2.17	0.76
1:C:4640:PHE:CG	1:C:4641:PRO:HD2	2.20	0.76
1:A:2465:LYS:NZ	1:A:2495:ASP:OD2	2.17	0.75
1:A:2832:THR:HG21	1:B:1290:PHE:HE2	1.50	0.75
1:B:4637:THR:HG22	1:B:4704:LYS:HG3	1.66	0.75
1:B:4640:PHE:CG	1:B:4641:PRO:HD2	2.20	0.75
1:A:4864:GLY:CA	1:D:4867:ILE:HG12	2.16	0.75
1:B:2760:TYR:OH	1:B:2772:ARG:NH1	2.18	0.75
1:C:2627:TRP:HB2	1:C:2630:PHE:HB2	1.69	0.75
1:D:2627:TRP:HB2	1:D:2630:PHE:HB2	1.69	0.75
1:D:3901:GLN:OE1	1:D:3904:ARG:NH2	2.20	0.75
1:A:2760:TYR:OH	1:A:2772:ARG:NH1	2.18	0.75
1:A:996:VAL:HG21	1:A:1051:ARG:HB3	1.67	0.74
1:D:2787:TRP:HD1	1:D:2906:GLY:H	1.34	0.74
1:A:3770:ASN:HB3	1:A:3773:VAL:HG12	1.69	0.74
1:B:996:VAL:HG21	1:B:1051:ARG:HB3	1.67	0.74
1:B:3770:ASN:HB3	1:B:3773:VAL:HG12	1.69	0.74
1:C:3770:ASN:HB3	1:C:3773:VAL:HG12	1.70	0.74
1:C:3901:GLN:OE1	1:C:3904:ARG:NH2	2.20	0.74
1:D:3770:ASN:HB3	1:D:3773:VAL:HG12	1.69	0.74
1:A:2627:TRP:HB2	1:A:2630:PHE:HB2	1.69	0.74
1:D:2760:TYR:OH	1:D:2772:ARG:NH1	2.18	0.74
1:C:2787:TRP:HD1	1:C:2906:GLY:H	1.34	0.74
1:A:1958:THR:HA	1:A:1961:LYS:HD2	1.70	0.74
1:B:2627:TRP:HB2	1:B:2630:PHE:HB2	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2787:TRP:HD1	1:A:2906:GLY:H	1.34	0.73
1:D:1958:THR:HA	1:D:1961:LYS:HD2	1.70	0.73
1:A:3901:GLN:OE1	1:A:3904:ARG:NH2	2.20	0.73
1:B:3901:GLN:OE1	1:B:3904:ARG:NH2	2.20	0.73
1:A:2793:ARG:NH1	1:A:2793:ARG:HG2	2.04	0.73
1:B:3051:GLU:OE1	1:B:3051:GLU:N	2.14	0.73
1:C:586:LEU:HD11	1:C:617:LEU:HA	1.71	0.73
1:D:2793:ARG:NH1	1:D:2793:ARG:HG2	2.04	0.73
1:C:1958:THR:HA	1:C:1961:LYS:HD2	1.70	0.72
1:D:2730:ASP:O	1:D:2734:MET:HG2	1.90	0.72
1:A:2730:ASP:O	1:A:2734:MET:HG2	1.90	0.72
1:B:1958:THR:HA	1:B:1961:LYS:HD2	1.70	0.72
1:B:4079:ASP:HB3	1:B:4082:GLU:HG2	1.72	0.72
1:D:586:LEU:HD11	1:D:617:LEU:HA	1.70	0.72
1:A:2436:ILE:HA	1:A:2465:LYS:HE3	1.72	0.72
1:A:2824:ARG:HE	1:B:1502:ASN:HB2	1.55	0.72
1:B:2730:ASP:O	1:B:2734:MET:HG2	1.89	0.72
1:B:2787:TRP:HD1	1:B:2906:GLY:H	1.34	0.72
1:B:2436:ILE:HA	1:B:2465:LYS:HE3	1.71	0.72
1:C:2436:ILE:HA	1:C:2465:LYS:HE3	1.71	0.72
1:C:2730:ASP:O	1:C:2734:MET:HG2	1.90	0.72
1:C:2552:VAL:HG13	1:C:2569:ILE:HD11	1.72	0.72
1:D:2436:ILE:HA	1:D:2465:LYS:HE3	1.72	0.72
1:A:586:LEU:HD11	1:A:617:LEU:HA	1.71	0.72
1:A:4079:ASP:HB3	1:A:4082:GLU:HG2	1.72	0.72
1:D:1166:VAL:HG23	1:D:1173:MET:HG2	1.72	0.72
1:C:1122:CYS:HA	1:C:1133:ARG:HD3	1.71	0.72
1:D:2552:VAL:HG13	1:D:2569:ILE:HD11	1.72	0.72
1:D:4079:ASP:HB3	1:D:4082:GLU:HG2	1.72	0.72
1:C:3051:GLU:OE1	1:C:3051:GLU:N	2.14	0.72
1:A:2552:VAL:HG13	1:A:2569:ILE:HD11	1.72	0.72
1:C:1129:GLY:HA3	1:C:1145:TRP:HB3	1.72	0.72
1:B:1122:CYS:HA	1:B:1133:ARG:HD3	1.71	0.71
1:C:1166:VAL:HG23	1:C:1173:MET:HG2	1.72	0.71
1:B:2976:LYS:O	1:B:2979:ARG:NH1	2.24	0.71
1:C:4079:ASP:HB3	1:C:4082:GLU:HG2	1.72	0.71
1:B:586:LEU:HD11	1:B:617:LEU:HA	1.71	0.71
1:D:2976:LYS:O	1:D:2979:ARG:NH1	2.24	0.71
1:A:2830:ASN:OD1	1:B:1549:SER:HB2	1.91	0.71
1:D:2736:LYS:HB3	1:D:2741:TRP:CD1	2.26	0.71
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2824:ARG:NH2	1:B:1502:ASN:O	2.24	0.71
1:D:3051:GLU:OE1	1:D:3051:GLU:N	2.14	0.71
1:A:1166:VAL:HG23	1:A:1173:MET:HG2	1.72	0.71
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	1.72	0.71
1:B:2552:VAL:HG13	1:B:2569:ILE:HD11	1.72	0.70
1:C:2793:ARG:NH1	1:C:2793:ARG:HG2	2.04	0.70
1:A:2736:LYS:HB3	1:A:2741:TRP:CD1	2.26	0.70
1:A:4818:TYR:HD1	1:B:4848:ILE:HD11	1.56	0.70
1:D:1122:CYS:HA	1:D:1133:ARG:HD3	1.72	0.70
1:D:799:LYS:NZ	1:D:1620:GLN:OE1	2.24	0.70
1:A:799:LYS:NZ	1:A:1620:GLN:OE1	2.24	0.70
1:C:1711:LEU:HB3	1:C:1831:MET:HE3	1.72	0.70
1:C:4814:MET:CE	1:D:4844:ILE:HD13	2.22	0.70
1:D:878:LEU:HG	1:D:940:LEU:HD12	1.74	0.70
1:B:1166:VAL:HG23	1:B:1173:MET:HG2	1.72	0.70
1:B:1711:LEU:HB3	1:B:1831:MET:HE3	1.72	0.70
1:A:878:LEU:HG	1:A:940:LEU:HD12	1.74	0.70
1:A:1122:CYS:HA	1:A:1133:ARG:HD3	1.72	0.70
1:B:2793:ARG:HG2	1:B:2793:ARG:NH1	2.04	0.70
1:C:878:LEU:HG	1:C:940:LEU:HD12	1.74	0.70
1:C:2788:ARG:HD3	1:C:2905:ARG:O	1.92	0.70
1:C:2976:LYS:O	1:C:2979:ARG:NH1	2.24	0.70
1:D:2788:ARG:HD3	1:D:2905:ARG:O	1.92	0.70
1:B:2788:ARG:HD3	1:B:2905:ARG:O	1.92	0.70
1:D:1711:LEU:HB3	1:D:1831:MET:HE3	1.74	0.70
1:B:799:LYS:NZ	1:B:1620:GLN:OE1	2.24	0.69
1:B:878:LEU:HG	1:B:940:LEU:HD12	1.74	0.69
1:D:2690:GLU:HB2	1:D:2692:GLN:OE1	1.92	0.69
1:B:2736:LYS:HB3	1:B:2741:TRP:CD1	2.26	0.69
1:C:2690:GLU:HB2	1:C:2692:GLN:OE1	1.92	0.69
1:C:2736:LYS:HB3	1:C:2741:TRP:CD1	2.26	0.69
1:A:2788:ARG:HD3	1:A:2905:ARG:O	1.92	0.69
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.26	0.69
1:A:2976:LYS:O	1:A:2979:ARG:NH1	2.24	0.69
1:B:2690:GLU:HB2	1:B:2692:GLN:OE1	1.92	0.69
1:B:2832:THR:OG1	1:C:1548:THR:O	2.09	0.69
1:C:799:LYS:NZ	1:C:1620:GLN:OE1	2.24	0.69
1:A:4872:GLU:HG2	1:D:4874:ARG:CD	2.22	0.69
1:C:2832:THR:OG1	1:D:1548:THR:O	2.10	0.69
1:B:1129:GLY:HA3	1:B:1145:TRP:HB3	1.72	0.69
1:D:1947:VAL:HG23	1:D:1961:LYS:HB3	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2332:GLY:H	1:D:2336:ARG:HH21	1.40	0.69
1:A:2690:GLU:HB2	1:A:2692:GLN:OE1	1.92	0.69
1:C:1144:ARG:NH1	1:C:1191:ALA:O	2.26	0.69
1:A:1947:VAL:HG23	1:A:1961:LYS:HB3	1.75	0.68
1:A:2332:GLY:H	1:A:2336:ARG:HH21	1.40	0.68
1:A:1144:ARG:NH1	1:A:1191:ALA:O	2.26	0.68
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.26	0.68
1:B:1898:LEU:HD23	1:B:1902:VAL:HG12	1.76	0.68
1:C:2711:ILE:HG21	1:C:2783:LEU:HB2	1.76	0.68
1:B:2332:GLY:H	1:B:2336:ARG:HH21	1.40	0.68
1:A:4521:LYS:NZ	1:B:4807:ASP:HB3	2.08	0.68
1:B:1035:TYR:HA	1:B:1038:LEU:HD12	1.76	0.68
1:B:1947:VAL:HG23	1:B:1961:LYS:HB3	1.75	0.68
1:C:1035:TYR:HA	1:C:1038:LEU:HD12	1.76	0.68
1:B:2782:MET:HG2	1:B:2783:LEU:HD12	1.76	0.67
1:C:1947:VAL:HG23	1:C:1961:LYS:HB3	1.75	0.67
1:A:2882:LYS:HB3	1:A:2886:ARG:HD3	1.76	0.67
1:B:2882:LYS:HB3	1:B:2886:ARG:HD3	1.76	0.67
1:C:2332:GLY:H	1:C:2336:ARG:HH21	1.40	0.67
1:A:4860:ALA:HB2	1:D:4863:GLN:HG2	1.76	0.67
1:B:3001:LYS:HD3	1:B:3044:THR:HG21	1.76	0.67
1:D:2782:MET:HG2	1:D:2783:LEU:HD12	1.76	0.67
1:D:1035:TYR:HA	1:D:1038:LEU:HD12	1.76	0.67
1:B:2576:ILE:O	1:B:2580:LEU:HB2	1.95	0.67
1:C:2782:MET:HG2	1:C:2783:LEU:HD12	1.76	0.67
1:A:1035:TYR:HA	1:A:1038:LEU:HD12	1.76	0.67
1:D:2711:ILE:HG21	1:D:2783:LEU:HB2	1.76	0.67
1:B:476:GLN:NE2	1:B:3677:THR:HA	2.10	0.67
1:B:2711:ILE:HG21	1:B:2783:LEU:HB2	1.76	0.67
1:C:2502:LEU:HD21	1:C:2516:LEU:HD23	1.77	0.67
1:A:166:SER:OG	1:A:168:GLN:OE1	2.13	0.67
1:A:4011:GLU:HG2	1:A:4121:LEU:HD21	1.77	0.67
1:D:476:GLN:NE2	1:D:3677:THR:HA	2.10	0.67
1:D:1898:LEU:HD23	1:D:1902:VAL:HG12	1.76	0.67
1:A:476:GLN:NE2	1:A:3677:THR:HA	2.10	0.66
1:D:2576:ILE:O	1:D:2580:LEU:HB2	1.95	0.66
1:A:2576:ILE:O	1:A:2580:LEU:HB2	1.95	0.66
1:A:4810:LEU:HD13	1:D:4518:LEU:HD21	1.75	0.66
1:B:1844:GLN:NE2	1:B:1853:GLU:OE1	2.26	0.66
1:D:3001:LYS:HD3	1:D:3044:THR:HG21	1.76	0.66
1:A:2711:ILE:HG21	1:A:2783:LEU:HB2	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2693:SER:OG	1:C:2704:GLN:NE2	2.28	0.66
1:D:2693:SER:OG	1:D:2704:GLN:NE2	2.28	0.66
1:D:4011:GLU:HG2	1:D:4121:LEU:HD21	1.77	0.66
1:B:4011:GLU:HG2	1:B:4121:LEU:HD21	1.77	0.66
1:A:2260:PRO:HA	1:A:2263:GLU:HG2	1.77	0.66
1:B:2756:LEU:HD13	1:B:2766:LYS:HE2	1.78	0.66
1:C:2576:ILE:O	1:C:2580:LEU:HB2	1.95	0.66
1:C:4011:GLU:HG2	1:C:4121:LEU:HD21	1.77	0.66
1:A:2693:SER:OG	1:A:2704:GLN:NE2	2.28	0.66
1:B:2693:SER:OG	1:B:2704:GLN:NE2	2.28	0.66
1:C:2756:LEU:HD13	1:C:2766:LYS:HE2	1.78	0.66
1:D:166:SER:OG	1:D:168:GLN:OE1	2.13	0.66
1:D:234:LEU:HD13	1:D:405:LEU:HD22	1.78	0.66
1:A:1898:LEU:HD23	1:A:1902:VAL:HG12	1.76	0.66
1:B:3900:GLU:OE2	1:B:3904:ARG:NH1	2.29	0.66
1:C:234:LEU:HD13	1:C:405:LEU:HD22	1.78	0.66
1:C:3900:GLU:OE2	1:C:3904:ARG:NH1	2.29	0.66
1:A:3001:LYS:HD3	1:A:3044:THR:HG21	1.76	0.66
1:A:3900:GLU:OE2	1:A:3904:ARG:NH1	2.29	0.66
1:C:2882:LYS:HB3	1:C:2886:ARG:HD3	1.76	0.66
1:D:2717:LEU:HD12	1:D:2779:LEU:HD13	1.77	0.66
1:C:166:SER:OG	1:C:168:GLN:OE1	2.13	0.66
1:C:1898:LEU:HD23	1:C:1902:VAL:HG12	1.76	0.66
1:C:2717:LEU:HD12	1:C:2779:LEU:HD13	1.77	0.66
1:C:2958:GLN:HA	1:C:2961:LYS:HE2	1.78	0.66
1:C:3001:LYS:HD3	1:C:3044:THR:HG21	1.76	0.66
1:D:887:GLU:HA	1:D:890:HIS:CD2	2.31	0.66
1:A:267:VAL:HA	1:A:270:HIS:HD2	1.61	0.66
2:E:22:THR:HG22	2:E:50:ARG:HG2	1.79	0.66
1:A:2782:MET:HG2	1:A:2783:LEU:HD12	1.76	0.65
1:D:3900:GLU:OE2	1:D:3904:ARG:NH1	2.29	0.65
1:A:2648:ILE:O	1:A:2652:LEU:HB2	1.97	0.65
1:B:669:GLN:HE22	1:B:862:PHE:H	1.44	0.65
1:B:2648:ILE:O	1:B:2652:LEU:HB2	1.97	0.65
1:C:476:GLN:NE2	1:C:3677:THR:HA	2.10	0.65
1:C:669:GLN:HE22	1:C:862:PHE:H	1.44	0.65
1:C:1052:GLU:HA	1:C:1055:ARG:HG2	1.79	0.65
1:D:2582:PRO:HA	1:D:2585:MET:HG3	1.79	0.65
1:B:267:VAL:HA	1:B:270:HIS:HD2	1.61	0.65
1:C:2648:ILE:O	1:C:2652:LEU:HB2	1.97	0.65
1:A:996:VAL:HG11	1:A:1051:ARG:HD2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:GLU:HA	1:A:1055:ARG:HG2	1.79	0.65
1:A:2502:LEU:HD21	1:A:2516:LEU:HD23	1.77	0.65
1:B:166:SER:OG	1:B:168:GLN:OE1	2.13	0.65
1:B:2717:LEU:HD12	1:B:2779:LEU:HD13	1.77	0.65
1:C:887:GLU:HA	1:C:890:HIS:CD2	2.31	0.65
1:C:2582:PRO:HA	1:C:2585:MET:HG3	1.79	0.65
1:B:996:VAL:HG11	1:B:1051:ARG:HD2	1.79	0.65
1:B:2154:VAL:HG13	1:B:2158:HIS:HD2	1.62	0.65
1:C:2933:VAL:HA	1:C:2963:PHE:HZ	1.62	0.65
1:D:1052:GLU:HA	1:D:1055:ARG:HG2	1.78	0.65
1:D:2648:ILE:O	1:D:2652:LEU:HB2	1.97	0.65
1:A:2958:GLN:HA	1:A:2961:LYS:HE2	1.78	0.65
2:F:22:THR:HG22	2:F:50:ARG:HG2	1.79	0.65
2:H:22:THR:HG22	2:H:50:ARG:HG2	1.79	0.65
1:B:1052:GLU:HA	1:B:1055:ARG:HG2	1.79	0.65
1:B:2502:LEU:HD21	1:B:2516:LEU:HD23	1.77	0.65
1:D:2882:LYS:HB3	1:D:2886:ARG:HD3	1.76	0.65
1:A:2756:LEU:HD13	1:A:2766:LYS:HE2	1.78	0.65
1:B:2958:GLN:HA	1:B:2961:LYS:HE2	1.78	0.65
1:B:4255:LEU:HB2	1:B:4293:THR:HG21	1.78	0.65
1:C:2154:VAL:HG13	1:C:2158:HIS:HD2	1.62	0.65
1:A:2717:LEU:HD12	1:A:2779:LEU:HD13	1.77	0.65
1:B:298:ARG:HH12	1:B:417:ARG:HH12	1.45	0.65
1:B:2582:PRO:HA	1:B:2585:MET:HG3	1.79	0.65
1:C:2260:PRO:HA	1:C:2263:GLU:HG2	1.77	0.65
1:D:2502:LEU:HD21	1:D:2516:LEU:HD23	1.77	0.65
1:A:298:ARG:HH12	1:A:417:ARG:HH12	1.45	0.65
1:A:2154:VAL:HG13	1:A:2158:HIS:HD2	1.62	0.65
1:D:298:ARG:HH12	1:D:417:ARG:HH12	1.45	0.65
1:D:2933:VAL:HA	1:D:2963:PHE:HZ	1.62	0.65
1:D:2958:GLN:HA	1:D:2961:LYS:HE2	1.78	0.65
1:D:4255:LEU:HB2	1:D:4293:THR:HG21	1.78	0.65
1:A:234:LEU:HD13	1:A:405:LEU:HD22	1.78	0.64
1:A:887:GLU:HA	1:A:890:HIS:CD2	2.31	0.64
1:B:234:LEU:HD13	1:B:405:LEU:HD22	1.78	0.64
1:D:2756:LEU:HD13	1:D:2766:LYS:HE2	1.78	0.64
1:A:669:GLN:HE22	1:A:862:PHE:H	1.44	0.64
1:C:1502:ASN:OD1	1:C:1503:ASN:N	2.30	0.64
1:D:1502:ASN:OD1	1:D:1503:ASN:N	2.30	0.64
1:A:1502:ASN:OD1	1:A:1503:ASN:N	2.30	0.64
1:A:4031:THR:HA	1:A:4034:GLU:HG2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2593:VAL:HA	1:B:2644:LEU:HD13	1.78	0.64
1:C:4031:THR:HA	1:C:4034:GLU:HG2	1.80	0.64
1:D:2260:PRO:HA	1:D:2263:GLU:HG2	1.77	0.64
1:A:2933:VAL:HA	1:A:2963:PHE:HZ	1.62	0.64
2:G:22:THR:HG22	2:G:50:ARG:HG2	1.79	0.64
1:C:298:ARG:HH12	1:C:417:ARG:HH12	1.45	0.64
1:D:2593:VAL:HA	1:D:2644:LEU:HD13	1.78	0.64
1:A:4255:LEU:HB2	1:A:4293:THR:HG21	1.78	0.64
1:B:2260:PRO:HA	1:B:2263:GLU:HG2	1.77	0.64
1:D:669:GLN:HE22	1:D:862:PHE:H	1.44	0.64
1:C:4049:HIS:HD2	1:C:4067:LEU:HD11	1.63	0.64
1:D:996:VAL:HG11	1:D:1051:ARG:HD2	1.78	0.64
1:B:887:GLU:HA	1:B:890:HIS:CD2	2.31	0.64
1:B:1502:ASN:OD1	1:B:1503:ASN:N	2.30	0.64
1:C:4255:LEU:HB2	1:C:4293:THR:HG21	1.78	0.64
1:D:267:VAL:HA	1:D:270:HIS:HD2	1.62	0.64
1:A:2582:PRO:HA	1:A:2585:MET:HG3	1.79	0.64
1:A:4618:THR:OG1	1:A:4619:GLU:OE1	2.15	0.64
1:D:4031:THR:HA	1:D:4034:GLU:HG2	1.80	0.64
1:B:4031:THR:HA	1:B:4034:GLU:HG2	1.80	0.64
1:C:2688:MET:HG2	1:C:2689:MET:HG3	1.80	0.64
1:D:1844:GLN:NE2	1:D:1853:GLU:OE1	2.26	0.64
1:D:2154:VAL:HG13	1:D:2158:HIS:HD2	1.62	0.64
1:A:2688:MET:HG2	1:A:2689:MET:HG3	1.80	0.64
1:B:2933:VAL:HA	1:B:2963:PHE:HZ	1.62	0.64
1:C:267:VAL:HA	1:C:270:HIS:HD2	1.61	0.64
1:A:2593:VAL:HA	1:A:2644:LEU:HD13	1.78	0.63
1:B:4049:HIS:HD2	1:B:4067:LEU:HD11	1.63	0.63
1:C:425:LEU:HD12	1:C:428:ARG:HD3	1.80	0.63
1:C:694:ARG:NH1	1:C:718:VAL:O	2.31	0.63
1:C:996:VAL:HG11	1:C:1051:ARG:HD2	1.78	0.63
1:C:2593:VAL:HA	1:C:2644:LEU:HD13	1.78	0.63
1:D:312:LYS:HG3	1:D:370:LEU:HD13	1.80	0.63
1:B:601:LEU:HB2	1:B:610:VAL:HG11	1.80	0.63
1:B:2793:ARG:HG2	1:B:2793:ARG:HH11	1.63	0.63
1:C:1989:PRO:HD2	1:C:1992:ILE:HD12	1.80	0.63
1:A:601:LEU:HB2	1:A:610:VAL:HG11	1.81	0.63
1:B:694:ARG:NH1	1:B:718:VAL:O	2.32	0.63
1:B:2688:MET:HG2	1:B:2689:MET:HG3	1.80	0.63
1:C:1844:GLN:NE2	1:C:1853:GLU:OE1	2.26	0.63
1:D:601:LEU:HB2	1:D:610:VAL:HG11	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1989:PRO:HD2	1:A:1992:ILE:HD12	1.80	0.63
1:D:2688:MET:HG2	1:D:2689:MET:HG3	1.80	0.63
1:B:194:LEU:HD11	1:B:201:LEU:HB3	1.81	0.63
1:B:425:LEU:HD12	1:B:428:ARG:HD3	1.80	0.63
1:A:2129:LEU:HA	1:A:2132:VAL:HG22	1.81	0.63
1:B:466:PRO:HG2	1:B:479:LEU:HD12	1.81	0.63
1:B:218:SER:HB3	1:B:286:GLY:HA3	1.80	0.63
1:B:776:GLN:OE1	1:B:776:GLN:N	2.32	0.63
1:A:694:ARG:NH1	1:A:718:VAL:O	2.32	0.62
1:A:4049:HIS:HD2	1:A:4067:LEU:HD11	1.63	0.62
1:D:776:GLN:N	1:D:776:GLN:OE1	2.32	0.62
1:A:1844:GLN:NE2	1:A:1853:GLU:OE1	2.26	0.62
1:A:4864:GLY:HA3	1:D:4867:ILE:HG12	1.79	0.62
1:D:218:SER:HB3	1:D:286:GLY:HA3	1.80	0.62
1:A:312:LYS:HG3	1:A:370:LEU:HD13	1.80	0.62
1:B:1482:ARG:NH1	1:B:1534:GLU:OE2	2.33	0.62
1:D:425:LEU:HD12	1:D:428:ARG:HD3	1.80	0.62
1:A:218:SER:HB3	1:A:286:GLY:HA3	1.80	0.62
1:A:466:PRO:HG2	1:A:479:LEU:HD12	1.81	0.62
1:A:4245:LEU:HD11	1:B:4626:ILE:HG13	1.82	0.62
1:C:194:LEU:HD11	1:C:201:LEU:HB3	1.81	0.62
1:D:998:LYS:HA	1:D:1001:GLU:HG2	1.81	0.62
1:D:2711:ILE:HG23	1:D:2783:LEU:HD22	1.81	0.62
1:D:4049:HIS:HD2	1:D:4067:LEU:HD11	1.63	0.62
1:A:882:ARG:NH1	1:A:933:LEU:HD22	2.15	0.62
1:C:218:SER:HB3	1:C:286:GLY:HA3	1.80	0.62
1:A:1026:ASN:HB3	1:A:1028:ARG:HG2	1.82	0.62
1:C:1113:MET:HB2	1:C:1156:TRP:CZ2	2.35	0.62
1:C:2129:LEU:HA	1:C:2132:VAL:HG22	1.81	0.62
1:C:2711:ILE:HG23	1:C:2783:LEU:HD22	1.81	0.62
1:C:4618:THR:OG1	1:C:4619:GLU:OE1	2.15	0.62
1:D:882:ARG:NH1	1:D:933:LEU:HD22	2.15	0.62
1:D:4046:ARG:NE	1:D:4046:ARG:HA	2.15	0.62
1:A:1113:MET:HB2	1:A:1156:TRP:CZ2	2.35	0.62
1:B:1989:PRO:HD2	1:B:1992:ILE:HD12	1.80	0.62
1:B:2322:ARG:HH12	1:C:189:GLU:HG3	1.64	0.62
1:B:4618:THR:OG1	1:B:4619:GLU:OE1	2.15	0.62
1:C:466:PRO:HG2	1:C:479:LEU:HD12	1.81	0.62
1:D:4617:ILE:HG12	1:D:4666:ILE:HD11	1.82	0.62
1:A:972:LEU:HD23	1:A:974:SER:H	1.65	0.62
1:C:882:ARG:NH1	1:C:933:LEU:HD22	2.15	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2793:ARG:HG2	1:C:2793:ARG:HH11	1.64	0.62
1:D:1113:MET:HB2	1:D:1156:TRP:CZ2	2.35	0.62
1:D:1989:PRO:HD2	1:D:1992:ILE:HD12	1.80	0.62
1:A:1482:ARG:NH1	1:A:1534:GLU:OE2	2.33	0.62
1:A:4872:GLU:HG2	1:D:4874:ARG:HD2	1.80	0.62
1:B:882:ARG:NH1	1:B:933:LEU:HD22	2.15	0.62
1:B:1303:ARG:NH1	1:B:1589:GLN:OE1	2.32	0.62
1:C:312:LYS:HG3	1:C:370:LEU:HD13	1.80	0.62
1:C:601:LEU:HB2	1:C:610:VAL:HG11	1.81	0.62
1:C:1303:ARG:NH1	1:C:1589:GLN:OE1	2.32	0.62
1:D:194:LEU:HD11	1:D:201:LEU:HB3	1.81	0.62
1:D:1026:ASN:HB3	1:D:1028:ARG:HG2	1.82	0.62
1:A:2793:ARG:HG2	1:A:2793:ARG:HH11	1.64	0.62
1:A:4617:ILE:HG12	1:A:4666:ILE:HD11	1.82	0.62
1:B:312:LYS:HG3	1:B:370:LEU:HD13	1.80	0.62
1:B:940:LEU:HA	1:B:943:LEU:HD12	1.82	0.62
1:B:2898:ILE:HG23	1:C:1500:ARG:HH22	1.64	0.62
1:B:4046:ARG:NE	1:B:4046:ARG:HA	2.15	0.62
1:B:4617:ILE:HG12	1:B:4666:ILE:HD11	1.82	0.62
1:C:972:LEU:HD23	1:C:974:SER:H	1.65	0.62
1:D:1303:ARG:NH1	1:D:1589:GLN:OE1	2.32	0.62
1:D:4819:VAL:HG12	1:D:4822:ARG:HH21	1.65	0.62
1:A:1434:PRO:O	1:D:2830:ASN:ND2	2.33	0.61
1:D:2129:LEU:HA	1:D:2132:VAL:HG22	1.81	0.61
1:A:2797:SER:HB3	1:A:2801:TYR:CE2	2.35	0.61
1:B:2797:SER:HB3	1:B:2801:TYR:CE2	2.35	0.61
1:B:2956:TYR:O	1:B:2960:ILE:HG22	2.00	0.61
1:C:4046:ARG:HA	1:C:4046:ARG:NE	2.15	0.61
1:D:4004:VAL:HG11	1:D:4114:ARG:HD2	1.82	0.61
1:A:317:MET:HE2	1:A:321:LYS:HG3	1.81	0.61
1:A:902:TRP:HZ2	1:A:915:HIS:HB3	1.65	0.61
1:A:998:LYS:HA	1:A:1001:GLU:HG2	1.82	0.61
1:A:4004:VAL:HG11	1:A:4114:ARG:HD2	1.83	0.61
1:A:4046:ARG:NE	1:A:4046:ARG:HA	2.15	0.61
1:B:2711:ILE:HG23	1:B:2783:LEU:HD22	1.81	0.61
1:C:940:LEU:HA	1:C:943:LEU:HD12	1.82	0.61
1:D:1482:ARG:NH1	1:D:1534:GLU:OE2	2.33	0.61
1:D:3729:ALA:HA	1:D:3732:HIS:CE1	2.36	0.61
1:A:1303:ARG:NH1	1:A:1589:GLN:OE1	2.33	0.61
1:B:2129:LEU:HA	1:B:2132:VAL:HG22	1.81	0.61
1:C:2797:SER:HB3	1:C:2801:TYR:CE2	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:694:ARG:NH1	1:D:718:VAL:O	2.31	0.61
1:A:425:LEU:HD12	1:A:428:ARG:HD3	1.80	0.61
1:B:4819:VAL:HG12	1:B:4822:ARG:HH21	1.65	0.61
1:C:776:GLN:OE1	1:C:776:GLN:N	2.32	0.61
1:C:902:TRP:HZ2	1:C:915:HIS:HB3	1.64	0.61
1:C:998:LYS:HA	1:C:1001:GLU:HG2	1.82	0.61
1:A:332:ARG:NH1	1:A:364:GLN:OE1	2.34	0.61
1:A:4814:MET:HA	1:A:4817:MET:HB2	1.83	0.61
1:B:3729:ALA:HA	1:B:3732:HIS:CE1	2.36	0.61
1:C:4819:VAL:HG12	1:C:4822:ARG:HH21	1.65	0.61
1:D:332:ARG:NH1	1:D:364:GLN:OE1	2.34	0.61
1:D:466:PRO:HG2	1:D:479:LEU:HD12	1.81	0.61
1:D:3034:HIS:O	1:D:3038:GLN:NE2	2.34	0.61
1:D:4618:THR:OG1	1:D:4619:GLU:OE1	2.15	0.61
1:A:194:LEU:HD11	1:A:201:LEU:HB3	1.81	0.61
1:A:4819:VAL:HG12	1:A:4822:ARG:HH21	1.65	0.61
1:B:972:LEU:HD23	1:B:974:SER:H	1.65	0.61
1:B:1113:MET:HB2	1:B:1156:TRP:CZ2	2.35	0.61
1:D:2779:LEU:O	1:D:2782:MET:HG2	2.01	0.61
1:B:4814:MET:HA	1:B:4817:MET:HB2	1.83	0.61
1:C:3034:HIS:O	1:C:3038:GLN:NE2	2.34	0.61
1:D:972:LEU:HD23	1:D:974:SER:H	1.65	0.61
1:A:2787:TRP:HD1	1:A:2906:GLY:N	1.99	0.61
1:B:902:TRP:HZ2	1:B:915:HIS:HB3	1.64	0.61
1:B:2779:LEU:O	1:B:2782:MET:HG2	2.01	0.61
1:A:776:GLN:N	1:A:776:GLN:OE1	2.32	0.61
1:A:842:GLN:HB2	1:A:1603:PHE:HB2	1.83	0.61
1:A:3034:HIS:O	1:A:3038:GLN:NE2	2.34	0.61
1:A:4864:GLY:HA2	1:D:4867:ILE:HG12	1.82	0.61
1:B:332:ARG:NH1	1:B:364:GLN:OE1	2.34	0.61
1:B:4004:VAL:HG11	1:B:4114:ARG:HD2	1.82	0.61
1:C:1026:ASN:HB3	1:C:1028:ARG:HG2	1.82	0.61
1:C:3729:ALA:HA	1:C:3732:HIS:CE1	2.36	0.61
1:C:4617:ILE:HG12	1:C:4666:ILE:HD11	1.82	0.61
1:D:2797:SER:HB3	1:D:2801:TYR:CE2	2.35	0.61
1:A:2779:LEU:O	1:A:2782:MET:HG2	2.01	0.60
1:B:3034:HIS:O	1:B:3038:GLN:NE2	2.34	0.60
1:C:1482:ARG:NH1	1:C:1534:GLU:OE2	2.33	0.60
1:D:2956:TYR:O	1:D:2960:ILE:HG22	2.00	0.60
1:A:2711:ILE:HG23	1:A:2783:LEU:HD22	1.81	0.60
1:B:1606:VAL:HG12	1:B:1621:CYS:HB2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2956:TYR:O	1:C:2960:ILE:HG22	2.00	0.60
1:D:2793:ARG:HG2	1:D:2793:ARG:HH11	1.64	0.60
1:A:2956:TYR:O	1:A:2960:ILE:HG22	2.00	0.60
1:A:940:LEU:HA	1:A:943:LEU:HD12	1.82	0.60
1:A:2187:ILE:HG13	1:A:2227:VAL:HG13	1.83	0.60
1:A:3729:ALA:HA	1:A:3732:HIS:CE1	2.36	0.60
1:C:2187:ILE:HG13	1:C:2227:VAL:HG13	1.83	0.60
1:C:3890:TRP:O	1:D:76:ARG:NH2	2.34	0.60
1:C:4004:VAL:HG11	1:C:4114:ARG:HD2	1.82	0.60
1:D:902:TRP:HZ2	1:D:915:HIS:HB3	1.65	0.60
1:D:2187:ILE:HG13	1:D:2227:VAL:HG13	1.83	0.60
1:A:1606:VAL:HG12	1:A:1621:CYS:HB2	1.83	0.60
1:B:998:LYS:HA	1:B:1001:GLU:HG2	1.82	0.60
1:D:2787:TRP:HD1	1:D:2906:GLY:N	1.99	0.60
1:A:4737:PHE:CD2	1:B:4783:VAL:HG13	2.36	0.60
1:B:1026:ASN:HB3	1:B:1028:ARG:HG2	1.82	0.60
1:C:332:ARG:NH1	1:C:364:GLN:OE1	2.34	0.60
1:D:2318:ASN:O	1:D:2322:ARG:HG3	2.01	0.60
1:D:940:LEU:HA	1:D:943:LEU:HD12	1.82	0.60
1:D:4814:MET:HA	1:D:4817:MET:HB2	1.83	0.60
1:A:2318:ASN:O	1:A:2322:ARG:HG3	2.01	0.60
1:B:1265:HIS:O	1:B:1288:LYS:NZ	2.27	0.60
1:C:1606:VAL:HG12	1:C:1621:CYS:HB2	1.83	0.60
1:B:2857:LYS:CE	1:B:2871:LEU:HD23	2.30	0.60
1:D:842:GLN:HB2	1:D:1603:PHE:HB2	1.83	0.60
1:A:1685:LEU:O	1:A:1689:ILE:HG12	2.02	0.59
1:A:1711:LEU:HB3	1:A:1831:MET:HE3	1.84	0.59
2:H:69:LEU:HA	2:H:104:LEU:HD23	1.84	0.59
1:B:1113:MET:HB2	1:B:1156:TRP:HZ2	1.67	0.59
1:B:1685:LEU:O	1:B:1689:ILE:HG12	2.02	0.59
1:C:1113:MET:HB2	1:C:1156:TRP:HZ2	1.67	0.59
1:C:2779:LEU:O	1:C:2782:MET:HG2	2.01	0.59
1:C:810:GLU:OE1	1:C:810:GLU:N	2.35	0.59
1:C:2787:TRP:HD1	1:C:2906:GLY:N	1.99	0.59
1:C:4814:MET:HA	1:C:4817:MET:HB2	1.83	0.59
2:F:69:LEU:HA	2:F:104:LEU:HD23	1.85	0.59
1:B:842:GLN:HB2	1:B:1603:PHE:HB2	1.83	0.59
1:D:1785:ASP:OD1	1:D:1786:ILE:N	2.36	0.59
1:C:2318:ASN:O	1:C:2322:ARG:HG3	2.01	0.59
1:A:1113:MET:HB2	1:A:1156:TRP:HZ2	1.67	0.59
1:B:2318:ASN:O	1:B:2322:ARG:HG3	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1606:VAL:HG12	1:D:1621:CYS:HB2	1.83	0.59
1:C:2146:LEU:O	1:C:2150:MET:HG2	2.03	0.59
1:A:4844:ILE:HG21	1:D:4814:MET:CE	2.33	0.59
1:B:2773:TRP:HB3	1:B:2774:PRO:HD3	1.85	0.59
1:A:2202:TYR:O	1:A:2206:ILE:HG12	2.03	0.59
1:A:2441:GLN:NE2	1:A:2442:MET:O	2.36	0.59
2:G:69:LEU:HA	2:G:104:LEU:HD23	1.85	0.59
1:B:810:GLU:N	1:B:810:GLU:OE1	2.35	0.59
1:C:1685:LEU:O	1:C:1689:ILE:HG12	2.02	0.59
1:C:2773:TRP:HB3	1:C:2774:PRO:HD3	1.85	0.59
1:D:810:GLU:OE1	1:D:810:GLU:N	2.35	0.59
1:D:1113:MET:HB2	1:D:1156:TRP:HZ2	1.67	0.59
1:D:2146:LEU:O	1:D:2150:MET:HG2	2.03	0.59
1:D:2441:GLN:NE2	1:D:2442:MET:O	2.36	0.59
2:E:69:LEU:HA	2:E:104:LEU:HD23	1.84	0.59
1:C:310:GLU:OE2	1:C:310:GLU:N	2.34	0.59
1:D:1950:ALA:HB1	1:D:1961:LYS:NZ	2.18	0.59
1:A:1785:ASP:OD1	1:A:1786:ILE:N	2.36	0.59
1:B:2187:ILE:HG13	1:B:2227:VAL:HG13	1.83	0.59
1:C:842:GLN:HB2	1:C:1603:PHE:HB2	1.83	0.59
1:C:4187:GLU:OE1	1:C:4949:TRP:NE1	2.35	0.59
1:A:191:TYR:CD1	1:A:209:GLN:HG3	2.38	0.58
1:C:2441:GLN:NE2	1:C:2442:MET:O	2.36	0.58
1:D:1685:LEU:O	1:D:1689:ILE:HG12	2.02	0.58
1:A:810:GLU:OE1	1:A:810:GLU:N	2.35	0.58
1:B:885:LEU:O	1:B:889:ILE:HG12	2.03	0.58
1:B:1043:LYS:HA	1:B:1046:ASN:HD21	1.68	0.58
1:C:1785:ASP:OD1	1:C:1786:ILE:N	2.36	0.58
1:D:191:TYR:CD1	1:D:209:GLN:HG3	2.38	0.58
1:D:1265:HIS:O	1:D:1288:LYS:NZ	2.27	0.58
1:A:1265:HIS:O	1:A:1288:LYS:NZ	2.27	0.58
1:A:2146:LEU:O	1:A:2150:MET:HG2	2.03	0.58
1:C:562:LEU:HG	1:C:600:LEU:HD13	1.85	0.58
1:C:1043:LYS:HA	1:C:1046:ASN:HD21	1.68	0.58
1:D:2773:TRP:HB3	1:D:2774:PRO:HD3	1.85	0.58
1:A:1950:ALA:HB1	1:A:1961:LYS:NZ	2.18	0.58
1:D:2202:TYR:O	1:D:2206:ILE:HG12	2.03	0.58
1:D:2905:ARG:HH11	1:D:2906:GLY:H	1.52	0.58
1:B:1670:HIS:O	1:B:1674:HIS:ND1	2.32	0.58
1:B:1950:ALA:HB1	1:B:1961:LYS:NZ	2.18	0.58
1:B:2441:GLN:NE2	1:B:2442:MET:O	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4517:LEU:HD21	1:D:4736:ASN:HB3	1.86	0.58
1:C:4517:LEU:HD21	1:C:4736:ASN:HB3	1.86	0.58
1:A:4818:TYR:CD1	1:B:4848:ILE:HD11	2.37	0.58
1:B:2146:LEU:O	1:B:2150:MET:HG2	2.03	0.58
1:C:2905:ARG:HH11	1:C:2906:GLY:H	1.52	0.58
1:D:1102:TYR:N	1:D:1237:GLU:O	2.37	0.58
1:A:76:ARG:NH2	1:D:3890:TRP:O	2.36	0.58
1:A:885:LEU:O	1:A:889:ILE:HG12	2.03	0.58
1:A:1255:LEU:HD11	1:A:1451:HIS:HB3	1.86	0.58
1:D:317:MET:HE2	1:D:321:LYS:HG3	1.85	0.58
1:D:2834:SER:OG	1:D:2836:ASP:OD1	2.19	0.58
1:A:3845:LEU:HD23	1:A:3848:GLU:HG3	1.86	0.58
1:B:4517:LEU:HD21	1:B:4736:ASN:HB3	1.86	0.58
1:C:2307:PHE:HB2	1:C:2401:ARG:HB3	1.86	0.58
1:C:4016:PHE:HA	1:C:4019:MET:HE3	1.85	0.58
1:D:881:ILE:HG13	1:D:885:LEU:HG	1.86	0.58
1:A:4870:PHE:HD2	1:B:4868:ASP:OD2	1.87	0.58
1:B:191:TYR:CD1	1:B:209:GLN:HG3	2.38	0.58
1:B:310:GLU:OE2	1:B:310:GLU:N	2.34	0.58
1:C:191:TYR:CD1	1:C:209:GLN:HG3	2.38	0.58
1:C:1102:TYR:N	1:C:1237:GLU:O	2.37	0.58
1:C:2202:TYR:O	1:C:2206:ILE:HG12	2.03	0.58
1:C:2877:LEU:O	1:C:2882:LYS:NZ	2.37	0.58
1:C:4116:GLN:HA	1:C:4119:LEU:HD12	1.85	0.58
1:D:562:LEU:HG	1:D:600:LEU:HD13	1.85	0.58
1:A:1043:LYS:HA	1:A:1046:ASN:HD21	1.68	0.57
1:A:2773:TRP:HB3	1:A:2774:PRO:HD3	1.85	0.57
1:B:1255:LEU:HD11	1:B:1451:HIS:HB3	1.86	0.57
1:B:1785:ASP:OD1	1:B:1786:ILE:N	2.36	0.57
1:B:2787:TRP:HD1	1:B:2906:GLY:N	1.99	0.57
1:B:2832:THR:HG21	1:C:1550:PRO:HD3	1.86	0.57
1:B:2877:LEU:O	1:B:2882:LYS:NZ	2.36	0.57
1:B:2905:ARG:HH11	1:B:2906:GLY:H	1.52	0.57
1:C:1950:ALA:HB1	1:C:1961:LYS:NZ	2.18	0.57
1:D:885:LEU:O	1:D:889:ILE:HG12	2.03	0.57
1:A:2877:LEU:O	1:A:2882:LYS:NZ	2.36	0.57
1:B:2202:TYR:O	1:B:2206:ILE:HG12	2.03	0.57
1:C:885:LEU:O	1:C:889:ILE:HG12	2.03	0.57
1:D:4116:GLN:HA	1:D:4119:LEU:HD12	1.85	0.57
1:A:2905:ARG:HH11	1:A:2906:GLY:H	1.52	0.57
1:A:4914:ASN:HB3	1:A:4917:ASN:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:LEU:HG	1:B:600:LEU:HD13	1.85	0.57
1:C:2894:LYS:O	1:C:2898:ILE:HG12	2.05	0.57
1:C:4144:ARG:NH2	1:C:4962:TYR:OH	2.34	0.57
1:D:1689:ILE:HA	1:D:1703:TYR:HE1	1.69	0.57
1:D:2790:GLU:N	1:D:2902:ALA:O	2.33	0.57
1:A:562:LEU:HG	1:A:600:LEU:HD13	1.85	0.57
1:A:4517:LEU:HD21	1:A:4736:ASN:HB3	1.86	0.57
1:C:3845:LEU:HD23	1:C:3848:GLU:HG3	1.86	0.57
1:D:4245:LEU:O	1:D:4249:ARG:HG3	2.04	0.57
1:A:881:ILE:HG13	1:A:885:LEU:HG	1.86	0.57
1:A:1689:ILE:HA	1:A:1703:TYR:HE1	1.69	0.57
1:B:891:GLU:O	1:B:895:MET:HG3	2.05	0.57
1:C:874:LEU:HD23	1:C:941:LYS:HD3	1.86	0.57
1:C:1255:LEU:HD11	1:C:1451:HIS:HB3	1.86	0.57
1:D:670:TYR:HD1	1:D:1017:THR:HG21	1.70	0.57
1:D:874:LEU:HD23	1:D:941:LYS:HD3	1.86	0.57
1:D:1043:LYS:HA	1:D:1046:ASN:HD21	1.68	0.57
1:D:4187:GLU:OE1	1:D:4949:TRP:NE1	2.35	0.57
1:A:4116:GLN:HA	1:A:4119:LEU:HD12	1.85	0.57
1:B:3778:LEU:HD13	1:B:3854:PHE:HD1	1.70	0.57
1:B:4116:GLN:HA	1:B:4119:LEU:HD12	1.85	0.57
1:B:4245:LEU:O	1:B:4249:ARG:HG3	2.04	0.57
1:C:881:ILE:HG13	1:C:885:LEU:HG	1.86	0.57
1:D:2877:LEU:O	1:D:2882:LYS:NZ	2.37	0.57
1:B:2307:PHE:HB2	1:B:2401:ARG:HB3	1.86	0.57
1:C:3778:LEU:HD13	1:C:3854:PHE:HD1	1.70	0.57
1:D:3845:LEU:HD23	1:D:3848:GLU:HG3	1.86	0.57
1:A:989:THR:OG1	1:A:992:GLN:HG3	2.05	0.57
1:A:2790:GLU:N	1:A:2902:ALA:O	2.33	0.57
1:B:262:TYR:HB2	1:B:389:ARG:HG3	1.86	0.57
1:B:317:MET:HE2	1:B:321:LYS:HG3	1.85	0.57
1:B:874:LEU:HD23	1:B:941:LYS:HD3	1.86	0.57
1:B:4914:ASN:HB3	1:B:4917:ASN:HB2	1.87	0.57
1:C:670:TYR:HD1	1:C:1017:THR:HG21	1.69	0.57
1:C:4245:LEU:O	1:C:4249:ARG:HG3	2.04	0.57
1:D:4197:ILE:HG23	1:D:4923:MET:HE2	1.87	0.57
1:D:4914:ASN:HB3	1:D:4917:ASN:HB2	1.87	0.57
1:A:2857:LYS:CE	1:A:2871:LEU:HD23	2.30	0.57
1:B:4481:TRP:CD1	1:B:4692:SER:HA	2.40	0.57
1:C:317:MET:HE2	1:C:321:LYS:HG3	1.86	0.57
1:D:2757:MET:O	1:D:2820:GLY:N	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:LEU:HD23	1:A:941:LYS:HD3	1.86	0.57
1:A:891:GLU:O	1:A:895:MET:HG3	2.05	0.57
1:A:2757:MET:O	1:A:2820:GLY:N	2.38	0.57
1:B:989:THR:OG1	1:B:992:GLN:HG3	2.05	0.57
1:C:891:GLU:O	1:C:895:MET:HG3	2.05	0.57
1:C:2757:MET:O	1:C:2820:GLY:N	2.38	0.57
1:C:4481:TRP:CD1	1:C:4692:SER:HA	2.40	0.57
1:D:891:GLU:HA	1:D:894:VAL:HG22	1.87	0.57
1:D:2307:PHE:HB2	1:D:2401:ARG:HB3	1.86	0.56
1:A:891:GLU:HA	1:A:894:VAL:HG22	1.87	0.56
1:B:1689:ILE:HA	1:B:1703:TYR:HE1	1.69	0.56
1:B:4026:LEU:HD13	1:B:4055:HIS:CG	2.40	0.56
1:C:204:ASP:OD1	1:C:205:ALA:N	2.38	0.56
1:C:1250:TRP:HE3	1:C:1596:TRP:HB3	1.70	0.56
1:D:989:THR:OG1	1:D:992:GLN:HG3	2.05	0.56
1:D:3022:PHE:HB2	1:D:3026:ALA:HB2	1.86	0.56
1:A:1250:TRP:HE3	1:A:1596:TRP:HB3	1.70	0.56
1:A:4026:LEU:HD13	1:A:4055:HIS:CG	2.40	0.56
1:A:4481:TRP:CD1	1:A:4692:SER:HA	2.40	0.56
1:A:4868:ASP:O	1:A:4872:GLU:HG3	2.05	0.56
1:B:204:ASP:OD1	1:B:205:ALA:N	2.38	0.56
1:B:2757:MET:O	1:B:2820:GLY:N	2.38	0.56
1:B:2855:LYS:HA	1:B:2858:MET:HG2	1.87	0.56
1:B:2894:LYS:O	1:B:2898:ILE:HG12	2.05	0.56
1:B:3022:PHE:HB2	1:B:3026:ALA:HB2	1.86	0.56
1:D:891:GLU:O	1:D:895:MET:HG3	2.05	0.56
1:D:1670:HIS:O	1:D:1674:HIS:ND1	2.32	0.56
1:D:2708:THR:O	1:D:2780:LYS:HD2	2.06	0.56
1:D:4026:LEU:HD13	1:D:4055:HIS:CG	2.40	0.56
1:D:4481:TRP:CD1	1:D:4692:SER:HA	2.40	0.56
1:A:204:ASP:OD1	1:A:205:ALA:N	2.38	0.56
1:A:262:TYR:HB2	1:A:389:ARG:HG3	1.86	0.56
1:A:4245:LEU:O	1:A:4249:ARG:HG3	2.04	0.56
1:B:881:ILE:HG13	1:B:885:LEU:HG	1.86	0.56
1:B:2440:PHE:HB3	1:B:2460:PHE:HD2	1.71	0.56
1:B:4868:ASP:O	1:B:4872:GLU:HG3	2.05	0.56
1:C:989:THR:OG1	1:C:992:GLN:HG3	2.05	0.56
1:C:1689:ILE:HA	1:C:1703:TYR:HE1	1.69	0.56
1:C:2440:PHE:HB3	1:C:2460:PHE:HD2	1.71	0.56
1:D:2855:LYS:HE3	1:D:2856:LYS:HZ2	1.70	0.56
1:D:2894:LYS:O	1:D:2898:ILE:HG12	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2307:PHE:HB2	1:A:2401:ARG:HB3	1.86	0.56
1:A:2440:PHE:HB3	1:A:2460:PHE:HD2	1.71	0.56
1:A:2855:LYS:HA	1:A:2858:MET:HG2	1.87	0.56
1:B:436:LEU:HG	1:B:445:VAL:HG11	1.88	0.56
1:B:670:TYR:HD1	1:B:1017:THR:HG21	1.69	0.56
1:B:3845:LEU:HD23	1:B:3848:GLU:HG3	1.86	0.56
1:C:985:PHE:H	1:C:985:PHE:HD2	1.53	0.56
1:C:3022:PHE:HB2	1:C:3026:ALA:HB2	1.86	0.56
1:C:4868:ASP:O	1:C:4872:GLU:HG3	2.05	0.56
1:D:1255:LEU:HD11	1:D:1451:HIS:HB3	1.86	0.56
2:H:88:HIS:NE2	1:D:1776:TYR:OH	2.30	0.56
1:B:1549:SER:OG	1:B:1551:ASN:O	2.24	0.56
1:C:4644:TYR:CE2	1:C:4646:ASP:HB3	2.41	0.56
1:D:4868:ASP:O	1:D:4872:GLU:HG3	2.05	0.56
1:B:1467:VAL:HG21	1:B:1482:ARG:HH21	1.71	0.56
1:C:398:HIS:HB3	1:C:400:ASP:H	1.70	0.56
1:C:436:LEU:HG	1:C:445:VAL:HG11	1.88	0.56
1:C:2708:THR:O	1:C:2780:LYS:HD2	2.06	0.56
1:C:2855:LYS:HA	1:C:2858:MET:HG2	1.86	0.56
1:C:4914:ASN:HB3	1:C:4917:ASN:HB2	1.87	0.56
1:D:204:ASP:OD1	1:D:205:ALA:N	2.38	0.56
1:A:398:HIS:HB3	1:A:400:ASP:H	1.70	0.56
1:A:670:TYR:HD1	1:A:1017:THR:HG21	1.70	0.56
1:A:1258:PHE:CG	1:A:1303:ARG:HD3	2.41	0.56
1:A:2480:VAL:HB	1:A:2483:PHE:HB3	1.88	0.56
1:A:3778:LEU:HD13	1:A:3854:PHE:HD1	1.69	0.56
1:B:4644:TYR:CE2	1:B:4646:ASP:HB3	2.41	0.56
1:C:262:TYR:HB2	1:C:389:ARG:HG3	1.86	0.56
1:D:1250:TRP:HE3	1:D:1596:TRP:HB3	1.71	0.56
1:D:2440:PHE:HB3	1:D:2460:PHE:HD2	1.71	0.56
1:A:3022:PHE:HB2	1:A:3026:ALA:HB2	1.86	0.56
1:B:1102:TYR:N	1:B:1237:GLU:O	2.37	0.56
1:B:2708:THR:O	1:B:2780:LYS:HD2	2.06	0.56
1:D:398:HIS:HB3	1:D:400:ASP:H	1.70	0.56
1:D:2855:LYS:HA	1:D:2858:MET:HG2	1.86	0.56
1:A:2195:ASN:HD22	1:A:2198:ARG:HH12	1.54	0.56
1:A:2894:LYS:O	1:A:2898:ILE:HG12	2.05	0.56
1:C:2195:ASN:HD22	1:C:2198:ARG:HH12	1.54	0.56
1:B:398:HIS:HB3	1:B:400:ASP:H	1.70	0.55
1:B:1258:PHE:CG	1:B:1303:ARG:HD3	2.41	0.55
1:C:1467:VAL:HG21	1:C:1482:ARG:HH21	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2635:GLU:HG2	1:C:2680:TYR:HE1	1.71	0.55
1:C:4026:LEU:HD13	1:C:4055:HIS:CG	2.40	0.55
1:D:436:LEU:HG	1:D:445:VAL:HG11	1.88	0.55
1:D:1467:VAL:HG21	1:D:1482:ARG:HH21	1.71	0.55
1:D:1929:SER:HG	1:D:3620:PHE:HD2	1.55	0.55
1:D:4016:PHE:HA	1:D:4019:MET:HE3	1.88	0.55
1:A:3962:SER:HB3	1:A:4071:GLU:HG2	1.88	0.55
1:A:4197:ILE:HG23	1:A:4923:MET:HE2	1.87	0.55
1:C:2659:GLN:OE1	1:C:2659:GLN:N	2.37	0.55
1:D:262:TYR:HB2	1:D:389:ARG:HG3	1.86	0.55
1:D:3778:LEU:HD13	1:D:3854:PHE:HD1	1.69	0.55
1:C:2480:VAL:HB	1:C:2483:PHE:HB3	1.88	0.55
1:A:2504:THR:O	1:A:2508:SER:N	2.40	0.55
1:A:4144:ARG:NH2	1:A:4962:TYR:OH	2.34	0.55
1:A:4521:LYS:HZ3	1:B:4807:ASP:HB3	1.70	0.55
1:B:3962:SER:HB3	1:B:4071:GLU:HG2	1.88	0.55
1:C:1724:GLU:HG2	1:C:2165:LEU:HD23	1.89	0.55
1:C:4197:ILE:HG23	1:C:4923:MET:HE2	1.88	0.55
1:D:756:SER:OG	1:D:769:ARG:O	2.25	0.55
1:D:3962:SER:HB3	1:D:4071:GLU:HG2	1.88	0.55
1:A:436:LEU:HG	1:A:445:VAL:HG11	1.88	0.55
1:A:985:PHE:H	1:A:985:PHE:HD2	1.53	0.55
1:A:1108:VAL:HB	1:A:1212:VAL:HG23	1.89	0.55
1:A:1724:GLU:HG2	1:A:2165:LEU:HD23	1.89	0.55
1:A:2635:GLU:HG2	1:A:2680:TYR:HE1	1.71	0.55
1:A:2708:THR:O	1:A:2780:LYS:HD2	2.06	0.55
1:A:4014:LEU:HD13	1:A:4122:ALA:HB2	1.88	0.55
1:B:857:LEU:HG	1:B:860:ALA:HB2	1.88	0.55
1:B:2195:ASN:HD22	1:B:2198:ARG:HH12	1.54	0.55
1:B:3622:GLN:O	1:B:3626:LYS:NZ	2.39	0.55
1:C:2619:LYS:HB2	1:C:2627:TRP:CH2	2.41	0.55
1:D:889:ILE:HA	1:D:892:LEU:HB2	1.88	0.55
1:D:1549:SER:OG	1:D:1551:ASN:O	2.24	0.55
1:B:2062:ILE:O	1:B:2066:MET:HG2	2.07	0.55
1:C:1258:PHE:CG	1:C:1303:ARG:HD3	2.41	0.55
1:D:894:VAL:HA	1:D:897:LYS:HG2	1.89	0.55
1:D:985:PHE:H	1:D:985:PHE:HD2	1.53	0.55
1:D:2195:ASN:HD22	1:D:2198:ARG:HH12	1.54	0.55
1:A:889:ILE:HA	1:A:892:LEU:HB2	1.88	0.55
1:A:1467:VAL:HG21	1:A:1482:ARG:HH21	1.71	0.55
1:C:2212:LYS:NZ	1:C:3822:GLU:OE1	2.32	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2521:CYS:HA	1:C:2525:LEU:HD12	1.89	0.55
1:D:1945:ASN:O	1:D:1949:GLN:HG2	2.07	0.55
1:D:2521:CYS:HA	1:D:2525:LEU:HD12	1.89	0.55
1:D:4093:ASP:OD1	1:D:4094:ILE:HD12	2.07	0.55
1:A:857:LEU:HG	1:A:860:ALA:HB2	1.88	0.55
1:B:1945:ASN:O	1:B:1949:GLN:HG2	2.07	0.55
1:B:4831:ILE:HG13	1:B:4843:ARG:NH2	2.21	0.55
1:C:1628:MET:HG3	1:C:1687:TYR:CD2	2.42	0.55
1:C:2062:ILE:O	1:C:2066:MET:HG2	2.07	0.55
1:C:2834:SER:OG	1:C:2836:ASP:OD1	2.20	0.55
1:D:625:VAL:HG12	1:D:628:ASN:H	1.72	0.55
1:D:919:VAL:HB	1:D:923:LYS:HG3	1.89	0.55
1:D:1258:PHE:CG	1:D:1303:ARG:HD3	2.41	0.55
1:D:2758:LYS:NZ	1:D:2762:LEU:O	2.40	0.55
1:D:4144:ARG:NH2	1:D:4962:TYR:OH	2.34	0.55
1:A:919:VAL:HB	1:A:923:LYS:HG3	1.89	0.55
1:A:1628:MET:HG3	1:A:1687:TYR:CD2	2.42	0.55
1:A:3622:GLN:O	1:A:3626:LYS:NZ	2.39	0.55
1:B:4827:ILE:O	1:B:4831:ILE:HG12	2.07	0.55
1:C:1610:ARG:HA	1:C:1617:TRP:HA	1.89	0.55
1:D:857:LEU:HG	1:D:860:ALA:HB2	1.88	0.55
1:D:1108:VAL:HB	1:D:1212:VAL:HG23	1.89	0.55
1:A:625:VAL:HG12	1:A:628:ASN:H	1.72	0.55
1:A:1102:TYR:N	1:A:1237:GLU:O	2.37	0.55
1:B:891:GLU:HA	1:B:894:VAL:HG22	1.87	0.55
1:B:1250:TRP:HE3	1:B:1596:TRP:HB3	1.70	0.55
1:B:1628:MET:HG3	1:B:1687:TYR:CD2	2.42	0.55
1:C:891:GLU:HA	1:C:894:VAL:HG22	1.87	0.55
1:D:2480:VAL:HB	1:D:2483:PHE:HB3	1.88	0.55
1:D:2619:LYS:HB2	1:D:2627:TRP:CH2	2.41	0.55
1:D:4014:LEU:HD13	1:D:4122:ALA:HB2	1.88	0.55
1:A:2605:MET:HB3	1:A:2606:PRO:HD3	1.89	0.54
1:A:4644:TYR:CE2	1:A:4646:ASP:HB3	2.41	0.54
1:B:2619:LYS:HB2	1:B:2627:TRP:CH2	2.41	0.54
1:B:2635:GLU:HG2	1:B:2680:TYR:HE1	1.71	0.54
1:B:2659:GLN:OE1	1:B:2659:GLN:N	2.37	0.54
1:B:2777:GLU:O	1:B:2781:THR:OG1	2.19	0.54
1:B:2998:ASN:OD1	1:B:2999:LYS:N	2.40	0.54
1:C:1670:HIS:O	1:C:1674:HIS:ND1	2.32	0.54
1:C:2790:GLU:N	1:C:2902:ALA:O	2.33	0.54
1:D:2160:ASN:OD1	1:D:2163:ARG:NH2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2605:MET:HB3	1:D:2606:PRO:HD3	1.89	0.54
1:D:2635:GLU:HG2	1:D:2680:TYR:HE1	1.71	0.54
1:D:2998:ASN:OD1	1:D:2999:LYS:N	2.40	0.54
1:D:3846:LEU:HB3	1:D:3854:PHE:CE2	2.42	0.54
1:A:894:VAL:HA	1:A:897:LYS:HG2	1.89	0.54
1:A:2619:LYS:HB2	1:A:2627:TRP:CH2	2.41	0.54
1:A:2998:ASN:OD1	1:A:2999:LYS:N	2.40	0.54
1:A:4183:LYS:HE2	1:D:4906:GLU:OE2	2.08	0.54
1:B:2480:VAL:HB	1:B:2483:PHE:HB3	1.88	0.54
1:B:2930:ILE:HA	1:B:3010:LYS:HZ1	1.73	0.54
1:C:857:LEU:HG	1:C:860:ALA:HB2	1.88	0.54
1:D:2062:ILE:O	1:D:2066:MET:HG2	2.07	0.54
1:D:2719:TYR:OH	1:D:2799:ALA:HB2	2.07	0.54
1:D:2768:LYS:O	1:D:2772:ARG:HD3	2.07	0.54
1:D:3013:VAL:O	1:D:3018:ARG:NH2	2.40	0.54
1:D:4644:TYR:CE2	1:D:4646:ASP:HB3	2.41	0.54
1:A:756:SER:OG	1:A:769:ARG:O	2.25	0.54
1:A:1945:ASN:O	1:A:1949:GLN:HG2	2.07	0.54
1:A:2719:TYR:OH	1:A:2799:ALA:HB2	2.07	0.54
1:B:756:SER:OG	1:B:769:ARG:O	2.25	0.54
1:B:2504:THR:O	1:B:2508:SER:N	2.40	0.54
1:B:2758:LYS:NZ	1:B:2762:LEU:O	2.40	0.54
1:D:1628:MET:HG3	1:D:1687:TYR:CD2	2.42	0.54
1:D:2767:GLU:O	1:D:2771:TYR:N	2.40	0.54
1:A:310:GLU:OE2	1:A:310:GLU:N	2.34	0.54
1:A:801:ARG:NH1	1:A:1615:GLN:O	2.40	0.54
1:A:1670:HIS:O	1:A:1674:HIS:ND1	2.32	0.54
1:A:2521:CYS:HA	1:A:2525:LEU:HD12	1.89	0.54
1:B:625:VAL:HG12	1:B:628:ASN:H	1.72	0.54
1:B:3013:VAL:O	1:B:3018:ARG:NH2	2.40	0.54
1:C:889:ILE:HA	1:C:892:LEU:HB2	1.88	0.54
1:C:1265:HIS:O	1:C:1288:LYS:NZ	2.27	0.54
1:C:1471:ASP:OD2	1:C:1473:LYS:NZ	2.40	0.54
1:C:2998:ASN:OD1	1:C:2999:LYS:N	2.40	0.54
1:D:1610:ARG:HA	1:D:1617:TRP:HA	1.89	0.54
1:A:2930:ILE:HA	1:A:3010:LYS:HZ1	1.73	0.54
1:A:4827:ILE:O	1:A:4831:ILE:HG12	2.07	0.54
2:H:80:ASP:OD1	2:H:81:VAL:N	2.41	0.54
1:B:2834:SER:OG	1:B:2836:ASP:OD1	2.20	0.54
1:C:801:ARG:NH1	1:C:1615:GLN:O	2.40	0.54
1:C:877:HIS:HA	1:C:880:ARG:CD	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:919:VAL:HB	1:C:923:LYS:HG3	1.89	0.54
1:C:2797:SER:HB3	1:C:2801:TYR:HE2	1.72	0.54
1:D:28:ILE:HG22	1:D:29:HIS:CD2	2.43	0.54
2:F:80:ASP:OD1	2:F:81:VAL:N	2.41	0.54
1:B:985:PHE:H	1:B:985:PHE:HD2	1.53	0.54
1:B:3846:LEU:HB3	1:B:3854:PHE:CE2	2.42	0.54
1:B:4014:LEU:HD13	1:B:4122:ALA:HB2	1.88	0.54
1:C:625:VAL:HG12	1:C:628:ASN:H	1.72	0.54
1:C:1440:ASN:HB3	1:C:1546:GLN:HB3	1.90	0.54
1:C:1896:MET:HB3	1:C:1898:LEU:HD11	1.90	0.54
1:C:2605:MET:HB3	1:C:2606:PRO:HD3	1.90	0.54
1:C:4093:ASP:OD1	1:C:4094:ILE:HD12	2.07	0.54
1:A:3846:LEU:HB3	1:A:3854:PHE:CE2	2.42	0.54
1:A:4093:ASP:OD1	1:A:4094:ILE:HD12	2.07	0.54
1:A:4520:TYR:CD1	1:A:4561:LEU:HD13	2.43	0.54
1:B:2160:ASN:OD1	1:B:2163:ARG:NH2	2.40	0.54
1:B:2719:TYR:OH	1:B:2799:ALA:HB2	2.07	0.54
1:C:28:ILE:HG22	1:C:29:HIS:CD2	2.43	0.54
1:C:28:ILE:HG22	1:C:29:HIS:HD2	1.73	0.54
1:C:1989:PRO:O	1:C:1993:ARG:HG3	2.08	0.54
1:C:3846:LEU:HB3	1:C:3854:PHE:CE2	2.42	0.54
1:C:3962:SER:HB3	1:C:4071:GLU:HG2	1.88	0.54
1:D:679:VAL:HA	1:D:800:VAL:HG12	1.90	0.54
1:D:1896:MET:HB3	1:D:1898:LEU:HD11	1.90	0.54
1:A:2855:LYS:HE3	1:A:2856:LYS:HZ2	1.73	0.54
2:F:16:PHE:O	2:F:18:LYS:NZ	2.37	0.54
1:B:1610:ARG:HA	1:B:1617:TRP:HA	1.89	0.54
1:B:1989:PRO:O	1:B:1993:ARG:HG3	2.08	0.54
1:B:2521:CYS:HA	1:B:2525:LEU:HD12	1.89	0.54
1:B:2832:THR:HG21	1:C:1290:PHE:HE2	1.73	0.54
1:C:20:VAL:HG12	1:C:216:PRO:HA	1.90	0.54
1:C:2768:LYS:O	1:C:2772:ARG:HD3	2.07	0.54
1:D:877:HIS:HA	1:D:880:ARG:CD	2.38	0.54
1:D:1440:ASN:HB3	1:D:1546:GLN:HB3	1.90	0.54
1:D:2092:TYR:CD2	1:D:3640:LEU:HD13	2.43	0.54
1:D:4827:ILE:O	1:D:4831:ILE:HG12	2.07	0.54
1:A:1303:ARG:HD2	1:A:1446:ILE:HD11	1.90	0.54
1:B:887:GLU:HB2	1:B:921:PHE:HZ	1.73	0.54
