Full wwPDB EM Validation Report (i)

May 18, 2024 – 10:01 AM EDT

PDB ID	:	6WOV
EMDB ID	:	EMD-21862
Title	:	Cryo-EM structure of recombinant mouse Ryanodine Receptor type 2 wild type in complex with FKBP12.6
Authors	:	Iyer, K.A.; Hu, Y.; Nayak, A.R.; Kurebayashi, N.; Murayama, T.; Samso, M.
Deposited on	:	2020-04-25
Resolution	:	5.10 Å(reported)
Based on initial model	:	5L1D

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 (i) 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 (i)) were used in the production of this report:

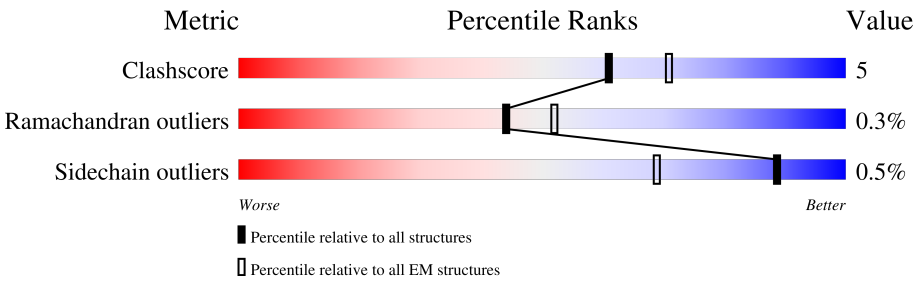
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.10 Å.

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



Metric	Whole archive (#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	4966	13% 69% 10% 21%
1	B	4966	13% 69% 10% 21%
1	C	4966	13% 69% 10% 21%
1	D	4966	13% 69% 10% 21%
2	E	107	18% 79% 21%
2	F	107	16% 79% 21%
2	G	107	18% 80% 20%
2	H	107	17% 79% 21%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 245656 atoms, of which 120412 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
			Total	C	H	N	O	S		
1	A	3921	59769	19350	29277	5253	5698	191	0	0
1	B	3921	59772	19350	29280	5253	5698	191	0	0
1	C	3921	59773	19350	29281	5253	5698	191	0	0
1	D	3921	59770	19350	29278	5253	5698	191	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	E	107	1642	516	824	144	154	4	0	0
2	F	107	1642	516	824	144	154	4	0	0
2	G	107	1642	516	824	144	154	4	0	0
2	H	107	1642	516	824	144	154	4	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

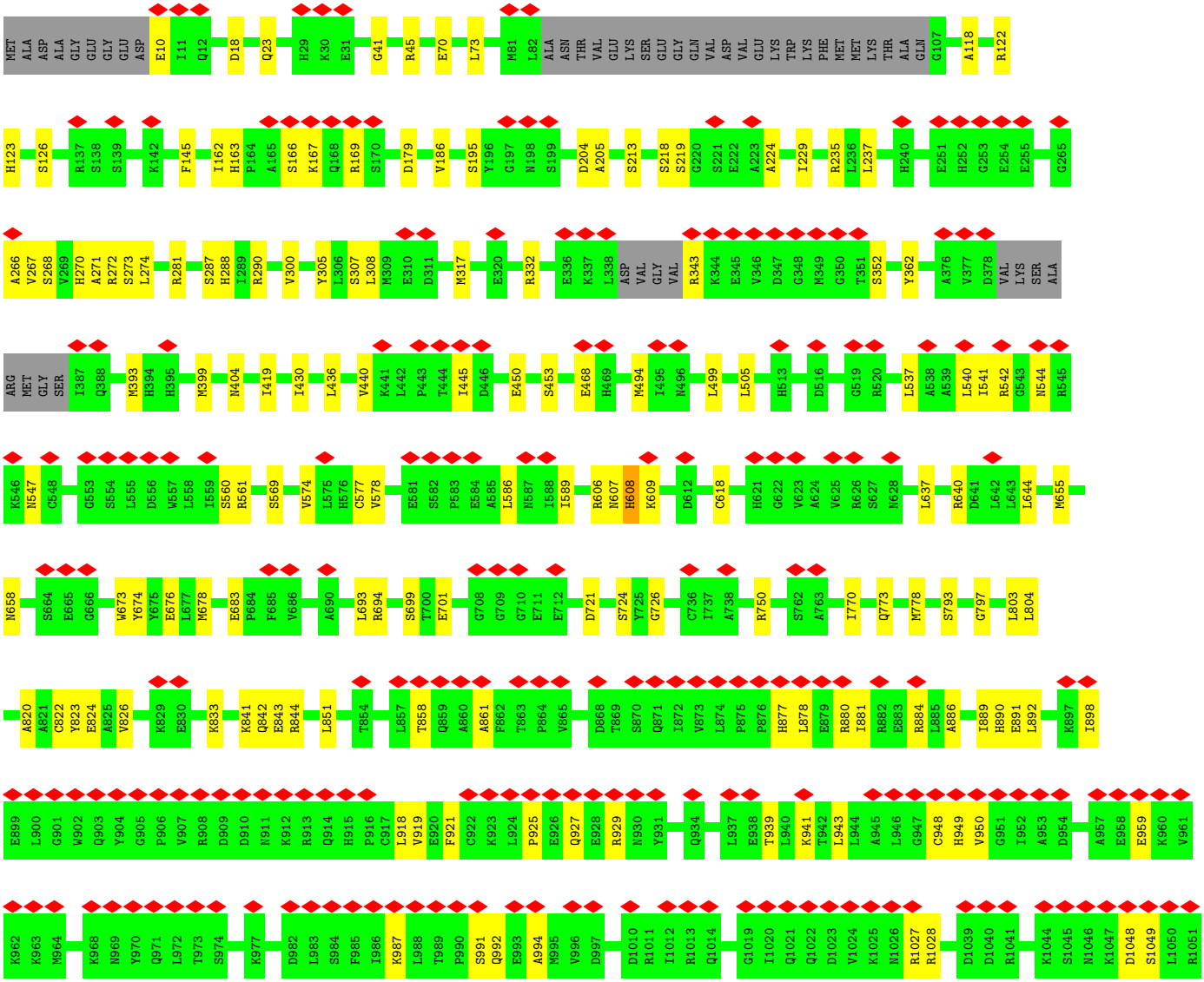
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	1	1	1	0
3	B	1	1	1	0
3	C	1	1	1	0
3	D	1	1	1	0

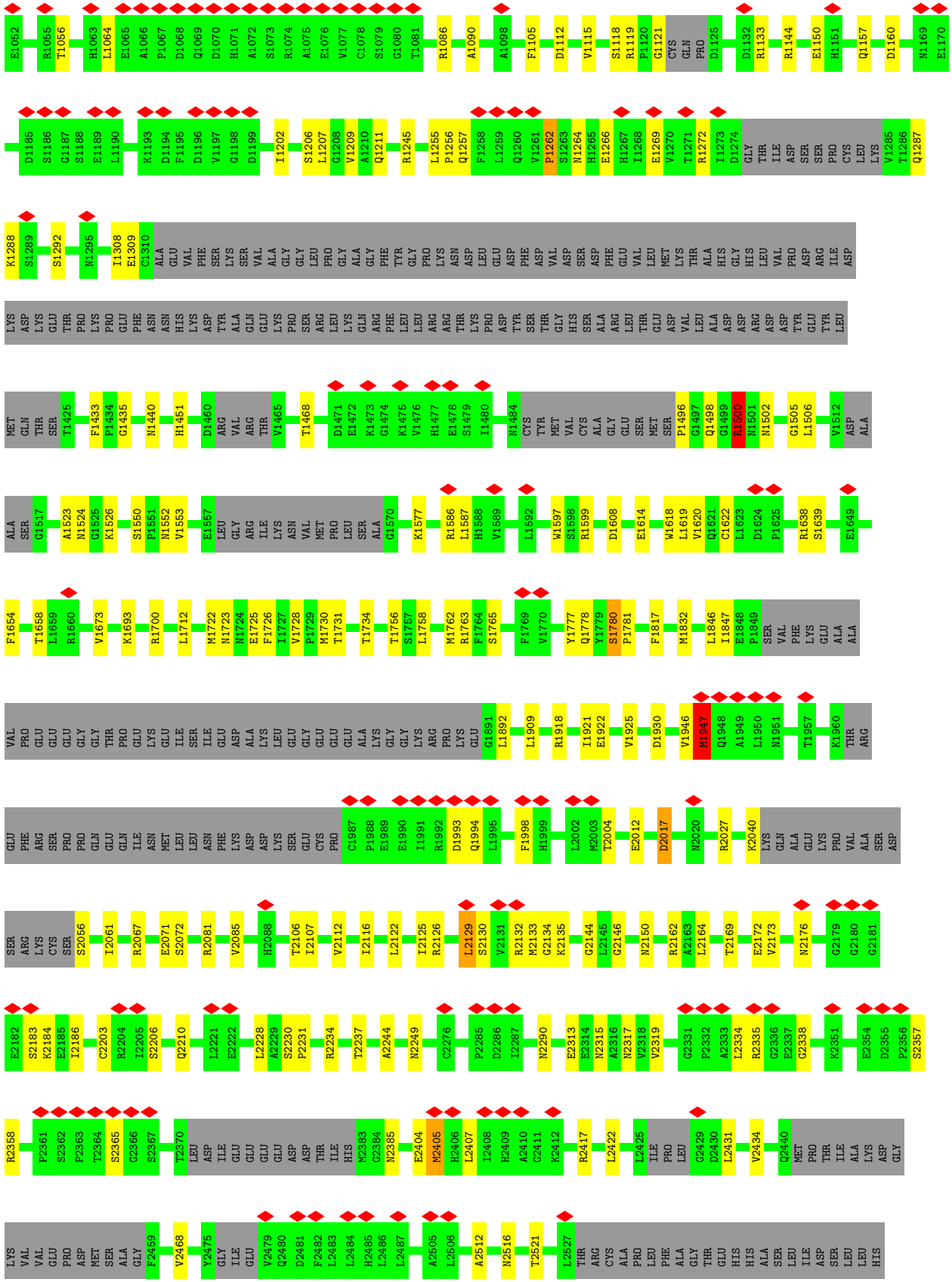
3 Residue-property plots (i)

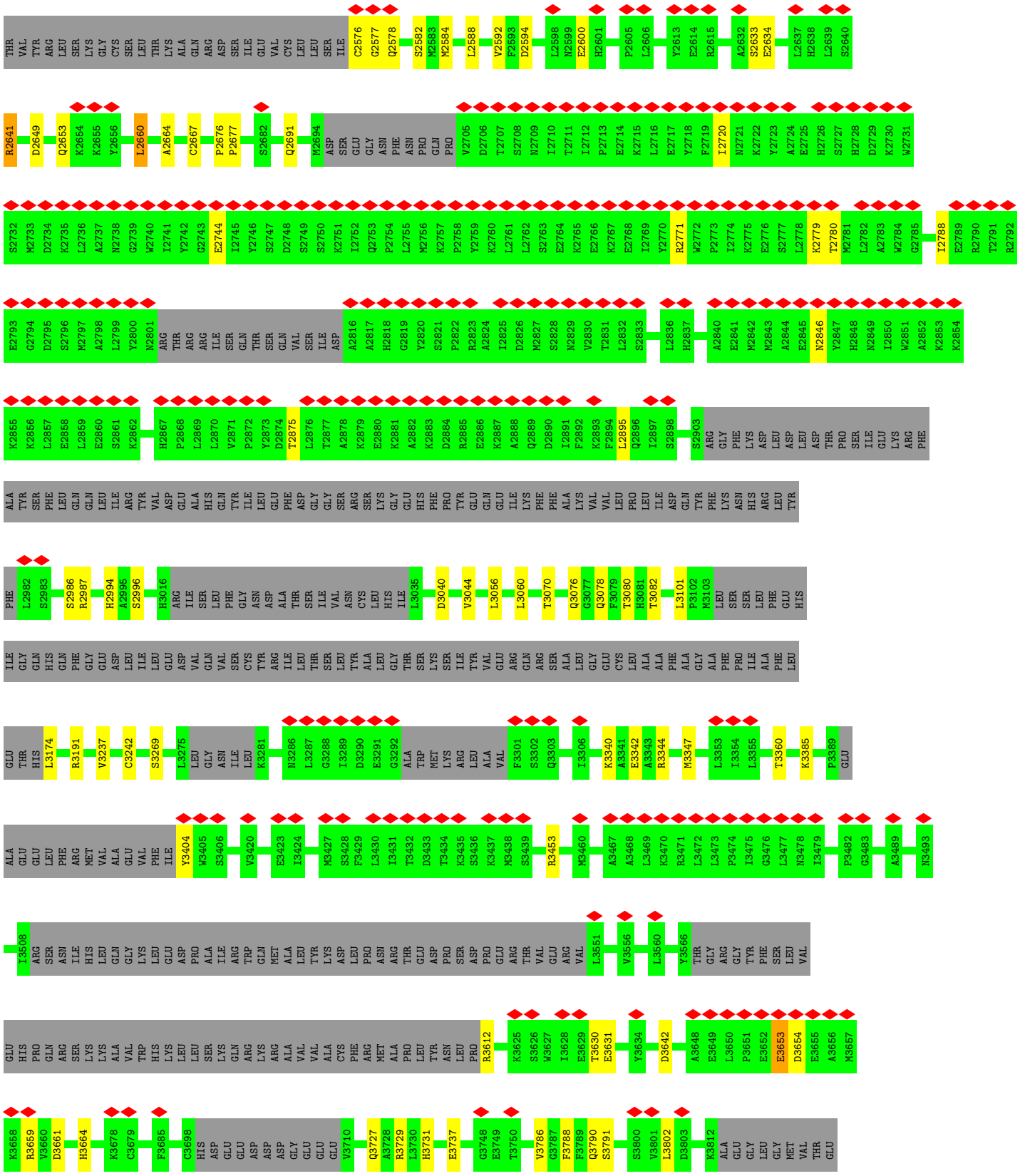
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

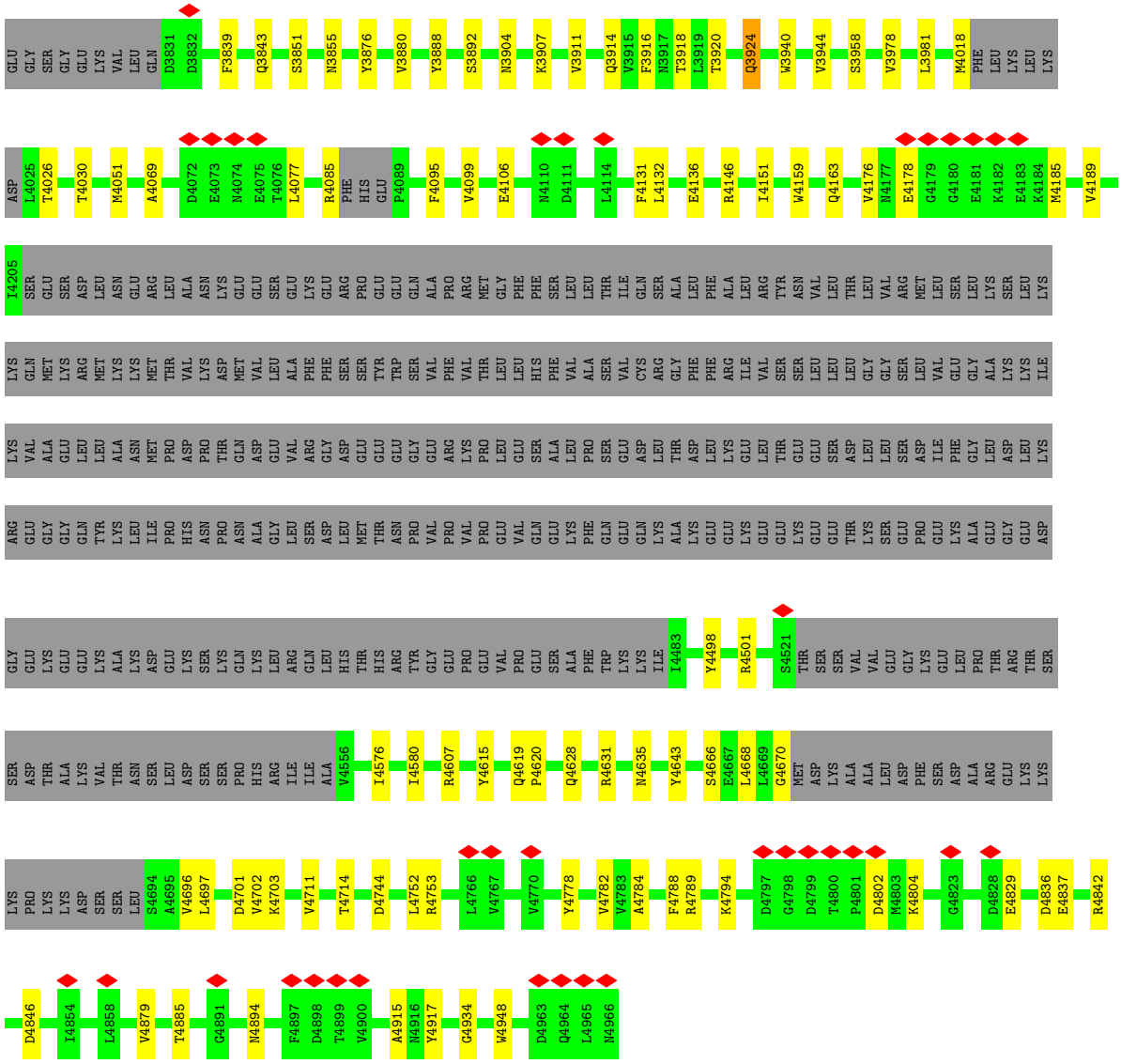
- Molecule 1: Ryanodine receptor 2

Chain A: 13% 69% 10% 21%



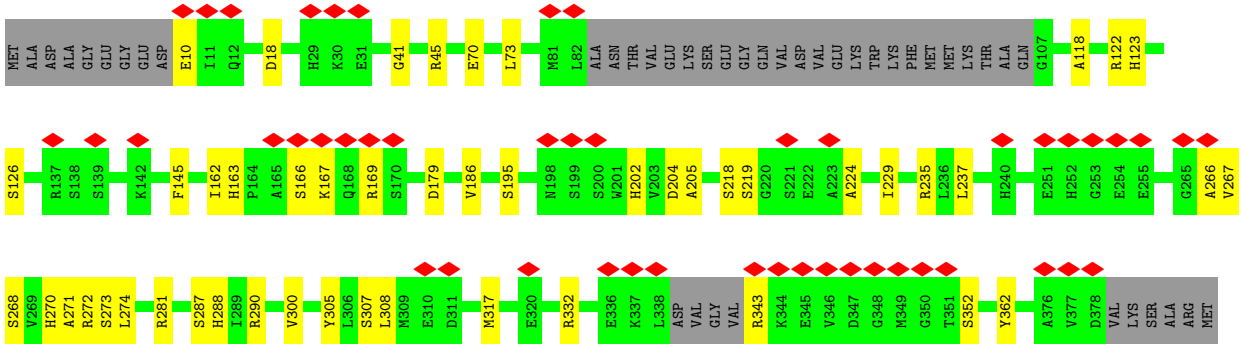

E1052 R1055 T1056 H1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 S1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 R1086 A1090 A1098 F1105 D1112 V1115 S1118 R1119 P1120 G1121 CYS GLN PRO D1125 D1132 R1133 R1144 E1150 H1151 Q1157 D1160 N1169 E1170
D1185 S1186 G1187 S1188 E1189 L1190 K1193 D1194 F1195 D1196 V1197 G1198 D1199 I1202 S1206 L1207 G1208 V1209 A1210 Q1211 R1245 L1255 P1256 Q1257 F1258 L1259 Q1260 V1261 P1262 S1263 N1264 H1265 E1266 H1267 I1268 E1269 V1270 T1271 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU LYS V1285 T1286 Q1287
K1288 S1289 S1292 N1295 I1308 E1309 C1310 ALA GLU VAL PHE SER LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS HIS LEU VAL PRO ASP ARG ILE ASP
LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR GLU TYR LEU
MET GLN THR SER T1425 F1433 P1434 G1435 N1440 H1451 D1460 ARG VAL ARG THR V1465 T1468 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 S1479 I1480 N1484 CYS TYR MET VAL CYS ALA GLY GLU SER MET SER P1496 G1497 Q1498 G1499 R1500 N1501 N1502 G1505 L1506 V1512 ASP ALA
ALA SER G1517 A1523 N1524 G1525 K1526 S1550 P1551 N1552 V1553 E1557 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER ALA G1570 K1577 R1586 L1587 H1588 V1589 L1592 W1597 S1598 R1599 D1608 E1614 W1618 L1619 V1620 Q1621 C1622 L1623 D1624 P1625 R1638 S1639 E1649
F1654 T1658 L1659 R1660 V1673 K1693 R1700 L1712 M1722 N1723 N1724 E1725 F1726 I1727 V1728 P1729 M1730 T1731 T1734 T1756 S1757 L1758 M1762 R1763 F1764 S1765 F1769 V1770 Y1777 Q1778 Y1779 S1780 P1781 F1817 M1832 L1846 I1847 E1848 P1849 SER VAL PHE LYS GLU ALA ALA
VAL PRO GLU GLU GLU GLY GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO LYS GLU G1891 L1892 L1909 R1918 I1921 E1922 V1925 D1930 V1946 M1947 Q1948 A1949 L1950 N1951 T1957 K1960 THR ARG
GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO C1987 P1988 E1989 E1990 I1991 R1992 D1993 Q1994 L1995 F1998 H1999 L2002 M2003 T2004 E2012 D2017 N2020 R2027 K2040 LYS GLN ALA GLU LYS PRO VAL ALA SER ASP
SER ARG LYS CYS SER S2056 I2061 R2067 E2071 S2072 R2081 V2085 H2088 T2106 I2107 V2112 I2116 L2122 I2125 R2126 L2129 S2130 V2131 R2132 M2133 G2134 K2135 G2144 L2145 G2146 N2150 R2162 A2163 L2164 T2169 E2172 V2173 N2176 G2179 G2180 G2181
E2182 S2183 K2184 E2185 I2186 C2203 R2204 I2205 S2206 Q2210 L2221 E2222 L2228 A2229 S2230 P2231 R2234 T2237 A2244 N2249 C2276 P2285 D2286 I2287 N2290 E2313 E2314 N2315 A2316 N2317 V2318 V2319 G2331 P2332 A2333 L2334 R2335 G2336 E2337 G2338 K2351 E2354 D2355 P2356 S2357
R2358 P2361 S2362 P2363 T2364 S2365 G2366 S2367 T2370 LEU ASP ILE GLU GLU GLU GLU ASP ASP THR ILE HIS M2383 G2384 N2385 E2404 M2405 H2406 L2407 I2408 H2409 A2410 G2411 K2412 R2417 L2422 L2425 ILE PRO LEU G2429 D2430 L2431 V2434 Q2440 MET PRO THR ILE ALA LYS ASP GLY
LYS VAL VAL GLU PRO ASP MET SER ALA GLY F2459 V2468 Y2475 GLY ILE GLU V2479 Q2480 D2481 F2482 L2483 L2484 H2485 L2486 L2487 A2505 L2506 A2512 N2516 T2521 L2527 THR ARG CYS ALA PRO LEU PHE ALA GLY THR GLU HIS HIS ALA SER LEU ILE ASP SER LEU LEU HIS