1:B:919:VAL:HB	1:B:923:LYS:HG3	1.89	0.54
1:C:3921:THR:O	1:C:3925:GLN:HG2	2.08	0.54
1:C:4520:TYR:CD1	1:C:4561:LEU:HD13	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:HG22	1:A:29:HIS:CD2	2.43	0.54
1:B:28:ILE:HG22	1:B:29:HIS:CD2	2.43	0.54
1:B:227:TYR:CG	1:B:352:SER:HB2	2.43	0.54
1:B:801:ARG:NH1	1:B:1615:GLN:O	2.40	0.54
1:B:1011:ARG:HH21	1:B:1014:GLN:NE2	2.06	0.54
1:B:1645:THR:HG22	1:B:1695:PRO:HG3	1.90	0.54
1:B:1896:MET:HB3	1:B:1898:LEU:HD11	1.90	0.54
1:B:2605:MET:HB3	1:B:2606:PRO:HD3	1.90	0.54
1:C:227:TYR:CG	1:C:352:SER:HB2	2.43	0.54
1:C:2526:PRO:HB3	1:C:2530:ARG:NH1	2.23	0.54
1:C:4827:ILE:O	1:C:4831:ILE:HG12	2.07	0.54
1:D:1724:GLU:HG2	1:D:2165:LEU:HD23	1.89	0.54
1:D:1989:PRO:O	1:D:1993:ARG:HG3	2.08	0.54
1:D:3622:GLN:O	1:D:3626:LYS:NZ	2.39	0.54
1:A:28:ILE:HG22	1:A:29:HIS:HD2	1.73	0.53
1:A:1429:SER:HB2	1:A:1556:GLU:HB2	1.90	0.53
1:A:3879:LEU:O	1:A:3882:GLN:HG3	2.08	0.53
1:B:966:LEU:HD12	1:B:979:ALA:HB2	1.90	0.53
1:B:1724:GLU:HG2	1:B:2165:LEU:HD23	1.89	0.53
1:B:2337:GLY:O	1:C:141:ASP:HA	2.08	0.53
1:B:2797:SER:HB3	1:B:2801:TYR:HE2	1.72	0.53
1:B:3879:LEU:O	1:B:3882:GLN:HG3	2.08	0.53
1:B:4881:LYS:O	1:B:4885:GLU:HG2	2.08	0.53
1:C:1023:ASP:HB2	1:C:1028:ARG:HB2	1.90	0.53
1:C:2092:TYR:CD2	1:C:3640:LEU:HD13	2.43	0.53
1:C:2719:TYR:OH	1:C:2799:ALA:HB2	2.08	0.53
1:D:2782:MET:CG	1:D:2783:LEU:HD12	2.38	0.53
1:A:679:VAL:HA	1:A:800:VAL:HG12	1.90	0.53
1:A:1014:GLN:O	1:A:1027:ARG:NH1	2.42	0.53
1:A:1896:MET:HB3	1:A:1898:LEU:HD11	1.90	0.53
1:A:2062:ILE:O	1:A:2066:MET:HG2	2.07	0.53
1:A:3013:VAL:O	1:A:3018:ARG:NH2	2.40	0.53
2:G:58:LYS:O	2:G:62:GLU:HG3	2.08	0.53
2:G:80:ASP:OD1	2:G:81:VAL:N	2.41	0.53
1:B:679:VAL:HA	1:B:800:VAL:HG12	1.90	0.53
1:B:894:VAL:HA	1:B:897:LYS:HG2	1.89	0.53
1:B:1303:ARG:HD2	1:B:1446:ILE:HD11	1.90	0.53
1:B:2729:HIS:NE2	1:B:2763:LEU:HD22	2.24	0.53
1:C:1097:LYS:NZ	1:C:1198:GLY:O	2.42	0.53
1:C:2782:MET:CG	1:C:2783:LEU:HD12	2.38	0.53
1:C:2857:LYS:CE	1:C:2871:LEU:HD23	2.30	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2930:ILE:HG23	1:C:3010:LYS:HZ3	1.73	0.53
1:C:4014:LEU:HD13	1:C:4122:ALA:HB2	1.88	0.53
1:D:1689:ILE:HA	1:D:1703:TYR:CE1	2.44	0.53
1:A:877:HIS:HA	1:A:880:ARG:CD	2.38	0.53
1:A:1477:HIS:CE1	1:A:1478:GLU:HG3	2.43	0.53
1:A:2782:MET:CG	1:A:2783:LEU:HD12	2.38	0.53
1:B:1023:ASP:HB2	1:B:1028:ARG:HB2	1.90	0.53
1:B:1108:VAL:HB	1:B:1212:VAL:HG23	1.89	0.53
1:B:1477:HIS:CE1	1:B:1478:GLU:HG3	2.43	0.53
1:C:1011:ARG:HH21	1:C:1014:GLN:NE2	2.06	0.53
1:C:1108:VAL:HB	1:C:1212:VAL:HG23	1.89	0.53
1:C:1945:ASN:O	1:C:1949:GLN:HG2	2.07	0.53
1:C:2832:THR:HG21	1:D:1550:PRO:HD3	1.90	0.53
1:D:310:GLU:OE2	1:D:310:GLU:N	2.34	0.53
1:D:2397:ASP:O	1:D:2401:ARG:HG2	2.09	0.53
1:D:2659:GLN:O	1:D:2965:LYS:NZ	2.41	0.53
1:D:2797:SER:HB3	1:D:2801:TYR:HE2	1.72	0.53
1:D:2857:LYS:CE	1:D:2871:LEU:HD23	2.30	0.53
1:D:4520:TYR:CD1	1:D:4561:LEU:HD13	2.43	0.53
1:A:1023:ASP:HB2	1:A:1028:ARG:HB2	1.90	0.53
1:A:2659:GLN:O	1:A:2965:LYS:NZ	2.41	0.53
1:A:2768:LYS:O	1:A:2772:ARG:HD3	2.07	0.53
2:G:16:PHE:O	2:G:18:LYS:NZ	2.37	0.53
1:B:1429:SER:HB2	1:B:1556:GLU:HB2	1.90	0.53
1:C:966:LEU:HD12	1:C:979:ALA:HB2	1.91	0.53
1:C:2127:ARG:NH2	1:C:2165:LEU:O	2.42	0.53
1:D:227:TYR:CG	1:D:352:SER:HB2	2.43	0.53
1:D:887:GLU:HB2	1:D:921:PHE:HZ	1.73	0.53
1:D:1014:GLN:O	1:D:1027:ARG:NH1	2.42	0.53
1:D:2729:HIS:NE2	1:D:2763:LEU:HD22	2.24	0.53
1:A:20:VAL:HG12	1:A:216:PRO:HA	1.90	0.53
1:A:966:LEU:HD12	1:A:979:ALA:HB2	1.90	0.53
1:A:1097:LYS:NZ	1:A:1198:GLY:O	2.42	0.53
1:A:2526:PRO:HB3	1:A:2530:ARG:NH1	2.23	0.53
1:B:877:HIS:HA	1:B:880:ARG:CD	2.38	0.53
1:B:889:ILE:HA	1:B:892:LEU:HB2	1.88	0.53
1:B:4520:TYR:CD1	1:B:4561:LEU:HD13	2.43	0.53
1:C:1477:HIS:CE1	1:C:1478:GLU:HG3	2.43	0.53
1:C:2729:HIS:NE2	1:C:2763:LEU:HD22	2.24	0.53
1:C:4265:LYS:O	1:C:4269:LYS:HG2	2.09	0.53
1:C:4831:ILE:HG13	1:C:4843:ARG:NH2	2.21	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4881:LYS:O	1:C:4885:GLU:HG2	2.08	0.53
1:D:966:LEU:HD12	1:D:979:ALA:HB2	1.90	0.53
1:D:1011:ARG:HH21	1:D:1014:GLN:NE2	2.06	0.53
1:D:1023:ASP:HB2	1:D:1028:ARG:HB2	1.90	0.53
1:D:1429:SER:HB2	1:D:1556:GLU:HB2	1.90	0.53
1:D:2127:ARG:NH2	1:D:2165:LEU:O	2.42	0.53
1:D:2868:HIS:CD2	1:D:2870:LEU:HB2	2.44	0.53
1:D:3668:ILE:HD12	1:D:3734:ARG:HB2	1.91	0.53
1:A:2729:HIS:NE2	1:A:2763:LEU:HD22	2.24	0.53
2:E:80:ASP:OD1	2:E:81:VAL:N	2.41	0.53
2:H:16:PHE:O	2:H:18:LYS:NZ	2.37	0.53
2:H:58:LYS:O	2:H:62:GLU:HG3	2.08	0.53
1:C:874:LEU:HB2	1:C:878:LEU:HD22	1.91	0.53
1:D:20:VAL:HG12	1:D:216:PRO:HA	1.90	0.53
1:D:28:ILE:HG22	1:D:29:HIS:HD2	1.73	0.53
1:D:1097:LYS:NZ	1:D:1198:GLY:O	2.42	0.53
1:A:1610:ARG:HA	1:A:1617:TRP:HA	1.89	0.53
1:A:1645:THR:HG22	1:A:1695:PRO:HG3	1.90	0.53
1:A:2832:THR:HG21	1:B:1290:PHE:CE2	2.39	0.53
2:E:58:LYS:O	2:E:62:GLU:HG3	2.08	0.53
1:B:874:LEU:HB2	1:B:878:LEU:HD22	1.91	0.53
1:B:2526:PRO:HB3	1:B:2530:ARG:NH1	2.23	0.53
1:C:679:VAL:HA	1:C:800:VAL:HG12	1.90	0.53
1:D:229:ILE:HG22	1:D:288:HIS:HD2	1.74	0.53
1:D:3921:THR:O	1:D:3925:GLN:HG2	2.08	0.53
1:D:4881:LYS:O	1:D:4885:GLU:HG2	2.08	0.53
1:A:887:GLU:HB2	1:A:921:PHE:HZ	1.73	0.53
1:A:2659:GLN:OE1	1:A:2659:GLN:N	2.37	0.53
1:A:4279:MET:HE2	1:B:4487:TYR:CD1	2.23	0.53
2:F:58:LYS:O	2:F:62:GLU:HG3	2.08	0.53
1:B:20:VAL:HG12	1:B:216:PRO:HA	1.90	0.53
1:B:1440:ASN:HB3	1:B:1546:GLN:HB3	1.90	0.53
1:B:2767:GLU:O	1:B:2771:TYR:N	2.40	0.53
1:B:2790:GLU:N	1:B:2902:ALA:O	2.33	0.53
1:C:894:VAL:HA	1:C:897:LYS:HG2	1.89	0.53
1:C:4287:TYR:HA	1:C:4290:ILE:HD12	1.91	0.53
1:D:4265:LYS:O	1:D:4269:LYS:HG2	2.09	0.53
1:A:1011:ARG:HH21	1:A:1014:GLN:NE2	2.06	0.53
1:A:3668:ILE:HD12	1:A:3734:ARG:HB2	1.91	0.53
1:B:1004:HIS:CE1	1:B:1038:LEU:HD21	2.44	0.53
1:B:2768:LYS:O	1:B:2772:ARG:HD3	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4093:ASP:OD1	1:B:4094:ILE:HD12	2.07	0.53
1:B:4187:GLU:OE1	1:B:4949:TRP:NE1	2.35	0.53
1:B:4287:TYR:HA	1:B:4290:ILE:HD12	1.91	0.53
1:C:1303:ARG:HD2	1:C:1446:ILE:HD11	1.90	0.53
1:C:1689:ILE:HA	1:C:1703:TYR:CE1	2.44	0.53
1:A:663:VAL:HG23	1:A:671:LYS:HE3	1.91	0.53
1:A:1689:ILE:HA	1:A:1703:TYR:CE1	2.44	0.53
1:A:1989:PRO:O	1:A:1993:ARG:HG3	2.08	0.53
1:A:2092:TYR:CD2	1:A:3640:LEU:HD13	2.43	0.53
1:A:2212:LYS:NZ	1:A:3822:GLU:OE1	2.32	0.53
1:A:4872:GLU:HG2	1:D:4874:ARG:HD3	1.91	0.53
2:G:12:ASP:OD1	2:G:68:SER:OG	2.27	0.53
1:B:2092:TYR:CD2	1:B:3640:LEU:HD13	2.43	0.53
1:B:2127:ARG:NH2	1:B:2165:LEU:O	2.42	0.53
1:B:2397:ASP:O	1:B:2401:ARG:HG2	2.09	0.53
1:B:3803:LEU:HB2	1:B:3884:SER:HB2	1.92	0.53
1:B:3921:THR:O	1:B:3925:GLN:HG2	2.08	0.53
1:B:4114:ARG:O	1:B:4117:THR:OG1	2.22	0.53
1:C:1014:GLN:O	1:C:1027:ARG:NH1	2.42	0.53
1:C:2504:THR:O	1:C:2508:SER:N	2.40	0.53
1:D:1181:ILE:HG22	1:D:1189:GLU:OE2	2.09	0.53
1:D:1477:HIS:CE1	1:D:1478:GLU:HG3	2.43	0.53
1:D:2526:PRO:HB3	1:D:2530:ARG:NH1	2.23	0.53
1:A:2724:TYR:HD1	1:A:2895:PHE:CD2	2.27	0.52
2:E:16:PHE:O	2:E:18:LYS:NZ	2.37	0.52
1:B:229:ILE:HG22	1:B:288:HIS:HD2	1.74	0.52
1:B:663:VAL:HG23	1:B:671:LYS:HE3	1.91	0.52
1:B:1087:ILE:HD11	1:B:1204:VAL:HG22	1.91	0.52
1:B:1689:ILE:HA	1:B:1703:TYR:CE1	2.44	0.52
1:B:2333:PRO:HA	1:B:2336:ARG:HG2	1.92	0.52
1:B:4016:PHE:HA	1:B:4019:MET:HE3	1.90	0.52
1:C:1181:ILE:HG22	1:C:1189:GLU:OE2	2.09	0.52
1:C:1429:SER:HB2	1:C:1556:GLU:HB2	1.90	0.52
1:C:2703:PRO:HB2	1:C:2854:LYS:HB2	1.91	0.52
1:D:3669:LEU:HB3	1:D:3673:ARG:HH21	1.74	0.52
1:A:229:ILE:HG22	1:A:288:HIS:HD2	1.74	0.52
1:A:1181:ILE:HG22	1:A:1189:GLU:OE2	2.09	0.52
1:A:1471:ASP:OD2	1:A:1473:LYS:NZ	2.40	0.52
1:A:2127:ARG:NH2	1:A:2165:LEU:O	2.42	0.52
1:A:2703:PRO:HB2	1:A:2854:LYS:HB2	1.91	0.52
1:B:1014:GLN:O	1:B:1027:ARG:NH1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4265:LYS:O	1:B:4269:LYS:HG2	2.09	0.52
1:C:1645:THR:HG22	1:C:1695:PRO:HG3	1.90	0.52
1:C:3803:LEU:HB2	1:C:3884:SER:HB2	1.92	0.52
1:D:663:VAL:HG23	1:D:671:LYS:HE3	1.91	0.52
1:D:1004:HIS:CE1	1:D:1038:LEU:HD21	2.44	0.52
1:D:1431:ARG:NE	1:D:1506:GLU:OE1	2.30	0.52
1:D:2333:PRO:HA	1:D:2336:ARG:HG2	1.92	0.52
1:A:1440:ASN:HB3	1:A:1546:GLN:HB3	1.90	0.52
1:A:2333:PRO:HA	1:A:2336:ARG:HG2	1.92	0.52
1:A:2729:HIS:CD2	1:A:2763:LEU:HD22	2.44	0.52
1:A:2868:HIS:CD2	1:A:2870:LEU:HB2	2.44	0.52
2:F:12:ASP:OD1	2:F:68:SER:OG	2.27	0.52
1:B:28:ILE:HG22	1:B:29:HIS:HD2	1.73	0.52
1:B:2729:HIS:CD2	1:B:2763:LEU:HD22	2.44	0.52
1:B:4144:ARG:NH2	1:B:4962:TYR:OH	2.34	0.52
1:C:663:VAL:HG23	1:C:671:LYS:HE3	1.91	0.52
1:C:887:GLU:HB2	1:C:921:PHE:HZ	1.73	0.52
1:D:1303:ARG:HD2	1:D:1446:ILE:HD11	1.90	0.52
1:D:1645:THR:HG22	1:D:1695:PRO:HG3	1.90	0.52
1:D:4831:ILE:HG13	1:D:4843:ARG:NH2	2.21	0.52
1:A:1549:SER:OG	1:A:1551:ASN:O	2.24	0.52
1:A:4640:PHE:HB3	1:A:4650:LYS:HE2	1.92	0.52
1:A:4881:LYS:O	1:A:4885:GLU:HG2	2.08	0.52
1:B:1097:LYS:NZ	1:B:1198:GLY:O	2.42	0.52
1:C:1549:SER:OG	1:C:1551:ASN:O	2.23	0.52
1:C:2397:ASP:O	1:C:2401:ARG:HG2	2.09	0.52
1:C:2729:HIS:CD2	1:C:2763:LEU:HD22	2.44	0.52
1:C:2868:HIS:CD2	1:C:2870:LEU:HB2	2.44	0.52
1:A:227:TYR:CG	1:A:352:SER:HB2	2.43	0.52
1:A:428:ARG:NH2	1:A:446:ASP:OD2	2.42	0.52
1:A:3921:THR:O	1:A:3925:GLN:HG2	2.08	0.52
1:B:428:ARG:NH2	1:B:446:ASP:OD2	2.43	0.52
1:C:367:ASP:OD1	1:C:368:THR:N	2.43	0.52
1:C:756:SER:OG	1:C:769:ARG:O	2.25	0.52
1:C:2333:PRO:HA	1:C:2336:ARG:HG2	1.92	0.52
1:C:3669:LEU:HB3	1:C:3673:ARG:HH21	1.74	0.52
1:D:332:ARG:NH1	1:D:339:ASP:OD1	2.43	0.52
1:D:2930:ILE:HA	1:D:3010:LYS:HZ1	1.75	0.52
1:A:1092:LYS:NZ	1:A:1646:GLU:OE1	2.39	0.52
1:A:2054:LYS:HE2	1:A:2056:SER:HA	1.92	0.52
1:B:332:ARG:NH1	1:B:339:ASP:OD1	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4197:ILE:HG23	1:B:4923:MET:HE2	1.90	0.52
1:C:4106:SER:HA	1:C:4115:LEU:HD21	1.92	0.52
1:C:4943:MET:HA	1:C:4946:GLU:HG2	1.91	0.52
1:A:4287:TYR:HA	1:A:4290:ILE:HD12	1.91	0.52
1:B:2054:LYS:HE2	1:B:2056:SER:HA	1.92	0.52
1:B:2868:HIS:CD2	1:B:2870:LEU:HB2	2.44	0.52
1:B:4702:ASP:O	1:B:4706:GLN:HG2	2.10	0.52
1:C:1087:ILE:HD11	1:C:1204:VAL:HG22	1.91	0.52
1:C:2659:GLN:O	1:C:2965:LYS:NZ	2.41	0.52
1:C:2724:TYR:HD1	1:C:2895:PHE:CD2	2.27	0.52
1:D:986:ILE:CD1	1:D:1055:ARG:HA	2.40	0.52
1:D:1471:ASP:OD2	1:D:1473:LYS:NZ	2.40	0.52
1:D:2724:TYR:HD1	1:D:2895:PHE:CD2	2.27	0.52
1:D:3803:LEU:HB2	1:D:3884:SER:HB2	1.92	0.52
1:D:4287:TYR:HA	1:D:4290:ILE:HD12	1.91	0.52
1:D:4664:ASP:N	1:D:4664:ASP:OD1	2.42	0.52
1:D:4702:ASP:O	1:D:4706:GLN:HG2	2.10	0.52
1:A:927:GLN:NE2	1:A:928:GLU:HG3	2.25	0.52
1:A:2397:ASP:O	1:A:2401:ARG:HG2	2.09	0.52
1:B:927:GLN:NE2	1:B:928:GLU:HG3	2.25	0.52
1:B:2782:MET:CG	1:B:2783:LEU:HD12	2.38	0.52
1:B:4664:ASP:OD1	1:B:4664:ASP:N	2.42	0.52
1:C:229:ILE:HG22	1:C:288:HIS:HD2	1.74	0.52
1:C:428:ARG:NH2	1:C:446:ASP:OD2	2.43	0.52
1:C:1004:HIS:CE1	1:C:1038:LEU:HD21	2.44	0.52
1:C:3823:GLU:HG3	1:C:3826:GLY:HA2	1.92	0.52
1:D:1087:ILE:HD11	1:D:1204:VAL:HG22	1.91	0.52
1:D:3879:LEU:O	1:D:3882:GLN:HG3	2.08	0.52
1:A:1087:ILE:HD11	1:A:1204:VAL:HG22	1.91	0.52
1:A:2160:ASN:OD1	1:A:2163:ARG:NH2	2.40	0.52
1:A:2767:GLU:O	1:A:2771:TYR:N	2.40	0.52
1:A:4943:MET:HA	1:A:4946:GLU:HG2	1.91	0.52
1:B:986:ILE:CD1	1:B:1055:ARG:HA	2.40	0.52
1:B:4640:PHE:HB3	1:B:4650:LYS:HE2	1.92	0.52
1:C:996:VAL:HG13	1:C:1047:LYS:HE2	1.91	0.52
1:C:3879:LEU:O	1:C:3882:GLN:HG3	2.08	0.52
1:D:428:ARG:NH2	1:D:446:ASP:OD2	2.42	0.52
1:D:2054:LYS:HE2	1:D:2056:SER:HA	1.92	0.52
1:D:4943:MET:HA	1:D:4946:GLU:HG2	1.91	0.52
1:A:902:TRP:HZ2	1:A:915:HIS:CB	2.23	0.52
1:A:1501:ASN:OD1	1:A:1502:ASN:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2581:ARG:HB3	1:A:2584:MET:HG2	1.92	0.52
2:E:12:ASP:OD1	2:E:68:SER:OG	2.27	0.52
1:B:902:TRP:HZ2	1:B:915:HIS:CB	2.23	0.52
1:B:2703:PRO:HB2	1:B:2854:LYS:HB2	1.91	0.52
1:B:4520:TYR:HD1	1:B:4561:LEU:HD13	1.75	0.52
1:C:986:ILE:CD1	1:C:1055:ARG:HA	2.40	0.52
1:C:3668:ILE:HD12	1:C:3734:ARG:HB2	1.91	0.52
1:A:1711:LEU:HB3	1:A:1831:MET:CE	2.40	0.51
1:A:4265:LYS:O	1:A:4269:LYS:HG2	2.09	0.51
1:A:4520:TYR:HD1	1:A:4561:LEU:HD13	1.75	0.51
1:B:848:ARG:NH1	1:B:1599:MET:SD	2.84	0.51
1:B:1181:ILE:HG22	1:B:1189:GLU:OE2	2.09	0.51
1:B:2581:ARG:HB3	1:B:2584:MET:HG2	1.92	0.51
1:D:801:ARG:NH1	1:D:1615:GLN:O	2.40	0.51
1:A:1004:HIS:CE1	1:A:1038:LEU:HD21	2.44	0.51
1:A:2758:LYS:NZ	1:A:2762:LEU:O	2.40	0.51
1:A:3823:GLU:HG3	1:A:3826:GLY:HA2	1.92	0.51
1:B:996:VAL:HG13	1:B:1047:LYS:HE2	1.91	0.51
1:B:2724:TYR:HD1	1:B:2895:PHE:CD2	2.27	0.51
1:B:2833:LEU:HB3	1:B:2838[A]:HIS:NE2	2.25	0.51
1:B:4943:MET:HA	1:B:4946:GLU:HG2	1.91	0.51
1:C:332:ARG:NH1	1:C:339:ASP:OD1	2.43	0.51
1:C:848:ARG:NH1	1:C:1599:MET:SD	2.83	0.51
1:C:2160:ASN:OD1	1:C:2163:ARG:NH2	2.40	0.51
1:C:2420:ARG:NH2	1:C:2475:VAL:O	2.44	0.51
1:D:874:LEU:HB2	1:D:878:LEU:HD22	1.91	0.51
1:D:2729:HIS:CD2	1:D:2763:LEU:HD22	2.44	0.51
1:A:2349:GLU:OE2	1:A:2359:ARG:NH2	2.42	0.51
1:A:4702:ASP:O	1:A:4706:GLN:HG2	2.10	0.51
1:C:2758:LYS:NZ	1:C:2762:LEU:O	2.40	0.51
1:C:2767:GLU:O	1:C:2771:TYR:N	2.40	0.51
1:C:3013:VAL:O	1:C:3018:ARG:NH2	2.40	0.51
1:C:4702:ASP:O	1:C:4706:GLN:HG2	2.10	0.51
1:D:927:GLN:NE2	1:D:928:GLU:HG3	2.25	0.51
1:D:2420:ARG:NH2	1:D:2475:VAL:O	2.44	0.51
1:D:4640:PHE:HB3	1:D:4650:LYS:HE2	1.92	0.51
1:A:2290:TRP:CZ2	1:A:2388:ILE:HG12	2.46	0.51
1:A:3803:LEU:HB2	1:A:3884:SER:HB2	1.92	0.51
1:B:367:ASP:OD1	1:B:368:THR:N	2.43	0.51
1:B:1501:ASN:OD1	1:B:1502:ASN:N	2.43	0.51
1:B:2349:GLU:OE2	1:B:2359:ARG:NH2	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3823:GLU:HG3	1:B:3826:GLY:HA2	1.92	0.51
1:C:2054:LYS:HE2	1:C:2056:SER:HA	1.92	0.51
1:D:848:ARG:NH1	1:D:1599:MET:SD	2.84	0.51
1:D:2503:ASP:HB3	1:D:2554:ARG:NH2	2.25	0.51
1:A:118:ALA:HA	1:A:161:THR:HA	1.93	0.51
1:A:874:LEU:HB2	1:A:878:LEU:HD22	1.91	0.51
1:A:996:VAL:HG13	1:A:1047:LYS:HE2	1.91	0.51
1:B:3668:ILE:HD12	1:B:3734:ARG:HB2	1.91	0.51
1:D:2290:TRP:CZ2	1:D:2388:ILE:HG12	2.46	0.51
1:A:332:ARG:NH1	1:A:339:ASP:OD1	2.43	0.51
1:A:848:ARG:NH1	1:A:1599:MET:SD	2.83	0.51
1:A:939:THR:O	1:A:943:LEU:HG	2.11	0.51
1:A:2420:ARG:NH2	1:A:2475:VAL:O	2.44	0.51
1:A:4664:ASP:N	1:A:4664:ASP:OD1	2.42	0.51
1:B:3669:LEU:HB3	1:B:3673:ARG:HH21	1.74	0.51
1:B:4106:SER:HA	1:B:4115:LEU:HD21	1.92	0.51
1:C:118:ALA:HA	1:C:161:THR:HA	1.93	0.51
1:C:902:TRP:HZ2	1:C:915:HIS:CB	2.23	0.51
1:C:2349:GLU:OE2	1:C:2359:ARG:NH2	2.42	0.51
1:C:2503:ASP:HB3	1:C:2554:ARG:NH2	2.25	0.51
1:D:538:ALA:O	1:D:542:ARG:HG3	2.11	0.51
1:D:1711:LEU:HB3	1:D:1831:MET:CE	2.40	0.51
1:D:3823:GLU:HG3	1:D:3826:GLY:HA2	1.92	0.51
1:D:4106:SER:HA	1:D:4115:LEU:HD21	1.92	0.51
1:A:2503:ASP:HB3	1:A:2554:ARG:NH2	2.25	0.51
1:A:3669:LEU:HB3	1:A:3673:ARG:HH21	1.74	0.51
1:B:2833:LEU:HB3	1:B:2838[B]:HIS:NE2	2.24	0.51
1:C:890:HIS:CE1	1:C:891:GLU:HG2	2.46	0.51
1:C:4569:GLU:HB3	1:C:4570:PRO:HD3	1.92	0.51
1:C:4943:MET:SD	1:C:4951:PHE:HB3	2.51	0.51
1:D:35:LEU:HD23	1:D:51:SER:HA	1.93	0.51
1:D:902:TRP:HZ2	1:D:915:HIS:CB	2.23	0.51
1:D:2504:THR:O	1:D:2508:SER:N	2.40	0.51
1:D:4520:TYR:HD1	1:D:4561:LEU:HD13	1.76	0.51
1:D:4569:GLU:HB3	1:D:4570:PRO:HD3	1.92	0.51
1:C:939:THR:O	1:C:943:LEU:HG	2.11	0.51
1:C:1431:ARG:NE	1:C:1506:GLU:OE1	2.30	0.51
1:C:2798:MET:SD	1:C:2799:ALA:N	2.84	0.51
1:C:4520:TYR:HD1	1:C:4561:LEU:HD13	1.76	0.51
1:C:4862:ILE:HD13	1:D:4852:PHE:HE1	1.75	0.51
1:D:890:HIS:CE1	1:D:891:GLU:HG2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1501:ASN:OD1	1:D:1502:ASN:N	2.43	0.51
1:D:2703:PRO:HB2	1:D:2854:LYS:HB2	1.91	0.51
1:D:2798:MET:SD	1:D:2799:ALA:N	2.84	0.51
1:D:4943:MET:SD	1:D:4951:PHE:HB3	2.51	0.51
1:B:1016:TRP:HA	1:B:1027:ARG:HB3	1.93	0.51
1:C:927:GLN:NE2	1:C:928:GLU:HG3	2.25	0.51
1:C:1501:ASN:OD1	1:C:1502:ASN:N	2.43	0.51
1:C:4631:ASP:O	1:C:4634:VAL:HG12	2.11	0.51
1:C:4640:PHE:CD2	1:C:4641:PRO:HD2	2.46	0.51
1:D:4631:ASP:O	1:D:4634:VAL:HG12	2.11	0.51
1:A:538:ALA:O	1:A:542:ARG:HG3	2.11	0.51
1:A:986:ILE:CD1	1:A:1055:ARG:HA	2.40	0.51
1:A:2797:SER:HB3	1:A:2801:TYR:HE2	1.72	0.51
1:A:4114:ARG:O	1:A:4117:THR:OG1	2.22	0.51
1:A:4187:GLU:OE1	1:A:4949:TRP:NE1	2.35	0.51
2:H:12:ASP:OD1	2:H:68:SER:OG	2.27	0.51
1:B:1432:ILE:HB	1:B:1505:LEU:HB3	1.94	0.51
1:B:1851:PHE:HZ	1:B:2058:LEU:HD13	1.76	0.51
1:C:35:LEU:HD23	1:C:51:SER:HA	1.93	0.51
1:C:1016:TRP:HA	1:C:1027:ARG:HB3	1.93	0.51
1:C:1432:ILE:HB	1:C:1505:LEU:HB3	1.94	0.51
1:C:2290:TRP:CZ2	1:C:2388:ILE:HG12	2.46	0.51
1:C:2794:GLU:O	1:C:2797:SER:HB2	2.11	0.51
1:D:1851:PHE:HZ	1:D:2058:LEU:HD13	1.76	0.51
1:D:2794:GLU:O	1:D:2797:SER:HB2	2.11	0.51
1:A:367:ASP:OD1	1:A:368:THR:N	2.43	0.50
1:A:890:HIS:CE1	1:A:891:GLU:HG2	2.46	0.50
1:A:1851:PHE:HZ	1:A:2058:LEU:HD13	1.76	0.50
1:A:1950:ALA:HB1	1:A:1961:LYS:HZ3	1.75	0.50
1:A:2839:ALA:O	1:A:2843:MET:HE3	2.11	0.50
1:A:4943:MET:SD	1:A:4951:PHE:HB3	2.51	0.50
1:B:538:ALA:O	1:B:542:ARG:HG3	2.11	0.50
1:B:2212:LYS:NZ	1:B:3822:GLU:OE1	2.32	0.50
1:C:2782:MET:HE1	1:C:2789:ILE:HB	1.94	0.50
1:C:4640:PHE:HB3	1:C:4650:LYS:HE2	1.92	0.50
1:A:2488:LEU:HD12	1:A:2492:PHE:HB2	1.93	0.50
1:A:2794:GLU:O	1:A:2797:SER:HB2	2.11	0.50
1:A:4569:GLU:HB3	1:A:4570:PRO:HD3	1.92	0.50
1:A:4631:ASP:O	1:A:4634:VAL:HG12	2.11	0.50
1:B:890:HIS:CE1	1:B:891:GLU:HG2	2.46	0.50
1:B:1243:THR:HG22	1:B:1808:ASP:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2290:TRP:CZ2	1:B:2388:ILE:HG12	2.46	0.50
1:B:2488:LEU:HD12	1:B:2492:PHE:HB2	1.93	0.50
1:B:2794:GLU:O	1:B:2797:SER:HB2	2.11	0.50
1:B:3097:THR:HA	1:B:3101:LEU:HD23	1.94	0.50
1:C:1685:LEU:HD22	1:C:1706:LEU:HB2	1.93	0.50
1:C:3996:GLY:O	1:C:4000:VAL:HG23	2.12	0.50
1:D:996:VAL:HG13	1:D:1047:LYS:HE2	1.91	0.50
1:D:2659:GLN:OE1	1:D:2659:GLN:N	2.37	0.50
1:D:2839:ALA:O	1:D:2843:MET:HE3	2.11	0.50
1:A:842:GLN:OE1	1:A:1603:PHE:N	2.43	0.50
1:A:1220:ASP:OD2	1:A:1222:SER:OG	2.30	0.50
1:A:1826:TYR:O	1:A:1830:ILE:HG12	2.12	0.50
1:A:2418:ARG:O	1:A:2422:ILE:HG12	2.12	0.50
1:A:4769:LEU:HB3	1:D:4753:LEU:CD2	2.41	0.50
1:B:67:PHE:HB3	1:B:121:LEU:HD22	1.93	0.50
1:B:1559:ARG:HD3	1:B:1565:PRO:HD3	1.93	0.50
1:B:1685:LEU:HD22	1:B:1706:LEU:HB2	1.93	0.50
1:B:4631:ASP:O	1:B:4634:VAL:HG12	2.11	0.50
1:C:929:ARG:HH22	1:C:933:LEU:HD21	1.75	0.50
1:C:2172:MET:O	1:C:2176:VAL:HG23	2.11	0.50
1:A:35:LEU:HD23	1:A:51:SER:HA	1.93	0.50
1:A:2933:VAL:HA	1:A:2963:PHE:CZ	2.46	0.50
1:A:4106:SER:HA	1:A:4115:LEU:HD21	1.92	0.50
1:B:2839:ALA:O	1:B:2843:MET:HE3	2.11	0.50
1:B:2856:LYS:O	1:B:2860:LEU:HD23	2.12	0.50
1:C:538:ALA:O	1:C:542:ARG:HG3	2.11	0.50
1:C:1559:ARG:HD3	1:C:1565:PRO:HD3	1.93	0.50
1:A:1947:VAL:HG11	1:A:1965:PHE:CE2	2.46	0.50
1:A:2129:LEU:HD23	1:A:2132:VAL:HG21	1.94	0.50
1:A:2172:MET:O	1:A:2176:VAL:HG23	2.11	0.50
1:B:1220:ASP:OD2	1:B:1222:SER:OG	2.30	0.50
1:B:2420:ARG:NH2	1:B:2475:VAL:O	2.44	0.50
1:B:4903:HIS:HB3	1:B:4906:GLU:OE2	2.12	0.50
1:C:1152:TYR:HD1	1:C:1184:ASP:HB3	1.76	0.50
1:C:1851:PHE:HZ	1:C:2058:LEU:HD13	1.76	0.50
1:C:1947:VAL:CG2	1:C:1961:LYS:HB3	2.42	0.50
1:C:2856:LYS:O	1:C:2860:LEU:HD23	2.12	0.50
1:D:398:HIS:HB3	1:D:400:ASP:N	2.26	0.50
1:D:939:THR:O	1:D:943:LEU:HG	2.11	0.50
1:D:1947:VAL:HG11	1:D:1965:PHE:CE2	2.46	0.50
1:D:2172:MET:O	1:D:2176:VAL:HG23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2798:MET:SD	1:A:2799:ALA:N	2.84	0.50
1:A:4245:LEU:CD1	1:B:4626:ILE:HG13	2.40	0.50
1:A:4844:ILE:HG21	1:D:4814:MET:HE2	1.93	0.50
1:B:118:ALA:HA	1:B:161:THR:HA	1.93	0.50
1:B:2798:MET:SD	1:B:2799:ALA:N	2.84	0.50
1:B:2933:VAL:HA	1:B:2963:PHE:CZ	2.46	0.50
1:B:3891:TYR:HA	1:C:76:ARG:NH2	2.25	0.50
1:C:1711:LEU:HB3	1:C:1831:MET:CE	2.40	0.50
1:C:2488:LEU:HD12	1:C:2492:PHE:HB2	1.93	0.50
1:D:1685:LEU:HD22	1:D:1706:LEU:HB2	1.93	0.50
1:D:2129:LEU:HD23	1:D:2132:VAL:HG21	1.94	0.50
1:A:4640:PHE:CD2	1:A:4641:PRO:HD2	2.46	0.50
1:B:132:CYS:H	1:B:157:ALA:HB1	1.77	0.50
1:B:939:THR:O	1:B:943:LEU:HG	2.11	0.50
1:B:1947:VAL:HG11	1:B:1965:PHE:CE2	2.46	0.50
1:B:2331:PHE:HB3	1:B:2335:LEU:HB2	1.94	0.50
1:B:2503:ASP:HB3	1:B:2554:ARG:NH2	2.25	0.50
1:B:4569:GLU:HB3	1:B:4570:PRO:HD3	1.92	0.50
1:C:1293:GLN:OE1	1:C:1294:ASN:N	2.45	0.50
1:C:2418:ARG:O	1:C:2422:ILE:HG12	2.12	0.50
1:C:2852:TRP:CZ2	1:C:2856:LYS:HE2	2.47	0.50
1:C:3622:GLN:O	1:C:3626:LYS:NZ	2.39	0.50
1:C:3944:VAL:HG11	1:C:4002:MET:HE1	1.94	0.50
1:D:118:ALA:HA	1:D:161:THR:HA	1.93	0.50
1:D:929:ARG:HH22	1:D:933:LEU:HD21	1.75	0.50
1:D:1826:TYR:O	1:D:1830:ILE:HG12	2.12	0.50
1:D:3912:VAL:O	1:D:3916:VAL:HG23	2.12	0.50
1:D:4903:HIS:HB3	1:D:4906:GLU:OE2	2.12	0.50
1:A:1293:GLN:OE1	1:A:1294:ASN:N	2.45	0.50
1:A:2777:GLU:O	1:A:2781:THR:OG1	2.19	0.50
1:B:929:ARG:HH22	1:B:933:LEU:HD21	1.75	0.50
1:B:2988:ARG:HB2	1:B:2989:PRO:HD3	1.94	0.50
1:C:398:HIS:HB3	1:C:400:ASP:N	2.26	0.50
1:C:625:VAL:HG22	1:C:2133:ARG:HD2	1.94	0.50
1:C:2129:LEU:HD23	1:C:2132:VAL:HG21	1.94	0.50
1:C:3097:THR:HA	1:C:3101:LEU:HD23	1.94	0.50
1:D:1559:ARG:HD3	1:D:1565:PRO:HD3	1.93	0.50
1:D:2856:LYS:O	1:D:2860:LEU:HD23	2.12	0.50
1:A:398:HIS:HB3	1:A:400:ASP:N	2.27	0.50
1:A:1432:ILE:HB	1:A:1505:LEU:HB3	1.93	0.50
1:A:1559:ARG:HD3	1:A:1565:PRO:HD3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1685:LEU:HD22	1:A:1706:LEU:HB2	1.93	0.50
1:A:2331:PHE:HB3	1:A:2335:LEU:HB2	1.94	0.50
1:A:2526:PRO:O	1:A:2529:THR:N	2.45	0.50
1:A:2833:LEU:HB3	1:A:2838[A]:HIS:CE1	2.47	0.50
1:A:3811:GLN:NE2	1:A:3823:GLU:OE2	2.45	0.50
1:B:1947:VAL:CG2	1:B:1961:LYS:HB3	2.42	0.50
1:B:2990:LEU:HB3	1:B:2993:GLY:O	2.12	0.50
1:B:4943:MET:SD	1:B:4951:PHE:HB3	2.51	0.50
1:C:2581:ARG:HB3	1:C:2584:MET:HG2	1.92	0.50
1:C:2839:ALA:O	1:C:2843:MET:HE3	2.11	0.50
1:C:3043:ARG:HB3	1:C:3047:LYS:NZ	2.27	0.50
1:D:1293:GLN:OE1	1:D:1294:ASN:N	2.45	0.50
1:D:1432:ILE:HB	1:D:1505:LEU:HB3	1.93	0.50
1:D:2888:LYS:HA	1:D:2891:ASP:OD2	2.12	0.50
1:D:3043:ARG:HB3	1:D:3047:LYS:NZ	2.27	0.50
1:A:929:ARG:HH22	1:A:933:LEU:HD21	1.75	0.49
1:A:2593:VAL:HG12	1:A:2644:LEU:HD22	1.94	0.49
1:A:3890:TRP:O	1:B:76:ARG:NH2	2.45	0.49
1:A:4831:ILE:HG13	1:A:4843:ARG:NH2	2.21	0.49
1:B:514:PHE:HD2	1:B:526:TRP:HB2	1.77	0.49
1:B:3996:GLY:O	1:B:4000:VAL:HG23	2.12	0.49
1:B:4930:GLU:OE2	1:B:4941:TRP:NE1	2.45	0.49
1:C:4903:HIS:HB3	1:C:4906:GLU:OE2	2.12	0.49
1:D:132:CYS:H	1:D:157:ALA:HB1	1.77	0.49
1:D:503:ASP:O	1:D:507:VAL:HG13	2.12	0.49
1:D:625:VAL:HG22	1:D:2133:ARG:HD2	1.94	0.49
1:D:1016:TRP:HA	1:D:1027:ARG:HB3	1.93	0.49
1:D:2581:ARG:HB3	1:D:2584:MET:HG2	1.92	0.49
1:D:2852:TRP:CZ2	1:D:2856:LYS:HE2	2.47	0.49
1:D:3996:GLY:O	1:D:4000:VAL:HG23	2.12	0.49
1:D:4267:GLN:O	1:D:4271:VAL:HG12	2.12	0.49
1:A:1016:TRP:HA	1:A:1027:ARG:HB3	1.93	0.49
1:A:2856:LYS:O	1:A:2860:LEU:HD23	2.12	0.49
1:A:2988:ARG:HB2	1:A:2989:PRO:HD3	1.94	0.49
1:A:3912:VAL:O	1:A:3916:VAL:HG23	2.12	0.49
1:A:4047:ASP:HA	1:A:4050:LYS:HG2	1.93	0.49
1:B:4267:GLN:O	1:B:4271:VAL:HG12	2.12	0.49
1:C:1243:THR:HG22	1:C:1808:ASP:HB2	1.93	0.49
1:C:4114:ARG:O	1:C:4117:THR:OG1	2.22	0.49
1:C:4664:ASP:N	1:C:4664:ASP:OD1	2.42	0.49
1:D:161:THR:HG23	1:D:186:VAL:HG22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2933:VAL:HA	1:D:2963:PHE:CZ	2.46	0.49
1:D:4047:ASP:HA	1:D:4050:LYS:HG2	1.93	0.49
1:D:4640:PHE:CD2	1:D:4641:PRO:HD2	2.46	0.49
1:A:161:THR:HG23	1:A:186:VAL:HG22	1.94	0.49
1:A:503:ASP:O	1:A:507:VAL:HG13	2.13	0.49
1:A:1152:TYR:HD1	1:A:1184:ASP:HB3	1.76	0.49
1:A:4903:HIS:HB3	1:A:4906:GLU:OE2	2.12	0.49
1:B:1293:GLN:OE1	1:B:1294:ASN:N	2.45	0.49
1:B:1298:ASP:OD1	1:B:1299:ILE:N	2.46	0.49
1:B:2885:ASP:O	1:B:2888:LYS:HG3	2.13	0.49
1:C:132:CYS:H	1:C:157:ALA:HB1	1.77	0.49
1:C:1042:THR:O	1:C:1046:ASN:ND2	2.46	0.49
1:C:3912:VAL:O	1:C:3916:VAL:HG23	2.12	0.49
1:C:4267:GLN:O	1:C:4271:VAL:HG12	2.12	0.49
1:D:67:PHE:HB3	1:D:121:LEU:HD22	1.93	0.49
1:D:1152:TYR:HD1	1:D:1184:ASP:HB3	1.76	0.49
1:D:1690:GLU:OE1	1:D:1790:LYS:NZ	2.42	0.49
1:D:4633:LEU:O	1:D:4637:THR:HG23	2.13	0.49
1:A:67:PHE:HB3	1:A:121:LEU:HD22	1.93	0.49
1:A:1042:THR:O	1:A:1046:ASN:ND2	2.46	0.49
1:A:1283:LEU:HB2	1:A:1555:PHE:HB2	1.94	0.49
1:A:1468:THR:HG22	1:A:1479:SER:HB2	1.95	0.49
1:A:3043:ARG:HB3	1:A:3047:LYS:NZ	2.27	0.49
1:A:3996:GLY:O	1:A:4000:VAL:HG23	2.12	0.49
1:A:4267:GLN:O	1:A:4271:VAL:HG12	2.12	0.49
1:B:35:LEU:HD23	1:B:51:SER:HA	1.93	0.49
1:B:971:GLN:HG3	1:B:978:PRO:HG2	1.94	0.49
1:B:2172:MET:O	1:B:2176:VAL:HG23	2.11	0.49
1:B:2418:ARG:O	1:B:2422:ILE:HG12	2.12	0.49
1:B:3042:ALA:HB3	1:B:3117:PHE:CE2	2.48	0.49
1:B:3074:ASN:OD1	1:B:3075:LEU:N	2.46	0.49
1:B:4633:LEU:HD22	1:B:4704:LYS:HE3	1.95	0.49
1:C:971:GLN:HG3	1:C:978:PRO:HG2	1.94	0.49
1:C:1102:TYR:HD2	1:C:1165:MET:HG2	1.77	0.49
1:C:2593:VAL:HG12	1:C:2644:LEU:HD22	1.94	0.49
1:C:4640:PHE:CD1	1:C:4641:PRO:HD2	2.47	0.49
1:D:1243:THR:HG22	1:D:1808:ASP:HB2	1.93	0.49
1:A:1243:THR:HG22	1:A:1808:ASP:HB2	1.93	0.49
1:A:2885:ASP:O	1:A:2888:LYS:HG3	2.13	0.49
1:A:4633:LEU:HD22	1:A:4704:LYS:HE3	1.95	0.49
1:B:842:GLN:OE1	1:B:1603:PHE:N	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1102:TYR:HD2	1:B:1165:MET:HG2	1.77	0.49
1:B:2129:LEU:HD23	1:B:2132:VAL:HG21	1.94	0.49
1:B:3811:GLN:NE2	1:B:3823:GLU:OE2	2.45	0.49
1:B:4640:PHE:CD1	1:B:4641:PRO:HD2	2.47	0.49
1:B:4640:PHE:CD2	1:B:4641:PRO:HD2	2.46	0.49
1:C:67:PHE:HB3	1:C:121:LEU:HD22	1.93	0.49
1:C:1826:TYR:O	1:C:1830:ILE:HG12	2.12	0.49
1:C:2930:ILE:HA	1:C:3010:LYS:HZ1	1.77	0.49
1:D:367:ASP:OD1	1:D:368:THR:N	2.43	0.49
1:D:1468:THR:HG22	1:D:1479:SER:HB2	1.95	0.49
1:D:2418:ARG:O	1:D:2422:ILE:HG12	2.12	0.49
1:D:2526:PRO:O	1:D:2529:THR:N	2.45	0.49
1:D:2990:LEU:HB3	1:D:2993:GLY:O	2.12	0.49
1:A:625:VAL:HG22	1:A:2133:ARG:HD2	1.94	0.49
1:A:1102:TYR:HD2	1:A:1165:MET:HG2	1.77	0.49
1:A:1298:ASP:OD1	1:A:1299:ILE:N	2.46	0.49
1:A:2852:TRP:CZ2	1:A:2856:LYS:HE2	2.47	0.49
1:A:3074:ASN:OD1	1:A:3075:LEU:N	2.46	0.49
1:A:3097:THR:HA	1:A:3101:LEU:HD23	1.94	0.49
1:B:161:THR:HG23	1:B:186:VAL:HG22	1.94	0.49
1:B:398:HIS:HB3	1:B:400:ASP:N	2.26	0.49
1:B:625:VAL:HG22	1:B:2133:ARG:HD2	1.94	0.49
1:B:1711:LEU:HB3	1:B:1831:MET:CE	2.40	0.49
1:B:2888:LYS:HA	1:B:2891:ASP:OD2	2.12	0.49
1:C:1947:VAL:HG11	1:C:1965:PHE:CE2	2.46	0.49
1:C:2933:VAL:HA	1:C:2963:PHE:CZ	2.46	0.49
1:C:3074:ASN:OD1	1:C:3075:LEU:N	2.46	0.49
1:C:3920:LEU:O	1:C:3924:ILE:HG12	2.13	0.49
1:C:4633:LEU:HD22	1:C:4704:LYS:HE3	1.95	0.49
1:D:926:GLU:O	1:D:929:ARG:HB3	2.13	0.49
1:D:1298:ASP:OD1	1:D:1299:ILE:N	2.46	0.49
1:D:3074:ASN:OD1	1:D:3075:LEU:N	2.46	0.49
1:D:4633:LEU:HD22	1:D:4704:LYS:HE3	1.95	0.49
1:D:4930:GLU:OE2	1:D:4941:TRP:NE1	2.45	0.49
2:H:35:LYS:NZ	1:D:640:ARG:O	2.46	0.49
1:B:503:ASP:O	1:B:507:VAL:HG13	2.12	0.49
1:B:1042:THR:O	1:B:1046:ASN:ND2	2.46	0.49
1:B:2593:VAL:HG12	1:B:2644:LEU:HD22	1.94	0.49
1:B:2659:GLN:O	1:B:2965:LYS:NZ	2.41	0.49
1:B:2929:LEU:O	1:B:2933:VAL:HG23	2.13	0.49
1:B:3912:VAL:O	1:B:3916:VAL:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:971:GLN:HG3	1:D:978:PRO:HG2	1.94	0.49
1:D:2229:LEU:O	1:D:2235:ARG:NH1	2.46	0.49
1:D:2711:ILE:CG2	1:D:2783:LEU:HD22	2.43	0.49
1:D:2988:ARG:HB2	1:D:2989:PRO:HD3	1.94	0.49
1:D:3811:GLN:NE2	1:D:3823:GLU:OE2	2.45	0.49
1:A:1564:MET:CE	1:A:1565:PRO:HD2	2.43	0.49
1:A:1788:LYS:O	1:A:1792:ILE:HG13	2.13	0.49
1:A:2868:HIS:CD2	1:A:2870:LEU:H	2.31	0.49
1:A:2888:LYS:HA	1:A:2891:ASP:OD2	2.12	0.49
1:B:2229:LEU:O	1:B:2235:ARG:NH1	2.46	0.49
1:C:1564:MET:CE	1:C:1565:PRO:HD2	2.43	0.49
1:C:2990:LEU:HB3	1:C:2993:GLY:O	2.12	0.49
1:C:3042:ALA:HB3	1:C:3117:PHE:CE2	2.48	0.49
1:D:1564:MET:CE	1:D:1565:PRO:HD2	2.43	0.49
1:D:1950:ALA:HB1	1:D:1961:LYS:HZ3	1.77	0.49
1:D:2331:PHE:HB3	1:D:2335:LEU:HB2	1.94	0.49
1:A:2711:ILE:CG2	1:A:2783:LEU:HD22	2.43	0.49
1:A:3763:ILE:HD11	1:A:3838:ASP:O	2.13	0.49
1:A:4633:LEU:O	1:A:4637:THR:HG23	2.13	0.49
1:A:4634:VAL:O	1:A:4637:THR:OG1	2.26	0.49
1:B:681:HIS:O	1:B:799:LYS:N	2.46	0.49
1:B:1089:ARG:HB3	1:B:1204:VAL:HG23	1.94	0.49
1:B:2982:PHE:O	1:B:3001:LYS:NZ	2.44	0.49
1:B:3043:ARG:HB3	1:B:3047:LYS:NZ	2.27	0.49
1:C:555:LEU:HD11	1:C:585:ALA:HB1	1.95	0.49
1:C:2526:PRO:O	1:C:2529:THR:N	2.45	0.49
1:C:3001:LYS:O	1:C:3005:THR:HG23	2.13	0.49
1:C:4047:ASP:HA	1:C:4050:LYS:HG2	1.93	0.49
1:D:2593:VAL:HG12	1:D:2644:LEU:HD22	1.94	0.49
1:D:3042:ALA:HB3	1:D:3117:PHE:CE2	2.48	0.49
1:D:4640:PHE:CD1	1:D:4641:PRO:HD2	2.47	0.49
1:A:681:HIS:O	1:A:799:LYS:N	2.46	0.49
1:A:1051:ARG:O	1:A:1055:ARG:HG2	2.13	0.49
1:A:3042:ALA:HB3	1:A:3117:PHE:CE2	2.48	0.49
1:A:3920:LEU:O	1:A:3924:ILE:HG12	2.13	0.49
1:A:4714:PHE:CD1	1:D:4294:LEU:HD12	2.48	0.49
1:B:1468:THR:HG22	1:B:1479:SER:HB2	1.95	0.49
1:B:2526:PRO:O	1:B:2529:THR:N	2.45	0.49
1:B:2553:TYR:HD2	1:B:2591:ARG:HH21	1.61	0.49
1:B:2826:ILE:HG22	1:C:1502:ASN:HA	1.94	0.49
1:B:3920:LEU:O	1:B:3924:ILE:HG12	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:681:HIS:O	1:C:799:LYS:N	2.46	0.49
1:C:926:GLU:O	1:C:929:ARG:HB3	2.13	0.49
1:C:1298:ASP:OD1	1:C:1299:ILE:N	2.46	0.49
1:C:2331:PHE:HB3	1:C:2335:LEU:HB2	1.94	0.49
1:C:2347:MET:O	1:C:2351:ILE:HG12	2.13	0.49
1:C:2868:HIS:CD2	1:C:2870:LEU:H	2.31	0.49
1:D:2349:GLU:OE2	1:D:2359:ARG:NH2	2.42	0.49
1:D:3920:LEU:O	1:D:3924:ILE:HG12	2.13	0.49
1:A:3001:LYS:O	1:A:3005:THR:HG23	2.13	0.48
1:A:4587:ILE:HG23	1:A:4719:PHE:HE1	1.78	0.48
1:A:4860:ALA:CB	1:D:4863:GLN:HG2	2.41	0.48
1:B:1152:TYR:HD1	1:B:1184:ASP:HB3	1.76	0.48
1:B:1471:ASP:OD2	1:B:1473:LYS:NZ	2.40	0.48
1:B:1826:TYR:O	1:B:1830:ILE:HG12	2.12	0.48
1:B:2852:TRP:CZ2	1:B:2856:LYS:HE2	2.47	0.48
1:B:3001:LYS:O	1:B:3005:THR:HG23	2.13	0.48
1:C:2885:ASP:O	1:C:2888:LYS:HG3	2.13	0.48
1:C:2888:LYS:HA	1:C:2891:ASP:OD2	2.12	0.48
1:C:3763:ILE:HD11	1:C:3838:ASP:O	2.13	0.48
1:C:4633:LEU:O	1:C:4637:THR:HG23	2.13	0.48
1:D:1089:ARG:HB3	1:D:1204:VAL:HG23	1.94	0.48
1:D:2488:LEU:HD12	1:D:2492:PHE:HB2	1.93	0.48
1:D:3097:THR:HA	1:D:3101:LEU:HD23	1.94	0.48
1:A:336:GLU:OE2	1:A:338:LEU:HB3	2.14	0.48
1:A:514:PHE:HD2	1:A:526:TRP:HB2	1.77	0.48
1:A:926:GLU:O	1:A:929:ARG:HB3	2.13	0.48
1:A:4640:PHE:CD1	1:A:4641:PRO:HD2	2.47	0.48
1:B:1051:ARG:O	1:B:1055:ARG:HG2	2.13	0.48
1:B:1564:MET:CE	1:B:1565:PRO:HD2	2.43	0.48
1:C:514:PHE:HD2	1:C:526:TRP:HB2	1.77	0.48
1:C:3811:GLN:NE2	1:C:3823:GLU:OE2	2.45	0.48
1:D:1042:THR:O	1:D:1046:ASN:ND2	2.46	0.48
1:D:1283:LEU:HB2	1:D:1555:PHE:HB2	1.94	0.48
1:D:2553:TYR:HD2	1:D:2591:ARG:HH21	1.61	0.48
1:A:132:CYS:H	1:A:157:ALA:HB1	1.77	0.48
1:A:555:LEU:HD11	1:A:585:ALA:HB1	1.95	0.48
1:A:1089:ARG:HB3	1:A:1204:VAL:HG23	1.94	0.48
1:B:1244:ASN:HD22	1:B:1801:GLU:HG2	1.78	0.48
1:B:2868:HIS:CD2	1:B:2870:LEU:H	2.31	0.48
1:B:2917:ILE:HD12	1:B:2920:ARG:HD2	1.95	0.48
1:B:3890:TRP:O	1:C:76:ARG:NH2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4587:ILE:HG23	1:B:4719:PHE:HE1	1.78	0.48
1:C:1051:ARG:O	1:C:1055:ARG:HG2	2.13	0.48
1:C:4930:GLU:OE2	1:C:4941:TRP:NE1	2.45	0.48
1:D:1051:ARG:O	1:D:1055:ARG:HG2	2.13	0.48
1:D:1102:TYR:HD2	1:D:1165:MET:HG2	1.77	0.48
1:D:1244:ASN:HD22	1:D:1801:GLU:HG2	1.78	0.48
1:D:1788:LYS:O	1:D:1792:ILE:HG13	2.13	0.48
1:D:2885:ASP:O	1:D:2888:LYS:HG3	2.13	0.48
1:A:1052:GLU:HA	1:A:1055:ARG:CG	2.44	0.48
1:A:1114:ARG:NH1	1:A:1128:LEU:O	2.39	0.48
1:A:1260:GLN:NE2	1:A:1261:VAL:O	2.47	0.48
1:B:555:LEU:HD11	1:B:585:ALA:HB1	1.95	0.48
1:B:1260:GLN:NE2	1:B:1261:VAL:O	2.47	0.48
1:B:1283:LEU:HB2	1:B:1555:PHE:HB2	1.94	0.48
1:B:2157:GLN:O	1:B:3615:ARG:NH2	2.44	0.48
1:B:2455:ASP:HB3	1:B:2458:ALA:HB3	1.95	0.48
1:B:3763:ILE:HD11	1:B:3838:ASP:O	2.13	0.48
1:B:4047:ASP:HA	1:B:4050:LYS:HG2	1.93	0.48
1:C:2455:ASP:HB3	1:C:2458:ALA:HB3	1.95	0.48
1:D:336:GLU:OE2	1:D:338:LEU:HB3	2.14	0.48
1:D:681:HIS:O	1:D:799:LYS:N	2.46	0.48
1:D:1052:GLU:HA	1:D:1055:ARG:CG	2.44	0.48
1:D:1518:LEU:HB2	1:D:1531:TYR:HB2	1.96	0.48
1:D:1947:VAL:CG2	1:D:1961:LYS:HB3	2.42	0.48
1:D:4109:MET:HB2	1:D:4115:LEU:HD22	1.96	0.48
1:C:1260:GLN:NE2	1:C:1261:VAL:O	2.47	0.48
1:C:1518:LEU:HB2	1:C:1531:TYR:HB2	1.96	0.48
1:C:2092:TYR:HD2	1:C:3640:LEU:HD13	1.78	0.48
1:C:2229:LEU:O	1:C:2235:ARG:NH1	2.46	0.48
1:C:2918:GLU:HA	1:C:2923:TYR:CD2	2.49	0.48
1:C:2929:LEU:O	1:C:2933:VAL:HG23	2.13	0.48
1:D:555:LEU:HD11	1:D:585:ALA:HB1	1.95	0.48
1:D:1092:LYS:NZ	1:D:1646:GLU:OE1	2.39	0.48
1:D:3763:ILE:HD11	1:D:3838:ASP:O	2.13	0.48
1:A:983:LEU:HD12	1:A:1055:ARG:HG3	1.96	0.48
1:A:2229:LEU:O	1:A:2235:ARG:NH1	2.46	0.48
1:A:2990:LEU:HB3	1:A:2993:GLY:O	2.12	0.48
1:A:3730:ARG:O	1:A:3734:ARG:NH1	2.47	0.48
2:F:12:ASP:OD2	2:F:15:THR:HG22	2.13	0.48
1:B:1788:LYS:O	1:B:1792:ILE:HG13	2.13	0.48
1:B:2711:ILE:CG2	1:B:2783:LEU:HD22	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3889:TYR:CD1	1:B:3954:MET:SD	3.07	0.48
1:C:2553:TYR:HD2	1:C:2591:ARG:HH21	1.61	0.48
1:C:2841:ALA:HB2	1:C:2893:LEU:HD21	1.96	0.48
1:C:2988:ARG:HB2	1:C:2989:PRO:HD3	1.94	0.48
1:C:2998:ASN:O	1:C:3002:GLU:HG2	2.13	0.48
1:A:1690:GLU:OE1	1:A:1790:LYS:NZ	2.42	0.48
1:A:2918:GLU:HA	1:A:2923:TYR:CD2	2.49	0.48
1:A:4930:GLU:OE2	1:A:4941:TRP:NE1	2.45	0.48
1:C:161:THR:HG23	1:C:186:VAL:HG22	1.94	0.48
1:C:1089:ARG:HB3	1:C:1204:VAL:HG23	1.94	0.48
1:C:2917:ILE:HD12	1:C:2920:ARG:HD2	1.95	0.48
1:C:3770:ASN:HB3	1:C:3773:VAL:CG1	2.42	0.48
1:C:4267:GLN:HA	1:C:4270:LYS:HE2	1.96	0.48
1:C:4587:ILE:HG23	1:C:4719:PHE:HE1	1.78	0.48
1:D:1220:ASP:OD2	1:D:1222:SER:OG	2.30	0.48
1:D:2868:HIS:CD2	1:D:2870:LEU:H	2.31	0.48
1:A:1947:VAL:CG2	1:A:1961:LYS:HB3	2.42	0.48
1:A:2497:ARG:HH22	1:A:2878:THR:N	2.12	0.48
1:A:4048:PHE:O	1:A:4052:MET:HG2	2.14	0.48
2:E:12:ASP:OD2	2:E:15:THR:HG22	2.13	0.48
1:B:614:LEU:HA	1:B:617:LEU:HD12	1.96	0.48
1:B:926:GLU:O	1:B:929:ARG:HB3	2.13	0.48
1:B:1518:LEU:HB2	1:B:1531:TYR:HB2	1.96	0.48
1:B:2347:MET:O	1:B:2351:ILE:HG12	2.13	0.48
1:C:336:GLU:OE2	1:C:338:LEU:HB3	2.13	0.48
1:C:718:VAL:HG23	1:C:793:SER:HB3	1.96	0.48
1:C:1468:THR:HG22	1:C:1479:SER:HB2	1.95	0.48
1:C:2432:LEU:O	1:C:2436:ILE:HG13	2.14	0.48
1:C:2855:LYS:HE3	1:C:2856:LYS:HZ2	1.78	0.48
1:C:4109:MET:HB2	1:C:4115:LEU:HD22	1.96	0.48
1:D:932:ASN:HA	1:D:935:MET:HG3	1.96	0.48
1:D:4048:PHE:O	1:D:4052:MET:HG2	2.14	0.48
1:A:971:GLN:HG3	1:A:978:PRO:HG2	1.94	0.48
1:A:1518:LEU:HB2	1:A:1531:TYR:HB2	1.96	0.48
1:A:2763:LEU:HG	1:A:2764:SER:N	2.29	0.48
1:A:4107:GLU:OE1	1:A:4149:TYR:OH	2.22	0.48
1:A:4109:MET:HB2	1:A:4115:LEU:HD22	1.96	0.48
2:G:50:ARG:N	2:G:55:GLU:OE2	2.37	0.48
1:B:932:ASN:HA	1:B:935:MET:HG3	1.96	0.48
1:B:2497:ARG:HH22	1:B:2878:THR:N	2.12	0.48
1:B:2855:LYS:HE3	1:B:2856:LYS:HZ2	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4048:PHE:O	1:B:4052:MET:HG2	2.14	0.48
1:B:4633:LEU:O	1:B:4637:THR:HG23	2.13	0.48
1:C:1787:LEU:HD23	1:C:1828:LEU:HD21	1.96	0.48
1:C:2763:LEU:HG	1:C:2764:SER:N	2.29	0.48
1:D:514:PHE:HD2	1:D:526:TRP:HB2	1.77	0.48
1:D:2929:LEU:O	1:D:2933:VAL:HG23	2.13	0.48
1:D:2930:ILE:HG23	1:D:3010:LYS:HZ3	1.79	0.48
1:D:4587:ILE:HG23	1:D:4719:PHE:HE1	1.78	0.48
1:D:4873:LEU:O	1:D:4877:GLN:HG2	2.14	0.48
1:A:2157:GLN:O	1:A:3615:ARG:NH2	2.44	0.48
1:A:2929:LEU:O	1:A:2933:VAL:HG23	2.13	0.48
1:A:4518:LEU:HD21	1:B:4810:LEU:HD13	1.96	0.48
2:G:12:ASP:OD2	2:G:15:THR:HG22	2.13	0.48
2:H:12:ASP:OD2	2:H:15:THR:HG22	2.13	0.48
1:B:2432:LEU:O	1:B:2436:ILE:HG13	2.14	0.48
1:B:4267:GLN:HA	1:B:4270:LYS:HE2	1.96	0.48
1:C:503:ASP:O	1:C:507:VAL:HG13	2.12	0.48
1:C:1911:GLN:OE1	1:C:2090:ARG:NH1	2.47	0.48
1:C:2791:ARG:HH21	1:C:2795:GLY:C	2.17	0.48
1:C:3889:TYR:CD1	1:C:3954:MET:SD	3.07	0.48
1:C:4008:ASN:OD1	1:C:4009:ASN:N	2.47	0.48
1:C:4730:VAL:HA	1:C:4733:HIS:HD2	1.78	0.48
1:C:4873:LEU:O	1:C:4877:GLN:HG2	2.14	0.48
1:D:448:PRO:HB2	1:D:451:SER:OG	2.14	0.48
1:D:614:LEU:HA	1:D:617:LEU:HD12	1.96	0.48
1:A:2834:SER:OG	1:A:2836:ASP:OD1	2.20	0.47
1:A:2841:ALA:HB2	1:A:2893:LEU:HD21	1.96	0.47
1:A:4008:ASN:OD1	1:A:4009:ASN:N	2.47	0.47
1:B:336:GLU:OE2	1:B:338:LEU:HB3	2.13	0.47
1:B:2685:TYR:CE1	1:B:2909:ASP:HB2	2.49	0.47
1:B:2763:LEU:HG	1:B:2764:SER:N	2.28	0.47
1:B:2791:ARG:HH21	1:B:2795:GLY:C	2.17	0.47
1:B:2905:ARG:HH11	1:B:2906:GLY:N	2.12	0.47
1:B:2998:ASN:O	1:B:3002:GLU:HG2	2.13	0.47
1:C:718:VAL:HG13	1:C:724:SER:HB2	1.96	0.47
1:C:932:ASN:HA	1:C:935:MET:HG3	1.96	0.47
1:C:1052:GLU:HA	1:C:1055:ARG:CG	2.44	0.47
1:C:1283:LEU:HB2	1:C:1555:PHE:HB2	1.94	0.47
1:D:718:VAL:HG23	1:D:793:SER:HB3	1.96	0.47
1:D:2982:PHE:O	1:D:3001:LYS:NZ	2.44	0.47
1:D:2998:ASN:O	1:D:3002:GLU:HG2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3662:ASP:O	1:D:3666:GLN:HG3	2.14	0.47
1:A:908:ARG:NH1	1:A:928:GLU:OE2	2.35	0.47
1:A:2526:PRO:HB3	1:A:2530:ARG:HH11	1.80	0.47
1:A:3004:VAL:O	1:A:3007:LEU:HG	2.15	0.47
1:A:4730:VAL:HA	1:A:4733:HIS:HD2	1.79	0.47
1:B:718:VAL:HG13	1:B:724:SER:HB2	1.96	0.47
1:B:1009:ARG:O	1:B:1013:ARG:HG2	2.15	0.47
1:B:1911:GLN:OE1	1:B:2090:ARG:NH1	2.47	0.47
1:B:2791:ARG:HH21	1:B:2796:ASP:N	2.12	0.47
1:C:1244:ASN:HD22	1:C:1801:GLU:HG2	1.78	0.47
1:C:2497:ARG:HH22	1:C:2878:THR:N	2.12	0.47
1:D:2497:ARG:HH22	1:D:2878:THR:N	2.12	0.47
1:D:2763:LEU:HG	1:D:2764:SER:N	2.29	0.47
1:D:2791:ARG:HH21	1:D:2795:GLY:C	2.17	0.47
1:D:2917:ILE:HD12	1:D:2920:ARG:HD2	1.95	0.47
1:A:2553:TYR:HD2	1:A:2591:ARG:HH21	1.61	0.47
1:B:983:LEU:HD12	1:B:1055:ARG:HG3	1.96	0.47
1:B:1007:TRP:O	1:B:1011:ARG:HG2	2.14	0.47
1:B:2092:TYR:HD2	1:B:3640:LEU:HD13	1.79	0.47
1:C:889:ILE:HA	1:C:892:LEU:HD12	1.97	0.47
1:C:1788:LYS:O	1:C:1792:ILE:HG13	2.13	0.47
1:C:4048:PHE:O	1:C:4052:MET:HG2	2.14	0.47
1:C:4120:GLU:HA	1:C:4123:GLU:HG2	1.97	0.47
1:D:983:LEU:HD12	1:D:1055:ARG:HG3	1.96	0.47
1:D:1260:GLN:NE2	1:D:1261:VAL:O	2.47	0.47
1:D:2212:LYS:NZ	1:D:3822:GLU:OE1	2.32	0.47
1:D:2775:ILE:O	1:D:2779:LEU:HG	2.14	0.47
1:D:3770:ASN:HB3	1:D:3773:VAL:CG1	2.42	0.47
1:D:4114:ARG:O	1:D:4117:THR:OG1	2.22	0.47
1:A:718:VAL:HG13	1:A:724:SER:HB2	1.96	0.47
1:A:1007:TRP:O	1:A:1011:ARG:HG2	2.14	0.47
1:A:1009:ARG:O	1:A:1013:ARG:HG2	2.14	0.47
1:A:2943:PHE:CE2	1:A:2947:SER:HB3	2.50	0.47
1:B:1954:SER:O	1:B:1958:THR:OG1	2.33	0.47
1:B:2775:ILE:O	1:B:2779:LEU:HG	2.14	0.47
1:B:4730:VAL:HA	1:B:4733:HIS:HD2	1.78	0.47
1:C:2791:ARG:HH21	1:C:2796:ASP:N	2.12	0.47
1:C:3701:ASP:OD2	1:C:3727:GLN:NE2	2.48	0.47
1:D:1911:GLN:OE1	1:D:2090:ARG:NH1	2.47	0.47
1:D:2526:PRO:HB3	1:D:2530:ARG:HH11	1.79	0.47
1:D:2918:GLU:HA	1:D:2923:TYR:CD2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3001:LYS:O	1:D:3005:THR:HG23	2.13	0.47
1:D:3016:ARG:O	1:D:3018:ARG:NH1	2.48	0.47
1:A:131:CYS:SG	1:A:150:GLN:HB2	2.55	0.47
1:A:920:GLU:O	1:A:924:LEU:N	2.48	0.47
1:A:1087:ILE:HG22	1:A:1252:SER:OG	2.15	0.47
1:A:1244:ASN:HD22	1:A:1801:GLU:HG2	1.78	0.47
1:A:3889:TYR:CD1	1:A:3954:MET:SD	3.07	0.47
1:B:232:ASP:OD2	1:B:407:ARG:NH1	2.48	0.47
1:B:1787:LEU:HD23	1:B:1828:LEU:HD21	1.95	0.47
1:B:2918:GLU:HA	1:B:2923:TYR:CD2	2.49	0.47
1:B:3016:ARG:O	1:B:3018:ARG:NH1	2.48	0.47
1:B:3730:ARG:O	1:B:3734:ARG:NH1	2.47	0.47
1:C:448:PRO:HB2	1:C:451:SER:OG	2.14	0.47
1:C:1954:SER:O	1:C:1958:THR:OG1	2.33	0.47
1:C:2711:ILE:CG2	1:C:2783:LEU:HD22	2.43	0.47
1:C:2886:ARG:O	1:C:2890:GLN:OE1	2.33	0.47
1:C:3004:VAL:O	1:C:3007:LEU:HG	2.15	0.47
1:C:3016:ARG:O	1:C:3018:ARG:NH1	2.48	0.47
1:D:718:VAL:HG13	1:D:724:SER:HB2	1.97	0.47
1:D:1787:LEU:HD23	1:D:1828:LEU:HD21	1.95	0.47
1:D:2347:MET:O	1:D:2351:ILE:HG12	2.13	0.47
1:D:2943:PHE:CE2	1:D:2947:SER:HB3	2.50	0.47
1:D:4730:VAL:HA	1:D:4733:HIS:HD2	1.78	0.47
1:A:889:ILE:HA	1:A:892:LEU:HD12	1.97	0.47
1:A:2791:ARG:HH21	1:A:2796:ASP:N	2.12	0.47
1:A:4873:LEU:O	1:A:4877:GLN:HG2	2.14	0.47
1:B:889:ILE:HA	1:B:892:LEU:HD12	1.97	0.47
1:B:1092:LYS:NZ	1:B:1646:GLU:OE1	2.39	0.47
1:B:2526:PRO:HB3	1:B:2530:ARG:HH11	1.80	0.47
1:B:2898:ILE:HG23	1:C:1500:ARG:NH2	2.27	0.47
1:B:3108:LEU:O	1:B:3112:ILE:HG12	2.15	0.47
1:C:4049:HIS:CD2	1:C:4067:LEU:HD11	2.47	0.47
1:D:1114:ARG:NH1	1:D:1128:LEU:O	2.39	0.47
1:D:1177:LEU:O	1:D:1180:GLU:HG3	2.15	0.47
1:D:2685:TYR:CE1	1:D:2909:ASP:HB2	2.49	0.47
1:D:2791:ARG:HH21	1:D:2796:ASP:N	2.12	0.47
1:D:2886:ARG:O	1:D:2890:GLN:OE1	2.33	0.47
1:D:3730:ARG:O	1:D:3734:ARG:NH1	2.47	0.47
1:A:232:ASP:OD2	1:A:407:ARG:NH1	2.48	0.47
1:A:932:ASN:HA	1:A:935:MET:HG3	1.96	0.47
1:A:1954:SER:O	1:A:1958:THR:OG1	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2775:ILE:O	1:A:2779:LEU:HG	2.14	0.47
1:A:2917:ILE:HD12	1:A:2920:ARG:HD2	1.95	0.47
1:A:2998:ASN:O	1:A:3002:GLU:HG2	2.13	0.47
1:A:3077:GLN:HG2	1:A:3078:GLY:N	2.30	0.47
1:A:4684:GLU:N	1:A:4684:GLU:OE2	2.48	0.47
1:B:2841:ALA:HB2	1:B:2893:LEU:HD21	1.96	0.47
1:B:2943:PHE:CE2	1:B:2947:SER:HB3	2.50	0.47
1:B:3701:ASP:OD2	1:B:3727:GLN:NE2	2.48	0.47
1:B:4109:MET:HB2	1:B:4115:LEU:HD22	1.96	0.47
1:B:4120:GLU:HA	1:B:4123:GLU:HG2	1.97	0.47
1:B:4873:LEU:O	1:B:4877:GLN:HG2	2.14	0.47
1:C:131:CYS:SG	1:C:150:GLN:HB2	2.55	0.47
1:C:1007:TRP:O	1:C:1011:ARG:HG2	2.14	0.47
1:C:1009:ARG:O	1:C:1013:ARG:HG2	2.14	0.47
1:C:1087:ILE:HG22	1:C:1252:SER:OG	2.15	0.47
1:C:1114:ARG:NH1	1:C:1128:LEU:O	2.39	0.47
1:C:3730:ARG:O	1:C:3734:ARG:NH1	2.47	0.47
1:D:474:ASP:O	1:D:478:ARG:HG2	2.15	0.47
1:D:1007:TRP:O	1:D:1011:ARG:HG2	2.14	0.47
1:D:1284:LYS:HZ1	1:D:1551:ASN:HB3	1.80	0.47
1:D:2432:LEU:O	1:D:2436:ILE:HG13	2.14	0.47
1:D:2841:ALA:HB2	1:D:2893:LEU:HD21	1.96	0.47
1:D:3889:TYR:CD1	1:D:3954:MET:SD	3.07	0.47
1:D:4120:GLU:HA	1:D:4123:GLU:HG2	1.97	0.47
1:A:1177:LEU:O	1:A:1180:GLU:HG3	2.15	0.47
1:A:1787:LEU:HD23	1:A:1828:LEU:HD21	1.96	0.47
1:B:1929:SER:HG	1:B:3620:PHE:HD2	1.63	0.47
1:B:3077:GLN:HG2	1:B:3078:GLY:N	2.30	0.47
1:C:423:VAL:HG23	1:C:497:LEU:HD22	1.97	0.47
1:C:874:LEU:HD13	1:C:878:LEU:HB3	1.96	0.47
1:C:1220:ASP:OD2	1:C:1222:SER:OG	2.30	0.47
1:C:2526:PRO:HB3	1:C:2530:ARG:HH11	1.79	0.47
1:C:2775:ILE:O	1:C:2779:LEU:HG	2.14	0.47
1:C:2789:ILE:HD12	1:C:2903:VAL:HA	1.96	0.47
1:D:889:ILE:HA	1:D:892:LEU:HD12	1.97	0.47
1:D:2092:TYR:HD2	1:D:3640:LEU:HD13	1.78	0.47
1:D:2629:ASN:OD1	1:D:2630:PHE:N	2.48	0.47
1:A:448:PRO:HB2	1:A:451:SER:OG	2.14	0.47
1:A:614:LEU:HA	1:A:617:LEU:HD12	1.96	0.47
1:A:1911:GLN:OE1	1:A:2090:ARG:NH1	2.47	0.47
1:A:2979:ARG:H	1:A:2979:ARG:HD3	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3662:ASP:O	1:A:3666:GLN:HG3	2.14	0.47
1:A:3770:ASN:HB3	1:A:3773:VAL:CG1	2.42	0.47
1:A:4049:HIS:CD2	1:A:4067:LEU:HD11	2.47	0.47
1:A:4187:GLU:OE2	1:A:4947:ARG:NH2	2.41	0.47
1:B:448:PRO:HB2	1:B:451:SER:OG	2.14	0.47
1:B:874:LEU:HD13	1:B:878:LEU:HB3	1.96	0.47
1:B:1611:ILE:HB	1:B:1615:GLN:HB2	1.97	0.47
1:B:2886:ARG:O	1:B:2890:GLN:OE1	2.33	0.47
1:B:3662:ASP:O	1:B:3666:GLN:HG3	2.14	0.47
1:B:3978:MET:HE3	1:B:3982:LEU:HD11	1.97	0.47
1:B:4502:MET:HE1	1:B:4585:PHE:HD2	1.80	0.47
1:C:983:LEU:HD12	1:C:1055:ARG:HG3	1.96	0.47
1:C:1611:ILE:HB	1:C:1615:GLN:HB2	1.97	0.47
1:D:874:LEU:HD13	1:D:878:LEU:HB3	1.96	0.47
1:D:2518:ARG:O	1:D:2522:THR:OG1	2.23	0.47
1:D:4269:LYS:HA	1:D:4272:LYS:HE3	1.96	0.47
1:A:2204:CYS:SG	1:A:2214:MET:HG2	2.55	0.47
1:A:2455:ASP:HB3	1:A:2458:ALA:HB3	1.95	0.47
1:A:4267:GLN:HA	1:A:4270:LYS:HE2	1.96	0.47
1:B:1431:ARG:NE	1:B:1506:GLU:OE1	2.30	0.47
1:B:2782:MET:O	1:B:2786:GLY:N	2.48	0.47
1:B:3728:GLN:O	1:B:3732:HIS:ND1	2.46	0.47
1:C:1177:LEU:O	1:C:1180:GLU:HG3	2.15	0.47
1:C:1940:GLN:OE1	1:C:3608:LEU:HB2	2.15	0.47
1:C:2943:PHE:CE2	1:C:2947:SER:HB3	2.50	0.47
1:C:4269:LYS:HA	1:C:4272:LYS:HE3	1.96	0.47
1:C:4639:SER:OG	1:C:4642:ASN:HB2	2.15	0.47
1:D:232:ASP:OD2	1:D:407:ARG:NH1	2.48	0.47
1:D:920:GLU:O	1:D:924:LEU:N	2.48	0.47
1:D:1009:ARG:O	1:D:1013:ARG:HG2	2.15	0.47
1:D:2204:CYS:SG	1:D:2214:MET:HG2	2.55	0.47
1:D:2526:PRO:O	1:D:2530:ARG:HG3	2.15	0.47
1:D:2610:LEU:HD13	1:D:2644:LEU:HD21	1.97	0.47
1:A:2629:ASN:OD1	1:A:2630:PHE:N	2.48	0.46
1:A:2791:ARG:HH21	1:A:2795:GLY:C	2.18	0.46
1:B:131:CYS:SG	1:B:150:GLN:HB2	2.55	0.46
1:B:1523:ASN:HB2	1:B:1525:LYS:NZ	2.30	0.46
1:B:2694:SER:O	1:B:2701:PHE:HA	2.15	0.46
1:C:920:GLU:O	1:C:924:LEU:N	2.48	0.46
1:C:2685:TYR:CE1	1:C:2909:ASP:HB2	2.49	0.46
1:C:3662:ASP:O	1:C:3666:GLN:HG3	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4502:MET:HE1	1:C:4585:PHE:HD2	1.80	0.46
1:D:131:CYS:SG	1:D:150:GLN:HB2	2.55	0.46
1:A:1118:SER:HB3	1:A:1204:VAL:HG11	1.97	0.46
1:A:1523:ASN:HB2	1:A:1525:LYS:NZ	2.30	0.46
1:A:1929:SER:HG	1:A:3620:PHE:HD2	1.63	0.46
1:A:1940:GLN:OE1	1:A:3608:LEU:HB2	2.15	0.46
1:A:2347:MET:O	1:A:2351:ILE:HG12	2.13	0.46
1:B:920:GLU:O	1:B:924:LEU:N	2.48	0.46
1:B:2629:ASN:OD1	1:B:2630:PHE:N	2.48	0.46
1:D:61:ASP:OD1	1:D:63:SER:OG	2.32	0.46
1:D:842:GLN:OE1	1:D:1603:PHE:N	2.43	0.46
1:D:1940:GLN:OE1	1:D:3608:LEU:HB2	2.15	0.46
1:D:1954:SER:O	1:D:1958:THR:OG1	2.33	0.46
1:D:3701:ASP:OD2	1:D:3727:GLN:NE2	2.48	0.46
1:D:4267:GLN:HA	1:D:4270:LYS:HE2	1.96	0.46
1:D:4796:SER:HB3	1:D:4803:ASP:HB3	1.97	0.46
1:B:61:ASP:OD1	1:B:63:SER:OG	2.32	0.46
1:B:718:VAL:HG23	1:B:793:SER:HB3	1.96	0.46
1:B:1052:GLU:HA	1:B:1055:ARG:CG	2.44	0.46
1:B:4008:ASN:OD1	1:B:4009:ASN:N	2.47	0.46
1:B:4684:GLU:N	1:B:4684:GLU:OE2	2.48	0.46
1:B:4796:SER:HB3	1:B:4803:ASP:HB3	1.98	0.46
1:C:2905:ARG:HH11	1:C:2906:GLY:N	2.12	0.46
1:C:3077:GLN:HG2	1:C:3078:GLY:N	2.30	0.46
1:D:1490:ALA:HA	1:D:1493:SER:HB2	1.98	0.46
1:D:2455:ASP:HB3	1:D:2458:ALA:HB3	1.95	0.46
1:D:2782:MET:O	1:D:2786:GLY:N	2.48	0.46
1:D:2905:ARG:HH11	1:D:2906:GLY:N	2.12	0.46
1:A:2303:ARG:NH1	1:A:2307:PHE:HB3	2.31	0.46
1:A:2526:PRO:O	1:A:2530:ARG:HG3	2.15	0.46
1:A:2666:LEU:HD13	1:A:2966:VAL:HA	1.97	0.46
1:A:2685:TYR:CE1	1:A:2909:ASP:HB2	2.49	0.46
1:A:4017:PHE:O	1:A:4021:LEU:HG	2.16	0.46
1:B:1118:SER:HB3	1:B:1204:VAL:HG11	1.97	0.46
1:B:1262:PRO:HD3	1:B:1590:PHE:HE1	1.81	0.46
1:B:3004:VAL:O	1:B:3007:LEU:HG	2.15	0.46
1:B:4017:PHE:O	1:B:4021:LEU:HG	2.16	0.46
1:B:4639:SER:OG	1:B:4642:ASN:HB2	2.15	0.46
1:C:1262:PRO:HD3	1:C:1590:PHE:HE1	1.81	0.46
1:C:2629:ASN:OD1	1:C:2630:PHE:N	2.48	0.46
1:C:2789:ILE:HD12	1:C:2903:VAL:CA	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4796:SER:HB3	1:C:4803:ASP:HB3	1.97	0.46
1:D:1087:ILE:HG22	1:D:1252:SER:OG	2.15	0.46
1:D:2789:ILE:HD12	1:D:2903:VAL:HA	1.96	0.46
1:D:3004:VAL:O	1:D:3007:LEU:HG	2.14	0.46
1:D:3108:LEU:O	1:D:3112:ILE:HG12	2.15	0.46
1:D:4008:ASN:OD1	1:D:4009:ASN:N	2.47	0.46
1:A:2092:TYR:HD2	1:A:3640:LEU:HD13	1.78	0.46
1:A:2905:ARG:HH11	1:A:2906:GLY:N	2.12	0.46
1:B:1494:MET:CE	1:B:1505:LEU:HD22	2.46	0.46
1:B:1523:ASN:HB2	1:B:1525:LYS:HZ1	1.81	0.46
1:B:2303:ARG:NH1	1:B:2307:PHE:HB3	2.31	0.46
1:B:2980:LEU:HD23	1:B:2990:LEU:HG	1.98	0.46
1:B:4815:PHE:O	1:B:4819:VAL:HG22	2.16	0.46
1:C:474:ASP:O	1:C:478:ARG:HG2	2.15	0.46
1:C:624:ALA:HB2	1:C:1667:LEU:HD12	1.97	0.46
1:C:2855:LYS:HE3	1:C:2856:LYS:NZ	2.31	0.46
1:C:4187:GLU:OE2	1:C:4947:ARG:NH2	2.41	0.46
1:D:1262:PRO:HD3	1:D:1590:PHE:HE1	1.81	0.46
1:D:2303:ARG:NH1	1:D:2307:PHE:HB3	2.31	0.46
1:D:2782:MET:HE1	1:D:2789:ILE:HB	1.97	0.46
1:D:3077:GLN:HG2	1:D:3078:GLY:N	2.30	0.46
1:D:4049:HIS:CD2	1:D:4067:LEU:HD11	2.47	0.46
1:D:4815:PHE:O	1:D:4819:VAL:HG22	2.16	0.46
1:A:474:ASP:O	1:A:478:ARG:HG2	2.15	0.46
1:A:1431:ARG:NE	1:A:1506:GLU:OE1	2.30	0.46
1:A:1490:ALA:HA	1:A:1493:SER:HB2	1.98	0.46
1:A:2432:LEU:O	1:A:2436:ILE:HG13	2.14	0.46
1:A:2610:LEU:HD13	1:A:2644:LEU:HD21	1.97	0.46
1:A:2782:MET:O	1:A:2786:GLY:N	2.48	0.46
1:A:2980:LEU:HD23	1:A:2990:LEU:HG	1.98	0.46
1:A:3016:ARG:O	1:A:3018:ARG:NH1	2.48	0.46
1:A:3108:LEU:O	1:A:3112:ILE:HG12	2.15	0.46
1:B:423:VAL:HG23	1:B:497:LEU:HD22	1.97	0.46
1:B:474:ASP:O	1:B:478:ARG:HG2	2.15	0.46
1:B:1114:ARG:NH1	1:B:1128:LEU:O	2.39	0.46
1:B:1953:MET:N	1:B:1953:MET:SD	2.89	0.46
1:B:2610:LEU:HD13	1:B:2644:LEU:HD21	1.97	0.46
1:B:2666:LEU:HD13	1:B:2966:VAL:HA	1.97	0.46
1:B:2979:ARG:HD3	1:B:2979:ARG:H	1.80	0.46
1:C:232:ASP:OD2	1:C:407:ARG:NH1	2.48	0.46
1:C:2526:PRO:O	1:C:2530:ARG:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2666:LEU:HD13	1:C:2966:VAL:HA	1.97	0.46
1:C:2782:MET:O	1:C:2786:GLY:N	2.48	0.46
1:C:3749:GLY:HA2	1:C:3796:LEU:HG	1.97	0.46
1:C:3961:ASP:OD2	1:C:3963:SER:OG	2.34	0.46
1:D:4017:PHE:O	1:D:4021:LEU:HG	2.16	0.46
1:A:1427:TYR:HB2	1:A:1563:VAL:HG11	1.98	0.46
1:A:2886:ARG:O	1:A:2890:GLN:OE1	2.33	0.46
1:A:4269:LYS:HA	1:A:4272:LYS:HE3	1.96	0.46
1:A:4796:SER:HB3	1:A:4803:ASP:HB3	1.98	0.46
1:B:624:ALA:HB2	1:B:1667:LEU:HD12	1.97	0.46
1:B:2789:ILE:HD12	1:B:2903:VAL:HA	1.96	0.46
1:B:4049:HIS:CD2	1:B:4067:LEU:HD11	2.47	0.46
1:B:4269:LYS:HA	1:B:4272:LYS:HE3	1.96	0.46
1:B:4751:LYS:HG3	1:B:4754:ARG:NH1	2.31	0.46
1:C:2979:ARG:H	1:C:2979:ARG:HD3	1.80	0.46
1:C:4684:GLU:N	1:C:4684:GLU:OE2	2.48	0.46
1:C:4815:PHE:O	1:C:4819:VAL:HG22	2.16	0.46
1:A:2772:ARG:O	1:A:2776:LYS:HG2	2.16	0.46
1:A:4120:GLU:HA	1:A:4123:GLU:HG2	1.97	0.46
1:B:504:ARG:O	1:B:507:VAL:HG22	2.16	0.46
1:B:1087:ILE:HG22	1:B:1252:SER:OG	2.15	0.46
1:B:1177:LEU:O	1:B:1180:GLU:HG3	2.15	0.46
1:B:3613:ARG:O	1:B:3617:VAL:HG23	2.16	0.46
1:C:61:ASP:OD1	1:C:63:SER:OG	2.32	0.46
1:C:614:LEU:HA	1:C:617:LEU:HD12	1.96	0.46
1:C:2204:CYS:SG	1:C:2214:MET:HG2	2.55	0.46
1:C:3108:LEU:O	1:C:3112:ILE:HG12	2.15	0.46
1:D:1523:ASN:HB2	1:D:1525:LYS:NZ	2.31	0.46
1:D:2979:ARG:H	1:D:2979:ARG:HD3	1.80	0.46
1:D:3693:ASP:O	1:D:3697:LYS:HG2	2.16	0.46
1:D:4684:GLU:N	1:D:4684:GLU:OE2	2.48	0.46
1:A:624:ALA:HB2	1:A:1667:LEU:HD12	1.97	0.46
1:A:2589:LEU:O	1:A:2593:VAL:HG13	2.16	0.46
1:A:2855:LYS:HE3	1:A:2856:LYS:NZ	2.31	0.46
1:A:3994:THR:HA	1:A:3997:LYS:HD2	1.98	0.46
1:B:2589:LEU:O	1:B:2593:VAL:HG13	2.16	0.46
1:B:2772:ARG:O	1:B:2776:LYS:HG2	2.16	0.46
1:C:1427:TYR:HB2	1:C:1563:VAL:HG11	1.98	0.46
1:C:2303:ARG:NH1	1:C:2307:PHE:HB3	2.31	0.46
1:D:1118:SER:HB3	1:D:1204:VAL:HG11	1.97	0.46
1:D:4639:SER:OG	1:D:4642:ASN:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:VAL:HG23	1:A:497:LEU:HD22	1.97	0.46
1:A:718:VAL:HG23	1:A:793:SER:HB3	1.96	0.46
1:A:2789:ILE:HD12	1:A:2903:VAL:HA	1.97	0.46
1:A:3728:GLN:O	1:A:3732:HIS:ND1	2.46	0.46
1:A:3891:TYR:HA	1:B:76:ARG:NH2	2.31	0.46
1:B:1284:LYS:HZ1	1:B:1551:ASN:HB3	1.81	0.46
1:B:1429:SER:HB3	1:B:1506:GLU:OE2	2.16	0.46
1:C:2157:GLN:O	1:C:3615:ARG:NH2	2.44	0.46
1:C:3613:ARG:O	1:C:3617:VAL:HG23	2.16	0.46
1:C:3693:ASP:O	1:C:3697:LYS:HG2	2.16	0.46
1:C:4862:ILE:HA	1:C:4865:LEU:HD12	1.98	0.46
1:D:423:VAL:HG23	1:D:497:LEU:HD22	1.97	0.46
1:D:624:ALA:HB2	1:D:1667:LEU:HD12	1.97	0.46
1:D:1611:ILE:HB	1:D:1615:GLN:HB2	1.97	0.46
1:D:2694:SER:O	1:D:2701:PHE:HA	2.15	0.46
1:D:3961:ASP:OD2	1:D:3963:SER:OG	2.34	0.46
1:D:4819:VAL:HG12	1:D:4822:ARG:NH2	2.31	0.46
1:D:4862:ILE:HA	1:D:4865:LEU:HD12	1.98	0.46
1:A:874:LEU:HD13	1:A:878:LEU:HB3	1.96	0.45
1:A:1960:ARG:H	1:A:1960:ARG:HG3	0.96	0.45
1:A:2789:ILE:HD12	1:A:2903:VAL:CA	2.46	0.45
1:A:3693:ASP:O	1:A:3697:LYS:HG2	2.16	0.45
1:A:4815:PHE:O	1:A:4819:VAL:HG22	2.16	0.45
1:B:1040:ASP:HA	1:B:1043:LYS:HG2	1.98	0.45
1:B:2526:PRO:O	1:B:2530:ARG:HG3	2.15	0.45
1:B:2789:ILE:HD12	1:B:2903:VAL:CA	2.46	0.45
1:C:942:THR:HA	1:C:945:ALA:HB3	1.98	0.45
1:C:2980:LEU:HD23	1:C:2990:LEU:HG	1.98	0.45
1:D:1106:GLU:HB3	1:D:1214:ARG:HB2	1.98	0.45
1:D:1953:MET:N	1:D:1953:MET:SD	2.89	0.45
1:D:2666:LEU:HD13	1:D:2966:VAL:HA	1.97	0.45
1:D:2980:LEU:HD23	1:D:2990:LEU:HG	1.98	0.45
1:D:3009:CYS:O	1:D:3013:VAL:HG23	2.17	0.45
1:D:3749:GLY:HA2	1:D:3796:LEU:HG	1.97	0.45
1:A:3613:ARG:O	1:A:3617:VAL:HG23	2.16	0.45
1:A:3701:ASP:OD2	1:A:3727:GLN:NE2	2.48	0.45
1:A:4016:PHE:HA	1:A:4019:MET:HE3	1.97	0.45
1:A:4862:ILE:HA	1:A:4865:LEU:HD12	1.98	0.45
1:B:1940:GLN:OE1	1:B:3608:LEU:HB2	2.15	0.45
1:B:2855:LYS:HE3	1:B:2856:LYS:NZ	2.31	0.45
1:B:2968:LEU:HD22	1:B:3029:ILE:HG23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3009:CYS:O	1:B:3013:VAL:HG23	2.17	0.45
1:B:3994:THR:HA	1:B:3997:LYS:HD2	1.98	0.45
1:C:1118:SER:HB3	1:C:1204:VAL:HG11	1.97	0.45
1:C:2973:GLN:O	1:C:2976:LYS:HG3	2.17	0.45
1:D:942:THR:HA	1:D:945:ALA:HB3	1.98	0.45
1:D:1427:TYR:HB2	1:D:1563:VAL:HG11	1.98	0.45
1:D:2973:GLN:O	1:D:2976:LYS:HG3	2.17	0.45
1:A:1052:GLU:O	1:A:1055:ARG:HB2	2.16	0.45
1:A:1262:PRO:HD3	1:A:1590:PHE:HE1	1.81	0.45
1:B:322:ALA:HB1	1:B:327:THR:HG21	1.99	0.45
1:B:942:THR:HA	1:B:945:ALA:HB3	1.98	0.45
1:B:4189:PHE:CE1	1:B:4915:LEU:HG	2.52	0.45
1:B:4249:ARG:O	1:B:4253:LEU:HD23	2.17	0.45
1:C:1523:ASN:HB2	1:C:1525:LYS:NZ	2.30	0.45
1:C:3019:ILE:HD12	1:C:3026:ALA:HB1	1.99	0.45
1:C:4751:LYS:HG3	1:C:4754:ARG:NH1	2.31	0.45
1:D:2154:VAL:HG13	1:D:2158:HIS:CD2	2.48	0.45
1:D:2192:MET:O	1:D:2192:MET:HG2	2.17	0.45
1:D:3019:ILE:HD12	1:D:3026:ALA:HB1	1.99	0.45
1:D:3797:MET:HG3	1:D:3839:LEU:HD21	1.98	0.45
1:A:1429:SER:HB3	1:A:1506:GLU:OE2	2.16	0.45
1:A:1494:MET:CE	1:A:1505:LEU:HD22	2.46	0.45
1:A:3009:CYS:O	1:A:3013:VAL:HG23	2.16	0.45
1:A:3878:LEU:HA	1:A:3881:VAL:HG12	1.99	0.45
1:A:4639:SER:OG	1:A:4642:ASN:HB2	2.15	0.45
1:B:468:GLU:HA	1:B:475:LYS:NZ	2.32	0.45
1:B:1490:ALA:HA	1:B:1493:SER:HB2	1.98	0.45
1:B:4862:ILE:HA	1:B:4865:LEU:HD12	1.98	0.45
1:C:1953:MET:SD	1:C:1953:MET:N	2.89	0.45
1:C:2694:SER:O	1:C:2701:PHE:HA	2.15	0.45
1:D:504:ARG:O	1:D:507:VAL:HG22	2.16	0.45
1:D:1307:PRO:HB3	1:D:1540:PHE:CE2	2.52	0.45
1:D:1415:ASP:OD2	1:D:1559:ARG:NH2	2.49	0.45
1:D:2157:GLN:O	1:D:3615:ARG:NH2	2.44	0.45
1:D:2789:ILE:HD12	1:D:2903:VAL:CA	2.46	0.45
1:D:2855:LYS:HE3	1:D:2856:LYS:NZ	2.31	0.45
1:A:322:ALA:HB1	1:A:327:THR:HG21	1.99	0.45
1:A:504:ARG:O	1:A:507:VAL:HG22	2.16	0.45
1:A:1611:ILE:HB	1:A:1615:GLN:HB2	1.97	0.45
1:A:1953:MET:N	1:A:1953:MET:SD	2.89	0.45
1:A:4249:ARG:O	1:A:4253:LEU:HD23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4751:LYS:HG3	1:A:4754:ARG:NH1	2.31	0.45
1:B:1052:GLU:O	1:B:1055:ARG:HB2	2.16	0.45
1:B:2204:CYS:SG	1:B:2214:MET:HG2	2.55	0.45
1:B:3749:GLY:HA2	1:B:3796:LEU:HG	1.97	0.45
1:B:3878:LEU:HA	1:B:3881:VAL:HG12	1.99	0.45
1:C:908:ARG:NH1	1:C:928:GLU:OE2	2.35	0.45
1:C:1052:GLU:O	1:C:1055:ARG:HB2	2.16	0.45
1:C:1092:LYS:NZ	1:C:1646:GLU:OE1	2.39	0.45
1:C:1284:LYS:HZ1	1:C:1551:ASN:HB3	1.82	0.45
1:C:2589:LEU:O	1:C:2593:VAL:HG13	2.16	0.45
1:C:2610:LEU:HD13	1:C:2644:LEU:HD21	1.97	0.45
1:C:2772:ARG:O	1:C:2776:LYS:HG2	2.16	0.45
1:C:3889:TYR:OH	1:C:3953:HIS:HB3	2.17	0.45
1:C:4921:PHE:HE2	1:C:4940:VAL:HG11	1.82	0.45
1:D:1040:ASP:HA	1:D:1043:LYS:HG2	1.98	0.45
1:D:3878:LEU:HA	1:D:3881:VAL:HG12	1.99	0.45
1:D:4751:LYS:HG3	1:D:4754:ARG:NH1	2.31	0.45
1:A:468:GLU:HA	1:A:475:LYS:NZ	2.32	0.45
1:A:2933:VAL:HB	1:A:3010:LYS:NZ	2.32	0.45
1:A:4819:VAL:HG12	1:A:4822:ARG:NH2	2.31	0.45
1:B:1727:VAL:HG11	1:B:1926:VAL:HG21	1.99	0.45
1:B:2973:GLN:O	1:B:2976:LYS:HG3	2.17	0.45
1:C:504:ARG:O	1:C:507:VAL:HG22	2.16	0.45
1:C:1494:MET:CE	1:C:1505:LEU:HD22	2.46	0.45
1:C:2192:MET:O	1:C:2192:MET:HG2	2.17	0.45
1:C:3009:CYS:O	1:C:3013:VAL:HG23	2.17	0.45
1:C:3878:LEU:HA	1:C:3881:VAL:HG12	1.99	0.45
1:C:3994:THR:HA	1:C:3997:LYS:HD2	1.98	0.45
1:C:4017:PHE:O	1:C:4021:LEU:HG	2.16	0.45
1:C:4249:ARG:O	1:C:4253:LEU:HD23	2.17	0.45
1:C:4819:VAL:HG12	1:C:4822:ARG:NH2	2.31	0.45
1:D:322:ALA:HB1	1:D:327:THR:HG21	1.99	0.45
1:D:2933:VAL:HB	1:D:3010:LYS:NZ	2.32	0.45
1:D:4249:ARG:O	1:D:4253:LEU:HD23	2.17	0.45
1:A:765:SER:HA	1:A:779:PHE:O	2.16	0.45
1:A:2694:SER:O	1:A:2701:PHE:HA	2.15	0.45
1:A:4262:LYS:HD2	1:A:4265:LYS:HD3	1.99	0.45
2:F:58:LYS:HB3	2:F:81:VAL:O	2.17	0.45
1:B:765:SER:HA	1:B:779:PHE:O	2.16	0.45
1:B:902:TRP:CZ2	1:B:915:HIS:HB3	2.50	0.45
1:B:3693:ASP:O	1:B:3697:LYS:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1307:PRO:HB3	1:C:1540:PHE:CE2	2.52	0.45
1:C:1490:ALA:HA	1:C:1493:SER:HB2	1.98	0.45
1:C:2968:LEU:HD22	1:C:3029:ILE:HG23	1.98	0.45
1:D:3994:THR:HA	1:D:3997:LYS:HD2	1.98	0.45
1:D:4262:LYS:HD2	1:D:4265:LYS:HD3	1.99	0.45
1:A:1106:GLU:HB3	1:A:1214:ARG:HB2	1.98	0.45
1:A:1825:PHE:CE1	1:A:1842:ILE:HD13	2.52	0.45
1:A:2332:GLY:N	1:A:2336:ARG:HH21	2.12	0.45
1:A:2973:GLN:O	1:A:2976:LYS:HG3	2.17	0.45
1:B:1307:PRO:HB3	1:B:1540:PHE:CE2	2.52	0.45
1:B:1427:TYR:HB2	1:B:1563:VAL:HG11	1.98	0.45
1:C:468:GLU:HA	1:C:475:LYS:NZ	2.32	0.45
1:D:468:GLU:HA	1:D:475:LYS:NZ	2.32	0.45
1:D:1052:GLU:O	1:D:1055:ARG:HB2	2.16	0.45
1:D:2176:VAL:HG22	1:D:2220:TYR:CE2	2.52	0.45
1:D:2589:LEU:O	1:D:2593:VAL:HG13	2.16	0.45
1:D:2772:ARG:O	1:D:2776:LYS:HG2	2.16	0.45
1:D:2968:LEU:HD22	1:D:3029:ILE:HG23	1.98	0.45
1:D:4189:PHE:CE1	1:D:4915:LEU:HG	2.52	0.45
1:D:4906:GLU:HA	1:D:4909:THR:OG1	2.16	0.45
1:A:2886:ARG:O	1:A:2889:ALA:HB3	2.17	0.45
1:A:3019:ILE:HD12	1:A:3026:ALA:HB1	1.99	0.45
1:A:4689:LYS:HD2	1:A:4696:ALA:HB2	1.99	0.45
1:A:4710:LEU:HD23	1:A:4710:LEU:HA	1.86	0.45
2:H:58:LYS:HB3	2:H:81:VAL:O	2.16	0.45
1:B:318:ASP:O	1:B:322:ALA:HB2	2.17	0.45
1:B:3961:ASP:OD2	1:B:3963:SER:OG	2.34	0.45
1:C:1106:GLU:HB3	1:C:1214:ARG:HB2	1.98	0.45
1:C:1429:SER:HB3	1:C:1506:GLU:OE2	2.16	0.45
1:C:2332:GLY:N	1:C:2336:ARG:HH21	2.13	0.45
1:D:2855:LYS:O	1:D:2858:MET:HG2	2.17	0.45
1:D:3889:TYR:OH	1:D:3953:HIS:HB3	2.17	0.45
1:A:317:MET:HB2	1:A:321:LYS:HZ2	1.82	0.45
1:A:942:THR:HA	1:A:945:ALA:HB3	1.98	0.45
1:A:1114:ARG:HB2	1:A:1206:SER:OG	2.18	0.45
1:A:2322:ARG:HH12	1:B:189:GLU:HG3	1.82	0.45
1:A:2581:ARG:HG3	1:A:2583:SER:H	1.82	0.45
1:A:3797:MET:HG3	1:A:3839:LEU:HD21	1.98	0.45
1:A:4071:GLU:HB2	1:A:4086:ARG:HH12	1.82	0.45
1:A:4189:PHE:CE1	1:A:4915:LEU:HG	2.52	0.45
1:B:816:PRO:HB2	1:B:819:TYR:CD1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2427:ILE:HD13	1:B:2471:PHE:CZ	2.52	0.45
1:B:3019:ILE:HD12	1:B:3026:ALA:HB1	1.99	0.45
1:B:3797:MET:HG3	1:B:3839:LEU:HD21	1.98	0.45
1:B:3889:TYR:OH	1:B:3953:HIS:HB3	2.17	0.45
1:B:4906:GLU:HA	1:B:4909:THR:OG1	2.16	0.45
1:B:4921:PHE:HE2	1:B:4940:VAL:HG11	1.82	0.45
1:C:765:SER:HA	1:C:779:PHE:O	2.16	0.45
1:C:1040:ASP:HA	1:C:1043:LYS:HG2	1.98	0.45
1:C:1100:ARG:NH2	1:C:1234:GLU:O	2.50	0.45
1:C:1415:ASP:OD2	1:C:1559:ARG:NH2	2.49	0.45
1:C:1523:ASN:HB2	1:C:1525:LYS:HZ1	1.81	0.45
1:C:1724:GLU:O	1:C:1919:ARG:NH2	2.50	0.45
1:C:1825:PHE:CE1	1:C:1842:ILE:HD13	2.52	0.45
1:C:2222:LEU:HD23	1:C:2222:LEU:HA	1.80	0.45
1:C:2855:LYS:O	1:C:2858:MET:HG2	2.17	0.45
1:C:2898:ILE:HG23	1:D:1500:ARG:HH22	1.81	0.45
1:C:3797:MET:HG3	1:C:3839:LEU:HD21	1.98	0.45
1:C:4071:GLU:OE1	1:C:4086:ARG:NH1	2.50	0.45
1:D:874:LEU:HA	1:D:875:PRO:HD3	1.82	0.45
1:D:1429:SER:HB3	1:D:1506:GLU:OE2	2.16	0.45
1:D:1494:MET:CE	1:D:1505:LEU:HD22	2.46	0.45
1:D:1564:MET:HE1	1:D:1578:PRO:HA	1.99	0.45
1:D:1727:VAL:HG11	1:D:1926:VAL:HG21	1.99	0.45
1:D:4921:PHE:HE2	1:D:4940:VAL:HG11	1.82	0.45
1:A:179:ASP:OD1	1:A:180:ASP:N	2.51	0.44
1:A:1040:ASP:HA	1:A:1043:LYS:HG2	1.98	0.44
1:A:1727:VAL:HG11	1:A:1926:VAL:HG21	1.99	0.44
1:A:2176:VAL:HG22	1:A:2220:TYR:CE2	2.52	0.44
1:A:3749:GLY:HA2	1:A:3796:LEU:HG	1.97	0.44
1:A:4071:GLU:OE1	1:A:4086:ARG:NH1	2.50	0.44
1:A:4906:GLU:HA	1:A:4909:THR:OG1	2.16	0.44
1:B:317:MET:HB2	1:B:321:LYS:HZ2	1.82	0.44
1:B:801:ARG:HG3	1:B:1618:LEU:HD13	2.00	0.44
1:B:4071:GLU:HB2	1:B:4086:ARG:HH12	1.82	0.44
1:B:4262:LYS:HD2	1:B:4265:LYS:HD3	1.99	0.44
1:B:4710:LEU:HD23	1:B:4710:LEU:HA	1.86	0.44
1:C:317:MET:HB2	1:C:321:LYS:HZ2	1.82	0.44
1:C:318:ASP:O	1:C:322:ALA:HB2	2.17	0.44
1:C:322:ALA:HB1	1:C:327:THR:HG21	1.99	0.44
1:C:816:PRO:HB2	1:C:819:TYR:CD1	2.52	0.44
1:C:4262:LYS:HD2	1:C:4265:LYS:HD3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:904:TYR:HB3	1:D:972:LEU:CD1	2.47	0.44
1:D:1724:GLU:O	1:D:1919:ARG:NH2	2.51	0.44
1:D:1825:PHE:CE1	1:D:1842:ILE:HD13	2.52	0.44
1:D:2581:ARG:HG3	1:D:2583:SER:H	1.82	0.44
1:D:2651:ALA:O	1:D:2655:LYS:HG2	2.17	0.44
1:D:3613:ARG:O	1:D:3617:VAL:HG23	2.16	0.44
1:D:3978:MET:HE3	1:D:3982:LEU:HD11	1.99	0.44
1:B:1106:GLU:HB3	1:B:1214:ARG:HB2	1.98	0.44
1:B:1114:ARG:HB2	1:B:1206:SER:OG	2.18	0.44
1:B:1255:LEU:HD12	1:B:1256:PRO:HD2	1.99	0.44
1:B:1724:GLU:O	1:B:1919:ARG:NH2	2.50	0.44
1:B:3968:LEU:O	1:B:3972:MET:HG2	2.18	0.44
1:C:904:TYR:HB3	1:C:972:LEU:CD1	2.47	0.44
1:C:1255:LEU:HD12	1:C:1256:PRO:HD2	1.99	0.44
1:C:3968:LEU:O	1:C:3972:MET:HG2	2.17	0.44
1:C:3978:MET:HE3	1:C:3982:LEU:HD11	1.99	0.44
1:C:4189:PHE:CE1	1:C:4915:LEU:HG	2.52	0.44
1:D:318:ASP:O	1:D:322:ALA:HB2	2.17	0.44
1:D:765:SER:HA	1:D:779:PHE:O	2.16	0.44
1:D:875:PRO:HB2	1:D:877:HIS:CE1	2.53	0.44
1:D:2383:HIS:CG	1:D:2458:ALA:HB2	2.53	0.44
1:D:3968:LEU:O	1:D:3972:MET:HG2	2.17	0.44
1:D:4187:GLU:OE2	1:D:4947:ARG:NH2	2.41	0.44
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.87	0.44
1:A:1523:ASN:HB2	1:A:1525:LYS:HZ1	1.82	0.44
1:A:2415:GLU:O	1:A:2419:ILE:HG12	2.18	0.44
1:A:2855:LYS:O	1:A:2858:MET:HG2	2.17	0.44
1:A:2968:LEU:HD22	1:A:3029:ILE:HG23	1.98	0.44
1:A:2985:ALA:HB2	1:A:3001:LYS:HE2	2.00	0.44
1:A:3889:TYR:OH	1:A:3953:HIS:HB3	2.17	0.44
1:A:4252:ILE:O	1:A:4256:MET:HG2	2.18	0.44
1:A:4521:LYS:HZ2	1:B:4807:ASP:HB3	1.80	0.44
1:B:120:LEU:HD12	1:B:120:LEU:HA	1.87	0.44
1:B:1853:GLU:OE1	1:B:1853:GLU:N	2.49	0.44
1:B:3077:GLN:HG2	1:B:3078:GLY:H	1.82	0.44
1:C:842:GLN:OE1	1:C:1603:PHE:N	2.43	0.44
1:C:1087:ILE:HG21	1:C:1124:PRO:HA	2.00	0.44
1:C:2581:ARG:HG3	1:C:2583:SER:H	1.82	0.44
1:C:3077:GLN:HG2	1:C:3078:GLY:H	1.83	0.44
1:C:4071:GLU:HB2	1:C:4086:ARG:HH12	1.82	0.44
1:C:4732:GLY:HA2	1:C:4738:PHE:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:801:ARG:HG3	1:D:1618:LEU:HD13	2.00	0.44
1:D:1087:ILE:HG21	1:D:1124:PRO:HA	2.00	0.44
1:D:2440:PHE:HB3	1:D:2460:PHE:CD2	2.51	0.44
1:D:4018:ASP:OD2	1:D:4022:LYS:NZ	2.38	0.44
1:A:703:TYR:HD2	1:A:858:THR:HG23	1.83	0.44
1:A:2440:PHE:HB3	1:A:2460:PHE:CD2	2.51	0.44
1:A:4047:ASP:HA	1:A:4050:LYS:HE3	2.00	0.44
1:A:4732:GLY:HA2	1:A:4738:PHE:HB2	1.98	0.44
1:A:4921:PHE:HE2	1:A:4940:VAL:HG11	1.82	0.44
1:B:921:PHE:HD1	1:B:929:ARG:NE	2.16	0.44
1:B:2195:ASN:ND2	1:B:2198:ARG:HH12	2.15	0.44
1:B:2554:ARG:HA	1:B:2554:ARG:HD2	1.85	0.44
1:B:2855:LYS:O	1:B:2858:MET:HG2	2.17	0.44
1:B:2886:ARG:O	1:B:2889:ALA:HB3	2.17	0.44
1:C:935:MET:HA	1:C:938:GLU:HG3	2.00	0.44
1:C:2176:VAL:HG22	1:C:2220:TYR:CE2	2.52	0.44
1:C:2383:HIS:CG	1:C:2458:ALA:HB2	2.53	0.44
1:C:2415:GLU:O	1:C:2419:ILE:HG12	2.18	0.44
1:C:2777:GLU:O	1:C:2781:THR:OG1	2.19	0.44
1:C:2789:ILE:HD11	1:C:2896:LEU:HD21	2.00	0.44
1:D:2222:LEU:HD23	1:D:2222:LEU:HA	1.80	0.44
1:D:2332:GLY:N	1:D:2336:ARG:HH21	2.13	0.44
1:D:3008:PHE:CD1	1:D:3040:LEU:HD11	2.53	0.44
1:D:4071:GLU:HB2	1:D:4086:ARG:HH12	1.82	0.44
1:A:904:TYR:HB3	1:A:972:LEU:CD1	2.48	0.44
1:A:2096:GLY:HA2	1:A:2099:VAL:HG22	1.99	0.44
1:A:2321:VAL:HG11	1:A:2419:ILE:HD12	2.00	0.44
1:A:3978:MET:HE3	1:A:3982:LEU:HD11	2.00	0.44
1:A:4769:LEU:HB3	1:D:4753:LEU:HD23	1.99	0.44
2:E:58:LYS:HB3	2:E:81:VAL:O	2.17	0.44
2:G:58:LYS:HB3	2:G:81:VAL:O	2.16	0.44
1:B:703:TYR:HD2	1:B:858:THR:HG23	1.83	0.44
1:B:875:PRO:HB2	1:B:877:HIS:CE1	2.53	0.44
1:B:1087:ILE:HG21	1:B:1124:PRO:HA	2.00	0.44
1:B:1100:ARG:NH2	1:B:1234:GLU:O	2.51	0.44
1:B:2581:ARG:HG3	1:B:2583:SER:H	1.82	0.44
1:B:2789:ILE:HD11	1:B:2896:LEU:HD21	2.00	0.44
1:B:3050:LEU:HD12	1:B:3051:GLU:OE1	2.18	0.44
1:B:3770:ASN:HB3	1:B:3773:VAL:CG1	2.42	0.44
1:B:4047:ASP:HA	1:B:4050:LYS:HE3	1.99	0.44
1:B:4071:GLU:OE1	1:B:4086:ARG:NH1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4689:LYS:HD2	1:B:4696:ALA:HB2	1.99	0.44
1:C:267:VAL:HG23	1:C:272:ARG:NH1	2.33	0.44
1:C:594:ILE:HD11	1:C:632:ILE:HG13	2.00	0.44
1:C:2933:VAL:HB	1:C:3010:LYS:NZ	2.32	0.44
1:C:3008:PHE:CD1	1:C:3040:LEU:HD11	2.53	0.44
1:C:4906:GLU:HA	1:C:4909:THR:OG1	2.16	0.44
1:D:1853:GLU:OE1	1:D:1853:GLU:N	2.49	0.44
1:D:2321:VAL:HG11	1:D:2419:ILE:HD12	2.00	0.44
1:D:4732:GLY:HA2	1:D:4738:PHE:HB2	1.98	0.44
1:A:61:ASP:OD1	1:A:63:SER:OG	2.32	0.44
1:A:640:ARG:O	2:E:35:LYS:NZ	2.49	0.44
1:A:711:GLU:OE1	1:A:716:ASN:HB2	2.18	0.44
1:A:1564:MET:HE1	1:A:1578:PRO:HA	2.00	0.44
1:A:4481:TRP:HA	1:A:4484:ILE:HG12	2.00	0.44
1:B:2176:VAL:HG22	1:B:2220:TYR:CE2	2.52	0.44
1:B:2933:VAL:HB	1:B:3010:LYS:NZ	2.32	0.44
1:B:4252:ILE:O	1:B:4256:MET:HG2	2.18	0.44
1:C:120:LEU:HD12	1:C:120:LEU:HA	1.87	0.44
1:C:515:ALA:HB2	1:C:523:GLY:HA3	2.00	0.44
1:C:703:TYR:HD2	1:C:858:THR:HG23	1.83	0.44
1:C:2427:ILE:HD13	1:C:2471:PHE:CZ	2.53	0.44
1:C:4689:LYS:HD2	1:C:4696:ALA:HB2	1.99	0.44
1:A:387:ILE:HD11	1:A:389:ARG:HH21	1.83	0.44
1:A:1307:PRO:HB3	1:A:1540:PHE:CE2	2.52	0.44
1:A:4752:THR:OG1	1:B:4766:GLN:OE1	2.36	0.44
1:B:1825:PHE:CE1	1:B:1842:ILE:HD13	2.52	0.44
1:B:2321:VAL:HG11	1:B:2419:ILE:HD12	2.00	0.44
1:B:3008:PHE:CD1	1:B:3040:LEU:HD11	2.53	0.44
1:B:4481:TRP:HA	1:B:4484:ILE:HG12	2.00	0.44
1:B:4819:VAL:HG12	1:B:4822:ARG:NH2	2.31	0.44
1:C:2886:ARG:O	1:C:2889:ALA:HB3	2.17	0.44
1:D:703:TYR:HD2	1:D:858:THR:HG23	1.83	0.44
1:D:1523:ASN:HB2	1:D:1525:LYS:HZ1	1.83	0.44
1:D:4071:GLU:OE1	1:D:4086:ARG:NH1	2.50	0.44
1:D:4481:TRP:HA	1:D:4484:ILE:HG12	2.00	0.44
1:A:21:VAL:HG12	1:A:66:THR:HA	2.00	0.44
1:A:2518:ARG:O	1:A:2522:THR:OG1	2.23	0.44
1:A:2651:ALA:O	1:A:2655:LYS:HG2	2.17	0.44
1:A:2877:LEU:HG	1:A:2882:LYS:HG3	2.00	0.44
1:A:3008:PHE:CD1	1:A:3040:LEU:HD11	2.53	0.44
1:B:308:LEU:HD13	1:B:393:MET:HG3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:ARG:HD3	1:B:733:TRP:CD1	2.53	0.44
1:B:935:MET:HA	1:B:938:GLU:HG3	1.99	0.44
1:B:1642:LEU:HD21	1:B:1691:ASN:ND2	2.33	0.44
1:B:1910:LEU:HD13	1:B:2062:ILE:HG12	1.99	0.44
1:B:2096:GLY:HA2	1:B:2099:VAL:HG22	1.99	0.44
1:B:2440:PHE:HB3	1:B:2460:PHE:CD2	2.51	0.44
1:B:2789:ILE:CD1	1:B:2903:VAL:HB	2.48	0.44
1:B:2887:GLU:HA	1:B:2890:GLN:OE1	2.18	0.44
1:B:2985:ALA:HB2	1:B:3001:LYS:HE2	2.00	0.44
1:B:3999:MET:HG3	1:B:4002:MET:HE3	2.00	0.44
1:B:4052:MET:HG3	1:B:4063:THR:HG23	2.00	0.44
1:B:4732:GLY:HA2	1:B:4738:PHE:HB2	1.98	0.44
1:C:921:PHE:HD1	1:C:929:ARG:NE	2.16	0.44
1:C:1114:ARG:HB2	1:C:1206:SER:OG	2.18	0.44
1:C:2760:TYR:HH	1:C:2772:ARG:HH12	1.59	0.44
1:C:3050:LEU:HD12	1:C:3051:GLU:OE1	2.18	0.44
1:D:1427:TYR:CE2	1:D:1560:ILE:HG23	2.53	0.44
1:D:1932:PHE:CE2	1:D:1996:LEU:HD22	2.53	0.44
1:D:2415:GLU:O	1:D:2419:ILE:HG12	2.18	0.44
1:A:308:LEU:HD13	1:A:393:MET:HG3	2.00	0.44
1:A:1415:ASP:OD2	1:A:1559:ARG:NH2	2.49	0.44
1:A:1566:LEU:O	1:A:1570:LEU:HG	2.18	0.44
1:A:2982:PHE:O	1:A:3001:LYS:NZ	2.44	0.44
1:A:3642:GLU:O	1:A:3646:LYS:HG3	2.18	0.44
1:A:4052:MET:HG3	1:A:4063:THR:HG23	2.00	0.44
1:A:4094:ILE:O	1:A:4098:VAL:HG23	2.18	0.44
2:E:50:ARG:N	2:E:55:GLU:OE2	2.37	0.44
2:H:26:HIS:CD2	2:H:105:LEU:HD11	2.53	0.44
1:B:794:PHE:CG	1:B:798:ILE:HD13	2.53	0.44
1:B:2877:LEU:HG	1:B:2882:LYS:HG3	2.00	0.44
1:B:2917:ILE:HG12	1:B:2999:LYS:HD3	2.00	0.44
1:C:1727:VAL:HG11	1:C:1926:VAL:HG21	1.99	0.44
1:C:2154:VAL:HG13	1:C:2158:HIS:CD2	2.48	0.44
1:C:4481:TRP:HA	1:C:4484:ILE:HG12	2.00	0.44
1:D:179:ASP:OD1	1:D:180:ASP:N	2.51	0.44
1:D:711:GLU:OE1	1:D:716:ASN:HB2	2.18	0.44
1:D:1566:LEU:O	1:D:1570:LEU:HG	2.18	0.44
1:D:2427:ILE:HD13	1:D:2471:PHE:CZ	2.52	0.44
1:D:3999:MET:HG3	1:D:4002:MET:HE3	2.00	0.44
1:D:4247:ALA:HA	1:D:4250:TYR:CE1	2.53	0.44
1:A:1724:GLU:O	1:A:1919:ARG:NH2	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1932:PHE:CE2	1:A:1996:LEU:HD22	2.53	0.43
1:A:2383:HIS:CG	1:A:2458:ALA:HB2	2.53	0.43
1:A:2427:ILE:HD13	1:A:2471:PHE:CZ	2.52	0.43
1:A:3961:ASP:OD2	1:A:3963:SER:OG	2.34	0.43
1:A:3968:LEU:O	1:A:3972:MET:HG2	2.17	0.43
1:A:4016:PHE:HA	1:A:4019:MET:CE	2.48	0.43
1:A:4611:GLU:HA	1:A:4653:VAL:HG22	2.00	0.43
2:E:26:HIS:CD2	2:E:105:LEU:HD11	2.53	0.43
1:B:594:ILE:HD11	1:B:632:ILE:HG13	2.00	0.43
1:B:1050:LEU:HD12	1:B:1050:LEU:HA	1.81	0.43
1:B:1947:VAL:HG11	1:B:1965:PHE:HE2	1.83	0.43
1:B:4634:VAL:O	1:B:4637:THR:OG1	2.26	0.43
1:C:308:LEU:HD13	1:C:393:MET:HG3	2.00	0.43
1:C:875:PRO:HB2	1:C:877:HIS:CE1	2.53	0.43
1:C:1642:LEU:HD21	1:C:1691:ASN:ND2	2.33	0.43
1:C:1749:PRO:HB2	1:C:1913:LEU:HD22	2.00	0.43
1:C:2887:GLU:HA	1:C:2890:GLN:OE1	2.18	0.43
1:C:4252:ILE:O	1:C:4256:MET:HG2	2.18	0.43
1:D:794:PHE:CG	1:D:798:ILE:HD13	2.53	0.43
1:D:816:PRO:HB2	1:D:819:TYR:CD1	2.52	0.43
1:D:1100:ARG:NH2	1:D:1234:GLU:O	2.51	0.43
1:D:1642:LEU:HD21	1:D:1691:ASN:ND2	2.33	0.43
1:D:1749:PRO:HB2	1:D:1913:LEU:HD22	2.00	0.43
1:D:2758:LYS:HE3	1:D:2763:LEU:HA	2.00	0.43
1:D:3077:GLN:HG2	1:D:3078:GLY:H	1.83	0.43
1:D:4052:MET:HG3	1:D:4063:THR:HG23	2.00	0.43
1:D:4689:LYS:HD2	1:D:4696:ALA:HB2	1.99	0.43
1:A:307:SER:OG	1:A:317:MET:HG2	2.19	0.43
1:A:935:MET:HA	1:A:938:GLU:HG3	1.99	0.43
1:A:1038:LEU:HB2	1:A:1043:LYS:HE2	2.00	0.43
1:A:1284:LYS:HZ1	1:A:1551:ASN:HB3	1.83	0.43
1:A:4748:MET:N	1:A:4748:MET:SD	2.92	0.43
1:A:4815:PHE:CZ	1:A:4819:VAL:HG21	2.53	0.43
1:B:387:ILE:HD11	1:B:389:ARG:HH21	1.83	0.43
1:B:658:ASN:HB2	1:B:832:LEU:HD12	2.00	0.43
1:B:1084:ARG:NH1	1:B:1127:GLU:OE1	2.50	0.43
1:B:4016:PHE:HA	1:B:4019:MET:CE	2.48	0.43
1:B:4748:MET:N	1:B:4748:MET:SD	2.92	0.43
1:C:658:ASN:HB2	1:C:832:LEU:HD12	2.00	0.43
1:C:1427:TYR:CE2	1:C:1560:ILE:HG23	2.53	0.43
1:C:4052:MET:HG3	1:C:4063:THR:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:MET:HB2	1:D:321:LYS:HZ2	1.83	0.43
1:D:515:ALA:HB2	1:D:523:GLY:HA3	2.00	0.43
1:D:594:ILE:HD11	1:D:632:ILE:HG13	2.00	0.43
1:D:1038:LEU:HB2	1:D:1043:LYS:HE2	2.00	0.43
1:D:1114:ARG:HB2	1:D:1206:SER:OG	2.18	0.43
1:D:1910:LEU:HD13	1:D:2062:ILE:HG12	1.99	0.43
1:D:2074:VAL:HG23	1:D:3660:ARG:HB2	2.01	0.43
1:D:4561:LEU:HD11	1:D:4563:GLU:OE2	2.19	0.43
1:D:4815:PHE:CZ	1:D:4819:VAL:HG21	2.53	0.43
1:A:658:ASN:HB2	1:A:832:LEU:HD12	2.00	0.43
1:A:794:PHE:CG	1:A:798:ILE:HD13	2.53	0.43
1:A:875:PRO:HB2	1:A:877:HIS:CE1	2.52	0.43
1:A:1034:PRO:HD2	1:A:1037:LEU:HD12	2.00	0.43
1:A:1087:ILE:HG21	1:A:1124:PRO:HA	2.00	0.43
1:A:1749:PRO:HB2	1:A:1913:LEU:HD22	2.00	0.43
1:A:2143:ILE:HG12	1:A:2195:ASN:OD1	2.18	0.43
1:A:2758:LYS:HE3	1:A:2763:LEU:HA	2.00	0.43
2:F:35:LYS:NZ	1:B:640:ARG:O	2.51	0.43
2:G:26:HIS:CD2	2:G:105:LEU:HD11	2.53	0.43
1:B:2383:HIS:CG	1:B:2458:ALA:HB2	2.53	0.43
1:B:3642:GLU:O	1:B:3646:LYS:HG3	2.18	0.43
1:C:179:ASP:OD1	1:C:180:ASP:N	2.51	0.43
1:C:711:GLU:OE1	1:C:716:ASN:HB2	2.18	0.43
1:C:1034:PRO:HD2	1:C:1037:LEU:HD12	2.00	0.43
1:C:1947:VAL:HG11	1:C:1965:PHE:HE2	1.83	0.43
1:C:2074:VAL:HG23	1:C:3660:ARG:HB2	2.00	0.43
1:C:2321:VAL:HG11	1:C:2419:ILE:HD12	2.00	0.43
1:C:4016:PHE:HA	1:C:4019:MET:CE	2.48	0.43
1:C:4561:LEU:HD11	1:C:4563:GLU:OE2	2.19	0.43
1:D:267:VAL:HG23	1:D:272:ARG:NH1	2.33	0.43
1:D:1641:ILE:HA	1:D:1644:LEU:HD13	2.00	0.43
1:D:2886:ARG:O	1:D:2889:ALA:HB3	2.17	0.43
1:D:4047:ASP:HA	1:D:4050:LYS:HE3	2.00	0.43
1:D:4611:GLU:HA	1:D:4653:VAL:HG22	2.00	0.43
1:A:52:THR:HG22	1:A:60:PRO:HB3	2.00	0.43
1:A:267:VAL:HG23	1:A:272:ARG:NH1	2.33	0.43
1:A:902:TRP:CZ2	1:A:915:HIS:HB3	2.50	0.43
1:A:1642:LEU:HD21	1:A:1691:ASN:ND2	2.33	0.43
1:A:1795:LEU:HD23	1:A:1842:ILE:HD11	2.01	0.43
1:A:2074:VAL:HG23	1:A:3660:ARG:HB2	2.00	0.43
1:A:4070:ALA:HB1	1:A:4078:LEU:HD22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:SER:OG	1:B:317:MET:HG2	2.19	0.43
1:B:1749:PRO:HB2	1:B:1913:LEU:HD22	2.00	0.43
1:B:1795:LEU:HD23	1:B:1842:ILE:HD11	2.01	0.43
1:B:4070:ALA:HB1	1:B:4078:LEU:HD22	2.01	0.43
1:B:4094:ILE:O	1:B:4098:VAL:HG23	2.18	0.43
1:B:4903:HIS:O	1:B:4907:THR:OG1	2.27	0.43
1:C:794:PHE:CG	1:C:798:ILE:HD13	2.53	0.43
1:C:1038:LEU:HB2	1:C:1043:LYS:HE2	2.00	0.43
1:C:1795:LEU:HD23	1:C:1842:ILE:HD11	2.01	0.43
1:C:4480:PHE:N	1:C:4482:LYS:HZ3	2.17	0.43
1:D:880:ARG:NH1	1:D:1062:TYR:OH	2.52	0.43
1:D:921:PHE:HD1	1:D:929:ARG:NE	2.16	0.43
1:D:2789:ILE:HD11	1:D:2896:LEU:HD21	2.00	0.43
1:D:4020:PHE:HA	1:D:4023:LEU:HB3	2.00	0.43
1:D:4252:ILE:O	1:D:4256:MET:HG2	2.18	0.43
1:D:4294:LEU:O	1:D:4298:VAL:HG23	2.19	0.43
1:A:816:PRO:HB2	1:A:819:TYR:CD1	2.52	0.43
1:A:1100:ARG:NH2	1:A:1234:GLU:O	2.51	0.43
1:A:1427:TYR:CE2	1:A:1560:ILE:HG23	2.53	0.43
1:A:1641:ILE:HA	1:A:1644:LEU:HD13	2.00	0.43
1:A:1947:VAL:HG11	1:A:1965:PHE:HE2	1.83	0.43
1:A:2789:ILE:HD11	1:A:2896:LEU:HD21	2.00	0.43
1:A:2833:LEU:HB3	1:A:2838[B]:HIS:CE1	2.53	0.43
1:A:4247:ALA:HA	1:A:4250:TYR:CE1	2.53	0.43
1:B:179:ASP:OD1	1:B:180:ASP:N	2.51	0.43
1:B:1415:ASP:OD2	1:B:1559:ARG:NH2	2.49	0.43
1:B:3060:PHE:HE2	1:B:3108:LEU:HD13	1.84	0.43
1:B:4247:ALA:HA	1:B:4250:TYR:CE1	2.53	0.43
1:C:21:VAL:HG12	1:C:66:THR:HA	2.00	0.43
1:C:747:HIS:HD2	1:C:750:ARG:HG3	1.84	0.43
1:C:880:ARG:NH1	1:C:1062:TYR:OH	2.52	0.43
1:C:2651:ALA:O	1:C:2655:LYS:HG2	2.17	0.43
1:C:2966:VAL:O	1:C:2970:LEU:N	2.46	0.43
1:C:4294:LEU:O	1:C:4298:VAL:HG23	2.19	0.43
1:C:4748:MET:N	1:C:4748:MET:SD	2.92	0.43
1:C:4815:PHE:CZ	1:C:4819:VAL:HG21	2.53	0.43
1:D:2887:GLU:HA	1:D:2890:GLN:OE1	2.18	0.43
1:D:3050:LEU:HD12	1:D:3051:GLU:OE1	2.18	0.43
1:D:3642:GLU:O	1:D:3646:LYS:HG3	2.18	0.43
1:D:4748:MET:N	1:D:4748:MET:SD	2.92	0.43
1:A:808:HIS:HA	1:A:1610:ARG:HH21	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:921:PHE:HD1	1:A:929:ARG:NE	2.16	0.43
1:A:1910:LEU:HD13	1:A:2062:ILE:HG12	1.99	0.43
1:A:3077:GLN:HG2	1:A:3078:GLY:H	1.83	0.43
1:A:4480:PHE:N	1:A:4482:LYS:HZ3	2.17	0.43
2:H:79:PRO:O	2:H:84:GLY:HA2	2.19	0.43
1:B:877:HIS:HA	1:B:880:ARG:NE	2.34	0.43
1:B:2074:VAL:HG23	1:B:3660:ARG:HB2	2.01	0.43
1:B:2192:MET:O	1:B:2192:MET:HG2	2.17	0.43
1:B:2651:ALA:O	1:B:2655:LYS:HG2	2.17	0.43
1:C:307:SER:OG	1:C:317:MET:HG2	2.18	0.43
1:C:694:ARG:HD3	1:C:733:TRP:CD1	2.53	0.43
1:C:877:HIS:HA	1:C:880:ARG:NE	2.34	0.43
1:C:1028:ARG:HA	1:C:1028:ARG:HD2	1.83	0.43
1:C:1050:LEU:HD12	1:C:1050:LEU:HA	1.81	0.43
1:C:1489:CYS:O	1:C:1493:SER:OG	2.27	0.43
1:C:1564:MET:HE1	1:C:1578:PRO:HA	1.99	0.43
1:C:1853:GLU:OE1	1:C:1853:GLU:N	2.49	0.43
1:C:1932:PHE:CE2	1:C:1996:LEU:HD22	2.53	0.43
1:C:2917:ILE:HG12	1:C:2999:LYS:HD3	2.00	0.43
1:C:3102:LEU:HA	1:C:3105:LEU:HG	2.00	0.43
1:D:387:ILE:HD11	1:D:389:ARG:HH21	1.83	0.43
1:D:747:HIS:HD2	1:D:750:ARG:HG3	1.84	0.43
1:D:1255:LEU:HD12	1:D:1256:PRO:HD2	1.99	0.43
1:D:2096:GLY:HA2	1:D:2099:VAL:HG22	1.99	0.43
1:D:2554:ARG:HA	1:D:2554:ARG:HD2	1.85	0.43
1:D:2789:ILE:CD1	1:D:2903:VAL:HB	2.48	0.43
1:D:2877:LEU:HG	1:D:2882:LYS:HG3	2.00	0.43
1:D:2985:ALA:HB2	1:D:3001:LYS:HE2	2.00	0.43
1:D:4016:PHE:HA	1:D:4019:MET:CE	2.48	0.43
1:D:4254:THR:HA	1:D:4257:ARG:HE	1.84	0.43
1:A:318:ASP:O	1:A:322:ALA:HB2	2.17	0.43
1:A:4561:LEU:HD11	1:A:4563:GLU:OE2	2.19	0.43
1:A:4690:LYS:HD3	1:A:4692:SER:OG	2.19	0.43
2:G:35:LYS:NZ	1:C:640:ARG:O	2.51	0.43
1:B:711:GLU:OE1	1:B:716:ASN:HB2	2.18	0.43
1:B:747:HIS:HD2	1:B:750:ARG:HG3	1.84	0.43
1:B:2691:LYS:O	1:B:2695:MET:HG3	2.19	0.43
1:B:2836:ASP:OD1	1:B:2836:ASP:N	2.52	0.43
1:B:4245:LEU:HD11	1:C:4626:ILE:HG13	2.00	0.43
1:B:4815:PHE:CZ	1:B:4819:VAL:HG21	2.53	0.43
1:C:52:THR:HG22	1:C:60:PRO:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:674:TYR:HE1	1:C:756:SER:HB2	1.84	0.43