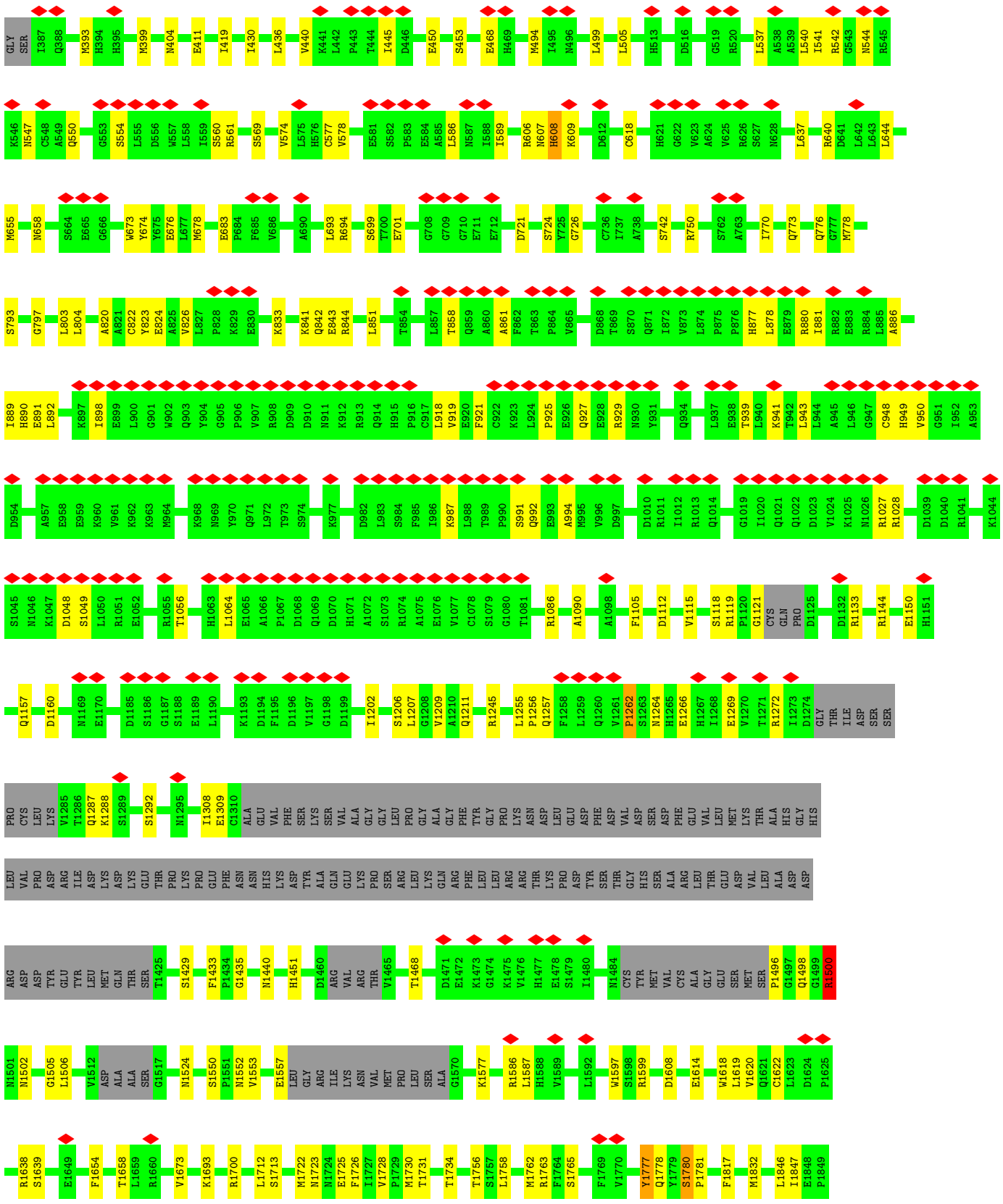

THR VAL TYR ARG LEU SER LYS GLY CYS SER LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU SER ILE C2576 G2577 Q2578 S2582 M2583 M2584 L2588 V2592 F2593 D2594 L2598 N2599 E2600 H2601 P2605 L2606 Y2613 E2614 R2615 A2632 S2633 E2634 L2637 H2638 L2639 S2640
R2641 D2649 Q2653 K2654 K2655 Y2656 L2660 A2664 C2667 P2676 P2677 S2682 Q2691 M2694 ASP SER GLU GLY ASN PHE ASN PRO GLN PRO V2705 D2706 T2707 S2708 N2709 I2710 T2711 I2712 P2713 E2714 K2715 L2716 E2717 Y2718 F2719 I2720 N2721 K2722 Y2723 A2724 E2725 H2726 S2727 H2728 D2729 K2730 W2731
S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 K2757 P2758 Y2759 K2760 L2761 L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782 A2783 W2784 G2785 I2788 E2789 R2790 T2791 R2792
E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP A2816 A2817 H2818 G2819 Y2820 S2821 P2822 R2823 A2824 I2825 D2826 M2827 S2828 N2829 V2830 T2831 L2832 S2833 L2836 H2837 A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854
K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 S2903 ARG GLY PHE LYS ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE
ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR
PHE L2982 S2983 S2986 R2987 H2994 A2995 S2996 H3016 ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE L3035 D3040 V3044 L3056 L3060 T3070 Q3076 G3077 Q3078 F3079 T3080 H3081 T3082 L3101 P3102 M3103 LEU SER SER LEU PHE GLU HIS
ILE GLY GLN HIS GLN PHE 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 ILE ALA PHE LEU
GLU THR HIS L3174 R3191 V3237 C3242 S3269 L3275 LEU GLY ASN ILE LEU K3281 N3286 L3287 G3288 I3289 D3290 E3291 G3292 ALA TRP MET LYS ARG LEU ALA VAL F3301 S3302 Q3303 I3306 K3340 A3341 E3342 A3343 R3344 M3347 L3353 I3354 L3355 T3360 K3385 P3389 GLU
ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE Y3404 W3405 S3406 V3420 E3423 I3424 M3427 S3428 P3429 L3430 I3431 T3432 D3433 T3434 K3435 S3436 K3437 M3438 S3439 R3453 M3460 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 L3477 N3478 I3479 P3482 G3483 A3489 N3493
I3508 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 GLU ASP PRO SER ASP PRO GLU ARG THR VAL GLU ARG VAL L3551 V3556 L3560 Y3566 THR GLY ARG GLY TYR PHE SER LEU VAL
GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET ALA PRO LEU TYR ASN LEU PRO R3612 K3625 S3626 W3627 I3628 E3629 T3630 E3631 Y3634 D3642 A3648 E3649 L3650 P3651 E3652 E3653 D3654 E3655 A3656 M3657
K3658 R3659 Y3660 D3661 H3664 K3678 C3679 F3685 C3698 HIS ASP GLU GLU ASP ASP GLY GLU GLU GLU V3710 Q3727 A3728 R3729 L3730 H3731 E3737 G3748 E3749 T3750 V3786 G3787 F3788 F3789 Q3790 S3791 S3800 Y3801 L3802 D3803 K3812 ALA GLU GLY LEU GLY MET VAL THR GLU



- Molecule 1: Ryanodine receptor 2

Chain B:

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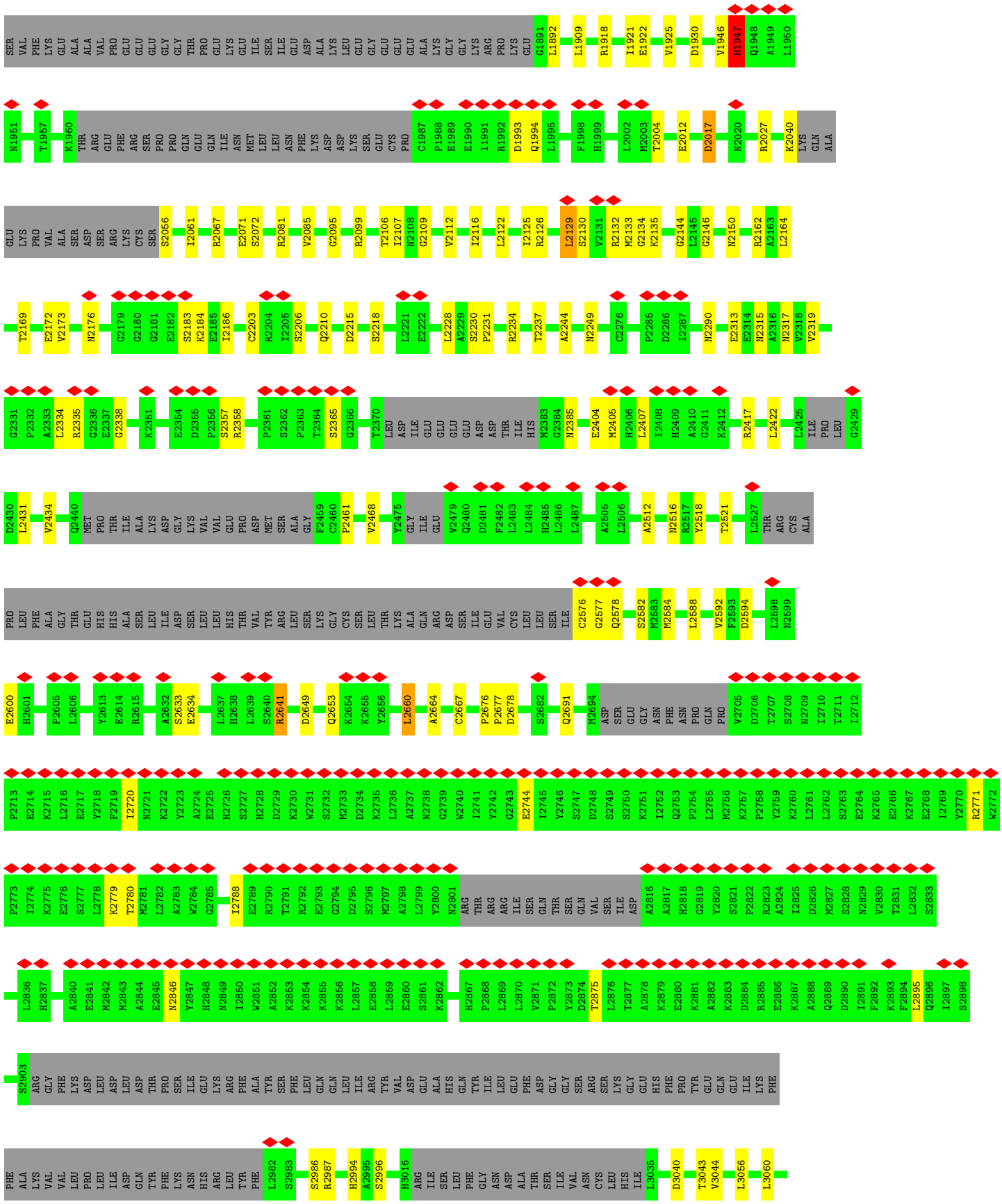
K546 N547 C548 A549 Q550 G553 S554 L555 D556 W557 L558 I559 S560 R561 S569 V574 L575 H576 C577 V578 E581 S582 P583 E584 A585 L586 N587 I588 I589 R606 N607 H608 K609 D612 C618 H621 G622 V623 A624 V625 R626 S627 N628 L637 R640 D641 L642 L643 L644
M655 N658 S664 E665 G666 W673 Y674 Y675 E676 L677 M678 E683 P684 F685 V686 A690 L693 R694 S699 T700 E701 G708 G709 G710 E711 E712 D721 S724 Y725 G726 C736 I737 A738 S742 R750 S762 A763 I770 Q773 Q776 G777 M778
S793 G797 L803 L804 A820 A821 C822 Y823 E824 A825 V826 L827 P828 K829 E830 K833 K841 Q842 E843 R844 L851 T854 L857 T858 Q859 A860 A861 F862 T863 P864 V865 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 R884 L885 A886
I889 H890 E891 L892 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 C922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 Q934 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 A953
D954 A957 E958 E959 K960 V961 K962 K963 M964 K968 N969 Y970 Q971 L972 T973 S974 K977 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 D997 D1010 R1011 I1012 R1013 Q1014 G1019 I1020 Q1021 Q1022 D1023 V1024 K1025 N1026 R1027 R1028 D1039 D1040 R1041 K1044
S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 R1055 T1056 H1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 S1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 R1086 A1090 A1098 F1105 D1112 V1115 S1118 R1119 P1120 G1121 CYS GLN PRO D1125 D1132 R1133 R1144 E1150 H1151
Q1157 D1160 N1169 E1170 D1185 S1186 G1187 S1188 E1189 L1190 K1193 D1194 F1195 D1196 V1197 G1198 D1199 I1202 S1206 L1207 G1208 V1209 A1210 Q1211 R1245 L1255 P1256 Q1257 F1258 L1259 Q1260 V1261 P1262 S1263 N1264 H1265 E1266 H1267 I1268 E1269 V1270 T1271 R1272 I1273 D1274 GLY THR ILE ASP SER SER
PRO CYS LEU LYS V1285 T1286 Q1287 K1288 S1289 S1292 N1295 I1308 E1309 C1310 ALA GLU VAL PHE SER LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS
LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU SER ASP VAL LEU ALA ASP ASP
ARG ASP ASP TYR GLU TYR LEU MET GLN THR SER T1425 S1429 F1433 P1434 G1435 N1440 H1451 D1460 ARG VAL ARG THR V1465 T1468 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 S1479 I1480 N1484 CYS TYR MET VAL CYS ALA GLY GLU SER MET SER P1496 G1497 Q1498 G1499 R1500
N1501 N1502 G1505 L1506 V1512 ASP ALA ALA SER G1517 N1524 S1550 P1551 N1552 V1553 E1557 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER ALA G1570 K1577 R1586 L1587 H1588 V1589 L1592 W1597 S1598 R1599 D1608 E1614 W1618 L1619 V1620 Q1621 C1622 L1623 D1624 P1625
R1638 S1639 E1649 F1654 T1658 L1659 R1660 V1673 K1693 R1700 L1712 S1713 M1722 N1723 N1724 E1725 F1726 I1727 V1728 P1729 M1730 T1731 T1734 T1756 S1757 L1758 M1762 R1763 F1764 S1765 F1769 V1770 Y1777 Q1778 Y1779 S1780 P1781 F1817 M1832 L1846 I1847 E1848 P1849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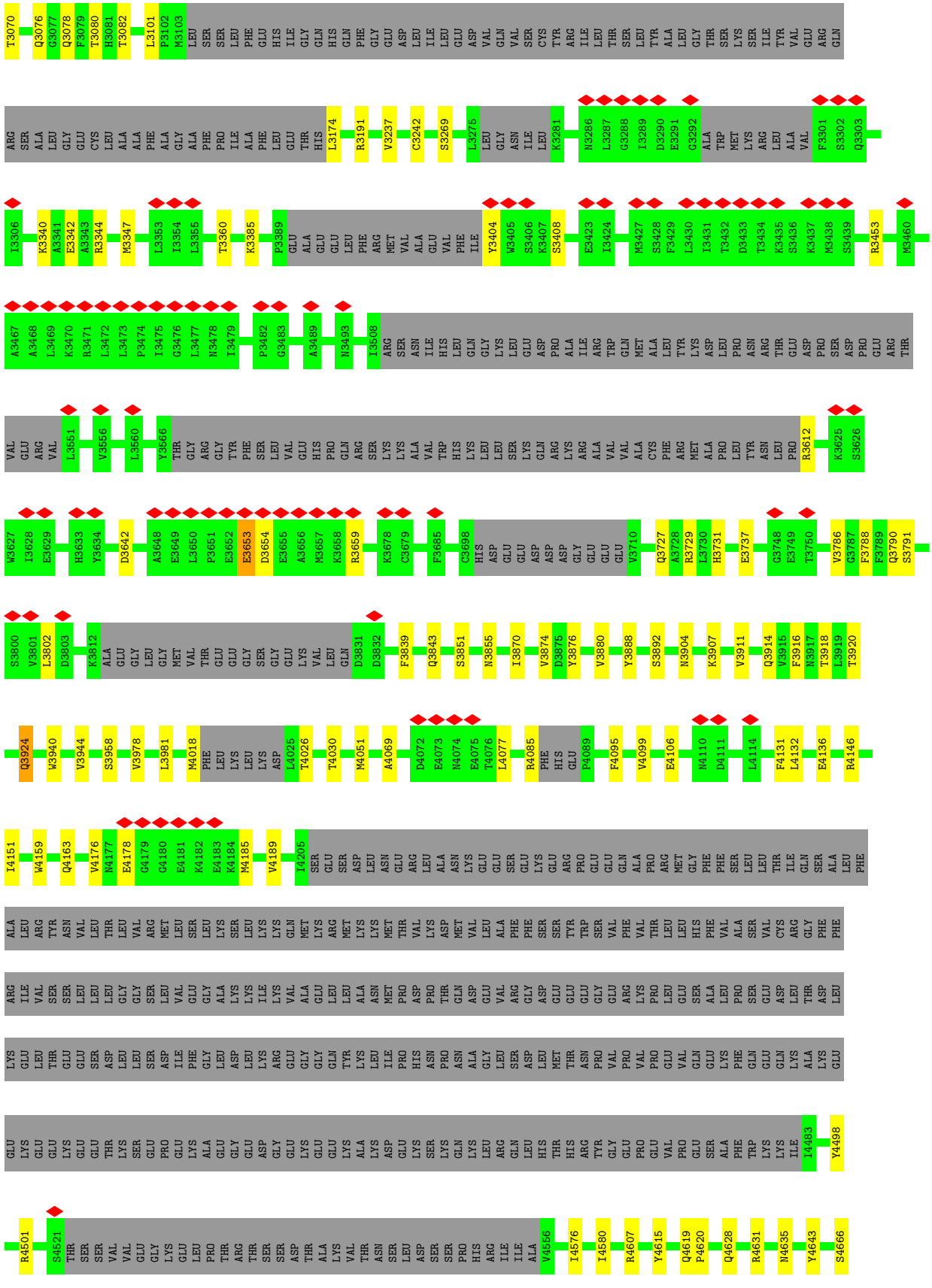
N1951 T1957 K1960 THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO G1987 P1988 E1989 E1990 I1991 R1992 D1993 Q1994 L1995 F1998 H1999 L2002 M2003 T2004 E2012 D2017 N2020 R2027 K2040 LYS GLN ALA
GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS SER S2056 I2061 R2067 E2071 S2072 R2081 V2085 G2095 R2099 T2106 I2107 N2108 G2109 V2112 I2116 L2122 I2125 R2126 L2129 S2130 V2131 R2132 M2133 G2134 K2135 G2144 L2145 G2146 N2150 R2162 A2163 L2164
T2169 E2172 V2173 N2176 G2179 G2180 G2181 E2182 S2183 K2184 E2185 I2186 C2203 R2204 I2205 S2206 Q2210 D2215 S2218 L2221 E2222 L2228 A2229 S2230 P2231 R2234 T2237 A2244 N2249 C2276 P2285 D2286 I2287 N2290 E2313 E2314 N2315 A2316 N2317 V2318 V2319
G2331 P2332 A2333 L2334 R2335 G2336 E2337 G2338 K2351 E2354 D2355 P2356 S2357 R2358 P2361 S2362 P2363 T2364 S2365 G2366 T2370 LEU ASP ILE GLU GLU GLU GLU ASP ASP THR ILE HIS M2383 G2384 N2385 E2404 M2405 H2406 L2407 I2408 H2409 A2410 G2411 K2412 R2417 L2422 L2425 ILE PRO LEU G2429
D2430 L2431 V2434 Q2440 MET PRO THR ILE ALA LYS ASP GLY LYS VAL VAL GLU PRO ASP MET SER ALA GLY F2459 C2460 P2461 V2468 Y2475 GLY ILE GLU V2479 Q2480 D2481 F2482 L2483 L2484 H2485 L2486 L2487 A2505 L2506 A2512 N2516 R2517 Y2518 T2521 L2527 THR ARG CYS ALA
PRO LEU PHE ALA GLY THR GLU HIS HIS ALA ALA SER LEU ILE ASP SER LEU LEU LEU HIS THR VAL TYR ARG LEU LEU SER LYS GLY CYS SER LEU LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU SER ILE C2576 G2577 Q2578 S2582 M2583 M2584 L2588 V2592 F2593 D2594 L2598 N2599
E2600 H2601 P2605 L2606 Y2613 E2614 R2615 A2632 S2633 E2634 L2637 H2638 L2639 S2640 R2641 D2649 Q2653 K2654 K2655 Y2656 L2660 A2664 C2667 P2676 P2677 D2678 S2682 Q2691 M2694 ASP SER GLU GLY ASN PHE ASN PRO GLN PRO V2705 D2706 T2707 S2708 N2709 I2710 T2711 I2712
P2713 E2714 K2715 L2716 E2717 Y2718 F2719 I2720 N2721 K2722 Y2723 A2724 E2725 H2726 S2727 H2728 D2729 K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 K2757 P2758 Y2759 K2760 L2761 L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772
P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782 A2783 W2784 G2785 I2788 E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP A2816 A2817 H2818 G2819 Y2820 S2821 P2822 R2823 A2824 I2825 D2826 M2827 S2828 N2829 V2830 T2831 L2832 S2833
L2836 H2837 A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898
S2903 ARG GLY PHE LYS ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE
PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE L2982 S2983 S2986 R2987 H2994 A2995 S2996 H3016 ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE L3035 D3040 T3043 V3044 L3056 L3060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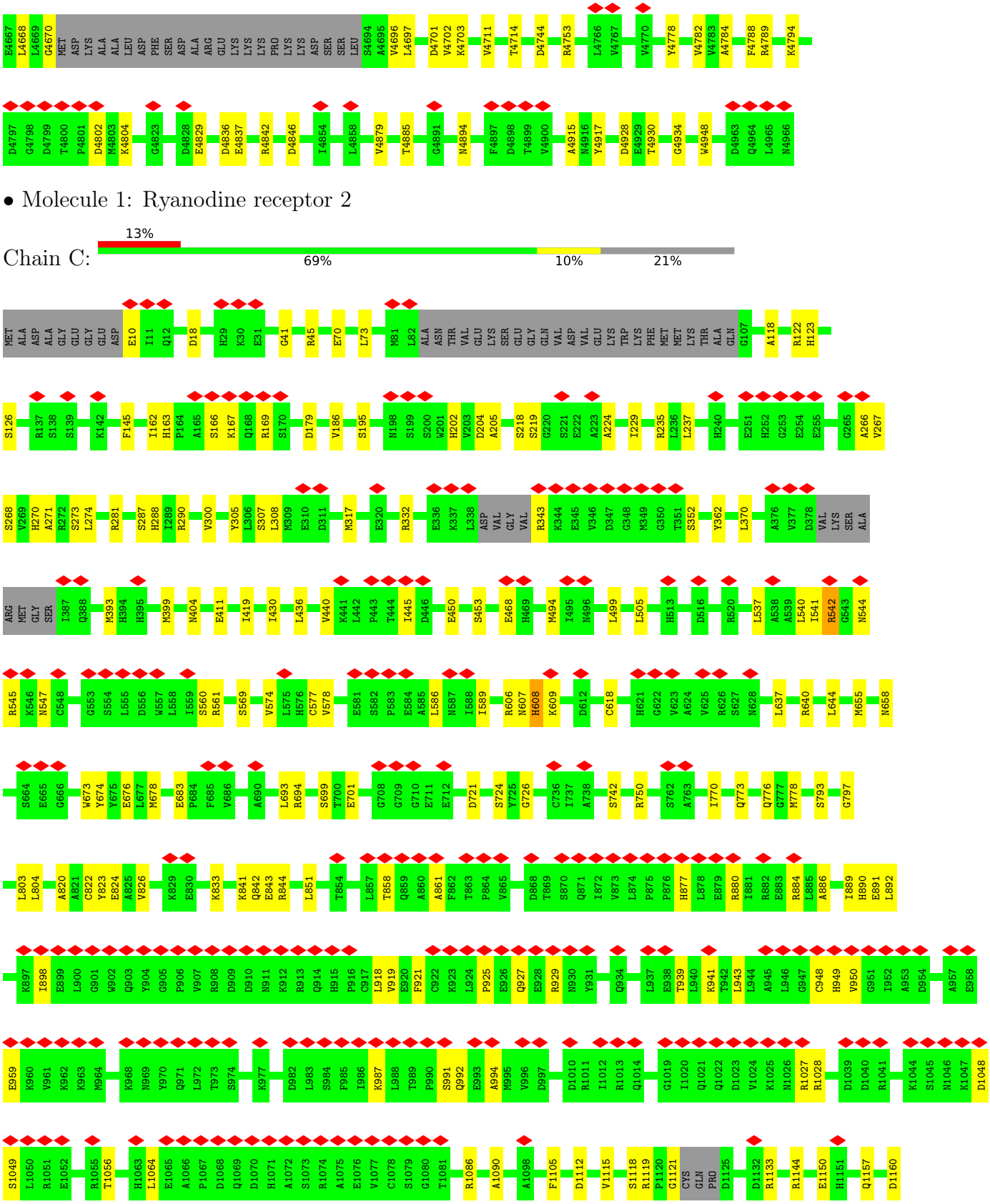
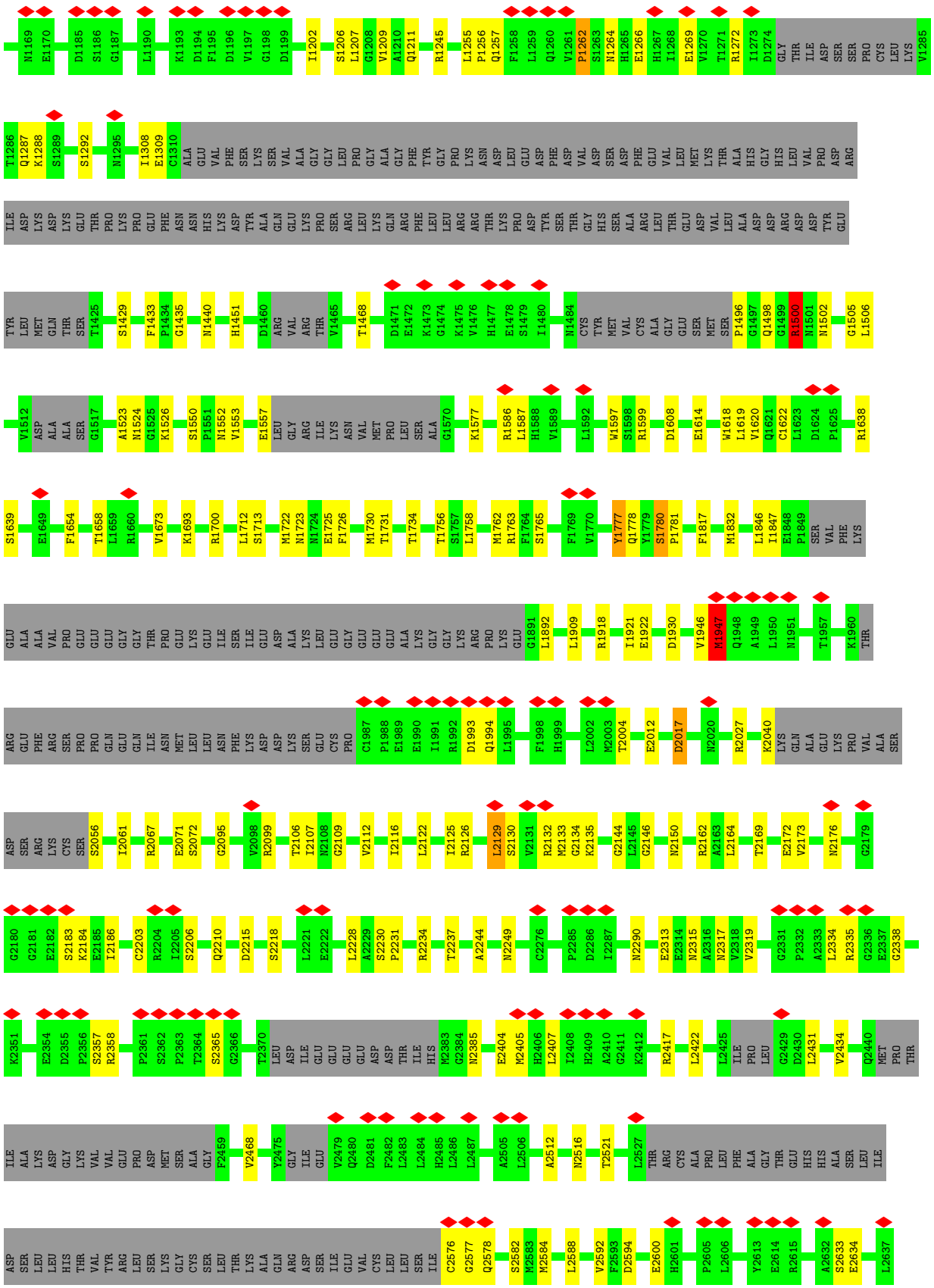
ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU THR HIS
L3174 R3191 V3237 C3242 S3269 L3275
LEU GLY ASN ILE LEU K3281
N3286 L3287 G3288 I3289 D3290 E3291 G3292
ALA TRP MET LYS ARG LEU ALA VAL F3301 S3302 Q3303
I3306 K3340 A3341 E3342 A3343 R3344 M3347 L3353 I3354 L3355 T3360 K3385 P3389
GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE
Y3404 W3405 S3406 K3407 S3408 E3423 I3424 M3427 S3428 F3429 L3430 I3431 T3432 D3433 T3434 K3435 S3436 K3437 M3438 S3439 R3453 M3460
A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 L3477 N3478 I3479 P3482 G3483 A3489 N3493 I3508
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 GLU ASP PRO SER ASP PRO GLU ARG THR
VAL GLU ARG VAL L3551 V3556 L3560 Y3566
THR GLY ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET ALA PRO LEU TYR ASN ASN LEU PRO R3612 K3625 S3626
W3627 I3628 E3629 H3633 Y3634 D3642 A3648 E3649 L3650 P3651 E3652 E3653 D3654 E3655 A3656 M3657 K3658 R3659 K3678 C3679 F3685 C3698
HIS ASP GLU GLU ASP ASP ASP GLY GLU GLU GLU V3710 Q3727 A3728 R3729 L3730 H3731 E3737 G3748 E3749 T3750 V3786 G3787 F3788 F3789 Q3790 S3791
S3800 V3801 L3802 D3803 K3812
ALA GLU GLY LEU GLY MET VAL THR GLU GLU GLY SER GLY GLU LYS VAL LEU GLN D3831 D3832 F3839 Q3843 S3851 N3855 I3870 V3874 D3875 Y3876 V3880 Y3888 S3892 N3904 K3907 V3911 Q3914 V3915 F3916 N3917 T3918 L3919 T3920
Q3924 W3940 V3944 S3958 V3978 L3981 M4018
PHE LEU LYS LEU LYS ASP L4025 T4026 T4030 M4051 A4069 D4072 E4073 N4074 E4075 T4076 L4077 R4085
PHE HIS GLU P4089 F4095 V4099 E4106 N4110 D4111 L4114 F4131 L4132 E4136 R4146
I4151 W4159 Q4163 V4176 N4177 E4178 G4179 G4180 E4181 K4182 E4183 K4184 M4185 V4189 I4205
SER GLU SER ASP LEU ASN GLU ARG LEU ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLN ALA PRO ARG MET GLY PHE PHE SER LEU LEU THR ILE GLN SER ALA LEU PHE
ALA LEU ARG TYR ASN VAL LEU THR LEU VAL ARG MET LEU SER LEU LYS SER LEU LYS LYS GLN MET LYS ARG MET LYS LYS MET THR VAL LYS ASP MET VAL LEU ALA PHE PHE SER SER TYR TRP SER VAL PHE VAL THR LEU LEU HIS PHE VAL ALA SER VAL CYS ARG GLY PHE PHE
ARG ILE VAL SER SER LEU LEU LEU GLY GLY SER LEU VAL GLU GLY SER LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLU GLU GLU GLY GLU ARG LYS PRO LEU GLU SER ALA LEU PRO SER GLU GLU ASP LEU THR ASP LEU
LYS GLU LEU THR GLU GLU SER ASP LEU SER ASP LEU PHE GLY LEU ASP LEU LYS ARG GLU GLY GLN TYR LYS LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET THR ASN PRO VAL PRO VAL PRO GLU VAL GLN GLU SER LYS PHE GLN GLU GLN LYS ALA GLU
GLU LYS GLU GLU LYS GLU GLU THR LYS SER GLU PRO GLU LYS ALA LYS ASP GLU LYS SER LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU SER ALA PHE TRP LYS LYS ILE I4483 Y4498
R4501 S4521
THR SER SER VAL VAL GLU GLY LYS GLU LEU PRO THR ARG THR SER SER ASP THR ALA ALA LYS VAL THR ASN SER LEU ASP SER SER PRO HIS ARG ILE ILE ALA V4556 I4576 I4580 R4607 Y4615 Q4619 P4620 Q4628 R4631 N4635 Y4643 S4666