1:C:986:ILE:HD11	1:C:1055:ARG:HA	2.01	0.43
1:C:2096:GLY:HA2	1:C:2099:VAL:HG22	1.99	0.43
1:D:52:THR:HG22	1:D:60:PRO:HB3	1.99	0.43
1:D:308:LEU:HD13	1:D:393:MET:HG3	2.00	0.43
1:D:608:HIS:HB2	1:D:1656:HIS:ND1	2.34	0.43
1:D:694:ARG:HD3	1:D:733:TRP:CD1	2.53	0.43
1:D:2691:LYS:O	1:D:2695:MET:HG3	2.19	0.43
1:D:2836:ASP:OD1	1:D:2836:ASP:N	2.52	0.43
1:A:50:GLU:CD	1:A:61:ASP:H	2.21	0.43
1:A:1190:LEU:HD11	1:A:1193:LYS:HA	2.01	0.43
1:A:1255:LEU:HD12	1:A:1256:PRO:HD2	1.99	0.43
1:A:2135:GLY:H	1:A:2138:GLU:HB2	1.84	0.43
1:A:2789:ILE:CD1	1:A:2903:VAL:HB	2.48	0.43
1:A:2917:ILE:HG12	1:A:2999:LYS:HD3	2.00	0.43
1:A:3050:LEU:HD12	1:A:3051:GLU:OE1	2.18	0.43
2:F:26:HIS:CD2	2:F:105:LEU:HD11	2.53	0.43
1:B:515:ALA:HB2	1:B:523:GLY:HA3	2.00	0.43
1:B:904:TYR:HB3	1:B:972:LEU:CD1	2.48	0.43
1:B:1690:GLU:OE1	1:B:1790:LYS:NZ	2.42	0.43
1:C:120:LEU:HD11	1:C:158:CYS:HB3	2.01	0.43
1:C:1566:LEU:O	1:C:1570:LEU:HG	2.18	0.43
1:C:1726:ILE:HD11	1:C:2161:LEU:HD11	2.01	0.43
1:C:2691:LYS:O	1:C:2695:MET:HG3	2.19	0.43
1:C:2763:LEU:HD23	1:C:2767:GLU:CD	2.39	0.43
1:C:3642:GLU:O	1:C:3646:LYS:HG3	2.18	0.43
1:D:21:VAL:HG12	1:D:66:THR:HA	2.00	0.43
1:D:658:ASN:HB2	1:D:832:LEU:HD12	2.00	0.43
1:D:674:TYR:HE1	1:D:756:SER:HB2	1.84	0.43
1:D:908:ARG:NH1	1:D:928:GLU:OE2	2.35	0.43
1:D:4094:ILE:O	1:D:4098:VAL:HG23	2.18	0.43
1:A:515:ALA:HB2	1:A:523:GLY:HA3	2.00	0.43
1:A:801:ARG:HG3	1:A:1618:LEU:HD13	2.00	0.43
1:A:1605:LYS:HE2	1:A:1623:ASP:OD2	2.19	0.43
1:A:2154:VAL:HG13	1:A:2158:HIS:CD2	2.48	0.43
1:A:2836:ASP:OD1	1:A:2836:ASP:N	2.52	0.43
1:A:3906:PHE:HB3	1:A:3967:LEU:HD11	2.01	0.43
1:A:4245:LEU:HD21	1:B:4629:GLN:HB3	2.01	0.43
1:B:267:VAL:HG23	1:B:272:ARG:NH1	2.33	0.43
1:B:591:GLU:O	1:B:594:ILE:HG22	2.19	0.43
1:B:732:LEU:HD23	1:B:732:LEU:HA	1.89	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1427:TYR:CE2	1:B:1560:ILE:HG23	2.53	0.43
1:B:2415:GLU:O	1:B:2419:ILE:HG12	2.18	0.43
1:B:4654:MET:HE3	1:B:4663:ARG:HH21	1.84	0.43
1:C:439:LYS:HD3	1:C:439:LYS:HA	1.73	0.43
1:C:801:ARG:HG3	1:C:1618:LEU:HD13	2.00	0.43
1:C:2758:LYS:HE3	1:C:2763:LEU:HA	2.00	0.43
1:C:4247:ALA:HA	1:C:4250:TYR:CE1	2.53	0.43
1:D:307:SER:OG	1:D:317:MET:HG2	2.18	0.43
1:D:732:LEU:HD23	1:D:732:LEU:HA	1.89	0.43
1:D:1034:PRO:HD2	1:D:1037:LEU:HD12	2.00	0.43
1:D:1726:ILE:HD11	1:D:2161:LEU:HD11	2.01	0.43
1:D:4480:PHE:N	1:D:4482:LYS:HZ3	2.16	0.43
1:A:2887:GLU:HA	1:A:2890:GLN:OE1	2.18	0.43
1:B:156:GLU:HB2	1:B:187:SER:HB3	2.01	0.43
1:B:675:TYR:HB3	1:B:822:CYS:SG	2.59	0.43
1:B:808:HIS:HA	1:B:1610:ARG:HH21	1.84	0.43
1:B:1566:LEU:O	1:B:1570:LEU:HG	2.18	0.43
1:B:1932:PHE:CE2	1:B:1996:LEU:HD22	2.53	0.43
1:B:2135:GLY:H	1:B:2138:GLU:HB2	1.84	0.43
1:B:4690:LYS:HD3	1:B:4692:SER:OG	2.19	0.43
1:C:675:TYR:HB3	1:C:822:CYS:SG	2.59	0.43
1:C:830:GLU:OE1	1:C:830:GLU:N	2.52	0.43
1:C:1426:TYR:HA	1:C:1564:MET:O	2.19	0.43
1:C:1960:ARG:H	1:C:1960:ARG:HG3	0.96	0.43
1:C:2440:PHE:HB3	1:C:2460:PHE:CD2	2.51	0.43
1:C:2937:HIS:O	1:C:2940:ILE:HG22	2.19	0.43
1:C:4047:ASP:HA	1:C:4050:LYS:HE3	2.00	0.43
1:D:156:GLU:HB2	1:D:187:SER:HB3	2.01	0.43
1:D:935:MET:HA	1:D:938:GLU:HG3	2.00	0.43
1:D:3960:GLN:HA	1:D:4069:CYS:HA	2.00	0.43
1:A:439:LYS:HA	1:A:439:LYS:HD3	1.73	0.42
1:A:694:ARG:HD3	1:A:733:TRP:CD1	2.53	0.42
1:A:830:GLU:OE1	1:A:830:GLU:N	2.52	0.42
1:A:874:LEU:HA	1:A:875:PRO:HD3	1.82	0.42
1:A:880:ARG:NH1	1:A:1062:TYR:OH	2.52	0.42
1:A:2066:MET:CE	1:A:2084:MET:HA	2.49	0.42
1:A:2704:GLN:O	1:A:2704:GLN:HG2	2.19	0.42
1:A:3999:MET:HG3	1:A:4002:MET:HE3	2.01	0.42
1:A:4654:MET:HE3	1:A:4663:ARG:HH21	1.84	0.42
2:G:19:LYS:HB2	2:G:19:LYS:HE3	1.83	0.42
1:B:1038:LEU:HB2	1:B:1043:LYS:HE2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1051:ARG:HA	1:B:1054:VAL:HG23	2.01	0.42
1:B:1564:MET:HE1	1:B:1578:PRO:HA	2.00	0.42
1:B:1605:LYS:HE2	1:B:1623:ASP:OD2	2.19	0.42
1:B:1732:GLU:O	1:B:1736:ILE:HG12	2.19	0.42
1:B:2763:LEU:HD23	1:B:2767:GLU:CD	2.39	0.42
1:B:3102:LEU:HA	1:B:3105:LEU:HG	2.00	0.42
1:B:4561:LEU:HD11	1:B:4563:GLU:OE2	2.19	0.42
1:C:165:ALA:HB2	1:C:182:ILE:HG23	2.01	0.42
1:C:1605:LYS:HE2	1:C:1623:ASP:OD2	2.19	0.42
1:C:2143:ILE:HG12	1:C:2195:ASN:OD1	2.18	0.42
1:C:2877:LEU:HG	1:C:2882:LYS:HG3	2.00	0.42
1:C:2985:ALA:HB2	1:C:3001:LYS:HE2	2.00	0.42
1:C:3036:LEU:O	1:C:3040:LEU:HG	2.19	0.42
1:C:4094:ILE:O	1:C:4098:VAL:HG23	2.18	0.42
1:D:82:LEU:HD13	1:D:156:GLU:HG2	2.01	0.42
1:D:120:LEU:HD11	1:D:158:CYS:HB3	2.01	0.42
1:D:308:LEU:HG	1:D:309:MET:O	2.19	0.42
1:D:2195:ASN:ND2	1:D:2198:ARG:HH12	2.15	0.42
1:D:2636:GLU:HG2	1:D:2637:GLU:N	2.34	0.42
1:D:2704:GLN:O	1:D:2704:GLN:HG2	2.19	0.42
1:D:3060:PHE:HE2	1:D:3108:LEU:HD13	1.84	0.42
1:A:608:HIS:HB2	1:A:1656:HIS:ND1	2.34	0.42
1:A:872:ILE:HG13	1:A:941:LYS:HE3	2.01	0.42
1:A:877:HIS:HA	1:A:880:ARG:NE	2.34	0.42
1:A:1426:TYR:HA	1:A:1564:MET:O	2.19	0.42
1:A:4055:HIS:O	1:B:4660:PHE:HE1	2.02	0.42
2:F:79:PRO:O	2:F:84:GLY:HA2	2.19	0.42
2:G:79:PRO:O	2:G:84:GLY:HA2	2.19	0.42
1:B:165:ALA:HB2	1:B:182:ILE:HG23	2.01	0.42
1:B:996:VAL:HG11	1:B:1051:ARG:CD	2.46	0.42
1:B:1034:PRO:HD2	1:B:1037:LEU:HD12	2.00	0.42
1:B:2143:ILE:HG12	1:B:2195:ASN:OD1	2.18	0.42
1:B:2937:HIS:O	1:B:2940:ILE:HG22	2.19	0.42
1:C:606:ARG:HB2	1:C:1653:PHE:CE1	2.55	0.42
1:C:1051:ARG:HA	1:C:1054:VAL:HG23	2.01	0.42
1:C:1732:GLU:O	1:C:1736:ILE:HG12	2.19	0.42
1:C:2636:GLU:HG2	1:C:2637:GLU:N	2.34	0.42
1:C:4611:GLU:HA	1:C:4653:VAL:HG22	2.00	0.42
1:D:872:ILE:HG13	1:D:941:LYS:HE3	2.01	0.42
1:D:877:HIS:HA	1:D:880:ARG:NE	2.34	0.42
1:D:1426:TYR:HA	1:D:1564:MET:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2143:ILE:HG12	1:D:2195:ASN:OD1	2.18	0.42
1:D:3102:LEU:HA	1:D:3105:LEU:HG	2.00	0.42
1:D:3728:GLN:O	1:D:3732:HIS:ND1	2.46	0.42
1:D:4208:GLU:OE1	1:D:4208:GLU:O	2.37	0.42
1:A:329:PHE:CE1	1:A:365:HIS:HD2	2.37	0.42
1:A:675:TYR:HB3	1:A:822:CYS:SG	2.59	0.42
1:A:3036:LEU:O	1:A:3040:LEU:HG	2.19	0.42
1:A:4020:PHE:HA	1:A:4023:LEU:HB3	2.00	0.42
1:A:4030:ASP:HA	1:A:4033:LYS:HE2	2.01	0.42
1:A:4732:GLY:HA2	1:A:4735:ASN:O	2.19	0.42
1:B:50:GLU:CD	1:B:61:ASP:H	2.21	0.42
1:B:880:ARG:NH1	1:B:1062:TYR:OH	2.52	0.42
1:B:1011:ARG:HB3	1:B:1016:TRP:HB2	2.00	0.42
1:B:1652:LYS:NZ	1:B:1656:HIS:HE1	2.17	0.42
1:C:308:LEU:HG	1:C:309:MET:O	2.19	0.42
1:C:3960:GLN:HA	1:C:4069:CYS:HA	2.00	0.42
1:C:4208:GLU:OE1	1:C:4208:GLU:O	2.37	0.42
1:C:4654:MET:HE3	1:C:4663:ARG:HH21	1.84	0.42
1:C:4862:ILE:HD13	1:D:4852:PHE:CE1	2.54	0.42
1:D:165:ALA:HB2	1:D:182:ILE:HG23	2.01	0.42
1:D:830:GLU:N	1:D:830:GLU:OE1	2.52	0.42
1:D:985:PHE:CD2	1:D:985:PHE:N	2.88	0.42
1:A:594:ILE:HD11	1:A:632:ILE:HG13	2.00	0.42
1:A:747:HIS:CD2	1:A:750:ARG:HG3	2.54	0.42
1:A:747:HIS:HD2	1:A:750:ARG:HG3	1.84	0.42
1:A:986:ILE:HD11	1:A:1055:ARG:HA	2.01	0.42
1:A:1011:ARG:HB3	1:A:1016:TRP:HB2	2.00	0.42
1:A:1652:LYS:NZ	1:A:1656:HIS:HE1	2.18	0.42
1:A:2678:PRO:HA	1:A:2921:PHE:HD2	1.84	0.42
1:A:2714:PRO:O	1:A:2718:GLU:HG2	2.20	0.42
1:A:2937:HIS:O	1:A:2940:ILE:HG22	2.19	0.42
1:A:3060:PHE:HE2	1:A:3108:LEU:HD13	1.84	0.42
1:A:4254:THR:HA	1:A:4257:ARG:HE	1.84	0.42
1:B:747:HIS:CD2	1:B:750:ARG:HG3	2.54	0.42
1:B:830:GLU:N	1:B:830:GLU:OE1	2.52	0.42
1:B:872:ILE:HG13	1:B:941:LYS:HE3	2.01	0.42
1:B:889:ILE:HG12	1:B:889:ILE:H	1.75	0.42
1:B:2678:PRO:HA	1:B:2921:PHE:HD2	1.84	0.42
1:B:3637:GLU:HG2	1:B:3697:LYS:HB2	2.02	0.42
1:B:4208:GLU:OE1	1:B:4208:GLU:O	2.37	0.42
1:B:4480:PHE:N	1:B:4482:LYS:HZ3	2.17	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:ILE:HD11	1:C:389:ARG:HH21	1.83	0.42
1:C:398:HIS:HB2	1:C:401:ASP:OD1	2.19	0.42
1:C:808:HIS:HA	1:C:1610:ARG:HH21	1.84	0.42
1:C:872:ILE:HG13	1:C:941:LYS:HE3	2.01	0.42
1:C:996:VAL:HG11	1:C:1051:ARG:CD	2.46	0.42
1:C:1011:ARG:HB3	1:C:1016:TRP:HB2	2.00	0.42
1:C:1690:GLU:OE1	1:C:1790:LYS:NZ	2.42	0.42
1:C:4254:THR:HA	1:C:4257:ARG:HE	1.84	0.42
1:D:808:HIS:HA	1:D:1610:ARG:HH21	1.84	0.42
1:D:1166:VAL:HG23	1:D:1173:MET:CG	2.46	0.42
1:D:2714:PRO:O	1:D:2718:GLU:HG2	2.20	0.42
1:D:4030:ASP:HA	1:D:4033:LYS:HE2	2.02	0.42
1:D:4502:MET:HE1	1:D:4585:PHE:HD2	1.85	0.42
1:D:4732:GLY:HA2	1:D:4735:ASN:O	2.20	0.42
1:A:120:LEU:HD11	1:A:158:CYS:HB3	2.01	0.42
1:A:165:ALA:HB2	1:A:182:ILE:HG23	2.01	0.42
1:A:674:TYR:HE1	1:A:756:SER:HB2	1.84	0.42
1:A:1952:ASN:HB2	1:A:1953:MET:HE1	2.01	0.42
1:A:2691:LYS:O	1:A:2695:MET:HG3	2.19	0.42
1:A:3960:GLN:HA	1:A:4069:CYS:HA	2.00	0.42
1:A:4503:ARG:NH2	1:A:4745:ASP:OD2	2.53	0.42
2:E:79:PRO:O	2:E:84:GLY:HA2	2.19	0.42
1:B:52:THR:HG22	1:B:60:PRO:HB3	2.00	0.42
1:B:163:HIS:HB2	1:B:182:ILE:HG13	2.02	0.42
1:B:882:ARG:HH11	1:B:933:LEU:HD22	1.85	0.42
1:B:2567:ASP:O	1:B:2571:VAL:HG23	2.20	0.42
1:B:3827:GLU:O	1:B:3831:GLN:HA	2.19	0.42
1:B:4030:ASP:HA	1:B:4033:LYS:HE2	2.02	0.42
1:B:4187:GLU:OE2	1:B:4947:ARG:NH2	2.41	0.42
1:B:4503:ARG:NH2	1:B:4745:ASP:OD2	2.53	0.42
1:C:591:GLU:O	1:C:594:ILE:HG22	2.19	0.42
1:C:1652:LYS:NZ	1:C:1656:HIS:HE1	2.18	0.42
1:C:1910:LEU:HD13	1:C:2062:ILE:HG12	1.99	0.42
1:C:2195:ASN:ND2	1:C:2198:ARG:HH12	2.15	0.42
1:C:2274:LEU:HD21	1:C:2329:GLU:HB2	2.01	0.42
1:C:2898:ILE:HD12	1:D:1500:ARG:HH22	1.84	0.42
1:C:4070:ALA:HB1	1:C:4078:LEU:HD22	2.01	0.42
1:C:4690:LYS:HD3	1:C:4692:SER:OG	2.19	0.42
1:D:606:ARG:HB2	1:D:1653:PHE:CE1	2.55	0.42
1:D:1050:LEU:HD12	1:D:1050:LEU:HA	1.81	0.42
1:D:1795:LEU:HD23	1:D:1842:ILE:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2917:ILE:HG12	1:D:2999:LYS:HD3	2.00	0.42
1:D:3637:GLU:HG2	1:D:3697:LYS:HB2	2.02	0.42
1:D:4070:ALA:HB1	1:D:4078:LEU:HD22	2.01	0.42
1:D:4135:ARG:HD2	1:D:4911:GLN:HB3	2.02	0.42
1:A:986:ILE:HD12	1:A:1058:LEU:HD12	2.01	0.42
1:A:1084:ARG:NH1	1:A:1127:GLU:OE1	2.50	0.42
1:A:1595:LEU:HD23	1:A:1595:LEU:HA	1.89	0.42
1:A:1611:ILE:HD11	1:A:1618:LEU:HD23	2.02	0.42
1:A:1649:GLU:HG2	1:A:1650:LEU:N	2.35	0.42
1:B:21:VAL:HG12	1:B:66:THR:HA	2.00	0.42
1:B:1190:LEU:HD11	1:B:1193:LYS:HA	2.01	0.42
1:B:1641:ILE:HA	1:B:1644:LEU:HD13	2.00	0.42
1:B:2636:GLU:HG2	1:B:2637:GLU:N	2.34	0.42
1:B:2701:PHE:CE2	1:B:2703:PRO:HG3	2.55	0.42
1:B:3698:SER:O	1:B:3727:GLN:NE2	2.49	0.42
1:B:4294:LEU:O	1:B:4298:VAL:HG23	2.18	0.42
1:C:329:PHE:CE1	1:C:365:HIS:HD2	2.37	0.42
1:C:2066:MET:CE	1:C:2084:MET:HA	2.49	0.42
1:C:2135:GLY:H	1:C:2138:GLU:HB2	1.84	0.42
1:C:2789:ILE:CD1	1:C:2903:VAL:HB	2.48	0.42
1:C:3637:GLU:HG2	1:C:3697:LYS:HB2	2.02	0.42
1:D:877:HIS:ND1	1:D:878:LEU:HD12	2.35	0.42
1:D:902:TRP:CZ2	1:D:915:HIS:HB3	2.50	0.42
1:D:1190:LEU:HD11	1:D:1193:LYS:HA	2.01	0.42
1:D:1552:VAL:HG12	1:D:1553:PHE:HD1	1.85	0.42
1:D:1649:GLU:HG2	1:D:1650:LEU:N	2.35	0.42
1:D:2937:HIS:O	1:D:2940:ILE:HG22	2.19	0.42
1:A:2129:LEU:HB2	1:A:2142:MET:HE1	2.01	0.42
1:A:3102:LEU:HA	1:A:3105:LEU:HG	2.00	0.42
1:A:4135:ARG:HD2	1:A:4911:GLN:HB3	2.02	0.42
1:A:4208:GLU:OE1	1:A:4208:GLU:O	2.37	0.42
1:B:506:HIS:CE1	1:B:530:LEU:HD21	2.55	0.42
1:B:2066:MET:CE	1:B:2084:MET:HA	2.49	0.42
1:B:2758:LYS:HE3	1:B:2763:LEU:HA	2.00	0.42
1:B:3821:THR:HG22	1:B:3823:GLU:H	1.85	0.42
1:B:4020:PHE:HA	1:B:4023:LEU:HB3	2.00	0.42
1:B:4611:GLU:HA	1:B:4653:VAL:HG22	2.00	0.42
1:C:874:LEU:HA	1:C:875:PRO:HD3	1.82	0.42
1:C:986:ILE:HD12	1:C:1058:LEU:HD12	2.01	0.42
1:C:1944:TYR:HA	1:C:1947:VAL:HG12	2.02	0.42
1:C:2701:PHE:CE2	1:C:2703:PRO:HG3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2714:PRO:O	1:C:2718:GLU:HG2	2.20	0.42
1:C:2836:ASP:OD1	1:C:2836:ASP:N	2.52	0.42
1:C:3060:PHE:HE2	1:C:3108:LEU:HD13	1.84	0.42
1:C:3821:THR:HG22	1:C:3823:GLU:H	1.85	0.42
1:C:4634:VAL:O	1:C:4637:THR:OG1	2.26	0.42
1:C:4732:GLY:HA2	1:C:4735:ASN:O	2.20	0.42
1:D:398:HIS:HB2	1:D:401:ASP:OD1	2.19	0.42
1:D:1732:GLU:O	1:D:1736:ILE:HG12	2.19	0.42
1:D:2274:LEU:HD21	1:D:2329:GLU:HB2	2.01	0.42
1:D:2567:ASP:O	1:D:2571:VAL:HG23	2.20	0.42
1:D:2857:LYS:O	1:D:2861:GLU:OE1	2.38	0.42
1:A:591:GLU:O	1:A:594:ILE:HG22	2.19	0.42
1:A:882:ARG:HH11	1:A:933:LEU:HD22	1.85	0.42
1:A:996:VAL:HG11	1:A:1051:ARG:CD	2.46	0.42
1:A:3642:GLU:HB3	1:A:3646:LYS:NZ	2.35	0.42
1:A:3827:GLU:O	1:A:3831:GLN:HA	2.20	0.42
1:B:120:LEU:HD11	1:B:158:CYS:HB3	2.01	0.42
1:B:398:HIS:HB2	1:B:401:ASP:OD1	2.19	0.42
1:B:608:HIS:HB2	1:B:1656:HIS:ND1	2.34	0.42
1:B:674:TYR:HE1	1:B:756:SER:HB2	1.84	0.42
1:B:955:GLU:HG3	1:B:959:ASP:OD2	2.20	0.42
1:B:1081:THR:HG23	1:B:1083:GLU:H	1.85	0.42
1:B:1426:TYR:HA	1:B:1564:MET:O	2.19	0.42
1:B:1726:ILE:HD11	1:B:2161:LEU:HD11	2.01	0.42
1:B:2154:VAL:HG13	1:B:2158:HIS:CD2	2.48	0.42
1:B:2714:PRO:O	1:B:2718:GLU:HG2	2.20	0.42
1:B:2782:MET:HB2	1:B:2782:MET:HE2	2.01	0.42
1:B:2857:LYS:O	1:B:2861:GLU:OE1	2.38	0.42
1:B:3906:PHE:HB3	1:B:3967:LEU:HD11	2.01	0.42
1:B:4018:ASP:OD2	1:B:4022:LYS:NZ	2.38	0.42
1:C:747:HIS:CD2	1:C:750:ARG:HG3	2.54	0.42
1:C:1552:VAL:HG12	1:C:1553:PHE:HD1	1.85	0.42
1:C:2129:LEU:HB2	1:C:2142:MET:HE1	2.02	0.42
1:D:675:TYR:HB3	1:D:822:CYS:SG	2.59	0.42
1:D:1944:TYR:HA	1:D:1947:VAL:HG12	2.02	0.42
1:D:2163:ARG:NH1	1:D:2209:GLN:HB3	2.35	0.42
1:D:2678:PRO:HA	1:D:2921:PHE:HD2	1.84	0.42
1:D:2763:LEU:HD23	1:D:2767:GLU:CD	2.39	0.42
1:A:191:TYR:CE1	1:A:209:GLN:HG3	2.55	0.42
1:A:985:PHE:CD2	1:A:985:PHE:N	2.88	0.42
1:A:1726:ILE:HD11	1:A:2161:LEU:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1914:CYS:O	1:A:1918:VAL:HG23	2.20	0.42
1:A:1931:ASP:OD1	1:A:1932:PHE:N	2.53	0.42
1:A:2659:GLN:C	1:A:2663:LYS:HZ2	2.23	0.42
1:A:2763:LEU:HD23	1:A:2767:GLU:CD	2.39	0.42
1:B:874:LEU:HA	1:B:875:PRO:HD3	1.82	0.42
1:B:986:ILE:HD11	1:B:1055:ARG:HA	2.01	0.42
1:B:986:ILE:HD13	1:B:1055:ARG:HA	2.02	0.42
1:B:1004:HIS:HE1	1:B:1038:LEU:HD21	1.84	0.42
1:B:1931:ASP:OD1	1:B:1932:PHE:N	2.53	0.42
1:B:1944:TYR:HA	1:B:1947:VAL:HG12	2.02	0.42
1:B:2163:ARG:NH1	1:B:2209:GLN:HB3	2.35	0.42
1:B:2704:GLN:O	1:B:2704:GLN:HG2	2.19	0.42
1:B:3960:GLN:HA	1:B:4069:CYS:HA	2.00	0.42
1:B:4254:THR:HA	1:B:4257:ARG:HE	1.84	0.42
1:C:483:LYS:HB2	1:C:483:LYS:HE3	1.84	0.42
1:C:506:HIS:CE1	1:C:530:LEU:HD21	2.55	0.42
1:C:955:GLU:HG3	1:C:959:ASP:OD2	2.20	0.42
1:C:2299:LEU:HD22	1:C:2395:LEU:HA	2.01	0.42
1:C:2552:VAL:HG11	1:C:2573:LEU:HD13	2.01	0.42
1:C:2678:PRO:HA	1:C:2921:PHE:HD2	1.84	0.42
1:C:2737:LEU:HD23	1:C:2737:LEU:HA	1.93	0.42
1:C:2857:LYS:O	1:C:2861:GLU:OE1	2.38	0.42
1:C:2982:PHE:O	1:C:3001:LYS:NZ	2.44	0.42
1:C:3827:GLU:O	1:C:3831:GLN:HA	2.19	0.42
1:C:4020:PHE:HA	1:C:4023:LEU:HB3	2.01	0.42
1:D:747:HIS:CD2	1:D:750:ARG:HG3	2.54	0.42
1:D:1475:LYS:HE3	1:D:1475:LYS:HB3	1.90	0.42
1:D:1605:LYS:HE2	1:D:1623:ASP:OD2	2.19	0.42
1:D:2066:MET:CE	1:D:2084:MET:HA	2.49	0.42
1:D:2765:GLU:HA	1:D:2768:LYS:HZ1	1.84	0.42
1:D:2777:GLU:O	1:D:2781:THR:OG1	2.19	0.42
1:D:3827:GLU:O	1:D:3831:GLN:HA	2.19	0.42
1:D:4654:MET:HE3	1:D:4663:ARG:HH21	1.84	0.42
1:A:606:ARG:HB2	1:A:1653:PHE:CE1	2.55	0.42
1:A:644:LEU:HD22	1:A:1630:LEU:HD21	2.02	0.42
1:A:1028:ARG:HA	1:A:1028:ARG:HD2	1.83	0.42
1:A:1502:ASN:O	1:D:2824:ARG:NH2	2.53	0.42
1:A:1944:TYR:HA	1:A:1947:VAL:HG12	2.02	0.42
1:B:82:LEU:HD13	1:B:156:GLU:HG2	2.01	0.42
1:B:1174:MET:HG3	1:B:1190:LEU:HA	2.02	0.42
1:B:1611:ILE:HD11	1:B:1618:LEU:HD23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1952:ASN:HB2	1:B:1953:MET:HE1	2.01	0.42
1:B:3036:LEU:O	1:B:3040:LEU:HG	2.19	0.42
1:B:4135:ARG:HD2	1:B:4911:GLN:HB3	2.02	0.42
1:C:163:HIS:HB2	1:C:182:ILE:HG13	2.02	0.42
1:C:608:HIS:HB2	1:C:1656:HIS:ND1	2.34	0.42
1:C:985:PHE:CD2	1:C:985:PHE:N	2.88	0.42
1:C:986:ILE:HD13	1:C:1055:ARG:HA	2.02	0.42
1:C:1190:LEU:HD11	1:C:1193:LYS:HA	2.01	0.42
1:C:1641:ILE:HA	1:C:1644:LEU:HD13	2.00	0.42
1:C:1649:GLU:HG2	1:C:1650:LEU:N	2.35	0.42
1:C:1952:ASN:HB2	1:C:1953:MET:HE1	2.01	0.42
1:C:2353:ILE:O	1:C:2360:ASP:HB2	2.20	0.42
1:C:2567:ASP:O	1:C:2571:VAL:HG23	2.20	0.42
1:C:4030:ASP:HA	1:C:4033:LYS:HE2	2.02	0.42
1:C:4814:MET:HE2	1:D:4844:ILE:HG21	2.02	0.42
1:D:191:TYR:CE1	1:D:209:GLN:HG3	2.55	0.42
1:D:591:GLU:O	1:D:594:ILE:HG22	2.19	0.42
1:D:644:LEU:HD22	1:D:1630:LEU:HD21	2.02	0.42
1:D:986:ILE:HD11	1:D:1055:ARG:HA	2.01	0.42
1:D:2353:ILE:O	1:D:2360:ASP:HB2	2.20	0.42
1:D:2552:VAL:HG11	1:D:2573:LEU:HD13	2.01	0.42
1:D:2659:GLN:C	1:D:2663:LYS:HZ2	2.23	0.42
1:D:2702:ASN:HA	1:D:2703:PRO:HD3	1.84	0.42
1:D:2841:ALA:HA	1:D:2844:MET:HG3	2.02	0.42
1:D:4690:LYS:HD3	1:D:4692:SER:OG	2.19	0.42
1:A:398:HIS:HB2	1:A:401:ASP:OD1	2.19	0.41
1:A:2636:GLU:HG2	1:A:2637:GLU:N	2.34	0.41
1:A:3948:LEU:HG	1:A:3978:MET:HE1	2.03	0.41
1:B:308:LEU:HG	1:B:309:MET:O	2.19	0.41
1:B:606:ARG:HB2	1:B:1653:PHE:CE1	2.55	0.41
1:B:2623:LEU:HB3	1:B:2626:GLY:HA2	2.02	0.41
1:B:4947:ARG:HA	1:B:4947:ARG:HD2	1.92	0.41
1:C:156:GLU:HB2	1:C:187:SER:HB3	2.01	0.41
1:C:2175:MET:HA	1:C:2178:VAL:HG12	2.02	0.41
1:C:2704:GLN:HG2	1:C:2704:GLN:O	2.19	0.41
1:C:3018:ARG:HG3	1:C:3021:LEU:HD22	2.02	0.41
1:C:3723:LYS:NZ	1:C:3727:GLN:OE1	2.52	0.41
1:C:4135:ARG:HD2	1:C:4911:GLN:HB3	2.02	0.41
1:D:50:GLU:CD	1:D:61:ASP:H	2.21	0.41
1:D:1483:SER:HB3	1:D:1486:TYR:CE1	2.55	0.41
1:D:2134:MET:HE3	1:D:2139:GLU:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2262:LEU:O	1:D:2266:VAL:HG23	2.20	0.41
1:D:3018:ARG:HG3	1:D:3021:LEU:HD22	2.02	0.41
1:D:3723:LYS:NZ	1:D:3727:GLN:OE1	2.52	0.41
1:A:506:HIS:CE1	1:A:530:LEU:HD21	2.55	0.41
1:A:586:LEU:HD22	1:A:620:CYS:HB2	2.02	0.41
1:A:921:PHE:HD1	1:A:929:ARG:CZ	2.34	0.41
1:A:1732:GLU:O	1:A:1736:ILE:HG12	2.19	0.41
1:A:2274:LEU:HD21	1:A:2329:GLU:HB2	2.01	0.41
1:A:2857:LYS:O	1:A:2861:GLU:OE1	2.38	0.41
1:A:3637:GLU:HG2	1:A:3697:LYS:HB2	2.02	0.41
1:A:4294:LEU:O	1:A:4298:VAL:HG23	2.18	0.41
1:B:165:ALA:HB1	1:B:211:LEU:HD22	2.03	0.41
1:B:329:PHE:CE1	1:B:365:HIS:HD2	2.37	0.41
1:B:1564:MET:HE3	1:B:1565:PRO:HD2	2.01	0.41
1:B:2175:MET:HA	1:B:2178:VAL:HG12	2.02	0.41
1:B:2353:ILE:O	1:B:2360:ASP:HB2	2.20	0.41
1:B:3065:ALA:O	1:B:3069:GLU:HG2	2.20	0.41
1:B:3677:THR:HB	1:B:3679:LYS:NZ	2.35	0.41
1:B:4038:ASP:OD2	1:B:4040:LYS:NZ	2.36	0.41
1:C:50:GLU:CD	1:C:61:ASP:H	2.21	0.41
1:C:1081:THR:HG23	1:C:1083:GLU:H	1.85	0.41
1:C:2163:ARG:NH1	1:C:2209:GLN:HB3	2.35	0.41
1:C:2623:LEU:HB3	1:C:2626:GLY:HA2	2.02	0.41
1:C:4710:LEU:HD23	1:C:4710:LEU:HA	1.86	0.41
1:D:1914:CYS:O	1:D:1918:VAL:HG23	2.20	0.41
1:D:1947:VAL:HG11	1:D:1965:PHE:HE2	1.83	0.41
1:D:2833:LEU:HB3	1:D:2838[B]:HIS:NE2	2.35	0.41
1:D:3036:LEU:O	1:D:3040:LEU:HG	2.19	0.41
1:D:3906:PHE:HB3	1:D:3967:LEU:HD11	2.01	0.41
1:D:4306:PHE:HA	1:D:4309:ILE:HG12	2.01	0.41
1:A:308:LEU:HG	1:A:309:MET:O	2.19	0.41
1:A:955:GLU:HG3	1:A:959:ASP:OD2	2.19	0.41
1:A:1161:VAL:HB	1:A:1226:TYR:HE2	1.85	0.41
1:A:1552:VAL:HG12	1:A:1553:PHE:HD1	1.85	0.41
1:A:2175:MET:HA	1:A:2178:VAL:HG12	2.02	0.41
1:A:2737:LEU:HD23	1:A:2737:LEU:HA	1.93	0.41
1:B:2552:VAL:HG11	1:B:2573:LEU:HD13	2.01	0.41
1:B:4818:TYR:HD1	1:C:4848:ILE:HD11	1.85	0.41
1:C:260:VAL:O	1:C:390:LYS:NZ	2.37	0.41
1:C:1931:ASP:OD1	1:C:1932:PHE:N	2.53	0.41
1:C:2837:LEU:HA	1:C:2840:MET:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2943:PHE:CE1	1:C:2952:GLU:HG2	2.55	0.41
1:C:2953:HIS:O	1:C:2953:HIS:CG	2.73	0.41
1:C:4568:MET:HA	1:C:4571:THR:HB	2.02	0.41
1:D:996:VAL:HG11	1:D:1051:ARG:CD	2.46	0.41
1:D:1011:ARG:HB3	1:D:1016:TRP:HB2	2.00	0.41
1:D:2135:GLY:H	1:D:2138:GLU:HB2	1.84	0.41
1:D:2943:PHE:CE2	1:D:3021:LEU:HD23	2.55	0.41
1:D:3642:GLU:HB3	1:D:3646:LYS:NZ	2.35	0.41
1:D:4107:GLU:OE1	1:D:4149:TYR:OH	2.22	0.41
1:D:4503:ARG:NH2	1:D:4745:ASP:OD2	2.53	0.41
1:A:82:LEU:HD13	1:A:156:GLU:HG2	2.01	0.41
1:A:163:HIS:HB2	1:A:182:ILE:HG13	2.02	0.41
1:A:1051:ARG:HA	1:A:1054:VAL:HG23	2.02	0.41
1:A:1312:GLU:OE1	2:E:32:GLN:HG2	2.20	0.41
1:A:2567:ASP:O	1:A:2571:VAL:HG23	2.20	0.41
1:A:2841:ALA:HA	1:A:2844:MET:HG3	2.02	0.41
1:A:4793:TYR:HH	1:A:4816:HIS:CE1	2.32	0.41
2:E:19:LYS:HE3	2:E:19:LYS:HB2	1.83	0.41
1:B:483:LYS:HB2	1:B:483:LYS:HE3	1.84	0.41
1:B:877:HIS:ND1	1:B:878:LEU:HD12	2.35	0.41
1:B:924:LEU:HD12	1:B:925:PRO:O	2.21	0.41
1:B:1190:LEU:HD11	1:B:1193:LYS:HD3	2.03	0.41
1:B:1234:GLU:H	1:B:1234:GLU:CD	2.23	0.41
1:B:1483:SER:HB3	1:B:1486:TYR:CE1	2.55	0.41
1:B:2943:PHE:CE2	1:B:3021:LEU:HD23	2.55	0.41
1:C:1084:ARG:NH1	1:C:1127:GLU:OE1	2.50	0.41
1:C:2238:THR:OG1	1:C:2241:ASP:OD2	2.24	0.41
1:C:3728:GLN:O	1:C:3732:HIS:ND1	2.46	0.41
1:D:955:GLU:HG3	1:D:959:ASP:OD2	2.20	0.41
1:D:2701:PHE:CE2	1:D:2703:PRO:HG3	2.55	0.41
1:D:2953:HIS:CG	1:D:2953:HIS:O	2.73	0.41
1:D:3821:THR:HG22	1:D:3823:GLU:H	1.85	0.41
1:A:156:GLU:HB2	1:A:187:SER:HB3	2.01	0.41
1:A:877:HIS:ND1	1:A:878:LEU:HD12	2.35	0.41
1:A:1004:HIS:HE1	1:A:1038:LEU:HD21	1.84	0.41
1:A:2195:ASN:ND2	1:A:2198:ARG:HH12	2.15	0.41
1:A:2460:PHE:CE2	1:A:2465:LYS:HD2	2.56	0.41
1:A:2701:PHE:CE2	1:A:2703:PRO:HG3	2.55	0.41
1:A:2857:LYS:HE3	1:A:2871:LEU:CD2	2.37	0.41
1:A:4306:PHE:HA	1:A:4309:ILE:HG12	2.02	0.41
1:A:4502:MET:HE1	1:A:4585:PHE:HD2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4858:LEU:HD23	1:A:4861:ILE:HD12	2.03	0.41
1:B:62:LEU:HD11	1:B:282:VAL:HG13	2.03	0.41
1:B:921:PHE:HD1	1:B:929:ARG:CZ	2.33	0.41
1:B:985:PHE:N	1:B:985:PHE:CD2	2.88	0.41
1:B:986:ILE:HD12	1:B:1058:LEU:HD12	2.01	0.41
1:B:1028:ARG:HA	1:B:1028:ARG:HD2	1.83	0.41
1:B:1304:LEU:HD23	1:B:1304:LEU:HA	1.95	0.41
1:B:1489:CYS:O	1:B:1493:SER:OG	2.27	0.41
1:B:2274:LEU:HD21	1:B:2329:GLU:HB2	2.01	0.41
1:B:2841:ALA:HA	1:B:2844:MET:HG3	2.02	0.41
1:B:2943:PHE:CE1	1:B:2952:GLU:HG2	2.56	0.41
1:B:4045:LYS:HE3	1:B:4067:LEU:HD22	2.03	0.41
1:B:4805:LYS:HA	1:B:4805:LYS:HD2	1.82	0.41
1:C:62:LEU:HD11	1:C:282:VAL:HG13	2.03	0.41
1:C:165:ALA:HB1	1:C:211:LEU:HD22	2.03	0.41
1:C:586:LEU:HD22	1:C:620:CYS:HB2	2.02	0.41
1:C:1074:ARG:NH1	1:C:1076:GLU:HA	2.36	0.41
1:C:1475:LYS:HE3	1:C:1475:LYS:HB3	1.90	0.41
1:C:2943:PHE:CE2	1:C:3021:LEU:HD23	2.56	0.41
1:C:3891:TYR:HA	1:D:76:ARG:NH2	2.36	0.41
1:D:329:PHE:CE1	1:D:365:HIS:HD2	2.37	0.41
1:D:506:HIS:CE1	1:D:530:LEU:HD21	2.55	0.41
1:D:1051:ARG:HA	1:D:1054:VAL:HG23	2.01	0.41
1:D:1174:MET:HG3	1:D:1190:LEU:HA	2.02	0.41
1:D:2966:VAL:O	1:D:2970:LEU:N	2.46	0.41
1:D:4045:LYS:HE3	1:D:4067:LEU:HD22	2.03	0.41
1:D:4908:HIS:CE1	1:D:4913:HIS:ND1	2.89	0.41
1:A:2192:MET:O	1:A:2192:MET:HG2	2.16	0.41
1:A:2262:LEU:O	1:A:2266:VAL:HG23	2.20	0.41
1:A:2552:VAL:HG11	1:A:2573:LEU:HD13	2.01	0.41
1:A:3065:ALA:O	1:A:3069:GLU:HG2	2.20	0.41
1:B:201:LEU:H	1:B:201:LEU:HD12	1.85	0.41
1:B:1074:ARG:NH1	1:B:1076:GLU:HA	2.36	0.41
1:B:1468:THR:HG22	1:B:1479:SER:CB	2.51	0.41
1:B:1950:ALA:HB1	1:B:1961:LYS:HZ3	1.85	0.41
1:B:2262:LEU:O	1:B:2266:VAL:HG23	2.20	0.41
1:B:2299:LEU:HD22	1:B:2395:LEU:HA	2.01	0.41
1:B:2460:PHE:CE2	1:B:2465:LYS:HD2	2.56	0.41
1:B:4306:PHE:HA	1:B:4309:ILE:HG12	2.01	0.41
1:B:4908:HIS:CE1	1:B:4913:HIS:ND1	2.89	0.41
1:C:39:ALA:O	1:C:64:ILE:HB	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:LEU:HD13	1:C:156:GLU:HG2	2.02	0.41
1:C:201:LEU:H	1:C:201:LEU:HD12	1.85	0.41
1:C:857:LEU:HD12	1:C:859:GLN:NE2	2.36	0.41
1:C:876:PRO:HA	1:C:879:GLU:OE1	2.21	0.41
1:C:1004:HIS:HE1	1:C:1038:LEU:HD21	1.84	0.41
1:C:1161:VAL:HB	1:C:1226:TYR:HE2	1.85	0.41
1:C:1174:MET:HG3	1:C:1190:LEU:HA	2.02	0.41
1:C:1483:SER:HB3	1:C:1486:TYR:CE1	2.55	0.41
1:C:1681:ASP:HB3	1:C:1683:PRO:HD2	2.03	0.41
1:C:2460:PHE:CE2	1:C:2465:LYS:HD2	2.56	0.41
1:C:2841:ALA:HA	1:C:2844:MET:HG3	2.02	0.41
1:C:3642:GLU:HB3	1:C:3646:LYS:NZ	2.35	0.41
1:C:3833:ASP:OD2	1:C:3908:LYS:HD2	2.21	0.41
1:D:439:LYS:HA	1:D:439:LYS:HD3	1.73	0.41
1:D:857:LEU:HD12	1:D:859:GLN:NE2	2.36	0.41
1:D:924:LEU:HD12	1:D:925:PRO:O	2.21	0.41
1:D:1004:HIS:HE1	1:D:1038:LEU:HD21	1.85	0.41
1:D:1652:LYS:NZ	1:D:1656:HIS:HE1	2.18	0.41
1:D:1948:MET:HA	1:D:1948:MET:CE	2.51	0.41
1:D:1979:PHE:CD1	1:D:1993:ARG:HG2	2.56	0.41
1:D:2299:LEU:HD22	1:D:2395:LEU:HA	2.01	0.41
1:D:2837:LEU:HA	1:D:2840:MET:HB2	2.02	0.41
1:D:4503:ARG:HD2	1:D:4503:ARG:HA	1.93	0.41
1:A:1564:MET:HE3	1:A:1565:PRO:HD2	2.03	0.41
1:A:1640:ASP:OD2	1:A:1641:ILE:N	2.54	0.41
1:A:1853:GLU:OE1	1:A:1853:GLU:N	2.49	0.41
1:A:1979:PHE:CD1	1:A:1993:ARG:HG2	2.56	0.41
1:A:2554:ARG:HH11	1:A:2557:LYS:HB2	1.86	0.41
1:A:2837:LEU:HA	1:A:2840:MET:HB2	2.02	0.41
1:A:2943:PHE:CE1	1:A:2952:GLU:HG2	2.56	0.41
1:A:2953:HIS:O	1:A:2953:HIS:CG	2.73	0.41
1:B:191:TYR:CE1	1:B:209:GLN:HG3	2.55	0.41
1:B:876:PRO:HA	1:B:879:GLU:OE1	2.21	0.41
1:B:1649:GLU:HG2	1:B:1650:LEU:N	2.35	0.41
1:B:1948:MET:CE	1:B:1948:MET:HA	2.51	0.41
1:B:2502:LEU:HD13	1:B:2513:ALA:HB1	2.03	0.41
1:B:2953:HIS:CG	1:B:2953:HIS:O	2.73	0.41
1:B:4061:SER:O	1:B:4064:GLU:HG3	2.21	0.41
1:B:4732:GLY:HA2	1:B:4735:ASN:O	2.20	0.41
1:B:4858:LEU:HD23	1:B:4861:ILE:HD12	2.03	0.41
1:C:709:GLY:HA3	1:C:723:PHE:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1152:TYR:CD1	1:C:1184:ASP:HB3	2.56	0.41
1:C:1234:GLU:H	1:C:1234:GLU:CD	2.23	0.41
1:C:4908:HIS:CE1	1:C:4913:HIS:ND1	2.89	0.41
1:D:3861:GLN:H	1:D:3867:THR:HG23	1.86	0.41
1:A:876:PRO:HA	1:A:879:GLU:OE1	2.21	0.41
1:A:986:ILE:HD13	1:A:1055:ARG:HA	2.02	0.41
1:A:1081:THR:HG23	1:A:1083:GLU:H	1.85	0.41
1:A:2782:MET:HB2	1:A:2782:MET:HE2	2.01	0.41
1:A:2943:PHE:CE2	1:A:3021:LEU:HD23	2.55	0.41
1:A:3833:ASP:OD2	1:A:3908:LYS:HD2	2.21	0.41
1:A:4177:VAL:HG11	1:A:4880:VAL:HA	2.03	0.41
1:B:585:ALA:O	1:B:588:ILE:HG22	2.21	0.41
1:B:603:LYS:HE3	1:B:603:LYS:HB3	1.94	0.41
1:C:62:LEU:O	1:C:66:THR:HG23	2.21	0.41
1:C:520:ARG:O	1:C:524:GLU:HG2	2.21	0.41
1:C:3065:ALA:O	1:C:3069:GLU:HG2	2.20	0.41
1:C:3861:GLN:H	1:C:3867:THR:HG23	1.86	0.41
1:D:1124:PRO:HD2	1:D:1594:VAL:HG23	2.03	0.41
1:D:1611:ILE:HD11	1:D:1618:LEU:HD23	2.02	0.41
1:D:1952:ASN:HB2	1:D:1953:MET:HE1	2.02	0.41
1:D:4480:PHE:N	1:D:4483:LYS:HZ3	2.18	0.41
1:A:165:ALA:HB1	1:A:211:LEU:HD22	2.02	0.41
1:A:201:LEU:HD12	1:A:201:LEU:H	1.85	0.41
1:A:1043:LYS:HA	1:A:1046:ASN:ND2	2.35	0.41
1:A:1050:LEU:HD12	1:A:1050:LEU:HA	1.81	0.41
1:A:1489:CYS:O	1:A:1493:SER:OG	2.27	0.41
1:A:1793:GLN:NE2	1:A:1797:GLU:OE2	2.54	0.41
1:A:2353:ILE:O	1:A:2360:ASP:HB2	2.20	0.41
1:A:2502:LEU:HD13	1:A:2513:ALA:HB1	2.03	0.41
1:A:2678:PRO:HB2	1:A:2981:TYR:CE1	2.56	0.41
1:A:2733:SER:HB3	1:A:2821:TYR:CZ	2.56	0.41
1:A:3107:SER:O	1:A:3110:GLU:HG3	2.21	0.41
1:A:3821:THR:HG22	1:A:3823:GLU:H	1.85	0.41
1:A:3861:GLN:H	1:A:3867:THR:HG23	1.86	0.41
1:A:4568:MET:HA	1:A:4571:THR:HB	2.02	0.41
1:A:4908:HIS:CE1	1:A:4913:HIS:ND1	2.89	0.41
1:B:513:HIS:O	1:B:517:VAL:HG23	2.21	0.41
1:B:680:ASP:N	1:B:799:LYS:O	2.54	0.41
1:B:1552:VAL:HG12	1:B:1553:PHE:HD1	1.85	0.41
1:B:1914:CYS:O	1:B:1918:VAL:HG23	2.20	0.41
1:B:1978:ASN:HB3	1:B:1983:LYS:HE2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1979:PHE:CD1	1:B:1993:ARG:HG2	2.56	0.41
1:B:2554:ARG:HH11	1:B:2557:LYS:HB2	1.86	0.41
1:B:2801:TYR:CE2	1:C:1496:PRO:O	2.74	0.41
1:B:3833:ASP:OD2	1:B:3908:LYS:HD2	2.21	0.41
1:B:4177:VAL:HG11	1:B:4880:VAL:HA	2.03	0.41
1:C:191:TYR:CE1	1:C:209:GLN:HG3	2.55	0.41
1:C:298:ARG:NH1	1:C:417:ARG:HH12	2.15	0.41
1:C:877:HIS:ND1	1:C:878:LEU:HD12	2.35	0.41
1:C:1166:VAL:HG23	1:C:1173:MET:CG	2.46	0.41
1:C:1630:LEU:HD13	1:C:1644:LEU:HD21	2.03	0.41
1:C:1793:GLN:NE2	1:C:1797:GLU:OE2	2.54	0.41
1:C:1914:CYS:O	1:C:1918:VAL:HG23	2.20	0.41
1:C:1979:PHE:CD1	1:C:1993:ARG:HG2	2.55	0.41
1:C:2087:LEU:O	1:C:2091:GLN:HG2	2.21	0.41
1:C:2555:LEU:HD12	1:C:2555:LEU:HA	1.97	0.41
1:C:2678:PRO:HB2	1:C:2981:TYR:CE1	2.56	0.41
1:C:3906:PHE:HB3	1:C:3967:LEU:HD11	2.01	0.41
1:C:4503:ARG:HD2	1:C:4503:ARG:HA	1.93	0.41
1:C:4503:ARG:NH2	1:C:4745:ASP:OD2	2.53	0.41
1:D:39:ALA:O	1:D:64:ILE:HB	2.21	0.41
1:D:163:HIS:HB2	1:D:182:ILE:HG13	2.02	0.41
1:D:513:HIS:O	1:D:517:VAL:HG23	2.21	0.41
1:D:709:GLY:HA3	1:D:723:PHE:CD2	2.55	0.41
1:D:986:ILE:HD12	1:D:1058:LEU:HD12	2.01	0.41
1:D:1102:TYR:CE1	1:D:1104:GLU:HG3	2.56	0.41
1:D:1161:VAL:HB	1:D:1226:TYR:HE2	1.85	0.41
1:D:1468:THR:HG22	1:D:1479:SER:CB	2.51	0.41
1:D:1681:ASP:HB3	1:D:1683:PRO:HD2	2.03	0.41
1:D:1793:GLN:NE2	1:D:1797:GLU:OE2	2.54	0.41
1:D:1931:ASP:OD1	1:D:1932:PHE:N	2.53	0.41
1:D:2175:MET:HA	1:D:2178:VAL:HG12	2.02	0.41
1:D:2678:PRO:HB2	1:D:2981:TYR:CE1	2.56	0.41
1:D:2721:ILE:HG21	1:D:2772:ARG:HG3	2.03	0.41
1:D:3065:ALA:O	1:D:3069:GLU:HG2	2.20	0.41
1:D:3698:SER:O	1:D:3727:GLN:NE2	2.50	0.41
1:D:3833:ASP:OD2	1:D:3908:LYS:HD2	2.21	0.41
1:D:4750:PHE:HD2	1:D:4753:LEU:HD12	1.86	0.41
1:A:924:LEU:HD12	1:A:925:PRO:O	2.21	0.41
1:A:1190:LEU:HD11	1:A:1193:LYS:HD3	2.03	0.41
1:A:1494:MET:HE3	1:A:1505:LEU:HD22	2.03	0.41
1:A:2163:ARG:NH1	1:A:2209:GLN:HB3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3018:ARG:HG3	1:A:3021:LEU:HD22	2.02	0.41
1:A:3639:LYS:NZ	1:A:3643:ASP:OD2	2.54	0.41
1:A:3677:THR:HB	1:A:3679:LYS:NZ	2.36	0.41
2:F:50:ARG:N	2:F:55:GLU:OE2	2.37	0.41
2:H:50:ARG:N	2:H:55:GLU:OE2	2.37	0.41
1:B:39:ALA:O	1:B:64:ILE:HB	2.21	0.41
1:B:709:GLY:HA3	1:B:723:PHE:CD2	2.56	0.41
1:B:1475:LYS:HB3	1:B:1475:LYS:HE3	1.90	0.41
1:B:2253:LEU:HD23	1:B:2253:LEU:HA	1.93	0.41
1:B:2344:LEU:HD22	1:B:2434:GLY:HA3	2.03	0.41
1:B:2733:SER:HB3	1:B:2821:TYR:CZ	2.56	0.41
1:B:3642:GLU:HB3	1:B:3646:LYS:NZ	2.35	0.41
1:B:3687:LEU:HD12	1:B:3687:LEU:HA	1.94	0.41
1:C:680:ASP:N	1:C:799:LYS:O	2.54	0.41
1:C:1640:ASP:OD2	1:C:1641:ILE:N	2.54	0.41
1:C:2262:LEU:O	1:C:2266:VAL:HG23	2.20	0.41
1:C:2765:GLU:HG2	1:C:2768:LYS:HZ2	1.86	0.41
1:C:4045:LYS:HE3	1:C:4067:LEU:HD22	2.03	0.41
1:C:4061:SER:O	1:C:4064:GLU:HG3	2.21	0.41
1:C:4306:PHE:HA	1:C:4309:ILE:HG12	2.02	0.41
1:D:876:PRO:HA	1:D:879:GLU:OE1	2.21	0.41
1:D:921:PHE:HD1	1:D:929:ARG:CZ	2.34	0.41
1:D:929:ARG:NH2	1:D:933:LEU:HD21	2.36	0.41
1:D:1152:TYR:CD1	1:D:1184:ASP:HB3	2.56	0.41
1:D:2943:PHE:CE1	1:D:2952:GLU:HG2	2.56	0.41
1:A:62:LEU:O	1:A:66:THR:HG23	2.21	0.40
1:A:520:ARG:O	1:A:524:GLU:HG2	2.21	0.40
1:A:585:ALA:O	1:A:588:ILE:HG22	2.21	0.40
1:A:709:GLY:HA3	1:A:723:PHE:CD2	2.55	0.40
1:A:1174:MET:HG3	1:A:1190:LEU:HA	2.02	0.40
1:A:1234:GLU:H	1:A:1234:GLU:CD	2.23	0.40
1:A:1483:SER:HB3	1:A:1486:TYR:CE1	2.55	0.40
1:A:2134:MET:HE3	1:A:2139:GLU:HB2	2.02	0.40
1:A:2299:LEU:HD22	1:A:2395:LEU:HA	2.01	0.40
1:A:2966:VAL:O	1:A:2970:LEU:N	2.46	0.40
1:A:4609:LYS:HD3	1:A:4615:LEU:HD13	2.03	0.40
1:B:644:LEU:HD22	1:B:1630:LEU:HD21	2.02	0.40
1:B:1161:VAL:HB	1:B:1226:TYR:HE2	1.85	0.40
1:B:1630:LEU:HD13	1:B:1644:LEU:HD21	2.03	0.40
1:B:1977:LEU:HD23	1:B:1977:LEU:HA	1.88	0.40
1:B:2087:LEU:O	1:B:2091:GLN:HG2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2837:LEU:HA	1:B:2840:MET:HB2	2.02	0.40
1:B:3882:GLN:HB3	1:B:3947:PHE:CE2	2.56	0.40
1:B:4609:LYS:HD3	1:B:4615:LEU:HD13	2.03	0.40
1:C:731:HIS:CE1	1:C:740:THR:HG22	2.57	0.40
1:C:892:LEU:HD13	1:C:1052:GLU:OE1	2.21	0.40
1:C:1102:TYR:CE1	1:C:1104:GLU:HG3	2.56	0.40
1:C:1611:ILE:HD11	1:C:1618:LEU:HD23	2.02	0.40
1:C:1948:MET:HA	1:C:1948:MET:CE	2.51	0.40
1:C:2502:LEU:HD13	1:C:2513:ALA:HB1	2.03	0.40
1:C:2721:ILE:HG21	1:C:2772:ARG:HG3	2.03	0.40
1:C:2733:SER:HB3	1:C:2821:TYR:CZ	2.56	0.40
1:C:3948:LEU:HG	1:C:3978:MET:HE1	2.03	0.40
1:C:4750:PHE:HD2	1:C:4753:LEU:HD12	1.86	0.40
1:D:165:ALA:HB1	1:D:211:LEU:HD22	2.02	0.40
1:D:586:LEU:HD22	1:D:620:CYS:HB2	2.02	0.40
1:D:674:TYR:CE1	1:D:756:SER:HB2	2.56	0.40
1:D:2146:LEU:HD23	1:D:2146:LEU:HA	1.94	0.40
1:D:2554:ARG:HH11	1:D:2557:LYS:HB2	1.86	0.40
1:D:2635:GLU:HG2	1:D:2680:TYR:CE1	2.55	0.40
1:D:3948:LEU:HG	1:D:3978:MET:HE1	2.03	0.40
1:D:4609:LYS:HD3	1:D:4615:LEU:HD13	2.03	0.40
1:A:2721:ILE:HG21	1:A:2772:ARG:HG3	2.03	0.40
1:A:2782:MET:HE1	1:A:2789:ILE:HB	2.02	0.40
1:A:3651:PRO:HB2	1:A:3652:PRO:HD3	2.04	0.40
1:A:4018:ASP:OD2	1:A:4022:LYS:NZ	2.38	0.40
1:A:4061:SER:O	1:A:4064:GLU:HG3	2.21	0.40
1:A:4172:PHE:CZ	1:A:4189:PHE:HA	2.57	0.40
1:A:4808:ASP:OD2	1:A:4810:LEU:HB3	2.22	0.40
1:B:731:HIS:CE1	1:B:740:THR:HG22	2.56	0.40
1:B:912:LYS:NZ	1:B:914:GLN:HG3	2.37	0.40
1:B:1640:ASP:OD2	1:B:1641:ILE:N	2.54	0.40
1:B:1681:ASP:HB3	1:B:1683:PRO:HD2	2.03	0.40
1:B:1793:GLN:NE2	1:B:1797:GLU:OE2	2.54	0.40
1:B:2659:GLN:C	1:B:2663:LYS:HZ2	2.23	0.40
1:B:4113:THR:O	1:B:4117:THR:HG23	2.21	0.40
1:C:824:GLU:OE2	1:C:1020:ILE:N	2.55	0.40
1:C:972:LEU:HG	1:C:973:THR:H	1.86	0.40
1:C:3651:PRO:HB2	1:C:3652:PRO:HD3	2.03	0.40
1:C:3872:ILE:O	1:C:3875:VAL:HG12	2.22	0.40
1:D:246:THR:HG21	1:D:267:VAL:HG21	2.03	0.40
1:D:288:HIS:CE1	1:D:352:SER:HB3	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ARG:NH1	1:D:417:ARG:HH12	2.15	0.40
1:D:1084:ARG:NH1	1:D:1127:GLU:OE1	2.50	0.40
1:D:1978:ASN:HB3	1:D:1983:LYS:HE2	2.03	0.40
1:D:2129:LEU:HB2	1:D:2142:MET:HE1	2.04	0.40
1:D:2502:LEU:HD13	1:D:2513:ALA:HB1	2.03	0.40
1:D:2733:SER:HB3	1:D:2821:TYR:CZ	2.56	0.40
1:D:2793:ARG:HH11	1:D:2793:ARG:CG	2.31	0.40
1:D:3107:SER:O	1:D:3110:GLU:HG3	2.21	0.40
1:D:3639:LYS:NZ	1:D:3643:ASP:OD2	2.54	0.40
1:D:4858:LEU:HD23	1:D:4861:ILE:HD12	2.03	0.40
1:A:163:HIS:HA	1:A:164:PRO:HD3	1.95	0.40
1:A:929:ARG:NH2	1:A:933:LEU:HD21	2.36	0.40
1:A:1166:VAL:HG23	1:A:1173:MET:CG	2.46	0.40
1:A:1948:MET:HA	1:A:1948:MET:CE	2.51	0.40
1:A:2623:LEU:HB3	1:A:2626:GLY:HA2	2.02	0.40
1:A:3882:GLN:HB3	1:A:3947:PHE:CE2	2.57	0.40
1:A:4045:LYS:HE3	1:A:4067:LEU:HD22	2.03	0.40
1:B:62:LEU:O	1:B:66:THR:HG23	2.21	0.40
1:B:857:LEU:HD12	1:B:859:GLN:NE2	2.36	0.40
1:B:880:ARG:NH1	1:B:881:ILE:HB	2.37	0.40
1:B:929:ARG:NH2	1:B:933:LEU:HD21	2.36	0.40
1:B:1786:ILE:O	1:B:1790:LYS:HG2	2.22	0.40
1:B:2678:PRO:HB2	1:B:2981:TYR:CE1	2.56	0.40
1:B:2966:VAL:O	1:B:2970:LEU:N	2.46	0.40
1:B:3018:ARG:HG3	1:B:3021:LEU:HD22	2.02	0.40
1:B:4568:MET:HA	1:B:4571:THR:HB	2.02	0.40
1:C:514:PHE:CD2	1:C:526:TRP:HB2	2.56	0.40
1:C:902:TRP:CZ2	1:C:915:HIS:HB3	2.50	0.40
1:C:921:PHE:HD1	1:C:929:ARG:CZ	2.34	0.40
1:C:1978:ASN:HB3	1:C:1983:LYS:HE2	2.03	0.40
1:C:2508:SER:HB3	1:C:2560:SER:OG	2.22	0.40
1:C:2659:GLN:C	1:C:2663:LYS:HZ2	2.24	0.40
1:C:3107:SER:O	1:C:3110:GLU:HG3	2.21	0.40
1:C:3677:THR:HB	1:C:3679:LYS:NZ	2.35	0.40
1:C:3882:GLN:HB3	1:C:3947:PHE:CE2	2.57	0.40
1:C:4858:LEU:HD23	1:C:4861:ILE:HD12	2.03	0.40
1:D:731:HIS:CE1	1:D:740:THR:HG22	2.56	0.40
1:D:1190:LEU:HD11	1:D:1193:LYS:HD3	2.03	0.40
1:D:1304:LEU:HD23	1:D:1304:LEU:HA	1.95	0.40
1:D:3651:PRO:HB2	1:D:3652:PRO:HD3	2.04	0.40
1:D:4042:VAL:HG12	1:D:4077:THR:HB	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4808:ASP:OD2	1:D:4810:LEU:HB3	2.21	0.40
1:A:880:ARG:NH1	1:A:881:ILE:HB	2.37	0.40
1:A:1468:THR:HG22	1:A:1479:SER:CB	2.51	0.40
1:A:1757:LEU:HD23	1:A:1757:LEU:HA	1.87	0.40
1:A:3043:ARG:HB3	1:A:3047:LYS:HZ1	1.86	0.40
1:A:3073:GLU:O	1:A:3077:GLN:OE1	2.40	0.40
1:A:4585:PHE:HA	1:A:4588:ILE:HD12	2.04	0.40
1:B:520:ARG:O	1:B:524:GLU:HG2	2.21	0.40
1:B:1102:TYR:CE1	1:B:1104:GLU:HG3	2.56	0.40
1:B:2086:VAL:HG22	1:B:3687:LEU:HD13	2.04	0.40
1:B:2721:ILE:HG21	1:B:2772:ARG:HG3	2.03	0.40
1:B:3639:LYS:NZ	1:B:3643:ASP:OD2	2.54	0.40
1:C:644:LEU:HD22	1:C:1630:LEU:HD21	2.02	0.40
1:C:924:LEU:HD12	1:C:925:PRO:O	2.21	0.40
1:C:2554:ARG:HH11	1:C:2557:LYS:HB2	1.86	0.40
1:C:2843:MET:O	1:C:2846:GLU:HG2	2.22	0.40
1:C:2844:MET:CE	1:C:2848:TYR:HE2	2.35	0.40
1:C:4177:VAL:HG11	1:C:4880:VAL:HA	2.03	0.40
1:C:4609:LYS:HD3	1:C:4615:LEU:HD13	2.03	0.40
1:D:587:ASN:OD1	1:D:2133:ARG:NH1	2.53	0.40
1:D:986:ILE:HD13	1:D:1055:ARG:HA	2.02	0.40
1:D:1234:GLU:H	1:D:1234:GLU:CD	2.23	0.40
1:D:1494:MET:HE3	1:D:1505:LEU:HD22	2.04	0.40
1:D:1640:ASP:OD2	1:D:1641:ILE:N	2.54	0.40
1:D:1960:ARG:H	1:D:1960:ARG:HG3	0.96	0.40
1:D:2460:PHE:CE2	1:D:2465:LYS:HD2	2.56	0.40
1:D:2844:MET:CE	1:D:2848:TYR:HE2	2.35	0.40
1:A:62:LEU:HD11	1:A:282:VAL:HG13	2.03	0.40
1:A:857:LEU:HD12	1:A:859:GLN:NE2	2.36	0.40
1:A:1786:ILE:O	1:A:1790:LYS:HG2	2.22	0.40
1:A:1977:LEU:HD23	1:A:1977:LEU:HA	1.88	0.40
1:A:2721:ILE:HG12	1:A:2775:ILE:CG2	2.52	0.40
1:A:3043:ARG:O	1:A:3047:LYS:HE2	2.22	0.40
1:A:3642:GLU:OE2	1:A:3730:ARG:NH1	2.55	0.40
1:B:586:LEU:HD22	1:B:620:CYS:HB2	2.02	0.40
1:B:1283:LEU:HD11	1:B:1582:CYS:SG	2.62	0.40
1:B:1850:VAL:HA	1:B:2054:LYS:HE3	2.03	0.40
1:B:2126:ILE:HA	1:B:2142:MET:HE1	2.04	0.40
1:B:2134:MET:HE3	1:B:2139:GLU:HB2	2.03	0.40
1:B:2721:ILE:HG12	1:B:2775:ILE:CG2	2.52	0.40
1:B:3642:GLU:OE2	1:B:3730:ARG:NH1	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4808:ASP:OD2	1:B:4810:LEU:HB3	2.21	0.40
1:C:513:HIS:O	1:C:517:VAL:HG23	2.21	0.40
1:C:929:ARG:NH2	1:C:933:LEU:HD21	2.36	0.40
1:C:1433:PHE:HE1	1:C:1554:GLN:HB2	1.87	0.40
1:C:1642:LEU:HD21	1:C:1691:ASN:HD21	1.87	0.40
1:C:1786:ILE:O	1:C:1790:LYS:HG2	2.22	0.40
1:C:2554:ARG:HA	1:C:2554:ARG:HD2	1.85	0.40
1:D:62:LEU:O	1:D:66:THR:HG23	2.21	0.40
1:D:201:LEU:HD12	1:D:201:LEU:H	1.85	0.40
1:D:1081:THR:HG23	1:D:1083:GLU:H	1.85	0.40
1:D:2623:LEU:HB3	1:D:2626:GLY:HA2	2.02	0.40
1:D:2635:GLU:HA	1:D:2638:LEU:HD12	2.03	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	3978/4967 (80%)	3861 (97%)	113 (3%)	4 (0%)	51 84
1	B	3978/4967 (80%)	3862 (97%)	112 (3%)	4 (0%)	51 84
1	C	3978/4967 (80%)	3861 (97%)	113 (3%)	4 (0%)	51 84
1	D	3978/4967 (80%)	3862 (97%)	112 (3%)	4 (0%)	51 84
2	E	105/108 (97%)	101 (96%)	4 (4%)	0	100 100
2	F	105/108 (97%)	101 (96%)	4 (4%)	0	100 100
2	G	105/108 (97%)	101 (96%)	4 (4%)	0	100 100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100 100
All	All	16332/20300 (80%)	15850 (97%)	466 (3%)	16 (0%)	54 84

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2988	ARG
1	A	3927	PRO
1	A	4641	PRO
1	B	2988	ARG
1	B	3927	PRO
1	B	4641	PRO
1	C	2988	ARG
1	C	3927	PRO
1	C	4641	PRO
1	D	2988	ARG
1	D	3927	PRO
1	D	4641	PRO
1	A	1081	THR
1	B	1081	THR
1	C	1081	THR
1	D	1081	THR

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	3513/4358 (81%)	3447 (98%)	66 (2%)	57	80
1	B	3513/4358 (81%)	3447 (98%)	66 (2%)	57	80
1	C	3513/4358 (81%)	3447 (98%)	66 (2%)	57	80
1	D	3513/4358 (81%)	3447 (98%)	66 (2%)	57	80
2	E	88/89 (99%)	85 (97%)	3 (3%)	37	68
2	F	88/89 (99%)	85 (97%)	3 (3%)	37	68
2	G	88/89 (99%)	85 (97%)	3 (3%)	37	68
2	H	88/89 (99%)	85 (97%)	3 (3%)	37	68
All	All	14404/17788 (81%)	14128 (98%)	276 (2%)	59	80

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	MET
1	A	317	MET
1	A	349	MET
1	A	398	HIS
1	A	778	MET
1	A	880	ARG
1	A	889	ILE
1	A	960	LYS
1	A	962	LYS
1	A	985	PHE
1	A	1025	LYS
1	A	1181	ILE
1	A	1249	MET
1	A	1293	GLN
1	A	1300	MET
1	A	1748	LEU
1	A	1939	ASN
1	A	1948	MET
1	A	1953	MET
1	A	1957	LEU
1	A	1960	ARG
1	A	2192	MET
1	A	2279	MET
1	A	2303	ARG
1	A	2347	MET
1	A	2384	MET
1	A	2482	ASP
1	A	2493	LEU
1	A	2530	ARG
1	A	2580	LEU
1	A	2689	MET
1	A	2695	MET
1	A	2730	ASP
1	A	2734	MET
1	A	2788	ARG
1	A	2793	ARG
1	A	2798	MET
1	A	2824	ARG
1	A	2828	MET
1	A	2843	MET
1	A	2855	LYS
1	A	2870	LEU
1	A	2880	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2884	LYS
1	A	2888	LYS
1	A	2897	GLN
1	A	2953	HIS
1	A	2963	PHE
1	A	2968	LEU
1	A	2976	LYS
1	A	3051	GLU
1	A	3105	LEU
1	A	3611	LEU
1	A	3739	MET
1	A	3999	MET
1	A	4046	ARG
1	A	4109	MET
1	A	4208	GLU
1	A	4292	MET
1	A	4306	PHE
1	A	4504	MET
1	A	4555	ILE
1	A	4648	PHE
1	A	4718	SER
1	A	4791	LYS
1	A	4817	MET
2	E	14	ARG
2	E	53	LYS
2	E	86	THR
2	F	14	ARG
2	F	53	LYS
2	F	86	THR
2	G	14	ARG
2	G	53	LYS
2	G	86	THR
2	H	14	ARG
2	H	53	LYS
2	H	86	THR
1	B	81	MET
1	B	317	MET
1	B	349	MET
1	B	398	HIS
1	B	778	MET
1	B	880	ARG
1	B	889	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	960	LYS
1	B	962	LYS
1	B	985	PHE
1	B	1025	LYS
1	B	1181	ILE
1	B	1249	MET
1	B	1293	GLN
1	B	1300	MET
1	B	1748	LEU
1	B	1939	ASN
1	B	1948	MET
1	B	1953	MET
1	B	1957	LEU
1	B	1960	ARG
1	B	2192	MET
1	B	2279	MET
1	B	2303	ARG
1	B	2347	MET
1	B	2384	MET
1	B	2482	ASP
1	B	2493	LEU
1	B	2530	ARG
1	B	2580	LEU
1	B	2689	MET
1	B	2695	MET
1	B	2730	ASP
1	B	2734	MET
1	B	2788	ARG
1	B	2793	ARG
1	B	2798	MET
1	B	2824	ARG
1	B	2828	MET
1	B	2843	MET
1	B	2855	LYS
1	B	2870	LEU
1	B	2880	LYS
1	B	2884	LYS
1	B	2888	LYS
1	B	2897	GLN
1	B	2953	HIS
1	B	2963	PHE
1	B	2968	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2976	LYS
1	B	3051	GLU
1	B	3105	LEU
1	B	3611	LEU
1	B	3739	MET
1	B	3999	MET
1	B	4046	ARG
1	B	4109	MET
1	B	4208	GLU
1	B	4292	MET
1	B	4306	PHE
1	B	4504	MET
1	B	4555	ILE
1	B	4648	PHE
1	B	4718	SER
1	B	4791	LYS
1	B	4817	MET
1	C	81	MET
1	C	317	MET
1	C	349	MET
1	C	398	HIS
1	C	778	MET
1	C	880	ARG
1	C	889	ILE
1	C	960	LYS
1	C	962	LYS
1	C	985	PHE
1	C	1025	LYS
1	C	1181	ILE
1	C	1249	MET
1	C	1293	GLN
1	C	1300	MET
1	C	1748	LEU
1	C	1939	ASN
1	C	1948	MET
1	C	1953	MET
1	C	1957	LEU
1	C	1960	ARG
1	C	2192	MET
1	C	2279	MET
1	C	2303	ARG
1	C	2347	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2384	MET
1	C	2482	ASP
1	C	2493	LEU
1	C	2530	ARG
1	C	2580	LEU
1	C	2689	MET
1	C	2695	MET
1	C	2730	ASP
1	C	2734	MET
1	C	2788	ARG
1	C	2793	ARG
1	C	2798	MET
1	C	2824	ARG
1	C	2828	MET
1	C	2843	MET
1	C	2855	LYS
1	C	2870	LEU
1	C	2880	LYS
1	C	2884	LYS
1	C	2888	LYS
1	C	2897	GLN
1	C	2953	HIS
1	C	2963	PHE
1	C	2968	LEU
1	C	2976	LYS
1	C	3051	GLU
1	C	3105	LEU
1	C	3611	LEU
1	C	3739	MET
1	C	3999	MET
1	C	4046	ARG
1	C	4109	MET
1	C	4208	GLU
1	C	4292	MET
1	C	4306	PHE
1	C	4504	MET
1	C	4555	ILE
1	C	4648	PHE
1	C	4718	SER
1	C	4791	LYS
1	C	4817	MET
1	D	81	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	317	MET
1	D	349	MET
1	D	398	HIS
1	D	778	MET
1	D	880	ARG
1	D	889	ILE
1	D	960	LYS
1	D	962	LYS
1	D	985	PHE
1	D	1025	LYS
1	D	1181	ILE
1	D	1249	MET
1	D	1293	GLN
1	D	1300	MET
1	D	1748	LEU
1	D	1939	ASN
1	D	1948	MET
1	D	1953	MET
1	D	1957	LEU
1	D	1960	ARG
1	D	2192	MET
1	D	2279	MET
1	D	2303	ARG
1	D	2347	MET
1	D	2384	MET
1	D	2482	ASP
1	D	2493	LEU
1	D	2530	ARG
1	D	2580	LEU
1	D	2689	MET
1	D	2695	MET
1	D	2730	ASP
1	D	2734	MET
1	D	2788	ARG
1	D	2793	ARG
1	D	2798	MET
1	D	2824	ARG
1	D	2828	MET
1	D	2843	MET
1	D	2855	LYS
1	D	2870	LEU
1	D	2880	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	2884	LYS
1	D	2888	LYS
1	D	2897	GLN
1	D	2953	HIS
1	D	2963	PHE
1	D	2968	LEU
1	D	2976	LYS
1	D	3051	GLU
1	D	3105	LEU
1	D	3611	LEU
1	D	3739	MET
1	D	3999	MET
1	D	4046	ARG
1	D	4109	MET
1	D	4208	GLU
1	D	4292	MET
1	D	4306	PHE
1	D	4504	MET
1	D	4555	ILE
1	D	4648	PHE
1	D	4718	SER
1	D	4791	LYS
1	D	4817	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	270	HIS
1	A	288	HIS
1	A	476	GLN
1	A	1004	HIS
1	A	1046	ASN
1	A	1656	HIS
1	A	2158	HIS
1	A	2702	ASN
1	A	2704	GLN
1	A	2868	HIS
1	A	2927	GLN
1	A	3038	GLN
1	A	3975	GLN
1	A	4049	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	23	GLN
1	B	270	HIS
1	B	288	HIS
1	B	476	GLN
1	B	1004	HIS
1	B	1046	ASN
1	B	1656	HIS
1	B	2158	HIS
1	B	2702	ASN
1	B	2704	GLN
1	B	2868	HIS
1	B	2927	GLN
1	B	3038	GLN
1	B	3975	GLN
1	B	4049	HIS
1	C	23	GLN
1	C	270	HIS
1	C	288	HIS
1	C	476	GLN
1	C	1004	HIS
1	C	1046	ASN
1	C	1656	HIS
1	C	2158	HIS
1	C	2702	ASN
1	C	2704	GLN
1	C	2868	HIS
1	C	2927	GLN
1	C	3038	GLN
1	C	3975	GLN
1	C	4049	HIS
1	D	23	GLN
1	D	270	HIS
1	D	288	HIS
1	D	476	GLN
1	D	1004	HIS
1	D	1046	ASN
1	D	1656	HIS
1	D	2158	HIS
1	D	2702	ASN
1	D	2704	GLN
1	D	2868	HIS
1	D	2927	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	3038	GLN
1	D	3975	GLN
1	D	4049	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	B	5004	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
4	ATP	A	5004	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
4	ATP	B	5002	-	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	0.74	2 (6%)
4	ATP	D	5004	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
4	ATP	A	5002	-	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
4	ATP	C	5002	-	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
4	ATP	C	5004	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	5004	-	-	8/18/38/38	0/3/3/3
4	ATP	A	5004	-	-	8/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	9/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	9/18/38/38	0/3/3/3
4	ATP	D	5004	-	-	8/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	9/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	9/18/38/38	0/3/3/3
4	ATP	C	5004	-	-	8/18/38/38	0/3/3/3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	5002	ATP	C5-C6-N6	2.31	123.86	120.35
4	A	5004	ATP	C5-C6-N6	2.30	123.85	120.35
4	B	5004	ATP	C5-C6-N6	2.30	123.85	120.35
4	A	5002	ATP	C5-C6-N6	2.30	123.85	120.35
4	C	5004	ATP	C5-C6-N6	2.30	123.85	120.35
4	D	5002	ATP	C5-C6-N6	2.30	123.85	120.35
4	D	5004	ATP	C5-C6-N6	2.28	123.82	120.35
4	B	5002	ATP	C5-C6-N6	2.26	123.79	120.35
4	D	5002	ATP	PB-O3B-PG	2.08	139.96	132.83
4	C	5002	ATP	PB-O3B-PG	2.07	139.93	132.83
4	A	5002	ATP	PB-O3B-PG	2.07	139.92	132.83
4	A	5004	ATP	PB-O3B-PG	2.06	139.91	132.83
4	B	5002	ATP	PB-O3B-PG	2.06	139.90	132.83
4	D	5004	ATP	PB-O3B-PG	2.05	139.87	132.83
4	C	5004	ATP	PB-O3B-PG	2.04	139.84	132.83
4	B	5004	ATP	PB-O3B-PG	2.04	139.84	132.83