- Molecule 1: Ryanodine receptor 2

Chain C: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T1286 Q1287 K1288 S1289 S1292 N1295 I1308 E1309 G1310 ALA GLU VAL PHE SER LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG
ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR GLU
TYR LEU MET GLN THR SER T1425 S1429 F1433 P1434 G1435 N1440 H1451 D1460 ARG VAL ARG THR V1465 T1468 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 S1479 I1480 N1484 CYS TYR MET VAL CYS ALA GLY GLU SER MET SER P1496 G1497 Q1498 G1499 R1500 N1501 N1502 G1505 L1506
V1512 ASP ALA ALA SER G1517 A1523 N1524 G1525 K1526 S1550 P1551 N1552 V1553 E1557 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER ALA G1570 K1577 R1586 L1587 H1588 V1589 L1592 W1597 S1598 R1599 D1608 E1614 W1618 L1619 V1620 Q1621 C1622 L1623 D1624 P1625 R1638
S1639 E1649 F1654 T1658 L1659 R1660 V1673 K1693 R1700 L1712 S1713 M1722 N1723 N1724 E1725 F1726 M1730 T1731 T1734 T1756 S1757 L1758 M1762 R1763 F1764 S1765 F1769 V1770 Y1777 Q1778 Y1779 S1780 P1781 F1817 M1832 L1846 I1847 E1848 P1849 SER VAL PHE LYS
GLU ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO LYS GLU G1891 L1892 L1909 R1918 I1921 E1922 D1930 V1946 M1947 Q1948 A1949 L1950 N1951 T1957 K1960 THR
ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO C1987 P1988 E1989 E1990 I1991 R1992 D1993 Q1994 L1995 F1998 H1999 L2002 M2003 T2004 E2012 D2017 N2020 R2027 K2040 LYS GLN ALA GLU LYS PRO VAL ALA SER
ASP SER ARG LYS CYS SER S2056 I2061 R2067 E2071 S2072 G2095 V2098 R2099 T2106 I2107 N2108 G2109 V2112 I2116 L2122 I2125 R2126 L2129 S2130 V2131 R2132 M2133 G2134 K2135 G2144 L2145 G2146 N2150 R2162 A2163 L2164 T2169 E2172 V2173 N2176 G2179
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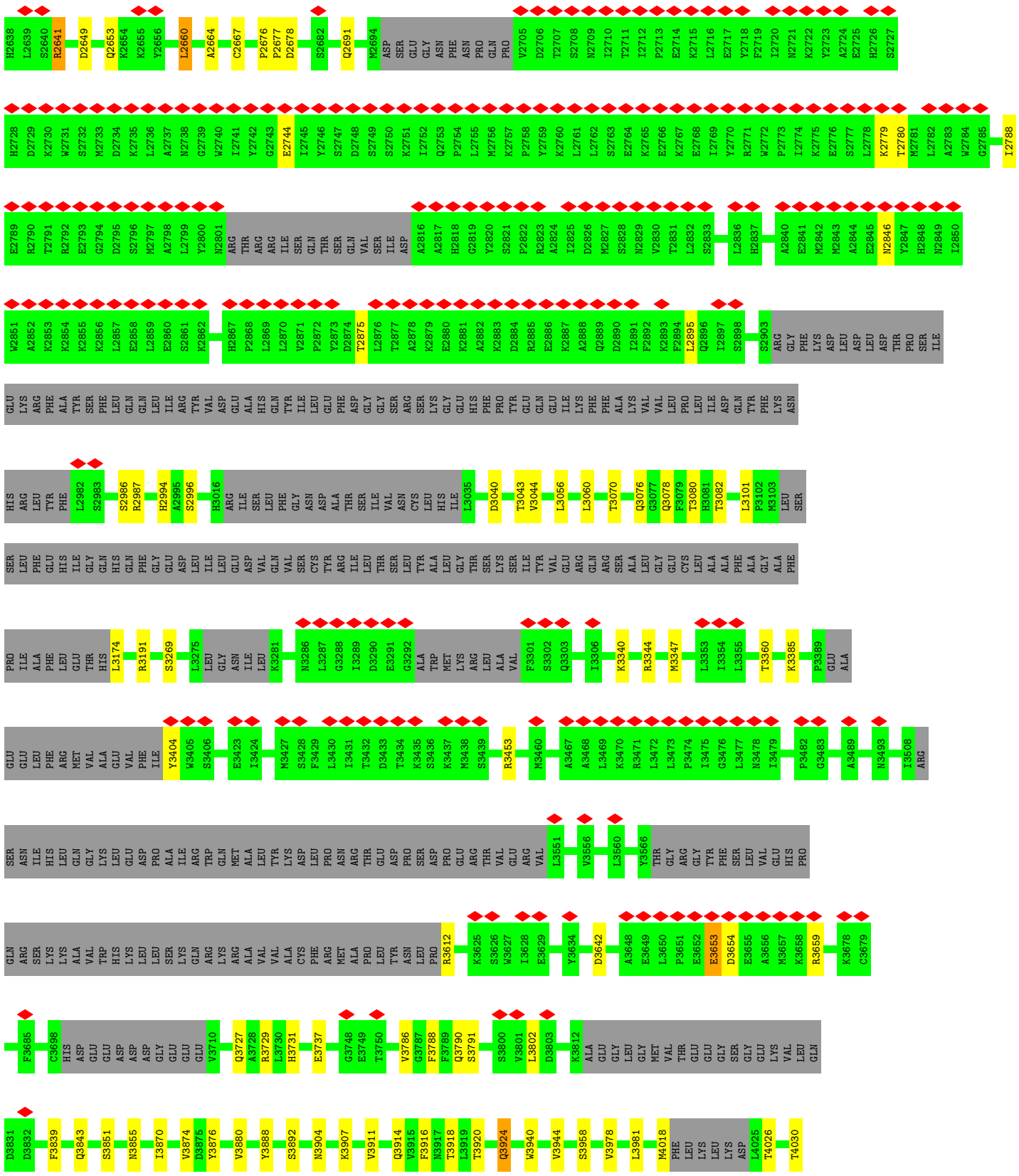
K2351 E2354 D2355 P2356 S2357 R2358 P2361 S2362 P2353 T2364 S2365 G2366 T2370 LEU ASP ILE GLU GLU GLU ASP ASP THR ILE HIS M2383 G2384 N2385 E2404 M2405 H2406 L2407 I2408 H2409 A2410 G2411 K2412 R2417 L2422 L2425 ILE PRO LEU G2429 D2430 L2431 V2434 Q2440 MET PRO THR
ILE ALA LYS ASP GLY LYS VAL VAL GLU PRO ASP MET SER ALA GLY F2459 V2468 Y2475 GLY ILE GLU V2479 Q2480 D2481 F2482 L2483 L2484 H2485 L2486 L2487 A2505 L2506 A2512 N2516 T2521 L2527 THR ARG CYS ALA PRO LEU PHE ALA GLY THR GLU HIS HIS ALA SER LEU ILE
ASP SER LEU LEU HIS THR VAL TYR ARG LEU SER LYS GLY CYS SER LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU SER ILE C2576 G2577 Q2578 S2582 M2583 M2584 L2588 V2592 F2593 D2594 E2600 H2601 P2605 L2606 Y2613 E2614 R2615 A2632 S2633 E2634 L2637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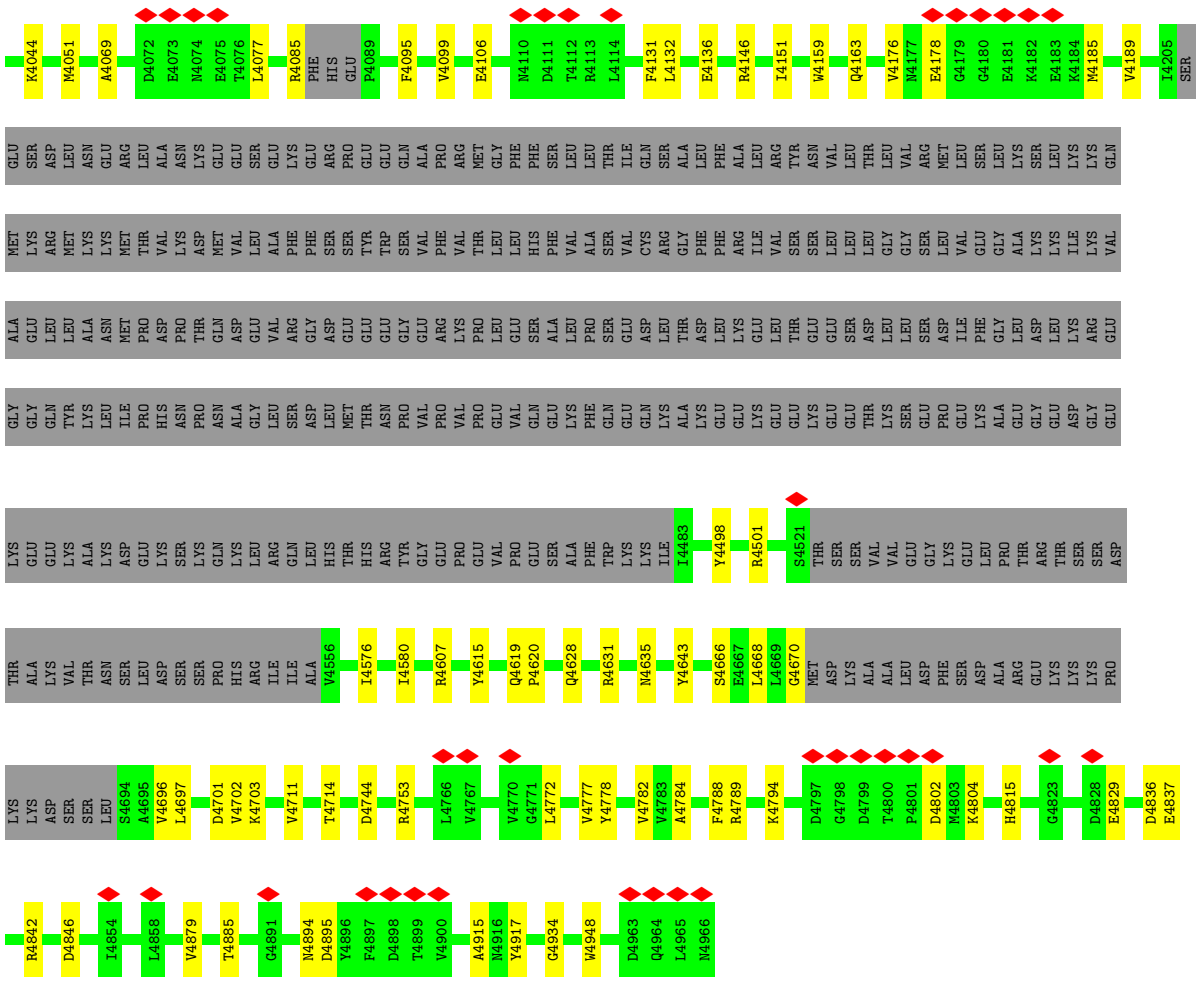
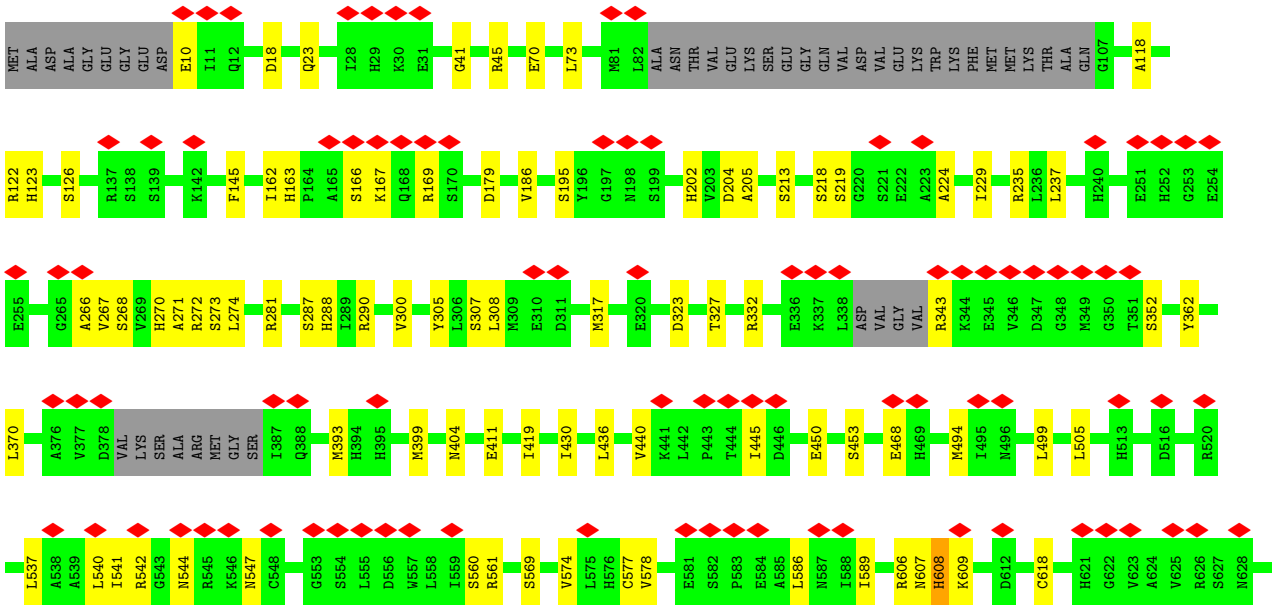
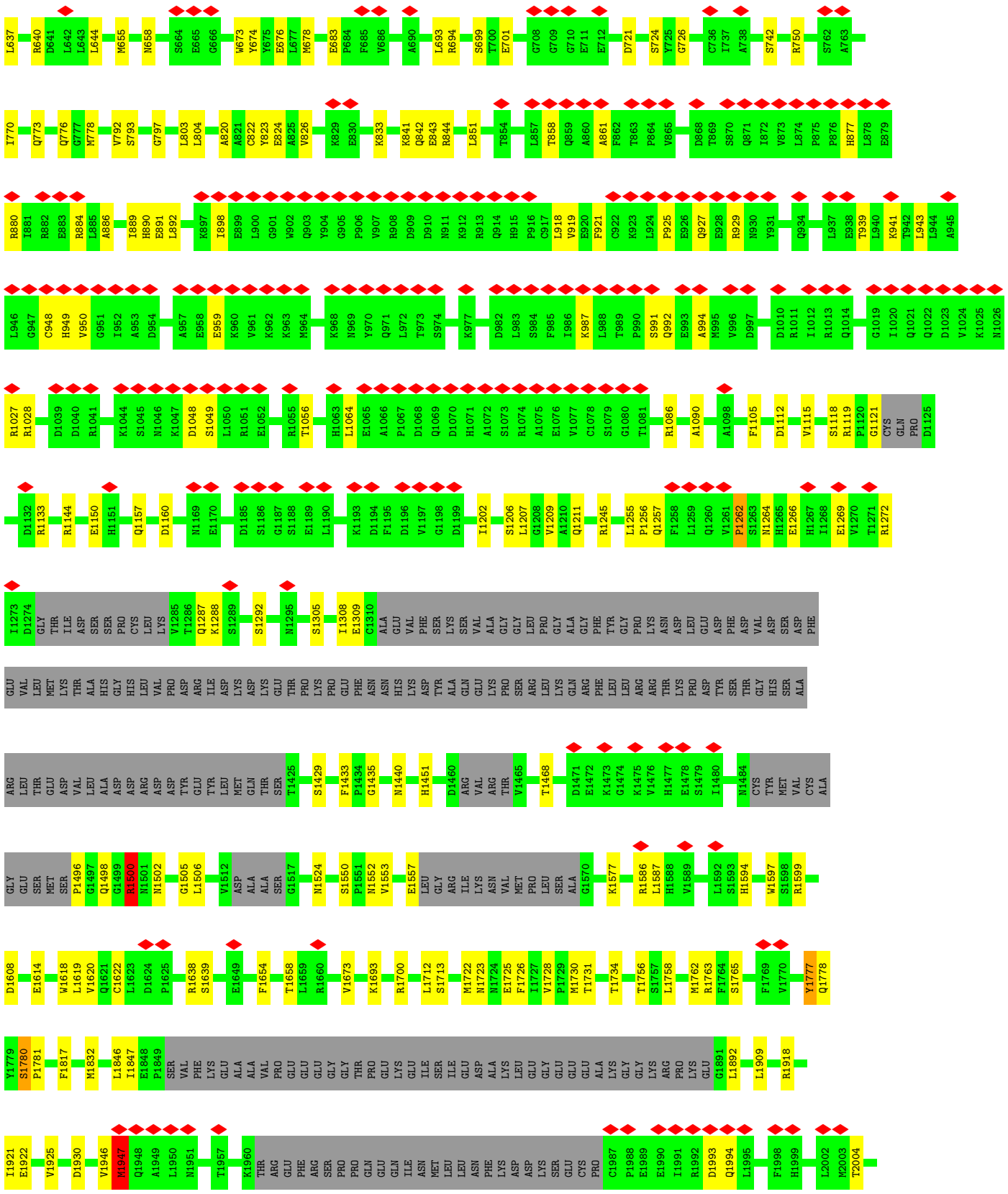
E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP A2816 A2817 H2818 G2819 Y2820 S2821 P2822 R2823 A2824 I2825 D2826 M2827 S2828 N2829 V2830 T2831 L2832 S2833 L2836 H2837 A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850
W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 S2903 ARG GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE
GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN
HIS ARG LEU TYR PHE L2982 S2983 S2986 R2987 H2994 A2995 S2996 H3016 ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE L3035 D3040 T3043 V3044 L3056 L3060 T3070 Q3076 G3077 Q3078 F3079 T3080 H3081 T3082 L3101 P3102 M3103 LEU SER
SER LEU PHE GLU HIS ILE GLY GLN HIS GLN PHE 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 ILE ALA PHE LEU GLU THR HIS L3174 R3191 S3269 L3275 LEU GLY ASN ILE LEU K3281 N3286 L3287 G3288 I3289 D3290 E3291 G3292 ALA TRP MET LYS ARG LEU ALA VAL F3301 S3302 Q3303 I3306 K3340 R3344 M3347 L3353 I3354 L3355 T3360 K3385 P3389 GLU ALA
GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE Y3404 W3405 S3406 E3423 I3424 M3427 S3428 F3429 L3430 I3431 T3432 D3433 T3434 K3435 S3436 K3437 M3438 S3439 R3453 M3460 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 L3477 N3478 I3479 P3482 G3483 A3489 N3493 I3508 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 GLU ASP PRO SER ASP PRO GLU ARG THR VAL GLU ARG VAL L3551 V3556 L3560 Y3566 THR GLY ARG GLY TYR PHE SER LEU VAL GLU HIS PRO
GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET ALA PRO LEU TYR ASN LEU PRO R3612 K3625 S3626 W3627 I3628 E3629 Y3634 D3642 A3648 E3649 L3650 P3651 E3652 E3653 D3654 E3655 A3656 M3657 K3658 R3659 K3678 C3679
F3685 C3698 HIS ASP GLU GLU ASP ASP ASP GLY GLU GLU GLU V3710 Q3727 A3728 R3729 L3730 H3731 E3737 G3748 E3749 T3750 V3786 G3787 F3788 F3789 Q3790 S3791 S3800 V3801 L3802 D3803 K3812 ALA GLU GLY LEU GLY MET VAL THR GLU GLU GLY SER GLY GLU LYS VAL LEU GLN
D3831 D3832 F3839 Q3843 S3851 N3855 I3870 V3874 D3875 Y3876 V3880 Y3888 S3892 N3904 K3907 V3911 Q3914 V3915 F3916 N3917 T3918 L3919 T3920 Q3924 W3940 V3944 S3958 V3978 L3981 M4018 PHE LEU LYS LEU LYS ASP L4025 T4026 T4030