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3B-PG-O3G
4	A	5002	ATP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O2A
4	A	5004	ATP	C5'-O5'-PA-O2A
4	B	5002	ATP	PB-O3B-PG-O3G
4	B	5002	ATP	C5'-O5'-PA-O1A
4	B	5002	ATP	C5'-O5'-PA-O2A
4	B	5002	ATP	C4'-C5'-O5'-PA
4	B	5004	ATP	C5'-O5'-PA-O2A
4	C	5002	ATP	PB-O3B-PG-O3G
4	C	5002	ATP	C5'-O5'-PA-O1A
4	C	5002	ATP	C5'-O5'-PA-O2A
4	C	5002	ATP	C4'-C5'-O5'-PA
4	C	5004	ATP	C5'-O5'-PA-O2A
4	D	5002	ATP	PB-O3B-PG-O3G
4	D	5002	ATP	C5'-O5'-PA-O1A
4	D	5002	ATP	C5'-O5'-PA-O2A
4	D	5004	ATP	C5'-O5'-PA-O2A
4	A	5004	ATP	O4'-C4'-C5'-O5'
4	B	5004	ATP	O4'-C4'-C5'-O5'
4	C	5004	ATP	O4'-C4'-C5'-O5'
4	D	5004	ATP	O4'-C4'-C5'-O5'
4	A	5002	ATP	C4'-C5'-O5'-PA
4	D	5002	ATP	C4'-C5'-O5'-PA
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
4	A	5004	ATP	PB-O3A-PA-O5'
4	B	5004	ATP	PB-O3A-PA-O5'
4	C	5004	ATP	PB-O3A-PA-O5'
4	D	5004	ATP	PB-O3A-PA-O5'
4	A	5004	ATP	C5'-O5'-PA-O3A
4	B	5004	ATP	C5'-O5'-PA-O3A
4	C	5004	ATP	C5'-O5'-PA-O3A
4	D	5004	ATP	C5'-O5'-PA-O3A
4	A	5004	ATP	PG-O3B-PB-O2B
4	B	5004	ATP	PG-O3B-PB-O2B
4	C	5004	ATP	PG-O3B-PB-O2B
4	D	5004	ATP	PG-O3B-PB-O2B
4	A	5004	ATP	C5'-O5'-PA-O1A
4	B	5004	ATP	C5'-O5'-PA-O1A
4	C	5004	ATP	C5'-O5'-PA-O1A
4	D	5004	ATP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

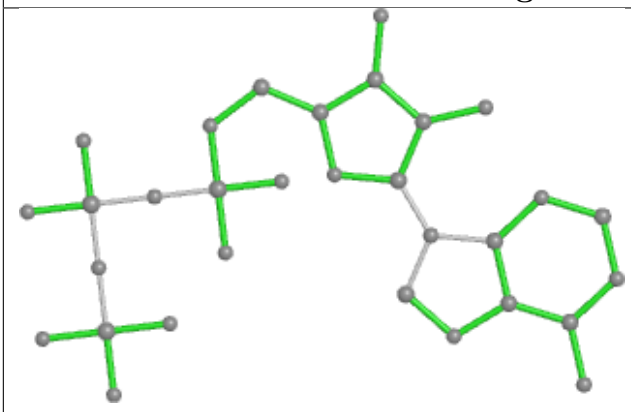
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	O4'-C4'-C5'-O5'
4	B	5002	ATP	O4'-C4'-C5'-O5'
4	C	5002	ATP	O4'-C4'-C5'-O5'
4	D	5002	ATP	O4'-C4'-C5'-O5'
4	A	5002	ATP	PB-O3B-PG-O1G
4	B	5002	ATP	PB-O3B-PG-O1G
4	C	5002	ATP	PB-O3B-PG-O1G
4	D	5002	ATP	PB-O3B-PG-O1G
4	A	5002	ATP	C5'-O5'-PA-O3A
4	B	5002	ATP	C5'-O5'-PA-O3A
4	C	5002	ATP	C5'-O5'-PA-O3A
4	D	5002	ATP	C5'-O5'-PA-O3A
4	A	5002	ATP	PA-O3A-PB-O1B
4	A	5004	ATP	PG-O3B-PB-O1B
4	A	5004	ATP	PB-O3A-PA-O1A
4	B	5002	ATP	PA-O3A-PB-O1B
4	B	5004	ATP	PG-O3B-PB-O1B
4	B	5004	ATP	PB-O3A-PA-O1A
4	C	5002	ATP	PA-O3A-PB-O1B
4	C	5004	ATP	PG-O3B-PB-O1B
4	C	5004	ATP	PB-O3A-PA-O1A
4	D	5002	ATP	PA-O3A-PB-O1B
4	D	5004	ATP	PG-O3B-PB-O1B
4	D	5004	ATP	PB-O3A-PA-O1A