- Molecule 1: Ryanodine receptor 2

Chain D:

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R880 I881 H882 E883 R884 L885 A886 I889 H890 E891 L892 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 C922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 Q934 L937 E938 T939 L940 K941 T942 L943 L944 A945
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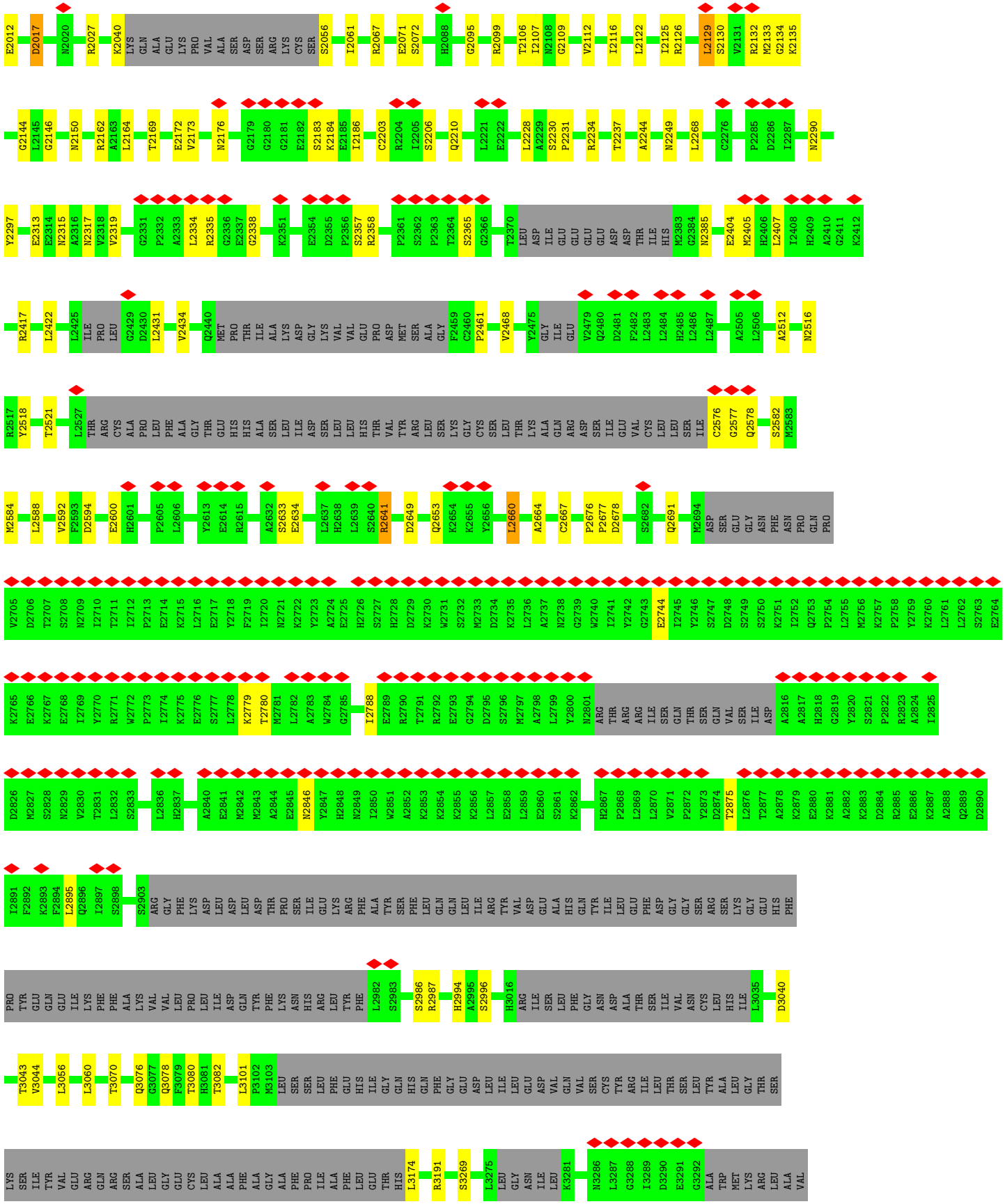
D1132 R1133 R1144 E1150 H1151 Q1157 D1160 N1169 E1170 D1185 S1186 G1187 S1188 E1189 L1190 K1193 D1194 F1195 D1196 V1197 G1198 D1199 I1202 S1206 L1207 G1208 V1209 A1210 Q1211 R1245 L1255 P1256 Q1257 F1258 L1259 Q1260 V1261 P1262 S1263 N1264 H1265 E1266 H1267 I1268 E1269 V1270 T1271 R1272
I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU LYS V1285 T1286 Q1287 K1288 S1289 S1292 N1295 S1305 I1308 E1309 C1310 ALA GLU VAL PHE SER LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE
GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS LYS GLN ARG PHE LEU LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA
ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ASP ASP TYR GLU TYR LEU MET GLN THR SER T1425 S1429 F1433 P1434 G1435 N1440 H1451 D1460 ARG VAL ARG THR V1465 T1468 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 S1479 I1480 N1484 CYS TYR MET VAL CYS ALA
GLY GLU SER MET SER P1496 G1497 Q1498 G1499 R1500 N1501 N1502 G1505 L1506 V1512 ASP ALA ALA SER G1517 N1524 S1550 P1551 N1552 V1553 E1557 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER ALA G1570 K1577 R1586 L1587 H1588 V1589 L1592 S1593 H1594 W1597 S1598 R1599
D1608 E1614 W1618 L1619 V1620 Q1621 C1622 L1623 D1624 P1625 R1638 S1639 E1649 F1654 T1658 L1659 R1660 V1673 K1693 R1700 L1712 S1713 M1722 N1723 N1724 E1725 F1726 I1727 V1728 P1729 M1730 T1731 T1734 T1756 S1757 L1758 M1762 R1763 F1764 S1765 F1769 V1770 Y1777 Q1778
Y1779 S1780 P1781 F1817 M1832 L1846 I1847 E1848 P1849 SER VAL PHE LYS GLU ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE ASN MET LEU LEU GLU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO G1891 L1892 L1909 R1918
I1921 E1922 V1925 D1930 V1946 M1947 Q1948 A1949 L1950 N1951 T1957 K1960 THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO C1987 P1988 E1989 E1990 I1991 R1992 D1993 Q1994 L1995 F1998 H1999 L2002 M2003 T2004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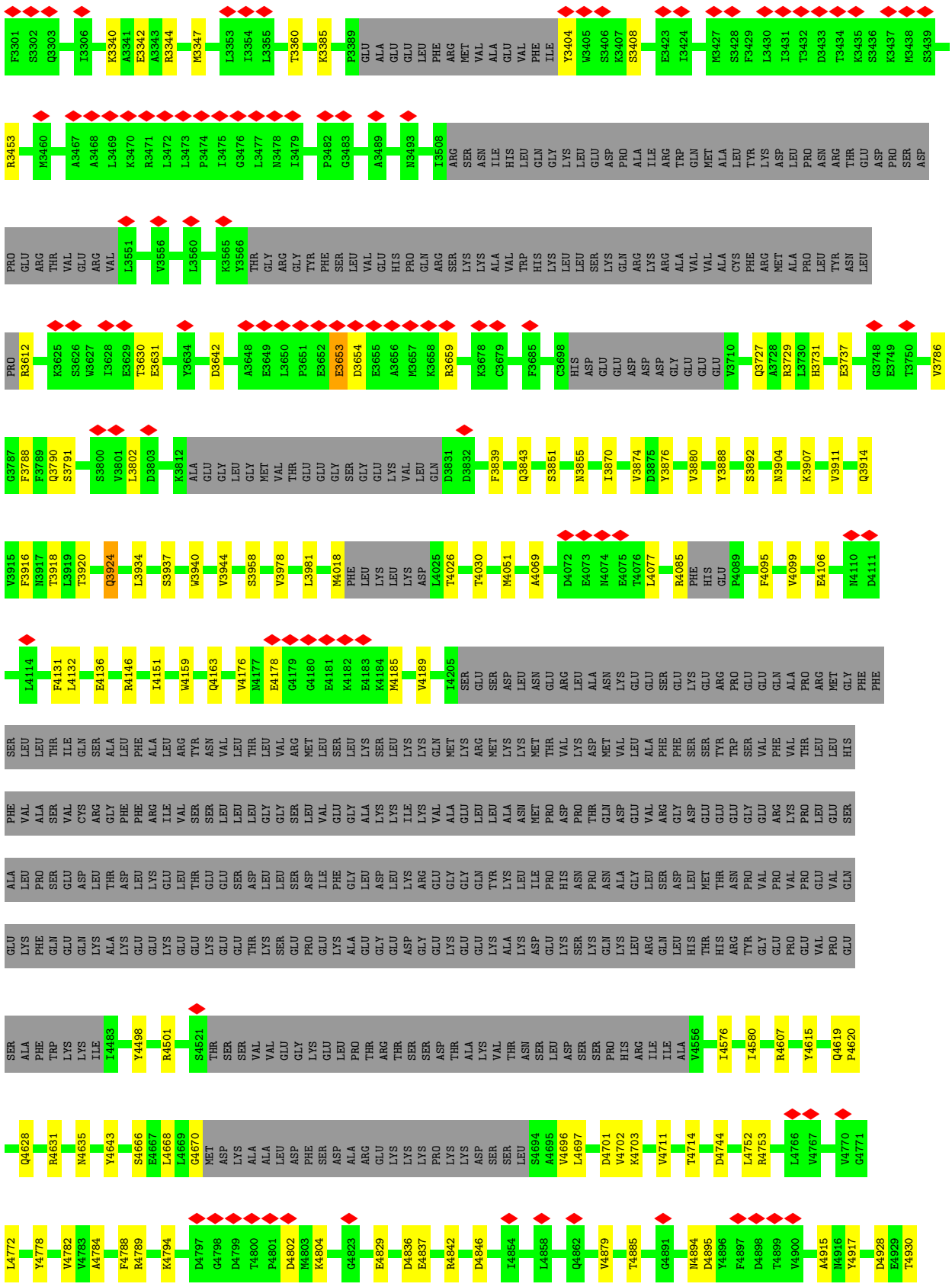
G2144 L2145 G2146 N2150 R2162 A2163 L2164 T2169 E2172 V2173 N2176 G2179 G2180 G2181 E2182 S2183 K2184 E2185 I2186 C2203 R2204 I2205 S2206 Q2210 L2221 E2222 L2228 A2229 S2230 P2231 R2234 T2237 A2244 N2249 L2268 C2276 P2285 D2286 I2287 N2290
Y2297 E2313 E2314 N2315 A2316 N2317 V2318 V2319 G2331 P2332 A2333 L2334 R2335 G2336 E2337 G2338 K2351 E2354 D2355 P2356 S2357 R2358 P2361 S2362 P2363 T2364 S2365 G2366 T2370 LEU ASP ILE GLU GLU GLU ASP ASP THR ILE HIS M2383 G2384 N2385 E2404 M2405 H2406 L2407 I2408 H2409 A2410 G2411 K2412
R2417 L2422 L2425 ILE PRO LEU G2429 D2430 L2431 V2434 Q2440 MET PRO THR ILE ALA LYS ASP GLY LYS VAL VAL GLU PRO ASP MET SER ALA GLY F2459 C2460 P2461 V2468 Y2475 GLY ILE GLU V2479 Q2480 D2481 F2482 L2483 L2484 H2485 L2486 L2487 A2505 L2506 A2512 N2516
R2517 Y2518 T2521 L2527 THR ARG CYS ALA PRO LEU PHE ALA GLY THR GLU HIS HIS ALA SER LEU ILE ASP SER LEU LEU LEU HIS THR VAL TYR ARG LEU SER LYS GLY CYS SER LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU SER ILE C2576 G2577 Q2578 S2582 M2583
M2584 L2588 V2592 F2593 D2594 E2600 H2601 P2605 L2606 Y2613 E2614 R2615 A2632 S2633 E2634 L2637 H2638 L2639 S2640 R2641 D2649 Q2653 K2654 K2655 Y2656 L2660 A2664 C2667 P2676 P2677 D2678 S2682 Q2691 M2694 ASP SER GLU GLY ASN PHE ASN PRO GLN PRO
V2705 D2706 T2707 S2708 N2709 I2710 T2711 I2712 P2713 E2714 K2715 L2716 E2717 Y2718 F2719 I2720 N2721 K2722 Y2723 A2724 E2725 H2726 S2727 H2728 D2729 K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 K2757 P2758 Y2759 K2760 L2761 L2762 S2763 E2764
K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782 A2783 W2784 G2785 I2788 E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP A2816 A2817 H2818 G2819 Y2820 S2821 P2822 R2823 A2824 I2825
D2826 M2827 S2828 N2829 V2830 T2831 L2832 S2833 L2836 H2837 A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890
I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 S2903 ARG GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE
PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE L2982 S2983 S2986 R2987 H2994 A2995 S2996 H3016 ARG ILE SER LEU PHE GLY L3035 D3040
T3043 V3044 L3056 L3060 T3070 Q3076 G3077 Q3078 F3079 T3080 H3081 T3082 L3101 P3102 M3103 LEU SER SER LEU PHE GLU HIS ILE GLY GLN HIS GLN PHE GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL SER 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 ILE ALA PHE LEU GLU THR HIS L3174 R3191 S3269 L3275 LEU GLY ASN ILE LEU K3281 N3286 L3287 G3288 I3289 D3290 E3291 G3292 ALA TRP MET LYS ARG LEU ALA VAL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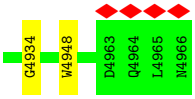
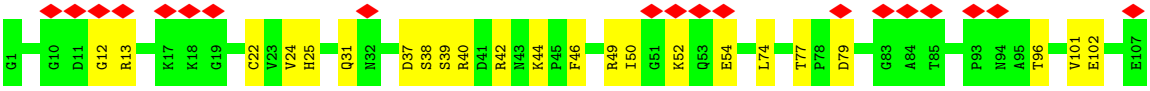
R3453 M3460 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 L3477 N3478 I3479 P3482 G3483 A3489 N3493 I3508 ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP PRO SER ASP
PRO GLU ARG THR VAL GLU ARG VAL L3551 V3556 L3560 K3565 Y3566 THR GLY ARG ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET ALA PRO LEU TYR ASN LEU
PRO R3612 K3625 S3626 W3627 I3628 E3629 T3630 E3631 Y3634 D3642 A3648 E3649 L3650 P3651 E3652 E3653 D3654 E3655 A3656 M3657 K3658 R3659 K3678 C3679 F3685 C3698 HIS ASP GLU GLU ASP ASP GLY GLU GLU GLU V3710 Q3727 A3728 R3729 L3730 H3731 E3737 G3748 E3749 T3750 V3786
G3787 F3788 F3789 Q3790 S3791 S3800 V3801 L3802 D3803 K3812 ALA GLU GLY LEU GLY MET VAL THR GLU GLU GLY SER GLY GLU LYS VAL LEU GLN D3831 D3832 F3839 Q3843 S3851 N3855 I3870 V3874 D3875 Y3876 V3880 Y3888 S3892 N3904 K3907 V3911 Q3914
V3915 F3916 N3917 T3918 L3919 T3920 Q3924 L3934 S3937 W3940 V3944 S3958 V3978 L3981 M4018 PHE LEU LYS LEU LYS ASP L4025 T4026 T4030 M4051 A4069 D4072 E4073 N4074 E4075 T4076 L4077 R4085 PHE HIS GLU P4089 F4095 V4099 E4106 N4110 D4111
L4114 F4131 L4132 E4136 R4146 I4151 W4159 Q4163 V4176 N4177 E4178 G4179 G4180 E4181 K4182 E4183 K4184 M4185 V4189 I4205 SER GLU SER ASP LEU ASN GLU ARG LEU ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLN ALA PRO ARG MET GLY PHE PHE
SER LEU LEU THR ILE GLN SER ALA LEU PHE ALA LEU ARG TYR ASN VAL LEU THR LEU VAL ARG MET LEU SER LEU LYS SER LEU LYS LYS GLN MET LYS ARG MET LYS LYS MET THR VAL LYS ASP MET VAL LEU ALA PHE PHE SER SER TYR TRP SER VAL PHE VAL THR LEU LEU HIS
PHE VAL ALA SER VAL CYS ARG GLY PHE PHE ARG ILE VAL SER SER LEU LEU LEU GLY GLY SER LEU LEU GLU GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLU GLU GLY GLU ARG LYS PRO LEU LEU GLU SER
ALA LEU PRO SER GLU ASP LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU SER ASP LEU LEU ASP LEU LYS ARG GLU GLY GLY GLN TYR LYS LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET THR ASN PRO VAL PRO VAL PRO GLU VAL GLN
GLU LYS PHE GLN GLU GLN LYS ALA LYS GLU GLU LYS GLU GLU LYS GLU THR LYS SER GLU PRO GLU LYS ALA GLU GLY GLU GLU LYS LYS GLU GLU ALA LYS ASP GLU LYS SER LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU
SER ALA PHE TRP LYS LYS ILE I4483 Y4498 R4501 S4521 THR SER SER VAL VAL GLU GLY LYS GLU LEU PRO THR ARG THR SER ASP THR ALA LYS VAL THR ASN SER LEU ASP SER SER PRO HIS ARG ILE ILE ALA V4556 I4576 I4580 R4607 Y4615 Q4619 P4620
Q4628 R4631 N4635 Y4643 S4666 E4667 L4668 L4669 G4670 MET ASP LYS ALA ALA LEU ASP PHE SER ASP ALA ARG GLU LYS LYS LYS PRO LYS LYS ASP SER SER LEU S4694 A4695 V4696 L4697 D4701 V4702 K4703 V4711 T4714 D4744 L4752 R4753 L4766 V4767 V4770 G4771
L4772 Y4778 V4782 V4783 A4784 F4788 R4789 K4794 D4797 G4798 D4799 T4800 P4801 D4802 M4803 K4804 G4823 E4829 D4836 E4837 R4842 D4846 I4854 L4858 Q4862 V4879 T4885 G4891 N4894 D4895 Y4896 F4897 D4898 T4899 V4900 A4915 N4916 Y4917 D4928 E4929 T4930



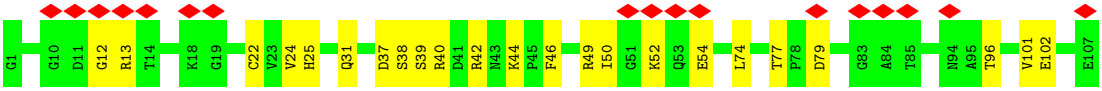
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



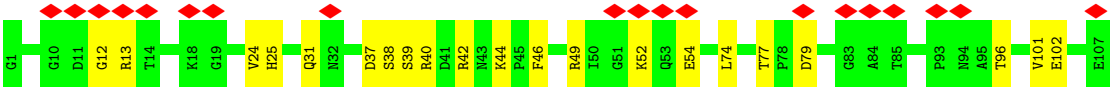
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



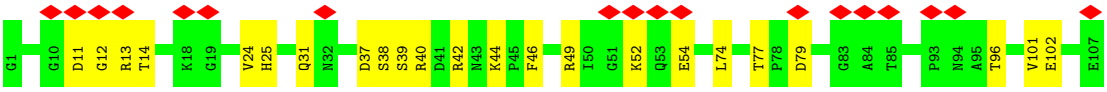
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

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, C4	Depositor
Number of particles used	103845	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	24.070	Depositor
Minimum map value	-7.125	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	484.70398, 484.70398, 484.70398	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.377, 1.377, 1.377	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.35	0/31108	0.68	15/42056 (0.0%)
1	B	0.35	0/31108	0.68	14/42056 (0.0%)
1	C	0.35	0/31108	0.68	13/42056 (0.0%)
1	D	0.35	0/31108	0.68	14/42056 (0.0%)
2	E	0.35	0/834	0.67	0/1123
2	F	0.35	0/834	0.67	0/1123
2	G	0.35	0/834	0.67	0/1123
2	H	0.35	0/834	0.67	0/1123
All	All	0.35	0/127768	0.68	56/172716 (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	15
1	B	0	15
1	C	0	15
1	D	0	15
All	All	0	60

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2660	LEU	CA-CB-CG	9.27	136.63	115.30
1	D	2660	LEU	CA-CB-CG	9.27	136.63	115.30
1	A	2660	LEU	CA-CB-CG	9.27	136.62	115.30
1	B	2660	LEU	CA-CB-CG	9.25	136.57	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1500	ARG	N-CA-C	7.46	131.14	111.00
1	C	1500	ARG	N-CA-C	7.46	131.14	111.00
1	D	1500	ARG	N-CA-C	7.45	131.12	111.00
1	A	1500	ARG	N-CA-C	7.45	131.12	111.00
1	C	1496	PRO	N-CA-CB	6.04	110.55	103.30
1	D	1086	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	4753	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	D	1496	PRO	N-CA-CB	6.03	110.54	103.30
1	B	1496	PRO	N-CA-CB	6.01	110.51	103.30
1	A	1496	PRO	N-CA-CB	6.01	110.51	103.30
1	B	1086	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	B	2067	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	2067	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	C	2067	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	1086	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	1086	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	2067	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	4753	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	D	4753	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	4753	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	2129	LEU	CA-CB-CG	5.75	128.53	115.30
1	A	2129	LEU	CA-CB-CG	5.75	128.52	115.30
1	C	2129	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	2129	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	750	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	750	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	750	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	4802	ASP	CB-CG-OD1	5.26	123.03	118.30
1	B	4802	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	4802	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	4802	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	750	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	272	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	2641	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	540	LEU	CA-CB-CG	5.16	127.16	115.30
1	D	540	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	540	LEU	CA-CB-CG	5.14	127.13	115.30
1	B	540	LEU	CA-CB-CG	5.12	127.08	115.30
1	B	2641	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	2641	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	D	2641	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	3653	GLU	CA-CB-CG	5.06	124.53	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	3653	GLU	CA-CB-CG	5.06	124.53	113.40
1	B	3653	GLU	CA-CB-CG	5.05	124.51	113.40
1	D	3653	GLU	CA-CB-CG	5.05	124.50	113.40
1	A	272	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	2133	MET	C-N-CA	5.03	132.86	122.30
1	D	2133	MET	C-N-CA	5.03	132.86	122.30
1	A	1998	PHE	CB-CG-CD2	5.02	124.32	120.80
1	B	2133	MET	C-N-CA	5.02	132.84	122.30
1	B	272	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	2133	MET	C-N-CA	5.01	132.83	122.30

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1266	GLU	Peptide
1	A	1500	ARG	Peptide
1	A	1502	ASN	Peptide
1	A	1552	ASN	Peptide
1	A	1777	TYR	Peptide
1	A	1780	SER	Peptide
1	A	1947	MET	Peptide
1	A	2132	ARG	Peptide
1	A	2134	GLY	Peptide
1	A	2234	ARG	Peptide
1	A	2385	ASN	Peptide
1	A	3924	GLN	Peptide
1	A	544	ASN	Peptide
1	A	608	HIS	Peptide
1	A	618	CYS	Peptide
1	B	1266	GLU	Peptide
1	B	1500	ARG	Peptide
1	B	1502	ASN	Peptide
1	B	1552	ASN	Peptide
1	B	1777	TYR	Peptide
1	B	1780	SER	Peptide
1	B	1947	MET	Peptide
1	B	2132	ARG	Peptide
1	B	2134	GLY	Peptide
1	B	2234	ARG	Peptide
1	B	2385	ASN	Peptide
1	B	3924	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	B	544	ASN	Peptide
1	B	608	HIS	Peptide
1	B	618	CYS	Peptide
1	C	1266	GLU	Peptide
1	C	1500	ARG	Peptide
1	C	1502	ASN	Peptide
1	C	1552	ASN	Peptide
1	C	1777	TYR	Peptide
1	C	1780	SER	Peptide
1	C	1947	MET	Peptide
1	C	2132	ARG	Peptide
1	C	2134	GLY	Peptide
1	C	2234	ARG	Peptide
1	C	2385	ASN	Peptide
1	C	3924	GLN	Peptide
1	C	544	ASN	Peptide
1	C	608	HIS	Peptide
1	C	618	CYS	Peptide
1	D	1266	GLU	Peptide
1	D	1500	ARG	Peptide
1	D	1502	ASN	Peptide
1	D	1552	ASN	Peptide
1	D	1777	TYR	Peptide
1	D	1780	SER	Peptide
1	D	1947	MET	Peptide
1	D	2132	ARG	Peptide
1	D	2134	GLY	Peptide
1	D	2234	ARG	Peptide
1	D	2385	ASN	Peptide
1	D	3924	GLN	Peptide
1	D	544	ASN	Peptide
1	D	608	HIS	Peptide
1	D	618	CYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30492	29277	29270	263	0
1	B	30492	29280	29270	272	0
1	C	30492	29281	29270	269	0
1	D	30492	29278	29270	276	0
2	E	818	824	824	14	0
2	F	818	824	824	14	0
2	G	818	824	824	13	0
2	H	818	824	824	14	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
All	All	125244	120412	120376	1129	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 5.

All (1129) 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:B:644:LEU:HD11	1:B:1658:THR:HG21	1.70	0.74
1:C:644:LEU:HD11	1:C:1658:THR:HG21	1.69	0.73
1:A:644:LEU:HD11	1:A:1658:THR:HG21	1.69	0.73
1:C:2106:THR:OG1	1:C:3612:ARG:O	2.06	0.73
1:B:288:HIS:O	1:B:290:ARG:NH1	2.22	0.72
1:D:644:LEU:HD11	1:D:1658:THR:HG21	1.69	0.72
1:D:288:HIS:O	1:D:290:ARG:NH1	2.22	0.72
1:C:288:HIS:O	1:C:290:ARG:NH1	2.22	0.72
1:A:288:HIS:O	1:A:290:ARG:NH1	2.22	0.71
1:A:2106:THR:OG1	1:A:3612:ARG:O	2.06	0.71
2:E:52:LYS:NZ	2:E:54:GLU:OE1	2.24	0.71
1:D:2106:THR:OG1	1:D:3612:ARG:O	2.06	0.71
1:A:778:MET:O	1:A:1468:THR:OG1	2.10	0.70
1:D:1713:SER:HG	1:D:1777:TYR:HH	1.38	0.70
2:F:52:LYS:NZ	2:F:54:GLU:OE1	2.24	0.70
1:C:778:MET:O	1:C:1468:THR:OG1	2.10	0.70
1:B:778:MET:O	1:B:1468:THR:OG1	2.10	0.70
1:D:778:MET:O	1:D:1468:THR:OG1	2.10	0.69
2:H:52:LYS:NZ	2:H:54:GLU:OE1	2.24	0.69
1:A:2313:GLU:O	1:A:2317:ASN:ND2	2.26	0.69
1:D:2313:GLU:O	1:D:2317:ASN:ND2	2.26	0.69
1:B:1700:ARG:NH1	1:B:1817:PHE:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1700:ARG:NH1	1:C:1817:PHE:O	2.26	0.69
1:B:890:HIS:NE2	1:B:919:VAL:O	2.26	0.69
1:D:890:HIS:NE2	1:D:919:VAL:O	2.26	0.69
2:G:52:LYS:NZ	2:G:54:GLU:OE1	2.24	0.69
1:A:890:HIS:NE2	1:A:919:VAL:O	2.26	0.68
1:B:2313:GLU:O	1:B:2317:ASN:ND2	2.26	0.68
1:C:890:HIS:NE2	1:C:919:VAL:O	2.26	0.68
1:D:4607:ARG:NE	1:D:4643:TYR:OH	2.27	0.68
1:C:2313:GLU:O	1:C:2317:ASN:ND2	2.26	0.68
1:D:1700:ARG:NH1	1:D:1817:PHE:O	2.26	0.68
1:A:1700:ARG:NH1	1:A:1817:PHE:O	2.26	0.68
1:A:721:ASP:O	1:A:724:SER:OG	2.12	0.68
1:C:1112:ASP:OD2	1:C:1211:GLN:NE2	2.27	0.68
1:B:858:THR:OG1	1:B:861:ALA:O	2.12	0.68
1:B:1112:ASP:OD2	1:B:1211:GLN:NE2	2.27	0.68
1:A:1112:ASP:OD2	1:A:1211:GLN:NE2	2.27	0.67
1:A:4607:ARG:NE	1:A:4643:TYR:OH	2.27	0.67
1:D:1756:THR:OG1	1:D:1922:GLU:OE2	2.12	0.67
1:D:1112:ASP:OD2	1:D:1211:GLN:NE2	2.27	0.67
1:B:721:ASP:O	1:B:724:SER:OG	2.12	0.67
1:B:4607:ARG:NE	1:B:4643:TYR:OH	2.27	0.67
1:C:2649:ASP:O	1:C:2653:GLN:NE2	2.28	0.67
1:D:858:THR:OG1	1:D:861:ALA:O	2.12	0.67
1:D:2004:THR:OG1	1:D:2012:GLU:OE1	2.13	0.67
1:D:2649:ASP:O	1:D:2653:GLN:NE2	2.28	0.67
1:B:1756:THR:OG1	1:B:1922:GLU:OE2	2.12	0.67
1:C:721:ASP:O	1:C:724:SER:OG	2.12	0.67
1:C:3101:LEU:O	1:C:3174:LEU:N	2.28	0.67
2:F:37:ASP:OD1	2:F:42:ARG:NH2	2.28	0.67
1:C:4607:ARG:NE	1:C:4643:TYR:OH	2.27	0.67
1:B:770:ILE:O	1:B:773:GLN:NE2	2.28	0.67
1:D:770:ILE:O	1:D:773:GLN:NE2	2.28	0.67
1:D:3101:LEU:O	1:D:3174:LEU:N	2.28	0.67
2:G:37:ASP:OD1	2:G:42:ARG:NH2	2.28	0.67
1:A:1756:THR:OG1	1:A:1922:GLU:OE2	2.12	0.66
1:B:2649:ASP:O	1:B:2653:GLN:NE2	2.28	0.66
1:A:797:GLY:N	1:A:1622:CYS:O	2.29	0.66
1:A:2649:ASP:O	1:A:2653:GLN:NE2	2.28	0.66
1:B:2106:THR:OG1	1:B:3612:ARG:O	2.06	0.66
1:D:721:ASP:O	1:D:724:SER:OG	2.12	0.66
2:H:37:ASP:OD1	2:H:42:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1257:GLN:O	1:C:1597:TRP:N	2.29	0.66
1:C:1287:GLN:NE2	1:C:1288:LYS:O	2.28	0.66
1:B:797:GLY:N	1:B:1622:CYS:O	2.29	0.66
1:B:1257:GLN:O	1:B:1597:TRP:N	2.29	0.66
1:A:770:ILE:O	1:A:773:GLN:NE2	2.28	0.66
1:C:4131:PHE:O	1:C:4151:ILE:N	2.28	0.66
1:D:4131:PHE:O	1:D:4151:ILE:N	2.28	0.66
2:E:37:ASP:OD1	2:E:42:ARG:NH2	2.28	0.66
1:A:858:THR:OG1	1:A:861:ALA:O	2.12	0.66
1:A:3851:SER:O	1:A:3855:ASN:ND2	2.29	0.66
1:D:1257:GLN:O	1:D:1597:TRP:N	2.29	0.66
1:A:1257:GLN:O	1:A:1597:TRP:N	2.29	0.66
1:B:3101:LEU:O	1:B:3174:LEU:N	2.28	0.66
1:C:1756:THR:OG1	1:C:1922:GLU:OE2	2.12	0.66
1:D:3851:SER:O	1:D:3855:ASN:ND2	2.29	0.66
1:C:797:GLY:N	1:C:1622:CYS:O	2.29	0.66
1:C:2004:THR:OG1	1:C:2012:GLU:OE1	2.13	0.66
1:A:4615:TYR:O	1:A:4619:GLN:NE2	2.29	0.66
1:B:2004:THR:OG1	1:B:2012:GLU:OE1	2.13	0.66
1:D:797:GLY:N	1:D:1622:CYS:O	2.29	0.66
2:F:24:VAL:O	2:F:46:PHE:N	2.29	0.66
1:A:4131:PHE:O	1:A:4151:ILE:N	2.28	0.66
1:B:4615:TYR:O	1:B:4619:GLN:NE2	2.29	0.65
1:A:1287:GLN:NE2	1:A:1288:LYS:O	2.28	0.65
1:A:2004:THR:OG1	1:A:2012:GLU:OE1	2.13	0.65
1:B:4131:PHE:O	1:B:4151:ILE:N	2.28	0.65
1:C:4615:TYR:O	1:C:4619:GLN:NE2	2.29	0.65
1:C:4136:GLU:O	1:C:4917:TYR:OH	2.15	0.65
1:D:4615:TYR:O	1:D:4619:GLN:NE2	2.29	0.65
1:A:3101:LEU:O	1:A:3174:LEU:N	2.28	0.65
1:C:3851:SER:O	1:C:3855:ASN:ND2	2.28	0.65
1:D:1287:GLN:NE2	1:D:1288:LYS:O	2.28	0.65
1:D:4136:GLU:O	1:D:4917:TYR:OH	2.15	0.65
2:G:24:VAL:O	2:G:46:PHE:N	2.29	0.65
2:H:24:VAL:O	2:H:46:PHE:N	2.29	0.65
1:C:770:ILE:O	1:C:773:GLN:NE2	2.28	0.65
1:B:4136:GLU:O	1:B:4917:TYR:OH	2.15	0.65
2:E:24:VAL:O	2:E:46:PHE:N	2.29	0.65
1:A:4136:GLU:O	1:A:4917:TYR:OH	2.15	0.65
1:B:1287:GLN:NE2	1:B:1288:LYS:O	2.28	0.65
1:B:3851:SER:O	1:B:3855:ASN:ND2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2576:CYS:SG	1:D:2578:GLN:NE2	2.70	0.65
1:A:2576:CYS:SG	1:A:2578:GLN:NE2	2.70	0.65
1:B:948:CYS:SG	1:B:949:HIS:N	2.70	0.64
1:C:2576:CYS:SG	1:C:2578:GLN:NE2	2.70	0.64
1:B:2576:CYS:SG	1:B:2578:GLN:NE2	2.70	0.64
1:C:948:CYS:SG	1:C:949:HIS:N	2.71	0.64
1:C:300:VAL:HG21	1:C:419:ILE:HD12	1.80	0.64
2:H:31:GLN:OE1	2:H:96:THR:OG1	2.15	0.64
1:D:300:VAL:HG21	1:D:419:ILE:HD12	1.80	0.64
2:F:31:GLN:OE1	2:F:96:THR:OG1	2.15	0.64
1:D:948:CYS:SG	1:D:949:HIS:N	2.70	0.64
1:A:948:CYS:SG	1:A:949:HIS:N	2.70	0.64
2:G:31:GLN:OE1	2:G:96:THR:OG1	2.15	0.64
1:B:300:VAL:HG21	1:B:419:ILE:HD12	1.80	0.64
1:A:1309:GLU:OE1	1:A:1577:LYS:N	2.31	0.64
1:C:858:THR:OG1	1:C:861:ALA:O	2.12	0.64
1:A:1027:ARG:NH2	1:A:1028:ARG:O	2.31	0.63
1:A:300:VAL:HG21	1:A:419:ILE:HD12	1.80	0.63
1:B:1027:ARG:NH2	1:B:1028:ARG:O	2.31	0.63
1:B:3191:ARG:NE	1:B:3191:ARG:O	2.32	0.63
1:D:1027:ARG:NH2	1:D:1028:ARG:O	2.31	0.63
2:E:31:GLN:OE1	2:E:96:THR:OG1	2.15	0.63
1:D:1309:GLU:OE1	1:D:1577:LYS:N	2.31	0.63
1:C:1713:SER:HG	1:C:1777:TYR:HH	1.46	0.63
1:C:4099:VAL:HG22	1:C:4132:LEU:HD13	1.80	0.63
1:A:362:TYR:OH	1:A:399:MET:O	2.16	0.63
1:C:1309:GLU:OE1	1:C:1577:LYS:N	2.31	0.63
1:A:3191:ARG:O	1:A:3191:ARG:NE	2.32	0.63
1:B:1713:SER:HG	1:B:1777:TYR:HH	1.46	0.63
1:C:1500:ARG:O	1:C:1524:ASN:ND2	2.32	0.63
1:C:1027:ARG:NH2	1:C:1028:ARG:O	2.31	0.62
1:D:3191:ARG:O	1:D:3191:ARG:NE	2.32	0.62
1:B:1500:ARG:O	1:B:1524:ASN:ND2	2.32	0.62
1:B:4099:VAL:HG22	1:B:4132:LEU:HD13	1.80	0.62
1:D:362:TYR:OH	1:D:399:MET:O	2.16	0.62
1:D:1500:ARG:O	1:D:1524:ASN:ND2	2.32	0.62
1:C:3191:ARG:O	1:C:3191:ARG:NE	2.32	0.62
1:B:1309:GLU:OE1	1:B:1577:LYS:N	2.31	0.62
1:C:3642:ASP:OD1	1:C:3729:ARG:NH1	2.33	0.62
1:C:362:TYR:OH	1:C:399:MET:O	2.16	0.62
1:A:1500:ARG:O	1:A:1524:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:HIS:ND1	1:B:126:SER:OG	2.33	0.62
1:D:4099:VAL:HG22	1:D:4132:LEU:HD13	1.80	0.62
1:D:3642:ASP:OD1	1:D:3729:ARG:NH1	2.33	0.62
1:A:4099:VAL:HG22	1:A:4132:LEU:HD13	1.80	0.61
1:B:145:PHE:O	1:B:205:ALA:N	2.33	0.61
1:B:3642:ASP:OD1	1:B:3729:ARG:NH1	2.33	0.61
1:D:2358:ARG:NH1	1:D:2365:SER:O	2.33	0.61
1:A:3642:ASP:OD1	1:A:3729:ARG:NH1	2.33	0.61
1:C:123:HIS:ND1	1:C:126:SER:OG	2.33	0.61
1:D:145:PHE:O	1:D:205:ALA:N	2.33	0.61
1:A:1765:SER:OG	1:A:1780:SER:O	2.18	0.61
1:D:3385:LYS:O	1:D:3453:ARG:NH1	2.34	0.61
1:A:3360:THR:O	1:A:3404:TYR:OH	2.18	0.61
1:A:3385:LYS:O	1:A:3453:ARG:NH1	2.34	0.61
1:B:281:ARG:NH2	1:B:287:SER:OG	2.34	0.61
1:C:1765:SER:OG	1:C:1780:SER:O	2.18	0.61
1:C:2334:LEU:N	1:C:2338:GLY:O	2.34	0.61
1:D:1209:VAL:O	1:D:1211:GLN:NE2	2.34	0.61
1:A:1209:VAL:O	1:A:1211:GLN:NE2	2.34	0.61
1:A:2334:LEU:N	1:A:2338:GLY:O	2.34	0.61
1:B:1209:VAL:O	1:B:1211:GLN:NE2	2.34	0.61
1:D:2334:LEU:N	1:D:2338:GLY:O	2.34	0.61
2:E:77:THR:OG1	2:E:79:ASP:OD2	2.09	0.61
1:B:2334:LEU:N	1:B:2338:GLY:O	2.34	0.61
1:C:2358:ARG:NH1	1:C:2365:SER:O	2.34	0.61
1:D:1763:ARG:O	1:D:1778:GLN:N	2.34	0.61
1:D:3360:THR:O	1:D:3404:TYR:OH	2.18	0.61
1:B:1765:SER:OG	1:B:1780:SER:O	2.18	0.61
1:B:2358:ARG:NH1	1:B:2365:SER:O	2.34	0.61
1:D:2678:ASP:OD2	1:D:3043:THR:OG1	2.14	0.61
1:A:145:PHE:O	1:A:205:ALA:N	2.33	0.60
1:B:362:TYR:OH	1:B:399:MET:O	2.16	0.60
1:B:694:ARG:NH2	1:B:726:GLY:O	2.34	0.60
1:C:145:PHE:O	1:C:205:ALA:N	2.33	0.60
1:C:699:SER:OG	1:C:721:ASP:OD2	2.19	0.60
1:C:3340:LYS:O	1:C:3344:ARG:CB	2.50	0.60
1:C:3385:LYS:O	1:C:3453:ARG:NH1	2.34	0.60
1:D:2588:LEU:O	1:D:2592:VAL:HG23	2.01	0.60
1:A:281:ARG:NH2	1:A:287:SER:OG	2.33	0.60
1:C:281:ARG:NH2	1:C:287:SER:OG	2.33	0.60
1:A:2588:LEU:O	1:A:2592:VAL:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3385:LYS:O	1:B:3453:ARG:NH1	2.34	0.60
1:C:1763:ARG:O	1:C:1778:GLN:N	2.34	0.60
1:D:699:SER:OG	1:D:721:ASP:OD2	2.20	0.60
1:C:3360:THR:O	1:C:3404:TYR:OH	2.18	0.60
1:D:281:ARG:NH2	1:D:287:SER:OG	2.33	0.60
1:D:3340:LYS:O	1:D:3344:ARG:CB	2.50	0.60
1:A:2358:ARG:NH1	1:A:2365:SER:O	2.34	0.60
1:C:2588:LEU:O	1:C:2592:VAL:HG23	2.02	0.60
1:A:637:LEU:HD13	1:A:1673:VAL:HG13	1.84	0.60
1:C:694:ARG:NH2	1:C:726:GLY:O	2.35	0.60
1:D:1765:SER:OG	1:D:1780:SER:O	2.18	0.60
1:A:694:ARG:NH2	1:A:726:GLY:O	2.35	0.60
1:B:2588:LEU:O	1:B:2592:VAL:HG23	2.02	0.60
1:A:1121:GLY:O	1:A:1133:ARG:NH1	2.35	0.60
1:C:1209:VAL:O	1:C:1211:GLN:NE2	2.34	0.60
1:D:694:ARG:NH2	1:D:726:GLY:O	2.35	0.60
1:D:1121:GLY:O	1:D:1133:ARG:NH1	2.35	0.60
1:A:1731:THR:O	1:A:1734:THR:OG1	2.19	0.60
1:A:3340:LYS:O	1:A:3344:ARG:CB	2.50	0.60
1:D:1429:SER:OG	1:D:1557:GLU:OE1	2.15	0.60
1:B:2215:ASP:O	1:B:2218:SER:OG	2.14	0.59
1:B:3340:LYS:O	1:B:3344:ARG:CB	2.50	0.59
1:B:637:LEU:HD13	1:B:1673:VAL:HG13	1.84	0.59
1:C:2146:GLY:O	1:C:2150:ASN:ND2	2.36	0.59
1:C:1722:MET:SD	1:C:2126:ARG:NH1	2.75	0.59
1:A:1722:MET:SD	1:A:2126:ARG:NH1	2.75	0.59
1:B:1763:ARG:O	1:B:1778:GLN:N	2.34	0.59
1:B:2146:GLY:O	1:B:2150:ASN:ND2	2.36	0.59
1:C:1121:GLY:O	1:C:1133:ARG:NH1	2.35	0.59
1:A:1144:ARG:N	1:A:1150:GLU:O	2.35	0.59
1:B:699:SER:OG	1:B:721:ASP:OD2	2.20	0.59
1:B:1121:GLY:O	1:B:1133:ARG:NH1	2.35	0.59
1:A:2146:GLY:O	1:A:2150:ASN:ND2	2.36	0.59
1:B:3360:THR:O	1:B:3404:TYR:OH	2.18	0.59
1:D:637:LEU:HD13	1:D:1673:VAL:HG13	1.84	0.59
1:C:1144:ARG:N	1:C:1150:GLU:O	2.35	0.59
1:D:2146:GLY:O	1:D:2150:ASN:ND2	2.36	0.59
1:A:699:SER:OG	1:A:721:ASP:OD2	2.20	0.59
1:B:305:TYR:O	1:B:317:MET:N	2.36	0.59
1:D:1722:MET:SD	1:D:2126:ARG:NH1	2.75	0.59
1:D:2660:LEU:O	1:D:2664:ALA:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1722:MET:SD	1:B:2126:ARG:NH1	2.75	0.58
1:C:2017:ASP:OD1	1:C:2017:ASP:N	2.37	0.58
1:A:305:TYR:O	1:A:317:MET:N	2.36	0.58
1:B:1586:ARG:NH2	1:B:1587:LEU:O	2.37	0.58
1:C:637:LEU:HD13	1:C:1673:VAL:HG13	1.84	0.58
1:A:1586:ARG:NH2	1:A:1587:LEU:O	2.37	0.58
1:D:2017:ASP:OD1	1:D:2017:ASP:N	2.37	0.58
1:B:1144:ARG:N	1:B:1150:GLU:O	2.35	0.58
1:D:1847:ILE:HG22	1:D:1892:LEU:HB3	1.86	0.58
1:A:1763:ARG:O	1:A:1778:GLN:N	2.34	0.58
1:A:4711:VAL:O	1:A:4714:THR:OG1	2.21	0.58
1:C:305:TYR:O	1:C:317:MET:N	2.36	0.58
1:D:123:HIS:ND1	1:D:126:SER:OG	2.33	0.58
1:D:305:TYR:O	1:D:317:MET:N	2.36	0.58
1:A:1847:ILE:HG22	1:A:1892:LEU:HB3	1.86	0.58
1:C:1586:ARG:NH2	1:C:1587:LEU:O	2.37	0.58
1:D:1144:ARG:N	1:D:1150:GLU:O	2.35	0.58
1:C:950:VAL:CG1	1:C:1064:LEU:HD13	2.34	0.57
1:D:1586:ARG:NH2	1:D:1587:LEU:O	2.37	0.57
1:D:4666:SER:O	1:D:4670:GLY:N	2.38	0.57
1:C:2660:LEU:O	1:C:2664:ALA:N	2.36	0.57
1:D:4711:VAL:O	1:D:4714:THR:OG1	2.21	0.57
1:B:2660:LEU:O	1:B:2664:ALA:N	2.36	0.57
1:C:2678:ASP:OD2	1:C:3043:THR:OG1	2.14	0.57
1:B:1847:ILE:HG22	1:B:1892:LEU:HB3	1.86	0.57
2:E:38:SER:O	2:E:42:ARG:NE	2.37	0.57
1:A:950:VAL:CG1	1:A:1064:LEU:HD13	2.34	0.57
1:A:2228:LEU:HD12	1:A:2237:THR:HB	1.87	0.57
1:B:1713:SER:OG	1:B:1777:TYR:OH	2.17	0.57
1:B:4711:VAL:O	1:B:4714:THR:OG1	2.21	0.57
1:D:950:VAL:CG1	1:D:1064:LEU:HD13	2.34	0.57
1:B:950:VAL:CG1	1:B:1064:LEU:HD13	2.34	0.57
1:C:1119:ARG:O	1:C:1133:ARG:NH2	2.37	0.57
1:C:4666:SER:O	1:C:4670:GLY:N	2.38	0.57
2:H:77:THR:OG1	2:H:79:ASP:OD2	2.09	0.57
1:A:1119:ARG:O	1:A:1133:ARG:NH2	2.38	0.57
1:B:2228:LEU:HD12	1:B:2237:THR:HB	1.87	0.57
1:D:4030:THR:HG21	1:D:4051:MET:SD	2.45	0.57
1:A:3078:GLN:O	1:A:3082:THR:OG1	2.18	0.57
1:B:1119:ARG:O	1:B:1133:ARG:NH2	2.38	0.57
1:B:1597:TRP:NE1	1:B:1599:ARG:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2017:ASP:OD1	1:B:2017:ASP:N	2.37	0.57
1:C:2228:LEU:HD12	1:C:2237:THR:HB	1.87	0.57
1:D:2228:LEU:HD12	1:D:2237:THR:HB	1.87	0.57
2:H:74:LEU:HD22	2:H:101:VAL:HG21	1.87	0.57
1:A:2017:ASP:N	1:A:2017:ASP:OD1	2.37	0.56
1:B:2404:GLU:H	1:B:2407:LEU:HD22	1.70	0.56
1:C:842:GLN:OE1	1:C:844:ARG:NH2	2.38	0.56
1:C:1731:THR:O	1:C:1734:THR:OG1	2.19	0.56
1:A:4163:GLN:OE1	1:A:4498:TYR:OH	2.12	0.56
1:B:4163:GLN:OE1	1:B:4498:TYR:OH	2.12	0.56
1:D:1731:THR:O	1:D:1734:THR:OG1	2.19	0.56
1:D:4696:VAL:HG13	1:D:4697:LEU:HG	1.88	0.56
1:A:1762:MET:SD	1:A:1778:GLN:NE2	2.78	0.56
1:A:4030:THR:HG21	1:A:4051:MET:SD	2.45	0.56
1:B:237:LEU:O	1:B:404:ASN:N	2.39	0.56
1:B:4696:VAL:HG13	1:B:4697:LEU:HG	1.87	0.56
1:C:1847:ILE:HG22	1:C:1892:LEU:HB3	1.86	0.56
1:C:4030:THR:HG21	1:C:4051:MET:SD	2.45	0.56
1:D:3076:GLN:O	1:D:3080:THR:HG23	2.06	0.56
1:A:4666:SER:O	1:A:4670:GLY:N	2.38	0.56