There are no ring outliers.

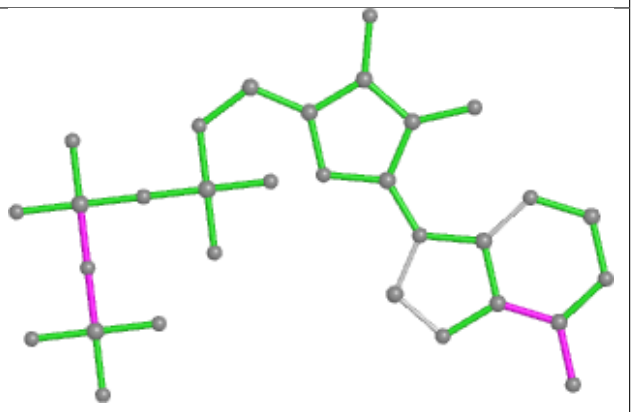
No monomer is involved in short contacts.

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

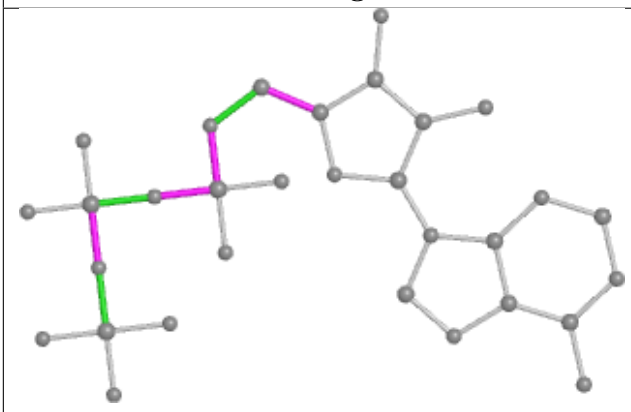
Ligand ATP B 5004



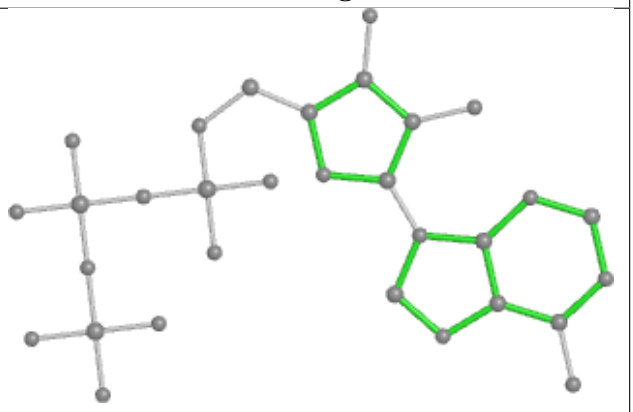
Bond lengths



Bond angles

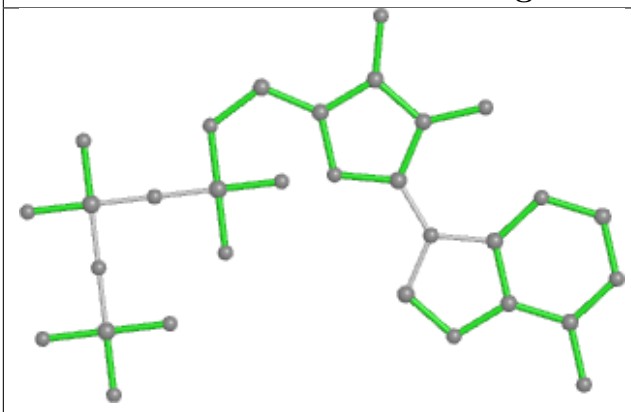


Torsions

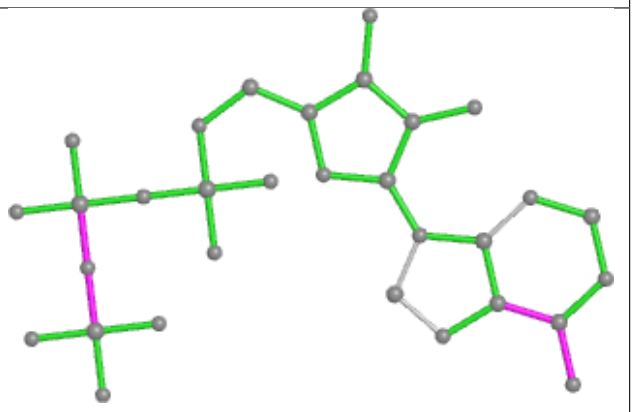


Rings

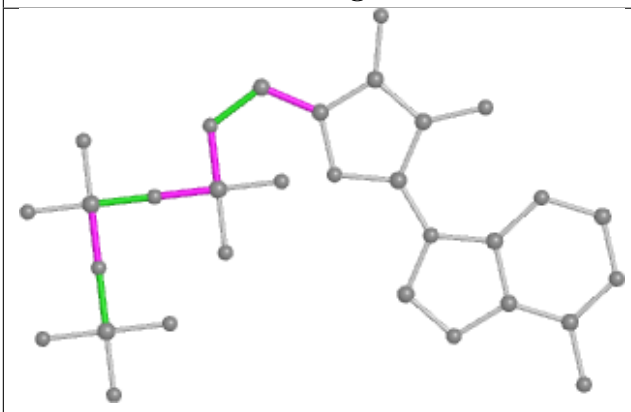
Ligand ATP A 5004



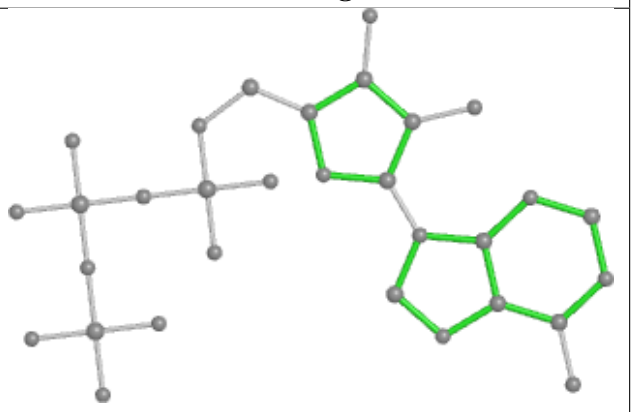
Bond lengths



Bond angles

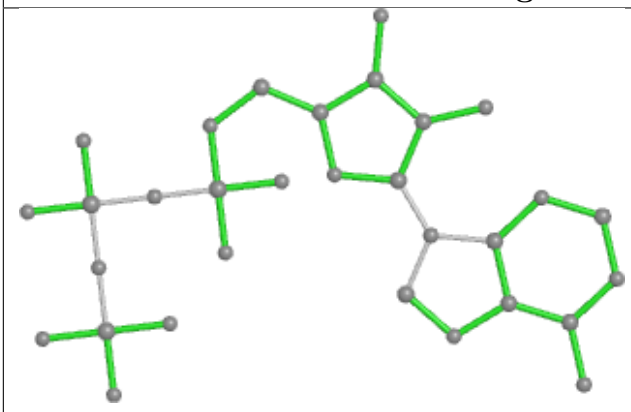


Torsions

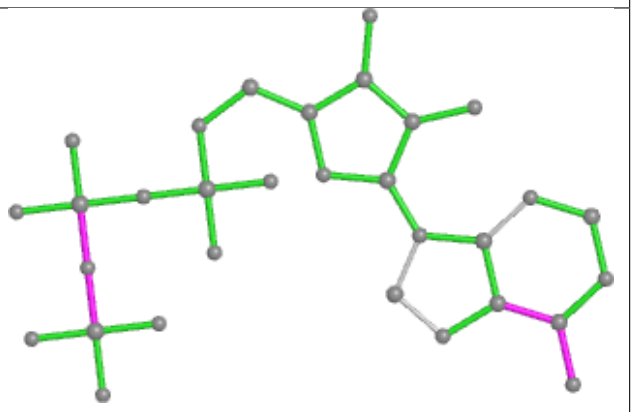


Rings

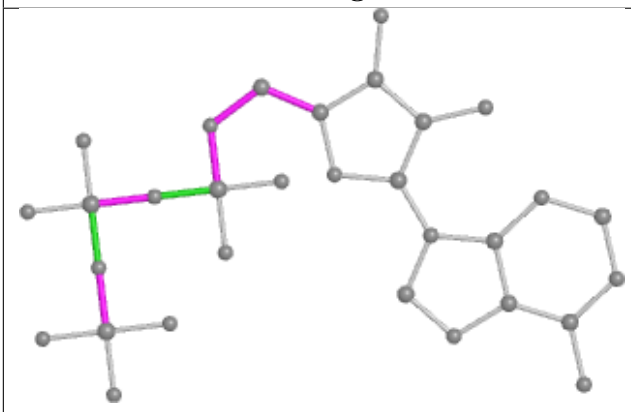
Ligand ATP B 5002



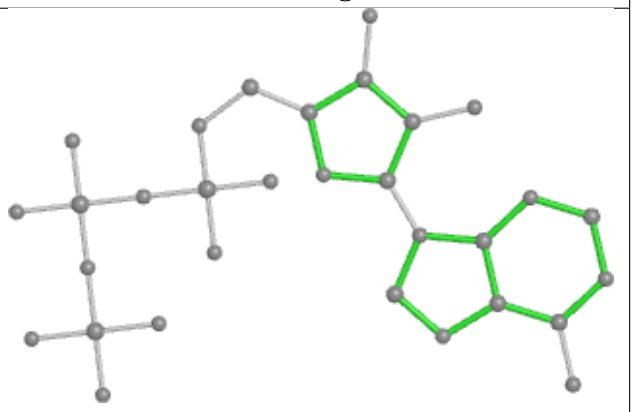
Bond lengths



Bond angles

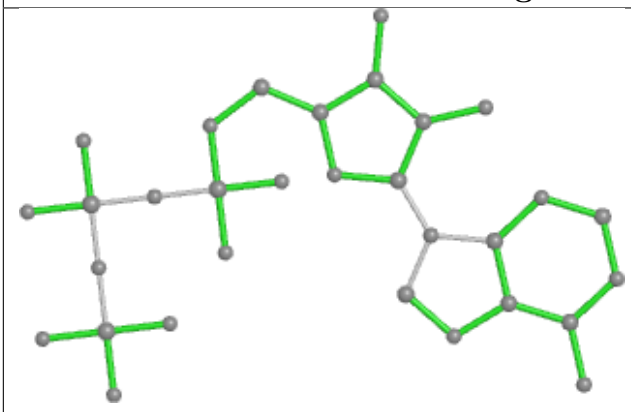


Torsions

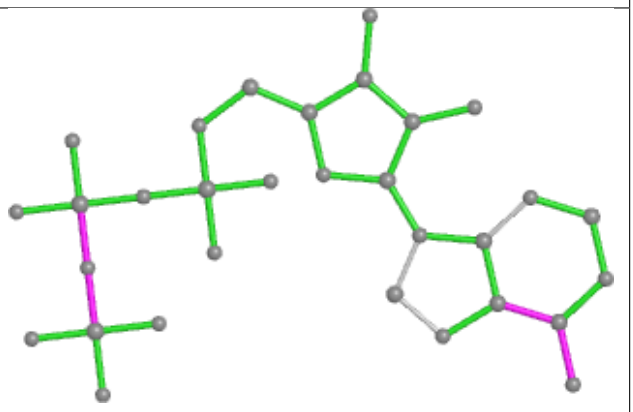


Rings

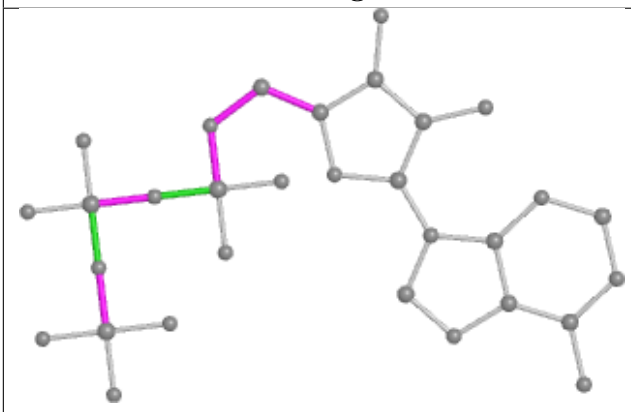
Ligand ATP D 5002



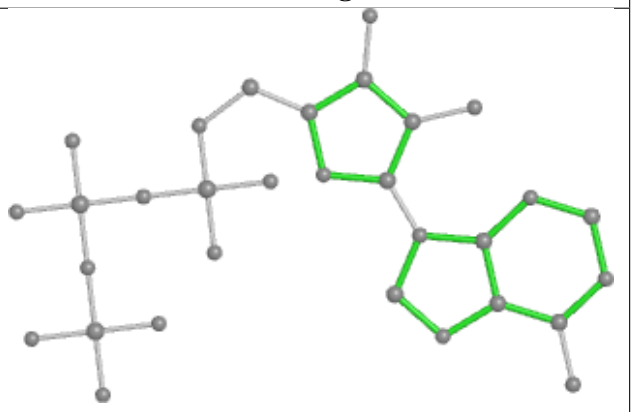
Bond lengths



Bond angles

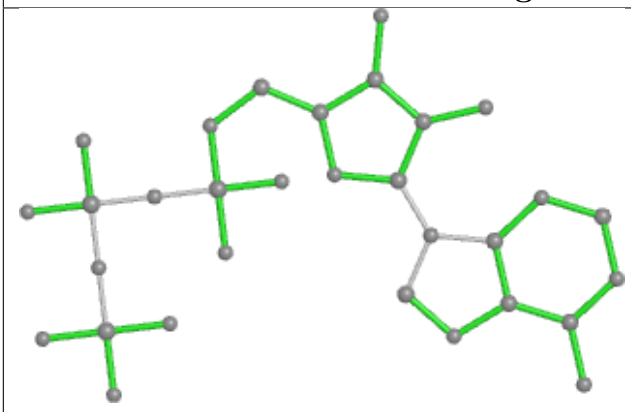


Torsions

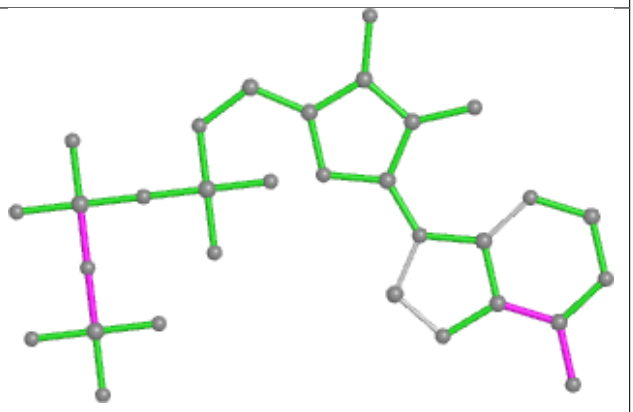


Rings

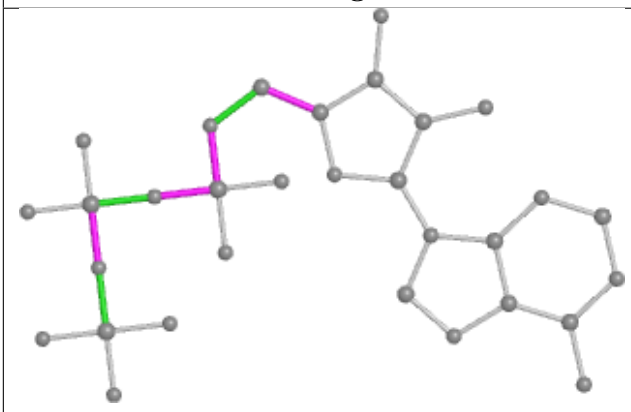
Ligand ATP D 5004



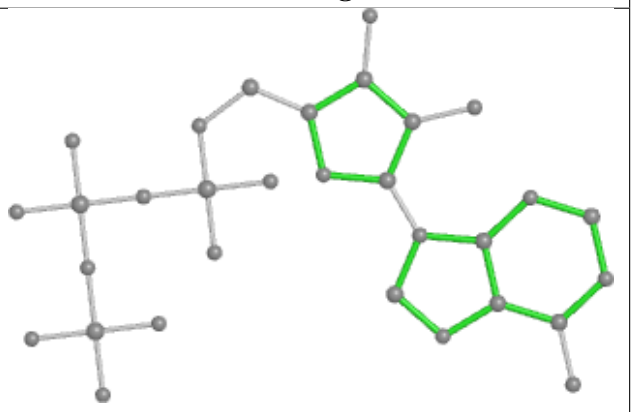
Bond lengths



Bond angles

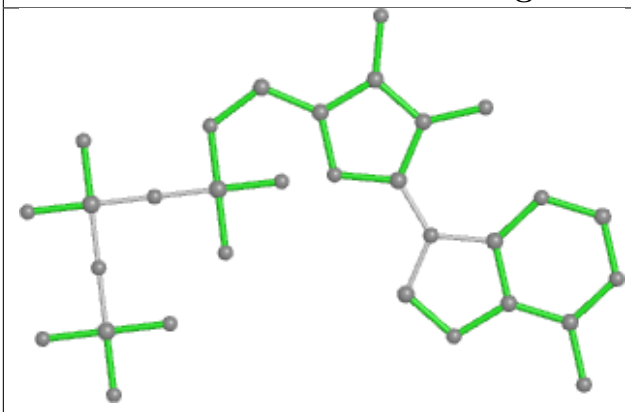


Torsions

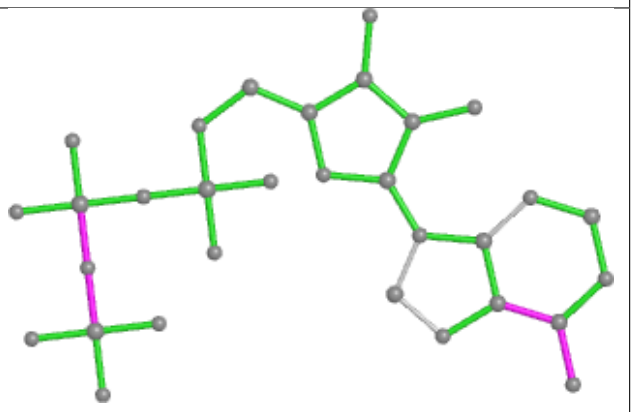


Rings

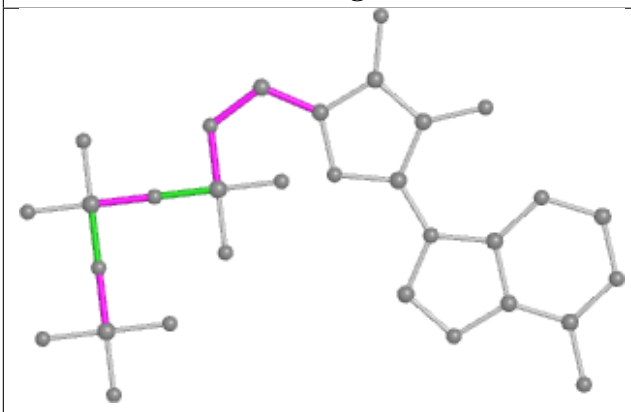
Ligand ATP A 5002



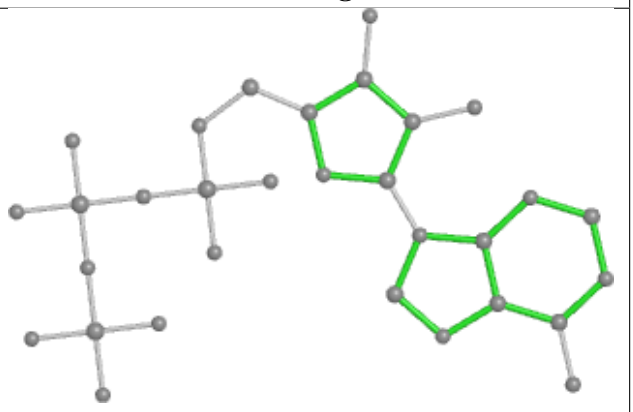
Bond lengths



Bond angles

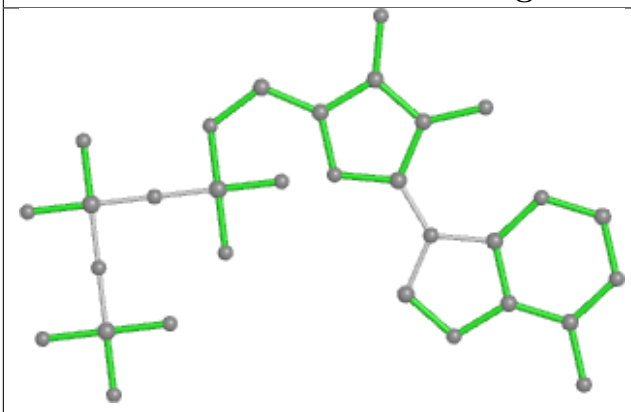


Torsions

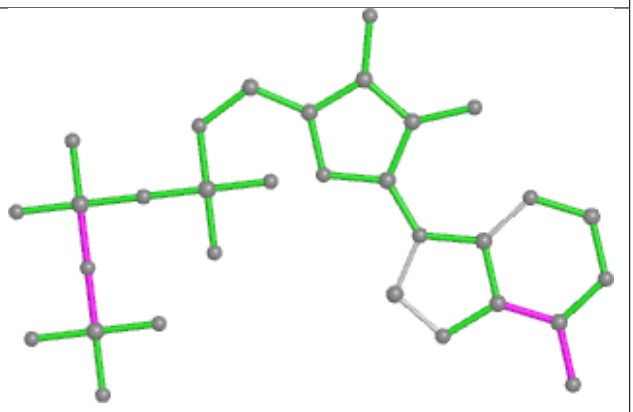


Rings

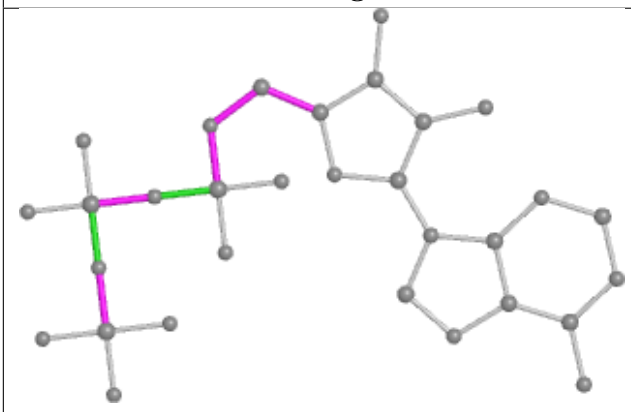
Ligand ATP C 5002



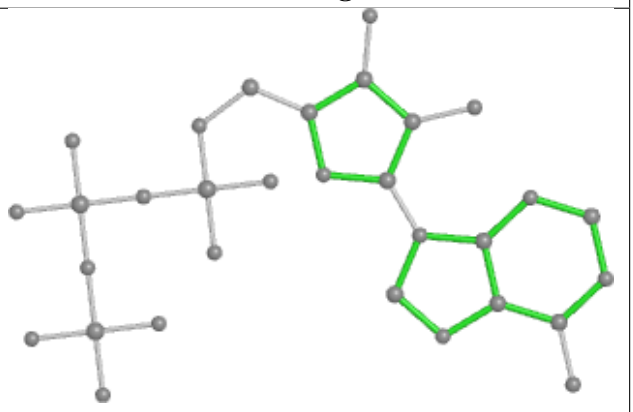
Bond lengths



Bond angles

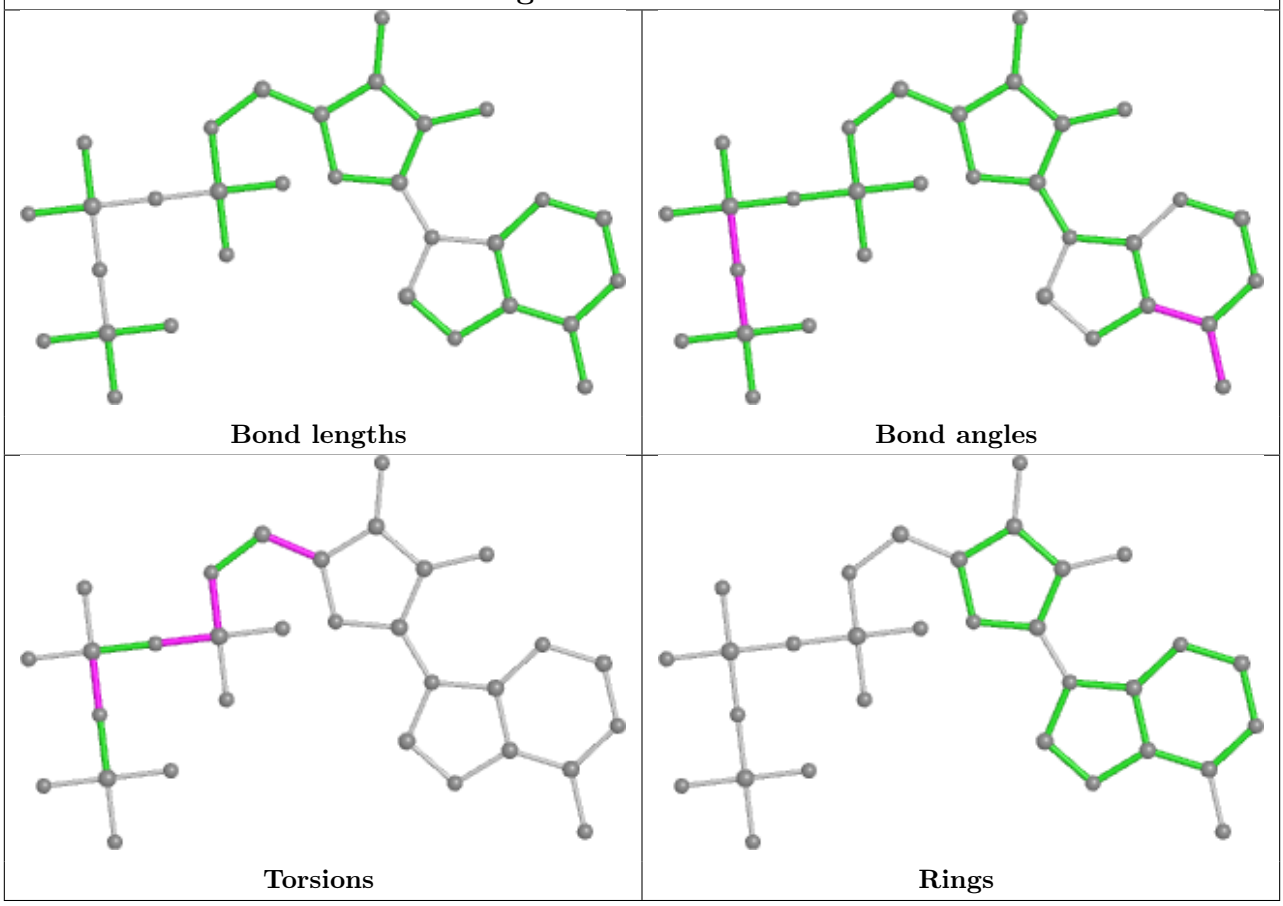


Torsions



Rings

Ligand ATP C 5004



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.

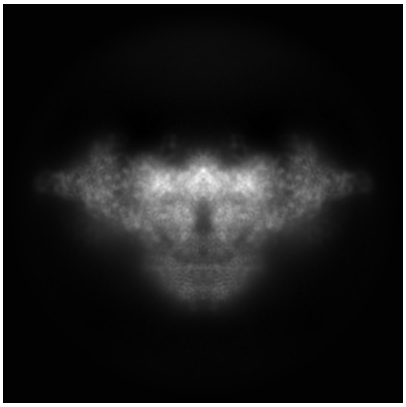
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42764. These allow visual inspection of the internal detail of the map and identification of artifacts.

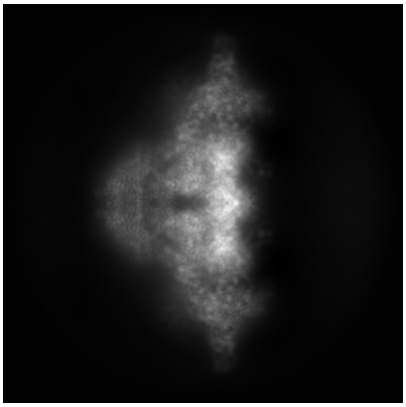
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

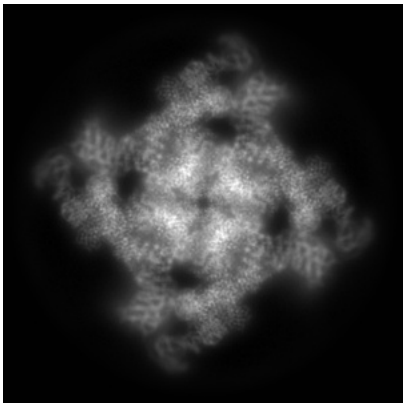
6.1.1 Primary map



X



Y

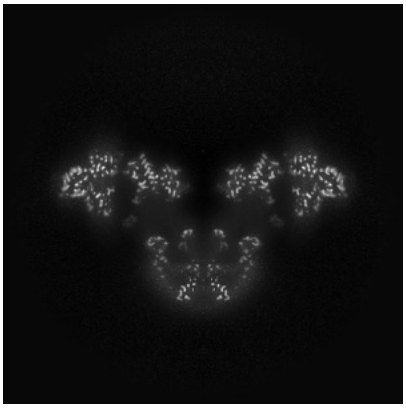


Z

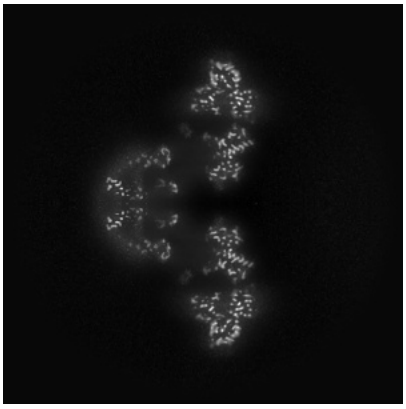
The images above show the map projected in three orthogonal directions.

6.2 Central slices

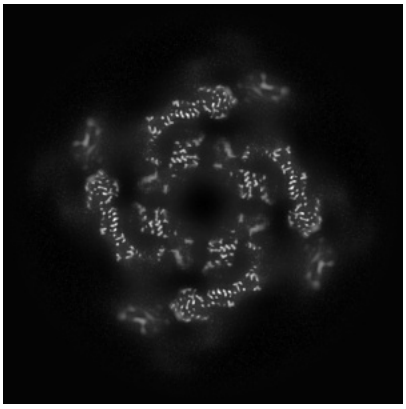
6.2.1 Primary map



X Index: 256



Y Index: 256

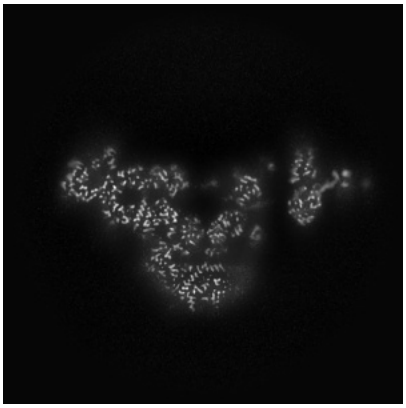


Z Index: 256

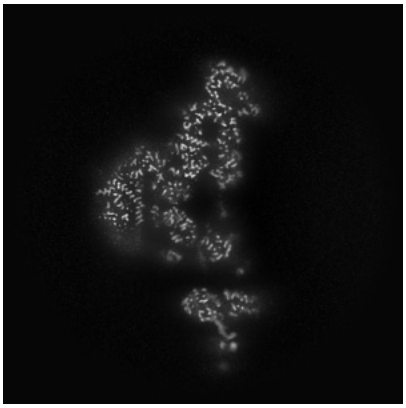
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

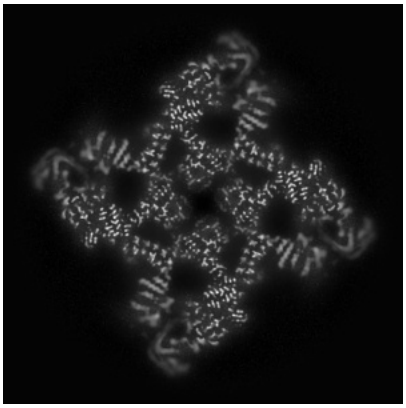
6.3.1 Primary map



X Index: 274



Y Index: 274



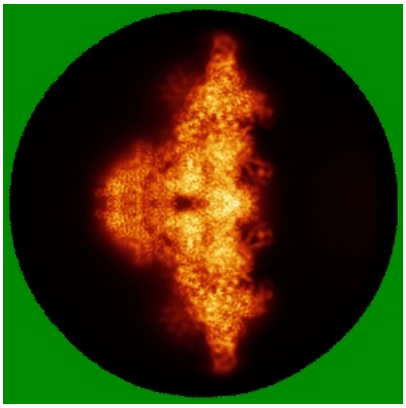
Z Index: 277

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

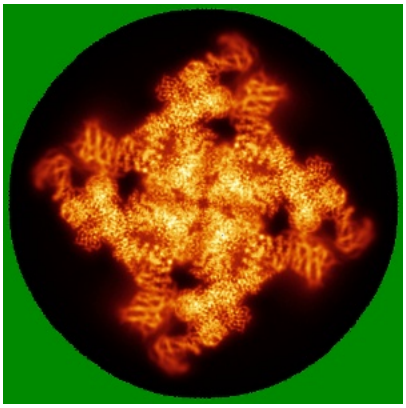
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

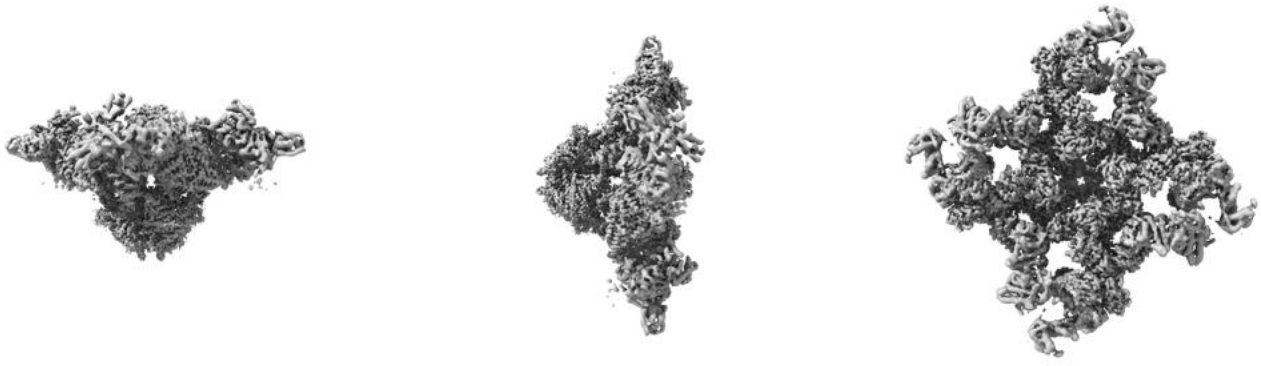


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

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

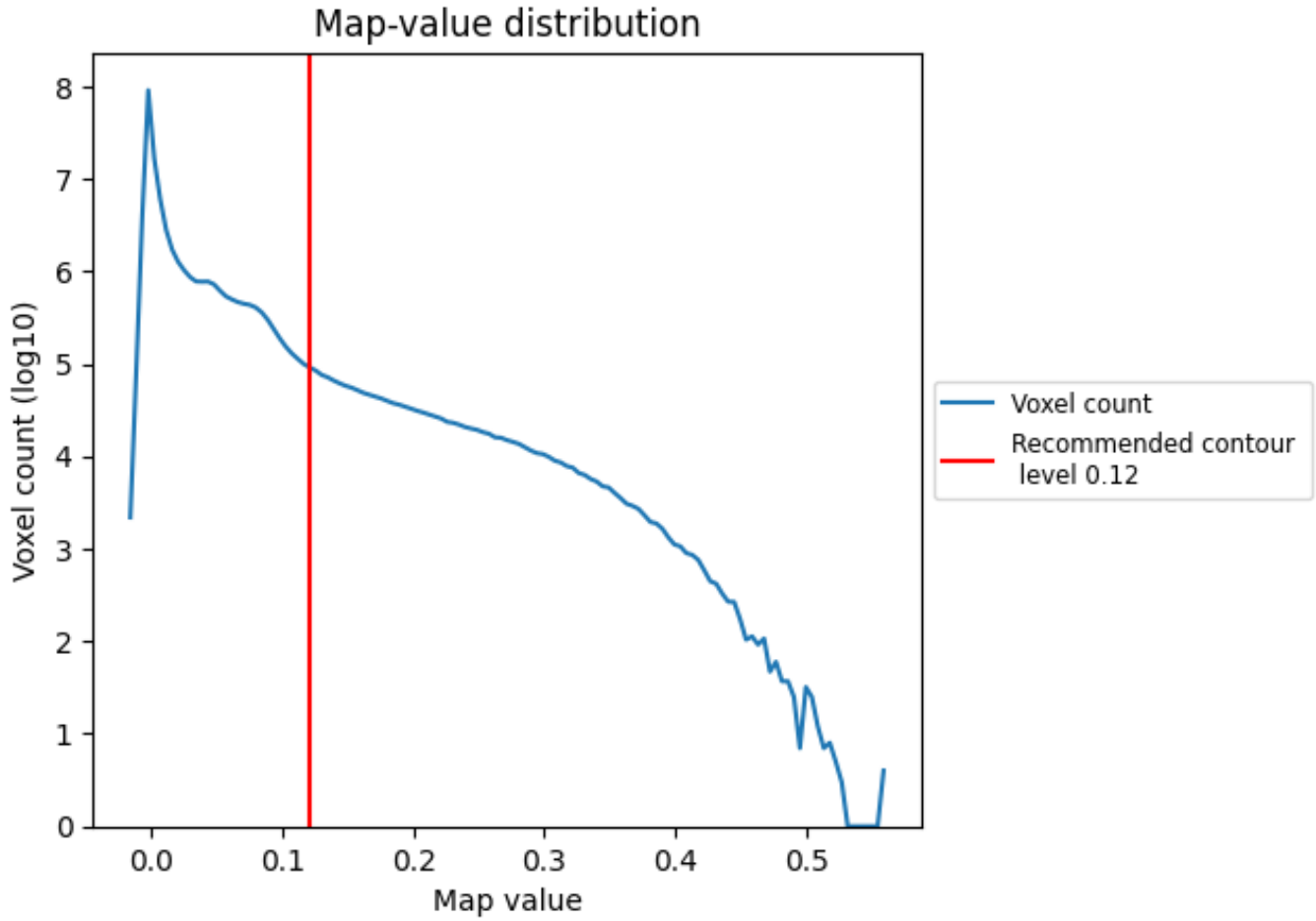
6.6 Mask visualisation (i)

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

7 Map analysis

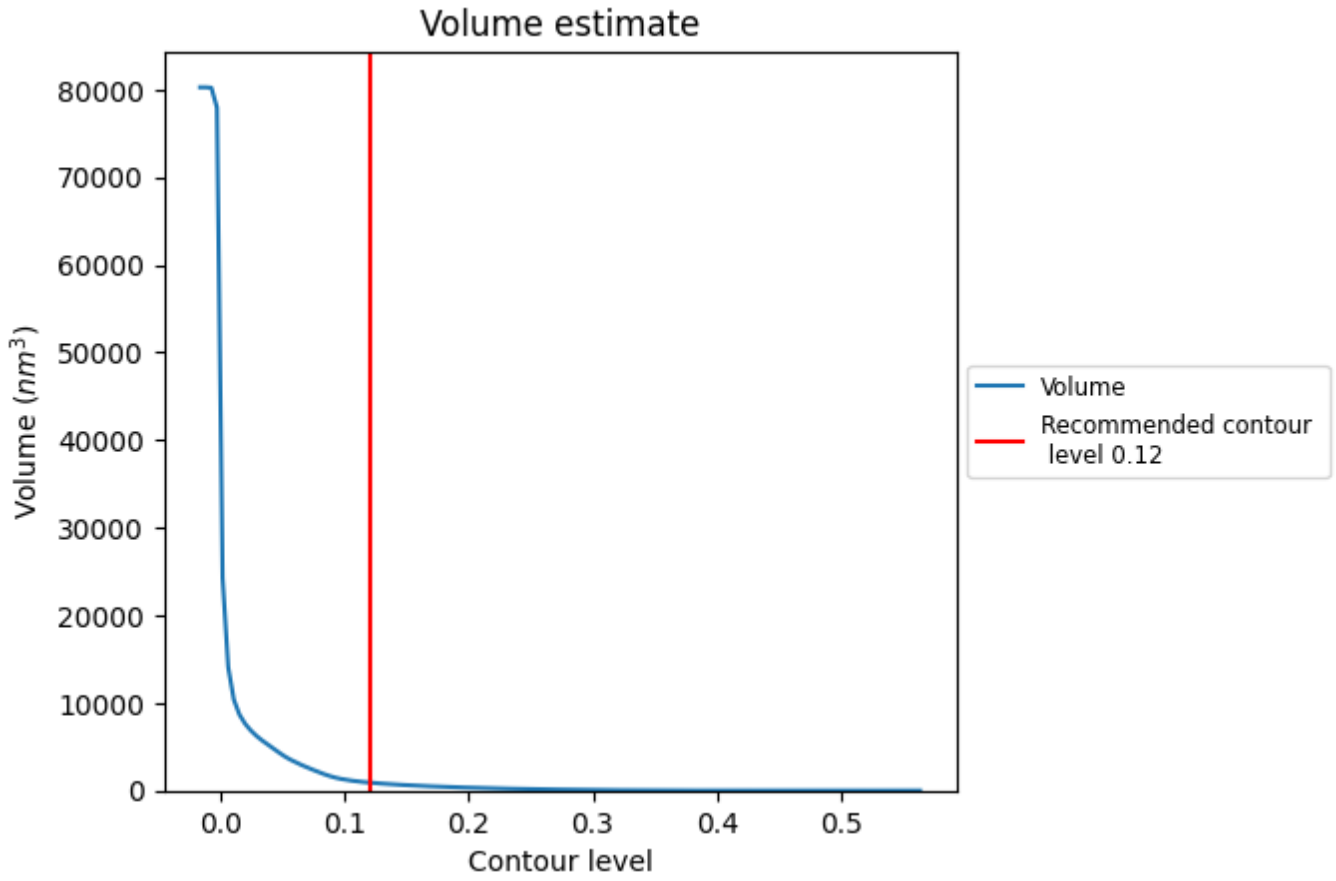
This section contains the results of statistical analysis of the map.

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.

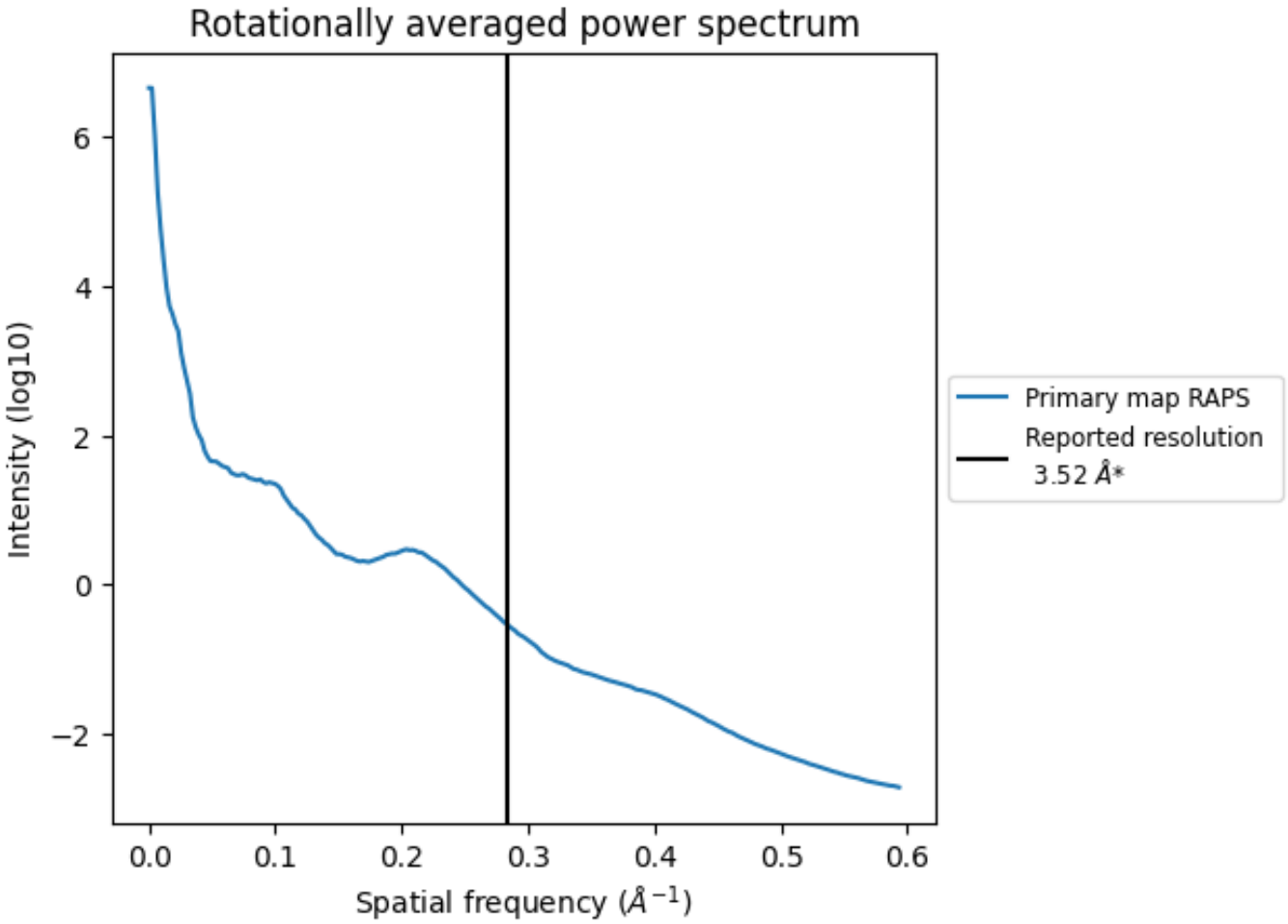
7.2 Volume estimate



The volume at the recommended contour level is 911 nm^3; this corresponds to an approximate mass of 823 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 0.284 Å^{-1}

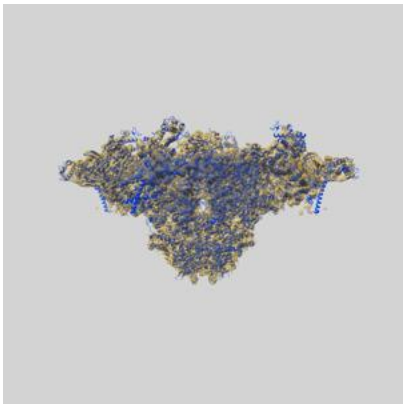
8 Fourier-Shell correlation

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

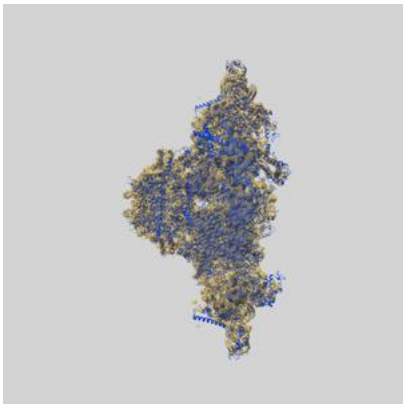
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42764 and PDB model 8UXH. Per-residue inclusion information can be found in section 3 on page 6.

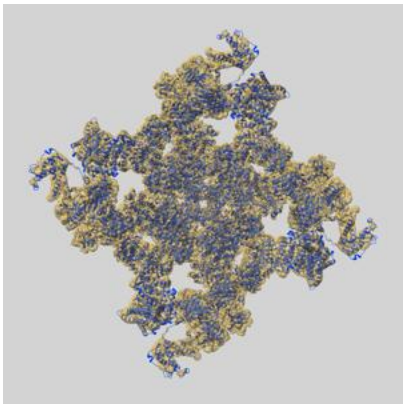
9.1 Map-model overlay



X



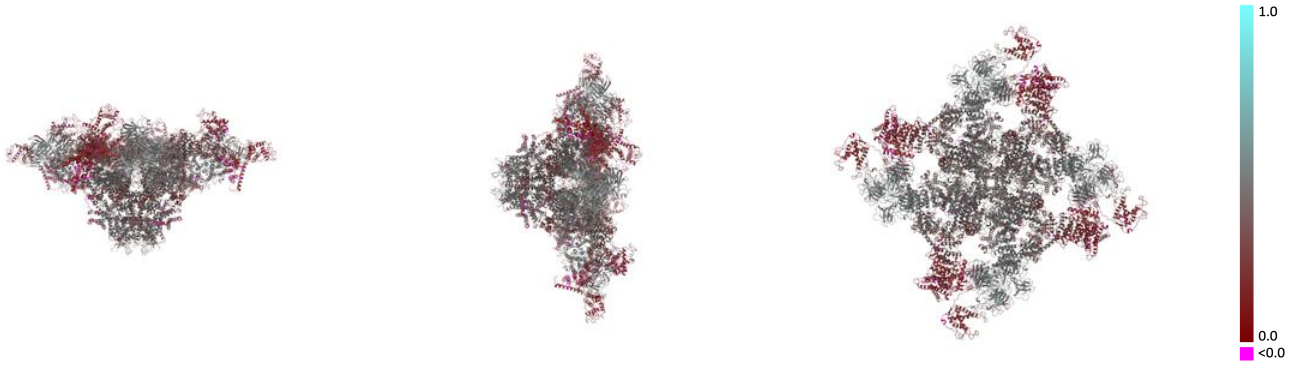
Y



Z

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

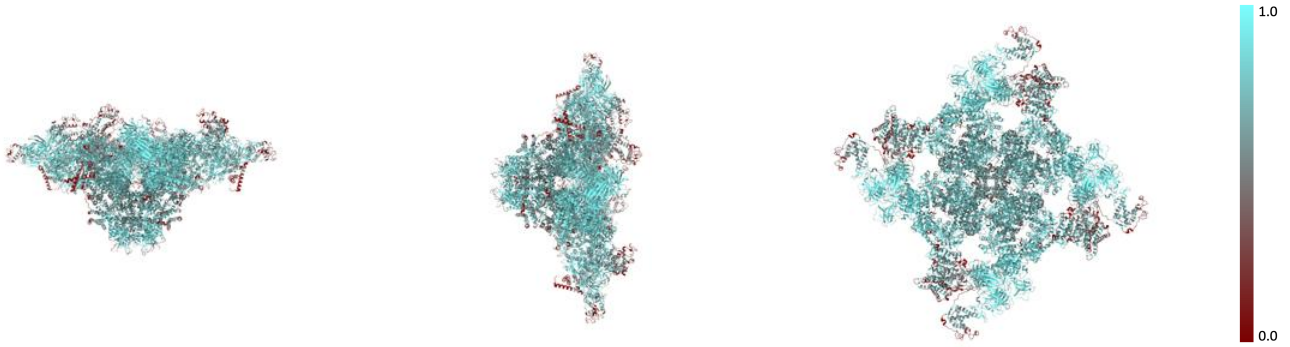
9.2 Q-score mapped to coordinate model



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.

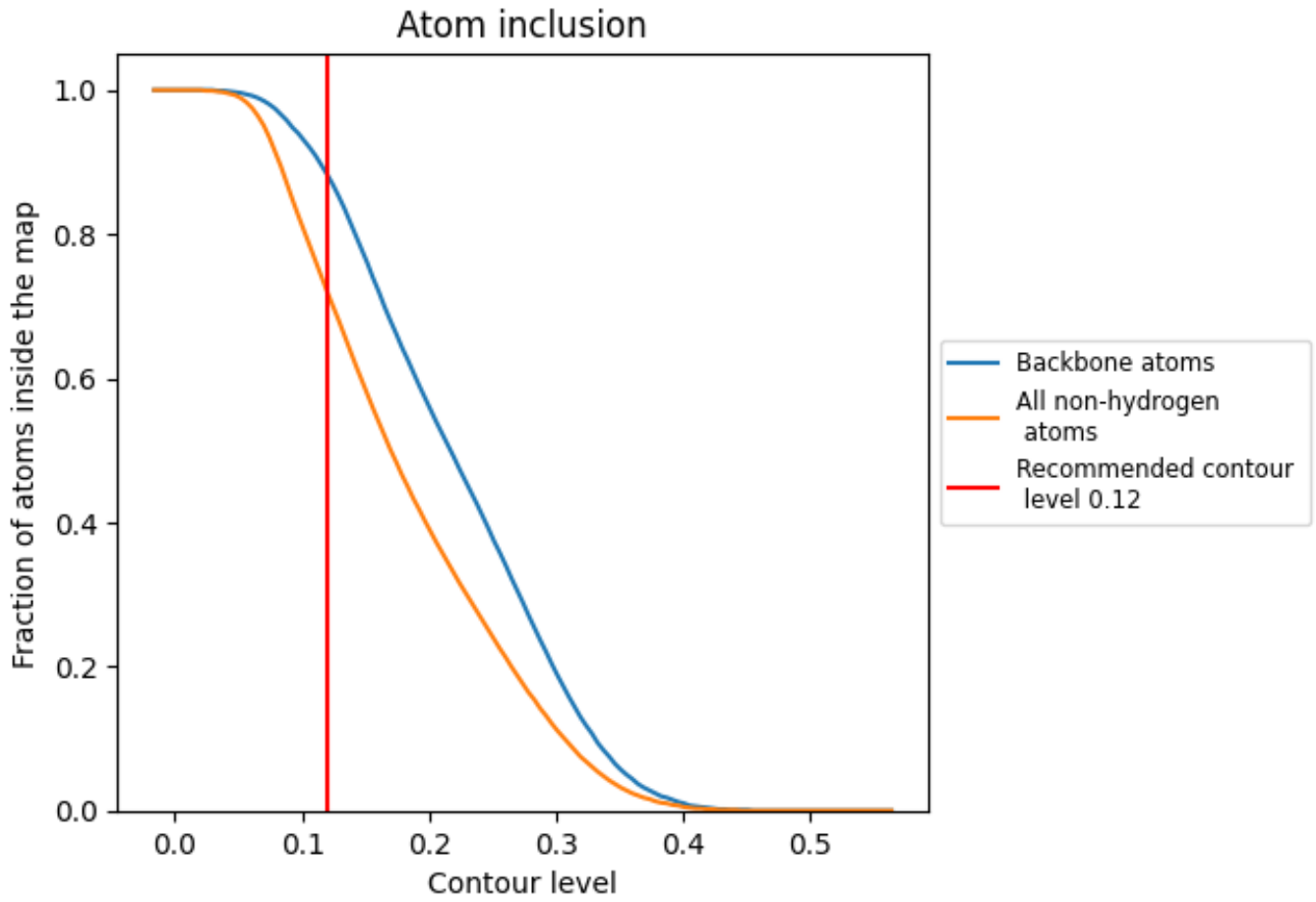
9.3 Atom inclusion mapped to coordinate model



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.7190	0.3660
A	0.7170	0.3650
B	0.7160	0.3640
C	0.7180	0.3660
D	0.7120	0.3560
E	0.8560	0.5050
F	0.8510	0.5030
G	0.8590	0.5060
H	0.8570	0.5040