1:B:4030:THR:HG21	1:B:4051:MET:SD	2.45	0.56
1:C:274:LEU:HD13	1:C:419:ILE:HD13	1.87	0.56
1:C:1762:MET:SD	1:C:1778:GLN:NE2	2.79	0.56
1:C:3076:GLN:O	1:C:3080:THR:HG23	2.06	0.56
1:A:2172:GLU:O	1:A:2176:ASN:ND2	2.38	0.56
1:B:842:GLN:OE1	1:B:844:ARG:NH2	2.38	0.56
1:B:1206:SER:O	1:B:1207:LEU:HD23	2.06	0.56
1:C:2172:GLU:O	1:C:2176:ASN:ND2	2.38	0.56
1:D:842:GLN:OE1	1:D:844:ARG:NH2	2.38	0.56
1:D:1119:ARG:O	1:D:1133:ARG:NH2	2.38	0.56
1:A:274:LEU:HD13	1:A:419:ILE:HD13	1.87	0.56
1:A:842:GLN:OE1	1:A:844:ARG:NH2	2.38	0.56
1:A:2660:LEU:O	1:A:2664:ALA:N	2.36	0.56
1:C:1206:SER:O	1:C:1207:LEU:HD23	2.06	0.56
1:C:2404:GLU:H	1:C:2407:LEU:HD22	1.70	0.56
1:D:1597:TRP:NE1	1:D:1599:ARG:O	2.38	0.56
2:E:74:LEU:HD22	2:E:101:VAL:HG21	1.87	0.56
2:F:40:ARG:NH2	2:F:102:GLU:OE1	2.39	0.56
1:A:3788:PHE:O	1:A:3791:SER:OG	2.22	0.56
1:D:1712:LEU:HD22	1:D:1832:MET:SD	2.46	0.56
1:A:1597:TRP:NE1	1:A:1599:ARG:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1712:LEU:HD22	1:A:1832:MET:SD	2.46	0.56
1:A:3076:GLN:O	1:A:3080:THR:HG23	2.06	0.56
1:D:237:LEU:O	1:D:404:ASN:N	2.39	0.56
1:D:4163:GLN:OE1	1:D:4498:TYR:OH	2.12	0.56
1:B:1712:LEU:HD22	1:B:1832:MET:SD	2.46	0.56
1:B:1731:THR:O	1:B:1734:THR:OG1	2.19	0.56
2:G:40:ARG:NH2	2:G:102:GLU:OE1	2.39	0.56
1:B:4666:SER:O	1:B:4670:GLY:N	2.38	0.55
1:C:237:LEU:O	1:C:404:ASN:N	2.39	0.55
1:D:2172:GLU:O	1:D:2176:ASN:ND2	2.38	0.55
1:D:2404:GLU:H	1:D:2407:LEU:HD22	1.70	0.55
2:E:40:ARG:NH2	2:E:102:GLU:OE1	2.39	0.55
2:F:74:LEU:HD22	2:F:101:VAL:HG21	1.87	0.55
1:A:237:LEU:O	1:A:404:ASN:N	2.39	0.55
1:A:1206:SER:O	1:A:1207:LEU:HD23	2.06	0.55
1:A:2404:GLU:H	1:A:2407:LEU:HD22	1.70	0.55
1:B:1762:MET:SD	1:B:1778:GLN:NE2	2.78	0.55
1:B:2172:GLU:O	1:B:2176:ASN:ND2	2.38	0.55
1:C:1597:TRP:NE1	1:C:1599:ARG:O	2.38	0.55
1:B:2071:GLU:O	1:B:3659:ARG:NH1	2.40	0.55
1:C:267:VAL:O	1:C:273:SER:OG	2.22	0.55
1:B:683:GLU:OE1	1:B:683:GLU:N	2.40	0.55
1:C:1429:SER:OG	1:C:1557:GLU:OE1	2.15	0.55
1:D:1730:MET:N	1:D:2107:ILE:O	2.40	0.55
2:G:74:LEU:HD22	2:G:101:VAL:HG21	1.87	0.55
1:C:169:ARG:NH1	1:C:179:ASP:OD2	2.40	0.55
1:C:683:GLU:N	1:C:683:GLU:OE1	2.40	0.55
1:D:169:ARG:NH1	1:D:179:ASP:OD2	2.40	0.55
1:D:274:LEU:HD13	1:D:419:ILE:HD13	1.87	0.55
1:A:2071:GLU:O	1:A:3659:ARG:NH1	2.40	0.55
1:D:1550:SER:HA	1:D:1553:VAL:HG12	1.88	0.55
1:D:1762:MET:SD	1:D:1778:GLN:NE2	2.79	0.55
1:B:1550:SER:HA	1:B:1553:VAL:HG12	1.88	0.55
1:C:1550:SER:HA	1:C:1553:VAL:HG12	1.88	0.55
1:D:1725:GLU:OE2	1:D:2126:ARG:NH1	2.40	0.55
1:B:274:LEU:HD13	1:B:419:ILE:HD13	1.87	0.55
1:B:1245:ARG:NH1	1:B:1693:LYS:O	2.40	0.55
1:B:2678:ASP:OD2	1:B:3043:THR:OG1	2.14	0.55
1:C:1245:ARG:NH1	1:C:1693:LYS:O	2.40	0.55
1:C:1712:LEU:HD22	1:C:1832:MET:SD	2.46	0.55
1:A:683:GLU:N	1:A:683:GLU:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4696:VAL:HG13	1:A:4697:LEU:HG	1.88	0.55
1:B:3076:GLN:O	1:B:3080:THR:HG23	2.06	0.55
1:C:2071:GLU:O	1:C:3659:ARG:NH1	2.40	0.55
1:C:4696:VAL:HG13	1:C:4697:LEU:HG	1.88	0.55
1:D:1206:SER:O	1:D:1207:LEU:HD23	2.06	0.55
2:H:40:ARG:NH2	2:H:102:GLU:OE1	2.39	0.55
1:A:1550:SER:HA	1:A:1553:VAL:HG12	1.88	0.55
1:A:169:ARG:NH1	1:A:179:ASP:OD2	2.40	0.54
1:A:693:LEU:HD12	1:A:793:SER:O	2.07	0.54
1:A:1725:GLU:OE2	1:A:2126:ARG:NH1	2.40	0.54
1:A:3786:VAL:HG12	1:A:3790:GLN:HG3	1.90	0.54
1:C:4106:GLU:OE2	1:C:4146:ARG:NH1	2.41	0.54
1:D:267:VAL:O	1:D:273:SER:OG	2.22	0.54
1:D:2071:GLU:O	1:D:3659:ARG:NH1	2.40	0.54
2:H:38:SER:O	2:H:42:ARG:NE	2.37	0.54
1:D:1245:ARG:NH1	1:D:1693:LYS:O	2.40	0.54
1:D:3786:VAL:HG12	1:D:3790:GLN:HG3	1.90	0.54
1:A:889:ILE:HD12	1:A:892:LEU:HD12	1.90	0.54
1:B:3786:VAL:HG12	1:B:3790:GLN:HG3	1.90	0.54
1:B:4106:GLU:OE2	1:B:4146:ARG:NH1	2.41	0.54
1:D:693:LEU:HD12	1:D:793:SER:O	2.07	0.54
1:B:169:ARG:NH1	1:B:179:ASP:OD2	2.40	0.54
1:D:1506:LEU:N	1:D:1524:ASN:OD1	2.41	0.54
1:B:1730:MET:N	1:B:2107:ILE:O	2.40	0.54
1:B:3958:SER:O	1:B:4085:ARG:NH2	2.41	0.54
1:C:3786:VAL:HG12	1:C:3790:GLN:HG3	1.90	0.54
1:A:3958:SER:O	1:A:4085:ARG:NH2	2.41	0.54
1:B:693:LEU:HD12	1:B:793:SER:O	2.07	0.54
1:B:823:TYR:O	1:B:826:VAL:HG23	2.08	0.54
1:C:3958:SER:O	1:C:4085:ARG:NH2	2.41	0.54
1:A:4106:GLU:OE2	1:A:4146:ARG:NH1	2.41	0.54
1:C:823:TYR:O	1:C:826:VAL:HG23	2.08	0.54
1:D:4106:GLU:OE2	1:D:4146:ARG:NH1	2.41	0.54
1:D:1269:GLU:N	1:D:1269:GLU:OE2	2.41	0.54
1:D:3802:LEU:HD11	1:D:3904:ASN:HB3	1.90	0.54
1:D:4784:ALA:O	1:D:4788:PHE:N	2.41	0.54
1:A:430:ILE:HG23	1:A:505:LEU:HD22	1.91	0.53
1:A:1245:ARG:NH1	1:A:1693:LYS:O	2.40	0.53
1:A:1730:MET:N	1:A:2107:ILE:O	2.40	0.53
1:A:3802:LEU:HD11	1:A:3904:ASN:HB3	1.90	0.53
1:A:4842:ARG:NH1	1:A:4846:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:ILE:HD12	1:B:892:LEU:HD12	1.90	0.53
1:B:3802:LEU:HD11	1:B:3904:ASN:HB3	1.90	0.53
1:C:3078:GLN:O	1:C:3082:THR:OG1	2.18	0.53
1:C:4163:GLN:OE1	1:C:4498:TYR:OH	2.12	0.53
1:D:3958:SER:O	1:D:4085:ARG:NH2	2.41	0.53
1:C:4842:ARG:NH1	1:C:4846:ASP:OD1	2.41	0.53
1:A:2576:CYS:SG	1:A:2577:GLY:N	2.82	0.53
1:B:2125:ILE:HD11	1:B:2144:GLY:HA3	1.90	0.53
1:B:4178:GLU:OE2	1:B:4178:GLU:N	2.42	0.53
1:C:430:ILE:HG23	1:C:505:LEU:HD22	1.91	0.53
1:D:655:MET:SD	1:D:1620:VAL:HG11	2.49	0.53
1:D:4842:ARG:NH1	1:D:4846:ASP:OD1	2.41	0.53
1:A:655:MET:SD	1:A:1620:VAL:HG11	2.49	0.53
1:A:1269:GLU:N	1:A:1269:GLU:OE2	2.41	0.53
1:B:70:GLU:OE2	1:B:122:ARG:NH2	2.42	0.53
1:B:4784:ALA:O	1:B:4788:PHE:N	2.42	0.53
1:C:693:LEU:HD12	1:C:793:SER:O	2.07	0.53
1:C:3802:LEU:HD11	1:C:3904:ASN:HB3	1.90	0.53
1:D:2125:ILE:HD11	1:D:2144:GLY:HA3	1.90	0.53
1:D:4885:THR:O	1:D:4894:ASN:N	2.42	0.53
2:E:39:SER:OG	2:E:44:LYS:O	2.26	0.53
2:H:39:SER:OG	2:H:44:LYS:O	2.26	0.53
1:A:823:TYR:O	1:A:826:VAL:HG23	2.08	0.53
1:C:4885:THR:O	1:C:4894:ASN:N	2.42	0.53
1:D:499:LEU:HD22	1:D:537:LEU:HD12	1.91	0.53
1:D:683:GLU:OE1	1:D:683:GLU:N	2.40	0.53
1:D:823:TYR:O	1:D:826:VAL:HG23	2.08	0.53
1:D:4178:GLU:OE2	1:D:4178:GLU:N	2.42	0.53
1:A:1118:SER:OG	1:A:1119:ARG:N	2.42	0.53
1:A:4784:ALA:O	1:A:4788:PHE:N	2.41	0.53
1:B:430:ILE:HG23	1:B:505:LEU:HD22	1.91	0.53
1:B:1723:ASN:O	1:B:1918:ARG:NH2	2.41	0.53
1:C:655:MET:SD	1:C:1620:VAL:HG11	2.49	0.53
1:C:1723:ASN:O	1:C:1918:ARG:NH2	2.41	0.53
2:G:39:SER:OG	2:G:44:LYS:O	2.26	0.53
1:B:2576:CYS:SG	1:B:2577:GLY:N	2.82	0.53
1:C:70:GLU:OE2	1:C:122:ARG:NH2	2.42	0.53
1:C:2125:ILE:HD11	1:C:2144:GLY:HA3	1.90	0.53
1:C:4711:VAL:O	1:C:4714:THR:OG1	2.21	0.53
1:B:499:LEU:HD22	1:B:537:LEU:HD12	1.91	0.53
1:B:2135:LYS:HE2	1:B:2186:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4842:ARG:NH1	1:B:4846:ASP:OD1	2.41	0.53
1:C:889:ILE:HD12	1:C:892:LEU:HD12	1.90	0.53
1:C:3788:PHE:O	1:C:3791:SER:OG	2.22	0.53
1:D:70:GLU:OE2	1:D:122:ARG:NH2	2.42	0.53
1:D:1118:SER:OG	1:D:1119:ARG:N	2.42	0.53
1:D:3788:PHE:O	1:D:3791:SER:OG	2.22	0.53
1:A:499:LEU:HD22	1:A:537:LEU:HD12	1.91	0.53
1:A:892:LEU:HD13	1:A:1056:THR:HG21	1.91	0.53
1:A:2135:LYS:HE2	1:A:2186:ILE:HD11	1.91	0.53
1:A:3269:SER:OG	1:A:3342:GLU:OE1	2.21	0.53
1:B:1269:GLU:N	1:B:1269:GLU:OE2	2.41	0.53
1:B:4885:THR:O	1:B:4894:ASN:N	2.42	0.53
1:C:2576:CYS:SG	1:C:2577:GLY:N	2.82	0.53
1:C:4784:ALA:O	1:C:4788:PHE:N	2.41	0.53
1:D:1723:ASN:O	1:D:1918:ARG:NH2	2.41	0.53
1:D:3078:GLN:O	1:D:3082:THR:OG1	2.18	0.53
1:B:267:VAL:O	1:B:273:SER:OG	2.21	0.53
1:B:1725:GLU:OE2	1:B:2126:ARG:NH1	2.40	0.53
1:C:499:LEU:HD22	1:C:537:LEU:HD12	1.91	0.53
1:C:1730:MET:N	1:C:2107:ILE:O	2.40	0.53
1:C:4178:GLU:N	1:C:4178:GLU:OE2	2.42	0.53
1:D:676:GLU:HB3	1:D:803:LEU:HD12	1.91	0.53
1:D:2576:CYS:SG	1:D:2577:GLY:N	2.82	0.53
1:A:1255:LEU:HD12	1:A:1256:PRO:HD2	1.91	0.52
1:A:1440:ASN:ND2	1:A:1498:GLN:O	2.42	0.52
1:A:2125:ILE:HD11	1:A:2144:GLY:HA3	1.90	0.52
1:A:4159:TRP:CH2	1:A:4915:ALA:HB2	2.45	0.52
1:A:4178:GLU:N	1:A:4178:GLU:OE2	2.42	0.52
1:A:4885:THR:O	1:A:4894:ASN:N	2.42	0.52
1:C:1118:SER:OG	1:C:1119:ARG:N	2.42	0.52
1:D:430:ILE:HG23	1:D:505:LEU:HD22	1.91	0.52
1:D:892:LEU:HD13	1:D:1056:THR:HG21	1.91	0.52
1:D:1255:LEU:HD12	1:D:1256:PRO:HD2	1.91	0.52
1:C:1440:ASN:ND2	1:C:1498:GLN:O	2.42	0.52
1:C:4159:TRP:CH2	1:C:4915:ALA:HB2	2.45	0.52
1:C:1269:GLU:OE2	1:C:1269:GLU:N	2.41	0.52
1:D:889:ILE:HD12	1:D:892:LEU:HD12	1.90	0.52
1:A:1723:ASN:O	1:A:1918:ARG:NH2	2.41	0.52
1:B:4159:TRP:CH2	1:B:4915:ALA:HB2	2.45	0.52
1:D:1440:ASN:ND2	1:D:1498:GLN:O	2.42	0.52
1:A:70:GLU:OE2	1:A:122:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:MET:SD	1:B:1620:VAL:HG11	2.49	0.52
1:A:676:GLU:HB3	1:A:803:LEU:HD12	1.91	0.52
1:A:2987:ARG:O	1:A:2994:HIS:NE2	2.43	0.52
1:B:892:LEU:HD13	1:B:1056:THR:HG21	1.91	0.52
1:C:1255:LEU:HD12	1:C:1256:PRO:HD2	1.91	0.52
1:D:1272:ARG:HH12	1:D:1308:ILE:HD11	1.75	0.52
1:D:4159:TRP:CH2	1:D:4915:ALA:HB2	2.45	0.52
2:H:25:HIS:O	2:H:40:ARG:NE	2.38	0.52
1:B:1118:SER:OG	1:B:1119:ARG:N	2.42	0.52
1:C:1725:GLU:OE2	1:C:2126:ARG:NH1	2.40	0.52
1:D:3269:SER:OG	1:D:3342:GLU:OE1	2.21	0.52
1:B:676:GLU:HB3	1:B:803:LEU:HD12	1.91	0.52
1:B:1255:LEU:HD12	1:B:1256:PRO:HD2	1.92	0.52
1:C:676:GLU:HB3	1:C:803:LEU:HD12	1.91	0.52
1:B:1440:ASN:ND2	1:B:1498:GLN:O	2.42	0.52
1:C:2135:LYS:HE2	1:C:2186:ILE:HD11	1.91	0.52
1:D:673:TRP:NE1	1:D:824:GLU:OE2	2.43	0.52
1:D:2135:LYS:HE2	1:D:2186:ILE:HD11	1.91	0.52
1:A:4620:PRO:O	1:A:4628:GLN:NE2	2.43	0.52
1:B:3788:PHE:O	1:B:3791:SER:OG	2.22	0.52
1:B:4620:PRO:O	1:B:4628:GLN:NE2	2.43	0.52
1:B:673:TRP:NE1	1:B:824:GLU:OE2	2.43	0.51
1:C:3269:SER:OG	1:C:3347:MET:SD	2.69	0.51
1:C:4620:PRO:O	1:C:4628:GLN:NE2	2.43	0.51
1:A:673:TRP:NE1	1:A:824:GLU:OE2	2.43	0.51
1:B:1272:ARG:HH12	1:B:1308:ILE:HD11	1.75	0.51
1:B:3078:GLN:O	1:B:3082:THR:OG1	2.18	0.51
1:C:673:TRP:NE1	1:C:824:GLU:OE2	2.43	0.51
1:C:1713:SER:OG	1:C:1777:TYR:OH	2.17	0.51
1:D:2987:ARG:O	1:D:2994:HIS:NE2	2.43	0.51
1:A:843:GLU:OE2	1:A:1608:ASP:N	2.43	0.51
1:A:1723:ASN:OD1	1:A:1918:ARG:NH2	2.43	0.51
1:B:3269:SER:OG	1:B:3347:MET:SD	2.69	0.51
1:C:892:LEU:HD13	1:C:1056:THR:HG21	1.91	0.51
1:D:4620:PRO:O	1:D:4628:GLN:NE2	2.43	0.51
1:A:436:LEU:HD23	1:A:440:VAL:HB	1.93	0.51
1:B:1429:SER:OG	1:B:1557:GLU:OE1	2.15	0.51
1:B:4189:VAL:HG21	1:B:4948:TRP:CZ3	2.46	0.51
1:C:606:ARG:O	1:C:608:HIS:ND1	2.44	0.51
1:D:3269:SER:OG	1:D:3347:MET:SD	2.69	0.51
2:F:39:SER:OG	2:F:44:LYS:O	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:38:SER:O	2:G:42:ARG:NE	2.37	0.51
1:D:925:PRO:O	1:D:929:ARG:N	2.44	0.51
1:D:4189:VAL:HG21	1:D:4948:TRP:CZ3	2.46	0.51
2:G:25:HIS:O	2:G:40:ARG:NE	2.38	0.51
1:B:891:GLU:N	1:B:891:GLU:OE1	2.44	0.51
1:B:1506:LEU:N	1:B:1524:ASN:OD1	2.41	0.51
1:B:2422:LEU:O	1:B:2431:LEU:HD11	2.11	0.51
1:C:843:GLU:OE2	1:C:1608:ASP:N	2.43	0.51
1:D:891:GLU:N	1:D:891:GLU:OE1	2.44	0.51
1:D:2422:LEU:O	1:D:2431:LEU:HD11	2.11	0.51
1:A:674:TYR:N	1:A:820:ALA:O	2.44	0.51
1:B:2667:CYS:SG	1:B:2691:GLN:NE2	2.84	0.51
1:B:2987:ARG:O	1:B:2994:HIS:NE2	2.43	0.51
1:D:2667:CYS:SG	1:D:2691:GLN:NE2	2.84	0.51
1:A:1272:ARG:HH12	1:A:1308:ILE:HD11	1.75	0.51
1:A:2667:CYS:SG	1:A:2691:GLN:NE2	2.84	0.51
1:A:4189:VAL:HG21	1:A:4948:TRP:CZ3	2.46	0.51
1:B:436:LEU:HD23	1:B:440:VAL:HB	1.93	0.51
1:B:843:GLU:OE2	1:B:1608:ASP:N	2.43	0.51
1:C:891:GLU:OE1	1:C:891:GLU:N	2.44	0.51
1:D:436:LEU:HD23	1:D:440:VAL:HB	1.93	0.51
1:B:4635:ASN:ND2	1:B:4668:LEU:O	2.44	0.50
2:G:77:THR:OG1	2:G:79:ASP:OD2	2.09	0.50
1:A:3916:PHE:O	1:A:3920:THR:HG23	2.12	0.50
1:D:162:ILE:O	1:D:163:HIS:ND1	2.45	0.50
1:A:3269:SER:OG	1:A:3347:MET:SD	2.69	0.50
1:A:4635:ASN:ND2	1:A:4668:LEU:O	2.44	0.50
1:C:2667:CYS:SG	1:C:2691:GLN:NE2	2.84	0.50
1:C:4189:VAL:HG21	1:C:4948:TRP:CZ3	2.46	0.50
1:D:1723:ASN:OD1	1:D:1918:ARG:NH2	2.43	0.50
1:B:674:TYR:N	1:B:820:ALA:O	2.44	0.50
1:C:2040:LYS:O	1:C:2056:SER:N	2.45	0.50
1:A:123:HIS:ND1	1:A:126:SER:OG	2.33	0.50
1:B:162:ILE:O	1:B:163:HIS:ND1	2.45	0.50
1:C:674:TYR:N	1:C:820:ALA:O	2.44	0.50
1:C:1272:ARG:HH12	1:C:1308:ILE:HD11	1.75	0.50
1:C:1946:VAL:HG12	1:C:1947:MET:H	1.77	0.50
1:C:3916:PHE:O	1:C:3920:THR:HG23	2.12	0.50
1:C:436:LEU:HD23	1:C:440:VAL:HB	1.93	0.50
1:D:674:TYR:N	1:D:820:ALA:O	2.44	0.50
1:D:3404:TYR:O	1:D:3408:SER:OG	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3916:PHE:O	1:D:3920:THR:HG23	2.12	0.50
1:B:1723:ASN:OD1	1:B:1918:ARG:NH2	2.43	0.50
1:B:2162:ARG:NH2	1:B:2206:SER:OG	2.45	0.50
1:C:436:LEU:HD21	1:C:445:ILE:HG22	1.93	0.50
1:C:1638:ARG:NH2	1:C:1639:SER:OG	2.45	0.50
1:C:2129:LEU:HD12	1:C:2130:SER:H	1.76	0.50
1:D:2129:LEU:HD12	1:D:2130:SER:H	1.76	0.50
1:A:925:PRO:O	1:A:929:ARG:N	2.44	0.50
1:A:2129:LEU:HD12	1:A:2130:SER:H	1.76	0.50
1:C:2162:ARG:NH2	1:C:2206:SER:OG	2.45	0.50
1:C:2422:LEU:O	1:C:2431:LEU:HD11	2.11	0.50
1:D:843:GLU:OE2	1:D:1608:ASP:N	2.43	0.50
1:D:2162:ARG:NH2	1:D:2206:SER:OG	2.45	0.50
1:D:2431:LEU:O	1:D:2434:VAL:HG22	2.12	0.50
1:A:162:ILE:O	1:A:163:HIS:ND1	2.45	0.50
1:A:891:GLU:OE1	1:A:891:GLU:N	2.44	0.50
1:A:2162:ARG:NH2	1:A:2206:SER:OG	2.45	0.50
1:B:1946:VAL:HG12	1:B:1947:MET:H	1.76	0.50
1:D:2040:LYS:O	1:D:2056:SER:N	2.45	0.50
1:A:436:LEU:HD21	1:A:445:ILE:HG22	1.93	0.49
1:B:166:SER:OG	1:B:167:LYS:N	2.45	0.49
1:B:436:LEU:HD21	1:B:445:ILE:HG22	1.93	0.49
1:B:2040:LYS:O	1:B:2056:SER:N	2.45	0.49
1:C:925:PRO:O	1:C:929:ARG:N	2.44	0.49
1:D:1946:VAL:HG12	1:D:1947:MET:H	1.77	0.49
1:D:4635:ASN:ND2	1:D:4668:LEU:O	2.44	0.49
1:A:606:ARG:O	1:A:608:HIS:ND1	2.44	0.49
1:A:2431:LEU:O	1:A:2434:VAL:HG22	2.12	0.49
1:B:3916:PHE:O	1:B:3920:THR:HG23	2.12	0.49
1:A:2422:LEU:O	1:A:2431:LEU:HD11	2.11	0.49
1:B:1638:ARG:NH2	1:B:1639:SER:OG	2.45	0.49
1:C:162:ILE:O	1:C:163:HIS:ND1	2.45	0.49
1:C:166:SER:OG	1:C:167:LYS:N	2.45	0.49
1:C:235:ARG:NE	1:C:268:SER:O	2.42	0.49
1:C:2987:ARG:O	1:C:2994:HIS:NE2	2.43	0.49
1:C:4635:ASN:ND2	1:C:4668:LEU:O	2.44	0.49
1:D:569:SER:O	1:D:609:LYS:NZ	2.40	0.49
1:B:606:ARG:O	1:B:608:HIS:ND1	2.44	0.49
1:A:267:VAL:O	1:A:273:SER:OG	2.21	0.49
1:B:1726:PHE:CD2	1:B:1921:ILE:HD11	2.48	0.49
1:B:4619:GLN:OE1	1:B:4631:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ALA:O	1:C:270:HIS:ND1	2.45	0.49
1:D:1105:PHE:CD2	1:D:1115:VAL:HG11	2.47	0.49
1:A:2040:LYS:O	1:A:2056:SER:N	2.45	0.49
1:B:300:VAL:CG2	1:B:419:ILE:HD12	2.43	0.49
1:C:1105:PHE:CD2	1:C:1115:VAL:HG11	2.47	0.49
1:D:1726:PHE:CD2	1:D:1921:ILE:HD11	2.48	0.49
1:A:1105:PHE:CD2	1:A:1115:VAL:HG11	2.47	0.49
1:B:2129:LEU:HD12	1:B:2130:SER:H	1.76	0.49
1:C:2169:THR:O	1:C:2173:VAL:HG23	2.13	0.49
1:C:4619:GLN:OE1	1:C:4631:ARG:NH1	2.46	0.49
1:A:877:HIS:O	1:A:880:ARG:NH1	2.46	0.49
1:C:2431:LEU:O	1:C:2434:VAL:HG22	2.12	0.49
1:D:1638:ARG:NH2	1:D:1639:SER:OG	2.45	0.49
1:A:166:SER:OG	1:A:167:LYS:N	2.46	0.49
1:A:4501:ARG:NH2	1:A:4744:ASP:OD1	2.46	0.49
1:B:3737:GLU:N	1:B:3737:GLU:OE2	2.46	0.49
1:B:3924:GLN:O	1:B:4934:GLY:N	2.46	0.49
1:C:841:LYS:HA	1:C:851:LEU:HD12	1.95	0.49
1:C:877:HIS:O	1:C:880:ARG:NH1	2.46	0.49
1:C:1723:ASN:OD1	1:C:1918:ARG:NH2	2.43	0.49
1:D:300:VAL:CG2	1:D:419:ILE:HD12	2.43	0.49
1:D:436:LEU:HD21	1:D:445:ILE:HG22	1.93	0.49
1:D:841:LYS:HA	1:D:851:LEU:HD12	1.95	0.49
1:D:877:HIS:O	1:D:880:ARG:NH1	2.46	0.49
1:A:1506:LEU:N	1:A:1524:ASN:OD1	2.41	0.49
1:A:1726:PHE:CD2	1:A:1921:ILE:HD11	2.48	0.49
1:A:1946:VAL:HG12	1:A:1947:MET:H	1.76	0.49
1:A:2169:THR:O	1:A:2173:VAL:HG23	2.13	0.49
1:A:3737:GLU:OE2	1:A:3737:GLU:N	2.46	0.49
1:B:678:MET:HB2	1:B:803:LEU:HD11	1.95	0.49
1:B:2468:VAL:HG11	1:B:2521:THR:HG22	1.95	0.49
1:D:166:SER:OG	1:D:167:LYS:N	2.45	0.49
1:D:2169:THR:O	1:D:2173:VAL:HG23	2.13	0.48
1:A:300:VAL:CG2	1:A:419:ILE:HD12	2.43	0.48
1:A:678:MET:HB2	1:A:803:LEU:HD11	1.95	0.48
1:B:877:HIS:O	1:B:880:ARG:NH1	2.46	0.48
1:C:300:VAL:CG2	1:C:419:ILE:HD12	2.43	0.48
1:B:1105:PHE:CD2	1:B:1115:VAL:HG11	2.47	0.48
1:B:3040:ASP:O	1:B:3044:VAL:HG22	2.14	0.48
1:D:606:ARG:O	1:D:608:HIS:ND1	2.44	0.48
1:D:3040:ASP:O	1:D:3044:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:38:SER:O	2:F:42:ARG:NE	2.37	0.48
1:A:569:SER:O	1:A:609:LYS:NZ	2.40	0.48
1:A:1638:ARG:NH2	1:A:1639:SER:OG	2.45	0.48
1:B:804:LEU:HD12	1:B:1618:TRP:CZ3	2.49	0.48
1:B:2431:LEU:O	1:B:2434:VAL:HG22	2.12	0.48
1:C:1505:GLY:O	1:C:1506:LEU:HD23	2.14	0.48
1:C:2780:THR:OG1	1:C:2846:ASN:ND2	2.47	0.48
1:C:3040:ASP:O	1:C:3044:VAL:HG22	2.14	0.48
1:A:4018:MET:O	1:A:4026:THR:OG1	2.29	0.48
1:B:1505:GLY:O	1:B:1506:LEU:HD23	2.14	0.48
1:B:2780:THR:OG1	1:B:2846:ASN:ND2	2.47	0.48
1:C:2468:VAL:HG11	1:C:2521:THR:HG22	1.95	0.48
1:C:3727:GLN:O	1:C:3731:HIS:ND1	2.46	0.48
1:C:3920:THR:O	1:C:3924:GLN:N	2.46	0.48
1:C:4501:ARG:NH2	1:C:4744:ASP:OD1	2.46	0.48
1:D:678:MET:HB2	1:D:803:LEU:HD11	1.95	0.48
1:D:3727:GLN:O	1:D:3731:HIS:ND1	2.46	0.48
1:D:4501:ARG:NH2	1:D:4744:ASP:OD1	2.46	0.48
1:A:186:VAL:O	1:B:2417:ARG:NH1	2.47	0.48
1:B:569:SER:O	1:B:609:LYS:NZ	2.40	0.48
1:B:2169:THR:O	1:B:2173:VAL:HG23	2.13	0.48
1:B:3727:GLN:O	1:B:3731:HIS:ND1	2.46	0.48
1:C:1726:PHE:CD2	1:C:1921:ILE:HD11	2.48	0.48
1:C:3737:GLU:OE2	1:C:3737:GLU:N	2.45	0.48
1:A:2357:SER:OG	1:A:2358:ARG:N	2.47	0.48
1:B:841:LYS:HA	1:B:851:LEU:HD12	1.95	0.48
1:C:1506:LEU:N	1:C:1524:ASN:OD1	2.41	0.48
1:D:3920:THR:O	1:D:3924:GLN:N	2.46	0.48
1:A:841:LYS:HA	1:A:851:LEU:HD12	1.95	0.48
1:A:2468:VAL:HG11	1:A:2521:THR:HG22	1.95	0.48
1:A:3040:ASP:O	1:A:3044:VAL:HG22	2.14	0.48
1:A:3727:GLN:O	1:A:3731:HIS:ND1	2.46	0.48
1:C:4044:LYS:NZ	1:C:4069:ALA:O	2.36	0.48
1:D:4018:MET:O	1:D:4026:THR:OG1	2.29	0.48
1:A:1505:GLY:O	1:A:1506:LEU:HD23	2.14	0.48
1:D:3737:GLU:OE2	1:D:3737:GLU:N	2.46	0.48
1:A:2417:ARG:NH1	1:D:186:VAL:O	2.47	0.47
1:C:2215:ASP:O	1:C:2218:SER:OG	2.14	0.47
1:C:2357:SER:OG	1:C:2358:ARG:N	2.47	0.47
1:D:804:LEU:HD12	1:D:1618:TRP:CZ3	2.48	0.47
1:A:266:ALA:O	1:A:270:HIS:ND1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ALA:HA	1:A:889:ILE:HG22	1.96	0.47
1:A:3920:THR:O	1:A:3924:GLN:N	2.46	0.47
1:B:4501:ARG:NH2	1:B:4744:ASP:OD1	2.46	0.47
1:D:2357:SER:OG	1:D:2358:ARG:N	2.47	0.47
1:A:2780:THR:OG1	1:A:2846:ASN:ND2	2.47	0.47
1:B:235:ARG:NE	1:B:268:SER:O	2.42	0.47
1:B:2357:SER:OG	1:B:2358:ARG:N	2.47	0.47
1:D:235:ARG:NE	1:D:268:SER:O	2.42	0.47
1:A:804:LEU:HD12	1:A:1618:TRP:CZ3	2.48	0.47
1:D:1614:GLU:N	1:D:1619:LEU:O	2.47	0.47
1:A:1614:GLU:N	1:A:1619:LEU:O	2.47	0.47
1:D:266:ALA:O	1:D:270:HIS:ND1	2.46	0.47
1:D:927:GLN:N	1:D:927:GLN:OE1	2.48	0.47
1:D:2780:THR:OG1	1:D:2846:ASN:ND2	2.46	0.47
2:F:77:THR:OG1	2:F:79:ASP:OD2	2.09	0.47
1:A:4619:GLN:OE1	1:A:4631:ARG:NH1	2.46	0.47
1:B:186:VAL:O	1:C:2417:ARG:NH1	2.47	0.47
1:C:678:MET:HB2	1:C:803:LEU:HD11	1.95	0.47
1:C:886:ALA:HA	1:C:889:ILE:HG22	1.96	0.47
1:D:2468:VAL:HG11	1:D:2521:THR:HG22	1.95	0.47
1:D:3934:LEU:O	1:D:3937:SER:OG	2.28	0.47
1:B:4836:ASP:OD1	1:B:4837:GLU:N	2.48	0.47
1:C:586:LEU:HD22	1:C:589:ILE:HD11	1.97	0.47
1:D:1505:GLY:O	1:D:1506:LEU:HD23	2.14	0.47
1:B:925:PRO:O	1:B:929:ARG:N	2.44	0.47
1:C:804:LEU:HD12	1:C:1618:TRP:CZ3	2.49	0.47
1:C:1614:GLU:N	1:C:1619:LEU:O	2.47	0.47
1:C:1909:LEU:HD22	1:C:2061:ILE:HD11	1.96	0.46
1:B:886:ALA:HA	1:B:889:ILE:HG22	1.96	0.46
1:B:2582:SER:HB2	1:B:2875:THR:HG22	1.97	0.46
1:B:4794:LYS:NZ	1:B:4829:GLU:OE1	2.49	0.46
1:C:186:VAL:O	1:D:2417:ARG:NH1	2.48	0.46
1:D:886:ALA:HA	1:D:889:ILE:HG22	1.96	0.46
1:A:1255:LEU:HD13	1:A:1451:HIS:ND1	2.31	0.46
1:B:1255:LEU:HD13	1:B:1451:HIS:ND1	2.31	0.46
1:D:3786:VAL:HG12	1:D:3790:GLN:CG	2.46	0.46
1:B:307:SER:OG	1:B:308:LEU:N	2.49	0.46
1:B:701:GLU:N	1:B:701:GLU:OE1	2.49	0.46
1:C:4794:LYS:NZ	1:C:4829:GLU:OE1	2.48	0.46
1:D:307:SER:OG	1:D:308:LEU:N	2.49	0.46
1:D:586:LEU:HD22	1:D:589:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:939:THR:O	1:D:943:LEU:HD13	2.16	0.46
1:A:701:GLU:N	1:A:701:GLU:OE1	2.49	0.46
1:A:2582:SER:HB2	1:A:2875:THR:HG22	1.97	0.46
1:B:3786:VAL:HG12	1:B:3790:GLN:CG	2.46	0.46
1:C:307:SER:OG	1:C:308:LEU:N	2.49	0.46
1:C:701:GLU:OE1	1:C:701:GLU:N	2.49	0.46
1:C:939:THR:O	1:C:943:LEU:HD13	2.16	0.46
1:D:1909:LEU:HD22	1:D:2061:ILE:HD11	1.96	0.46
1:A:4794:LYS:NZ	1:A:4829:GLU:OE1	2.49	0.46
1:B:927:GLN:OE1	1:B:927:GLN:N	2.48	0.46
1:B:1909:LEU:HD22	1:B:2061:ILE:HD11	1.96	0.46
1:D:73:LEU:O	1:D:118:ALA:N	2.49	0.46
1:A:3786:VAL:HG12	1:A:3790:GLN:CG	2.46	0.46
1:A:4836:ASP:OD1	1:A:4837:GLU:N	2.48	0.46
1:D:3924:GLN:O	1:D:4934:GLY:N	2.46	0.46
1:A:1157:GLN:NE2	1:A:1160:ASP:OD2	2.49	0.46
1:A:3888:TYR:O	1:A:3892:SER:N	2.49	0.46
1:A:4136:GLU:OE2	1:A:4146:ARG:NH2	2.48	0.46
1:B:560:SER:OG	1:B:561:ARG:NH2	2.49	0.46
1:B:1614:GLU:N	1:B:1619:LEU:O	2.47	0.46
1:C:1255:LEU:HD13	1:C:1451:HIS:ND1	2.31	0.46
1:D:195:SER:OG	1:D:204:ASP:OD2	2.34	0.46
1:D:701:GLU:N	1:D:701:GLU:OE1	2.49	0.46
1:B:586:LEU:HD22	1:B:589:ILE:HD11	1.97	0.46
1:C:927:GLN:OE1	1:C:927:GLN:N	2.48	0.46
1:C:3786:VAL:HG12	1:C:3790:GLN:CG	2.46	0.46
2:F:25:HIS:O	2:F:40:ARG:NE	2.38	0.46
1:A:939:THR:O	1:A:943:LEU:HD13	2.16	0.45
1:B:450:GLU:O	1:B:453:SER:OG	2.32	0.45
1:B:3920:THR:O	1:B:3924:GLN:N	2.46	0.45
1:B:4136:GLU:OE2	1:B:4146:ARG:NH2	2.48	0.45
1:D:4176:VAL:HG13	1:D:4879:VAL:HG12	1.98	0.45
1:D:4836:ASP:OD1	1:D:4837:GLU:N	2.48	0.45
1:D:4928:ASP:OD2	1:D:4930:THR:OG1	2.25	0.45
1:A:307:SER:OG	1:A:308:LEU:N	2.49	0.45
1:A:494:MET:CE	1:A:499:LEU:HD21	2.46	0.45
1:A:1909:LEU:HD22	1:A:2061:ILE:HD11	1.96	0.45
1:B:266:ALA:O	1:B:270:HIS:ND1	2.46	0.45
1:C:494:MET:CE	1:C:499:LEU:HD21	2.46	0.45
1:C:1157:GLN:NE2	1:C:1160:ASP:OD2	2.49	0.45
1:C:4176:VAL:HG13	1:C:4879:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:494:MET:CE	1:D:499:LEU:HD21	2.46	0.45
1:D:898:ILE:HD11	1:D:918:LEU:HD22	1.99	0.45
1:D:1157:GLN:NE2	1:D:1160:ASP:OD2	2.49	0.45
1:D:1255:LEU:HD13	1:D:1451:HIS:ND1	2.31	0.45
1:A:195:SER:OG	1:A:204:ASP:OD2	2.34	0.45
1:A:898:ILE:HD11	1:A:918:LEU:HD22	1.99	0.45
1:C:886:ALA:HB1	1:C:921:PHE:CE1	2.52	0.45
1:D:560:SER:OG	1:D:561:ARG:NH2	2.49	0.45
1:A:73:LEU:O	1:A:118:ALA:N	2.49	0.45
1:A:4176:VAL:HG13	1:A:4879:VAL:HG12	1.98	0.45
1:B:939:THR:O	1:B:943:LEU:HD13	2.16	0.45
1:C:73:LEU:O	1:C:118:ALA:N	2.49	0.45
1:C:560:SER:OG	1:C:561:ARG:NH2	2.49	0.45
1:B:1157:GLN:NE2	1:B:1160:ASP:OD2	2.49	0.45
1:C:2582:SER:HB2	1:C:2875:THR:HG22	1.97	0.45
1:C:4836:ASP:OD1	1:C:4837:GLU:N	2.48	0.45
1:A:560:SER:OG	1:A:561:ARG:NH2	2.49	0.45
1:A:586:LEU:HD22	1:A:589:ILE:HD11	1.97	0.45
1:A:927:GLN:OE1	1:A:927:GLN:N	2.48	0.45
1:B:886:ALA:HB1	1:B:921:PHE:CE1	2.52	0.45
1:B:898:ILE:HD11	1:B:918:LEU:HD22	1.99	0.45
1:C:674:TYR:O	1:C:822:CYS:N	2.48	0.45
1:C:3978:VAL:HA	1:C:3981:LEU:HD12	1.99	0.45
1:B:10:GLU:OE2	1:B:10:GLU:N	2.50	0.45
1:B:4176:VAL:HG13	1:B:4879:VAL:HG12	1.98	0.45
1:C:1262:PRO:O	1:C:1264:ASN:ND2	2.49	0.45
1:C:1930:ASP:OD1	1:C:2027:ARG:NH2	2.49	0.45
1:D:3940:TRP:O	1:D:3944:VAL:HG13	2.17	0.45
1:C:898:ILE:HD11	1:C:918:LEU:HD22	1.99	0.45
1:A:3940:TRP:O	1:A:3944:VAL:HG13	2.17	0.45
1:B:1105:PHE:CE2	1:B:1115:VAL:HG11	2.52	0.45
1:B:4018:MET:O	1:B:4026:THR:OG1	2.29	0.45
1:C:3940:TRP:O	1:C:3944:VAL:HG13	2.17	0.45
1:D:886:ALA:HB1	1:D:921:PHE:CE1	2.52	0.45
1:D:4185:MET:O	1:D:4189:VAL:HG23	2.17	0.45
1:D:4794:LYS:NZ	1:D:4829:GLU:OE1	2.48	0.45
1:A:235:ARG:NE	1:A:268:SER:O	2.42	0.44
1:A:1105:PHE:CE2	1:A:1115:VAL:HG11	2.52	0.44
1:A:4185:MET:O	1:A:4189:VAL:HG23	2.17	0.44
1:B:1262:PRO:O	1:B:1264:ASN:ND2	2.49	0.44
1:B:2129:LEU:HD12	1:B:2130:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ARG:HH21	1:C:287:SER:HG	1.66	0.44
1:C:1105:PHE:CE2	1:C:1115:VAL:HG11	2.53	0.44
1:C:4018:MET:O	1:C:4026:THR:OG1	2.29	0.44
1:D:1930:ASP:OD1	1:D:2027:ARG:NH2	2.49	0.44
1:D:2582:SER:HB2	1:D:2875:THR:HG22	1.97	0.44
1:B:73:LEU:O	1:B:118:ALA:N	2.49	0.44
1:B:494:MET:CE	1:B:499:LEU:HD21	2.46	0.44
1:C:2183:SER:OG	1:C:2184:LYS:N	2.50	0.44
1:D:1105:PHE:CE2	1:D:1115:VAL:HG11	2.52	0.44
1:D:3888:TYR:O	1:D:3892:SER:N	2.49	0.44
1:A:1262:PRO:O	1:A:1264:ASN:ND2	2.49	0.44
1:B:3888:TYR:O	1:B:3892:SER:N	2.49	0.44
1:B:3940:TRP:O	1:B:3944:VAL:HG13	2.17	0.44
1:C:2129:LEU:HD12	1:C:2130:SER:N	2.32	0.44
1:C:3924:GLN:O	1:C:4934:GLY:N	2.46	0.44
1:D:674:TYR:O	1:D:822:CYS:N	2.48	0.44
1:D:2290:ASN:OD1	1:D:2290:ASN:N	2.51	0.44
1:D:4619:GLN:OE1	1:D:4631:ARG:NH1	2.46	0.44
1:A:886:ALA:HB1	1:A:921:PHE:CE1	2.52	0.44
1:A:2129:LEU:HD12	1:A:2130:SER:N	2.32	0.44
1:C:10:GLU:N	1:C:10:GLU:OE2	2.50	0.44
1:C:2290:ASN:OD1	1:C:2290:ASN:N	2.51	0.44
1:C:4069:ALA:HB1	1:C:4077:LEU:HD13	1.99	0.44
1:D:2129:LEU:HD12	1:D:2130:SER:N	2.32	0.44
2:E:25:HIS:O	2:E:40:ARG:NE	2.38	0.44
1:A:3924:GLN:O	1:A:4934:GLY:N	2.46	0.44
1:B:1930:ASP:OD1	1:B:2027:ARG:NH2	2.49	0.44
1:B:2290:ASN:N	1:B:2290:ASN:OD1	2.51	0.44
1:C:2584:MET:SD	1:C:2584:MET:N	2.91	0.44
1:C:3888:TYR:O	1:C:3892:SER:N	2.49	0.44
1:D:3978:VAL:HA	1:D:3981:LEU:HD12	1.99	0.44
2:H:24:VAL:N	2:H:46:PHE:O	2.50	0.44
1:A:10:GLU:N	1:A:10:GLU:OE2	2.50	0.44
1:A:2592:VAL:HG22	1:A:2641:ARG:NH2	2.33	0.44
1:A:4069:ALA:HB1	1:A:4077:LEU:HD13	1.99	0.44
1:B:2584:MET:SD	1:B:2584:MET:N	2.91	0.44
1:B:4069:ALA:HB1	1:B:4077:LEU:HD13	1.99	0.44
1:C:195:SER:OG	1:C:204:ASP:OD2	2.34	0.44
1:C:4185:MET:O	1:C:4189:VAL:HG23	2.17	0.44
1:D:2183:SER:OG	1:D:2184:LYS:N	2.50	0.44
1:B:1846:LEU:HB2	1:B:1847:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:GLU:N	1:D:10:GLU:OE2	2.50	0.44
1:B:271:ALA:HA	1:B:274:LEU:HD12	2.00	0.44
1:B:2592:VAL:HG22	1:B:2641:ARG:NH2	2.33	0.44
1:B:3978:VAL:HA	1:B:3981:LEU:HD12	1.99	0.44
1:D:4069:ALA:HB1	1:D:4077:LEU:HD13	1.99	0.44
1:A:1048:ASP:OD2	1:A:1049:SER:N	2.51	0.44
1:A:224:ALA:HB2	1:A:229:ILE:HD12	2.00	0.43
1:A:878:LEU:O	1:A:881:ILE:N	2.50	0.43
1:B:2183:SER:OG	1:B:2184:LYS:N	2.50	0.43
1:C:271:ALA:HA	1:C:274:LEU:HD12	2.00	0.43
1:C:1846:LEU:HB2	1:C:1847:ILE:HG23	2.00	0.43
1:C:4789:ARG:O	1:C:4804:LYS:NZ	2.50	0.43
1:D:271:ALA:HA	1:D:274:LEU:HD12	2.00	0.43
1:D:1048:ASP:OD2	1:D:1049:SER:N	2.51	0.43
1:A:3978:VAL:HA	1:A:3981:LEU:HD12	1.99	0.43
1:B:195:SER:OG	1:B:204:ASP:OD2	2.34	0.43
1:B:218:SER:OG	1:B:219:SER:N	2.51	0.43
1:D:308:LEU:HD22	1:D:393:MET:HG3	2.00	0.43
1:D:2584:MET:SD	1:D:2584:MET:N	2.91	0.43
1:D:2592:VAL:HG22	1:D:2641:ARG:NH2	2.33	0.43
1:A:41:GLY:O	1:A:45:ARG:NH1	2.52	0.43
1:A:271:ALA:HA	1:A:274:LEU:HD12	2.00	0.43
1:D:281:ARG:HH21	1:D:287:SER:HG	1.66	0.43
1:D:1262:PRO:O	1:D:1264:ASN:ND2	2.49	0.43
1:A:218:SER:OG	1:A:219:SER:N	2.51	0.43
1:A:2996:SER:OG	1:A:3070:THR:HG21	2.19	0.43
1:B:541:ILE:HG23	1:B:547:ASN:O	2.19	0.43
1:C:2315:ASN:O	1:C:2319:VAL:HG23	2.19	0.43
1:B:41:GLY:O	1:B:45:ARG:NH1	2.52	0.43
1:B:4185:MET:O	1:B:4189:VAL:HG23	2.17	0.43
1:D:2122:LEU:CD2	1:D:2164:LEU:HD13	2.49	0.43
1:A:1930:ASP:OD1	1:A:2027:ARG:NH2	2.49	0.43
1:A:4099:VAL:HG22	1:A:4132:LEU:CD1	2.47	0.43
1:B:1048:ASP:OD2	1:B:1049:SER:N	2.51	0.43
1:B:2122:LEU:CD2	1:B:2164:LEU:HD13	2.49	0.43
1:B:3839:PHE:HB3	1:B:3918:THR:HG21	2.00	0.43
1:B:4701:ASP:OD1	1:B:4703:LYS:N	2.52	0.43
1:C:2122:LEU:CD2	1:C:2164:LEU:HD13	2.49	0.43
1:C:3056:LEU:O	1:C:3060:LEU:N	2.52	0.43
1:C:4136:GLU:OE2	1:C:4146:ARG:NH2	2.48	0.43
1:D:218:SER:OG	1:D:219:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ALA:HB2	1:D:229:ILE:HD12	2.00	0.43
2:E:12:GLY:O	2:E:13:ARG:NE	2.52	0.43
2:H:12:GLY:O	2:H:13:ARG:NE	2.52	0.43
1:A:290:ARG:NH2	1:A:352:SER:OG	2.52	0.43
1:A:541:ILE:HG23	1:A:547:ASN:O	2.19	0.43
1:A:991:SER:O	1:A:994:ALA:N	2.52	0.43
1:A:1846:LEU:HB2	1:A:1847:ILE:HG23	2.00	0.43
1:A:2183:SER:OG	1:A:2184:LYS:N	2.50	0.43
1:A:4789:ARG:O	1:A:4804:LYS:NZ	2.50	0.43
1:B:308:LEU:HD22	1:B:393:MET:HG3	2.01	0.43
1:B:991:SER:O	1:B:994:ALA:N	2.52	0.43
1:D:1758:LEU:HD22	1:D:2116:ILE:HD11	2.01	0.43
1:A:3056:LEU:O	1:A:3060:LEU:N	2.52	0.43
1:C:41:GLY:O	1:C:45:ARG:NH1	2.51	0.43
1:C:218:SER:OG	1:C:219:SER:N	2.51	0.43
1:C:411:GLU:OE1	1:C:411:GLU:N	2.49	0.43
1:C:569:SER:O	1:C:609:LYS:NZ	2.40	0.43
1:C:1048:ASP:OD2	1:C:1049:SER:N	2.51	0.43
1:C:2592:VAL:HG22	1:C:2641:ARG:NH2	2.33	0.43
1:D:2461:PRO:O	1:D:2518:TYR:OH	2.28	0.43
2:F:24:VAL:N	2:F:46:PHE:O	2.50	0.43
1:B:2986:SER:OG	1:B:2987:ARG:N	2.52	0.43
1:B:3269:SER:OG	1:B:3342:GLU:OE1	2.21	0.43
1:D:4701:ASP:OD1	1:D:4703:LYS:N	2.52	0.43
2:F:12:GLY:O	2:F:13:ARG:NE	2.52	0.43
1:A:2290:ASN:OD1	1:A:2290:ASN:N	2.51	0.43
1:A:2584:MET:SD	1:A:2584:MET:N	2.91	0.43
1:B:224:ALA:HB2	1:B:229:ILE:HD12	2.00	0.43
1:B:2720:ILE:O	1:B:2771:ARG:NE	2.44	0.43
1:B:2996:SER:OG	1:B:3070:THR:HG21	2.19	0.43
1:C:541:ILE:HG23	1:C:547:ASN:O	2.19	0.43
1:C:742:SER:O	1:C:776:GLN:N	2.51	0.43
1:C:991:SER:O	1:C:994:ALA:N	2.52	0.43
1:C:3839:PHE:HB3	1:C:3918:THR:HG21	2.00	0.43
1:D:1846:LEU:HB2	1:D:1847:ILE:HG23	2.00	0.43
1:D:4136:GLU:OE2	1:D:4146:ARG:NH2	2.48	0.43
2:G:12:GLY:O	2:G:13:ARG:NE	2.52	0.43
1:A:658:ASN:N	1:A:833:LYS:O	2.53	0.42
1:A:2122:LEU:CD2	1:A:2164:LEU:HD13	2.49	0.42
1:A:2315:ASN:O	1:A:2319:VAL:HG23	2.19	0.42
1:A:2986:SER:OG	1:A:2987:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ARG:NH2	1:B:352:SER:OG	2.52	0.42
1:B:2315:ASN:O	1:B:2319:VAL:HG23	2.19	0.42
1:C:2112:VAL:O	1:C:2116:ILE:HD12	2.19	0.42
1:D:991:SER:O	1:D:994:ALA:N	2.52	0.42
1:A:4701:ASP:OD1	1:A:4703:LYS:N	2.52	0.42
1:A:4778:TYR:O	1:A:4782:VAL:HG23	2.19	0.42
1:B:2112:VAL:O	1:B:2116:ILE:HD12	2.19	0.42
1:B:2210:GLN:NE2	1:B:2244:ALA:O	2.52	0.42
1:C:224:ALA:HB2	1:C:229:ILE:HD12	2.00	0.42
1:C:290:ARG:NH2	1:C:352:SER:OG	2.52	0.42
1:D:450:GLU:O	1:D:453:SER:OG	2.33	0.42
1:D:884:ARG:NH2	1:D:959:GLU:OE1	2.52	0.42
1:D:1292:SER:H	1:D:1553:VAL:HG22	1.84	0.42
1:D:2996:SER:OG	1:D:3070:THR:HG21	2.19	0.42
1:A:3661:ASP:OD2	1:A:3664:HIS:N	2.50	0.42
1:B:3914:GLN:O	1:B:3918:THR:HG23	2.20	0.42
1:C:4701:ASP:OD1	1:C:4703:LYS:N	2.52	0.42
1:D:41:GLY:O	1:D:45:ARG:NH1	2.52	0.42
2:F:37:ASP:OD1	2:F:38:SER:N	2.53	0.42
1:A:1758:LEU:HD22	1:A:2116:ILE:HD11	2.01	0.42
1:A:2210:GLN:NE2	1:A:2244:ALA:O	2.52	0.42
1:C:1758:LEU:HD22	1:C:2116:ILE:HD11	2.01	0.42
1:C:2210:GLN:NE2	1:C:2244:ALA:O	2.52	0.42
1:A:308:LEU:HD22	1:A:393:MET:HG3	2.01	0.42
1:B:2633:SER:OG	1:B:2634:GLU:N	2.53	0.42
1:C:2986:SER:OG	1:C:2987:ARG:N	2.52	0.42
1:C:2996:SER:OG	1:C:3070:THR:HG21	2.19	0.42
1:C:4778:TYR:O	1:C:4782:VAL:HG23	2.19	0.42
1:D:411:GLU:OE1	1:D:411:GLU:N	2.49	0.42
2:G:24:VAL:N	2:G:46:PHE:O	2.50	0.42
1:A:1090:ALA:HB3	1:A:1202:ILE:HD11	2.02	0.42
1:A:3914:GLN:O	1:A:3918:THR:HG23	2.20	0.42
1:B:4778:TYR:O	1:B:4782:VAL:HG23	2.19	0.42
1:B:4789:ARG:O	1:B:4804:LYS:NZ	2.50	0.42
1:C:3914:GLN:O	1:C:3918:THR:HG23	2.19	0.42
1:C:4099:VAL:HG22	1:C:4132:LEU:CD1	2.47	0.42
1:C:4576:ILE:HG22	1:C:4580:ILE:HD12	2.02	0.42
1:D:541:ILE:HG23	1:D:547:ASN:O	2.19	0.42
1:D:658:ASN:N	1:D:833:LYS:O	2.53	0.42
1:A:281:ARG:HH21	1:A:287:SER:HG	1.67	0.42
1:A:2512:ALA:O	1:A:2516:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2594:ASP:OD2	1:A:2600:GLU:N	2.53	0.42
1:A:3237:VAL:O	1:A:3242:CYS:N	2.51	0.42
1:A:3839:PHE:HB3	1:A:3918:THR:HG21	2.00	0.42
1:C:1292:SER:H	1:C:1553:VAL:HG22	1.84	0.42
1:D:290:ARG:NH2	1:D:352:SER:OG	2.52	0.42
1:D:3056:LEU:O	1:D:3060:LEU:N	2.52	0.42
1:D:4778:TYR:O	1:D:4782:VAL:HG23	2.19	0.42
1:B:742:SER:O	1:B:776:GLN:N	2.51	0.42
1:D:742:SER:O	1:D:776:GLN:N	2.51	0.42
1:D:2112:VAL:O	1:D:2116:ILE:HD12	2.19	0.42
1:D:2594:ASP:OD2	1:D:2600:GLU:N	2.53	0.42
1:D:3839:PHE:HB3	1:D:3918:THR:HG21	2.00	0.42
1:A:541:ILE:HG22	1:A:577:CYS:SG	2.60	0.42
1:B:658:ASN:N	1:B:833:LYS:O	2.53	0.42
1:B:892:LEU:HD13	1:B:1056:THR:CG2	2.50	0.42
1:B:4099:VAL:HG22	1:B:4132:LEU:CD1	2.47	0.42
1:C:308:LEU:HD22	1:C:393:MET:HG3	2.01	0.42
1:C:1090:ALA:HB3	1:C:1202:ILE:HD11	2.02	0.42
1:C:2633:SER:OG	1:C:2634:GLU:N	2.53	0.42
1:D:2315:ASN:O	1:D:2319:VAL:HG23	2.19	0.42
1:D:3914:GLN:O	1:D:3918:THR:HG23	2.20	0.42
2:E:37:ASP:OD1	2:E:38:SER:N	2.53	0.42
1:A:1433:PHE:O	1:A:1435:GLY:N	2.53	0.42
1:A:3876:TYR:O	1:A:3880:VAL:HG23	2.20	0.42
1:B:3056:LEU:O	1:B:3060:LEU:N	2.52	0.42
1:C:3876:TYR:O	1:C:3880:VAL:HG23	2.20	0.42
1:D:3876:TYR:O	1:D:3880:VAL:HG23	2.20	0.42
2:G:37:ASP:OD1	2:G:38:SER:N	2.53	0.42
2:H:11:ASP:OD2	2:H:14:THR:OG1	2.28	0.42
1:A:4576:ILE:HG22	1:A:4580:ILE:HD12	2.01	0.41
1:B:550:GLN:O	1:B:554:SER:N	2.53	0.41
1:B:674:TYR:O	1:B:822:CYS:N	2.48	0.41
1:B:1090:ALA:HB3	1:B:1202:ILE:HD11	2.02	0.41
1:C:1433:PHE:O	1:C:1435:GLY:N	2.53	0.41
1:C:4895:ASP:OD1	1:C:4895:ASP:N	2.53	0.41
1:D:2210:GLN:NE2	1:D:2244:ALA:O	2.52	0.41
1:A:450:GLU:O	1:A:453:SER:OG	2.32	0.41
1:A:2720:ILE:O	1:A:2771:ARG:NE	2.44	0.41
1:B:195:SER:OG	1:B:202:HIS:O	2.38	0.41
1:D:892:LEU:HD13	1:D:1056:THR:CG2	2.50	0.41
1:D:1433:PHE:O	1:D:1435:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2633:SER:OG	1:D:2634:GLU:N	2.53	0.41
1:D:2986:SER:OG	1:D:2987:ARG:N	2.52	0.41
1:D:3630:THR:OG1	1:D:3631:GLU:N	2.53	0.41
1:A:18:ASP:N	1:A:18:ASP:OD1	2.54	0.41
1:A:2633:SER:OG	1:A:2634:GLU:N	2.53	0.41
1:B:878:LEU:O	1:B:881:ILE:N	2.50	0.41
1:B:1433:PHE:O	1:B:1435:GLY:N	2.53	0.41
1:B:1758:LEU:HD22	1:B:2116:ILE:HD11	2.01	0.41
1:B:3237:VAL:O	1:B:3242:CYS:N	2.51	0.41
1:C:195:SER:OG	1:C:202:HIS:O	2.38	0.41
1:C:658:ASN:N	1:C:833:LYS:O	2.53	0.41
1:D:4895:ASP:OD1	1:D:4895:ASP:N	2.53	0.41
1:A:1292:SER:H	1:A:1553:VAL:HG22	1.84	0.41
1:A:2112:VAL:O	1:A:2116:ILE:HD12	2.19	0.41
1:B:541:ILE:HG22	1:B:577:CYS:SG	2.60	0.41
1:B:1292:SER:H	1:B:1553:VAL:HG22	1.84	0.41
1:B:2461:PRO:O	1:B:2518:TYR:OH	2.28	0.41
1:B:4576:ILE:HG22	1:B:4580:ILE:HD12	2.02	0.41
1:B:4928:ASP:OD2	1:B:4930:THR:OG1	2.25	0.41
1:D:541:ILE:HG22	1:D:577:CYS:SG	2.60	0.41
1:D:4789:ARG:O	1:D:4804:LYS:NZ	2.50	0.41
2:H:37:ASP:OD1	2:H:38:SER:N	2.53	0.41
1:A:674:TYR:O	1:A:822:CYS:N	2.48	0.41
1:A:2405:MET:SD	1:A:2405:MET:N	2.89	0.41
1:C:892:LEU:HD13	1:C:1056:THR:CG2	2.50	0.41
1:C:2210:GLN:OE1	1:C:2249:ASN:ND2	2.54	0.41
1:C:4701:ASP:OD1	1:C:4702:VAL:N	2.53	0.41
1:D:195:SER:OG	1:D:202:HIS:O	2.38	0.41
1:D:1090:ALA:HB3	1:D:1202:ILE:HD11	2.02	0.41
1:A:2081:ARG:O	1:A:2085:VAL:HG23	2.21	0.41
1:A:2788:ILE:HD11	1:A:2895:LEU:HD11	2.03	0.41
1:A:3907:LYS:O	1:A:3911:VAL:HG23	2.21	0.41
1:B:332:ARG:N	1:B:362:TYR:O	2.54	0.41
1:B:2512:ALA:O	1:B:2516:ASN:ND2	2.53	0.41
1:C:332:ARG:N	1:C:362:TYR:O	2.54	0.41
1:C:3843:GLN:HB2	1:C:3918:THR:HG22	2.03	0.41
1:D:332:ARG:N	1:D:362:TYR:O	2.54	0.41
1:D:2512:ALA:O	1:D:2516:ASN:ND2	2.53	0.41
1:D:3843:GLN:HB2	1:D:3918:THR:HG22	2.03	0.41
1:D:4701:ASP:OD1	1:D:4702:VAL:N	2.53	0.41
1:A:332:ARG:N	1:A:362:TYR:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:991:SER:OG	1:A:992:GLN:N	2.54	0.41
1:B:2081:ARG:O	1:B:2085:VAL:HG23	2.21	0.41
1:C:2512:ALA:O	1:C:2516:ASN:ND2	2.53	0.41
1:D:18:ASP:N	1:D:18:ASP:OD1	2.54	0.41
1:D:991:SER:OG	1:D:992:GLN:N	2.54	0.41
1:D:2210:GLN:OE1	1:D:2249:ASN:ND2	2.54	0.41
1:A:884:ARG:NH2	1:A:959:GLU:OE1	2.52	0.41
1:A:1523:ALA:O	1:A:1526:LYS:NZ	2.52	0.41
1:B:3907:LYS:O	1:B:3911:VAL:HG23	2.21	0.41
1:C:541:ILE:HG22	1:C:577:CYS:SG	2.60	0.41
1:C:2788:ILE:HD11	1:C:2895:LEU:HD11	2.03	0.41
1:A:1728:VAL:HG11	1:A:1925:VAL:HG11	2.03	0.41
1:A:2210:GLN:OE1	1:A:2249:ASN:ND2	2.54	0.41
1:A:2365:SER:O	1:A:2365:SER:OG	2.37	0.41
1:A:4701:ASP:OD1	1:A:4702:VAL:N	2.53	0.41
1:B:2210:GLN:OE1	1:B:2249:ASN:ND2	2.54	0.41
1:B:2594:ASP:OD2	1:B:2600:GLU:N	2.53	0.41
1:B:3876:TYR:O	1:B:3880:VAL:HG23	2.20	0.41
1:C:1993:ASP:OD2	1:C:1994:GLN:N	2.54	0.41
1:C:2594:ASP:OD2	1:C:2600:GLU:N	2.53	0.41
1:C:3907:LYS:O	1:C:3911:VAL:HG23	2.21	0.41
1:C:4095:PHE:O	1:C:4099:VAL:HG23	2.21	0.41
1:D:2109:GLY:O	1:D:2112:VAL:HG22	2.21	0.41
1:D:3907:LYS:O	1:D:3911:VAL:HG23	2.21	0.41
1:D:4095:PHE:O	1:D:4099:VAL:HG23	2.21	0.41
1:D:4576:ILE:HG22	1:D:4580:ILE:HD12	2.02	0.41
1:B:237:LEU:N	1:B:404:ASN:O	2.52	0.41
1:B:574:VAL:O	1:B:578:VAL:HG23	2.21	0.41
1:B:2788:ILE:HD11	1:B:2895:LEU:HD11	2.03	0.41
1:B:3404:TYR:O	1:B:3408:SER:OG	2.21	0.41
1:B:4701:ASP:OD1	1:B:4702:VAL:N	2.53	0.41
1:C:450:GLU:O	1:C:453:SER:OG	2.32	0.41
1:D:327:THR:O	1:D:327:THR:OG1	2.38	0.41
1:D:655:MET:N	1:D:792:VAL:O	2.54	0.41
1:A:1654:PHE:O	1:A:1658:THR:HG23	2.21	0.40
1:A:3630:THR:OG1	1:A:3631:GLU:N	2.53	0.40
1:B:18:ASP:N	1:B:18:ASP:OD1	2.54	0.40
1:B:991:SER:OG	1:B:992:GLN:N	2.54	0.40
1:B:1728:VAL:HG11	1:B:1925:VAL:HG11	2.03	0.40
1:B:3843:GLN:HB2	1:B:3918:THR:HG22	2.03	0.40
1:C:1654:PHE:O	1:C:1658:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4772:LEU:HD21	1:D:4752:LEU:CD1	2.51	0.40
1:D:323:ASP:N	1:D:323:ASP:OD1	2.54	0.40
1:D:1305:SER:HG	1:D:1594:HIS:CE1	2.40	0.40
1:A:574:VAL:O	1:A:578:VAL:HG23	2.22	0.40
1:B:948:CYS:SG	1:B:1064:LEU:HD12	2.62	0.40
1:C:574:VAL:O	1:C:578:VAL:HG23	2.22	0.40
1:C:884:ARG:NH2	1:C:959:GLU:OE1	2.51	0.40
1:C:991:SER:OG	1:C:992:GLN:N	2.54	0.40
1:C:2109:GLY:O	1:C:2112:VAL:HG22	2.21	0.40
1:C:3870:ILE:O	1:C:3874:VAL:HG23	2.21	0.40
1:A:23:GLN:O	1:A:213:SER:N	2.52	0.40
1:A:4095:PHE:O	1:A:4099:VAL:HG23	2.21	0.40
1:A:4752:LEU:CD1	1:D:4772:LEU:HD21	2.51	0.40
1:B:1993:ASP:OD2	1:B:1994:GLN:N	2.54	0.40
1:C:542:ARG:O	1:C:545:ARG:NH1	2.55	0.40
1:C:2095:GLY:O	1:C:2099:ARG:NH1	2.55	0.40
1:D:2268:LEU:HD21	1:D:2297:TYR:HB2	2.04	0.40
1:D:3870:ILE:O	1:D:3874:VAL:HG23	2.22	0.40
2:E:22:CYS:SG	2:E:50:ILE:HD11	2.62	0.40
2:F:22:CYS:SG	2:F:50:ILE:HD11	2.62	0.40
1:A:3843:GLN:HB2	1:A:3918:THR:HG22	2.03	0.40
1:B:411:GLU:OE1	1:B:411:GLU:N	2.49	0.40
1:B:1654:PHE:O	1:B:1658:THR:HG23	2.21	0.40
1:B:2095:GLY:O	1:B:2099:ARG:NH1	2.55	0.40
1:B:2109:GLY:O	1:B:2112:VAL:HG22	2.21	0.40
1:B:4095:PHE:O	1:B:4099:VAL:HG23	2.21	0.40
1:C:18:ASP:OD1	1:C:18:ASP:N	2.54	0.40
1:D:23:GLN:N	1:D:213:SER:O	2.54	0.40
1:D:308:LEU:HD21	1:D:370:LEU:HD12	2.04	0.40
1:D:1654:PHE:O	1:D:1658:THR:HG23	2.21	0.40
1:D:1993:ASP:OD2	1:D:1994:GLN:N	2.54	0.40
1:D:2095:GLY:O	1:D:2099:ARG:NH1	2.55	0.40
1:D:2788:ILE:HD11	1:D:2895:LEU:HD11	2.03	0.40
2:E:24:VAL:N	2:E:46:PHE:O	2.50	0.40
1:A:1993:ASP:OD2	1:A:1994:GLN:N	2.54	0.40
1:B:3870:ILE:O	1:B:3874:VAL:HG23	2.21	0.40
1:C:308:LEU:HD21	1:C:370:LEU:HD12	2.03	0.40
1:C:1523:ALA:O	1:C:1526:LYS:NZ	2.52	0.40
1:C:4777:VAL:HG13	1:C:4815:HIS:HB3	2.04	0.40
1:D:574:VAL:O	1:D:578:VAL:HG23	2.21	0.40
1:D:1728:VAL:HG11	1:D:1925:VAL:HG11	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	3849/4966 (78%)	3357 (87%)	482 (12%)	10 (0%)	41	76
1	B	3849/4966 (78%)	3358 (87%)	481 (12%)	10 (0%)	41	76
1	C	3849/4966 (78%)	3358 (87%)	481 (12%)	10 (0%)	41	76
1	D	3849/4966 (78%)	3359 (87%)	480 (12%)	10 (0%)	41	76
2	E	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	F	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	G	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	H	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
All	All	15816/20292 (78%)	13816 (87%)	1960 (12%)	40 (0%)	44	76

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1500	ARG
1	B	1500	ARG
1	C	1500	ARG
1	D	1500	ARG
1	A	607	ASN
1	B	607	ASN
1	C	607	ASN
1	D	607	ASN
1	A	2677	PRO
1	B	2677	PRO
1	C	2677	PRO
1	D	2677	PRO
1	A	2230	SER
1	B	2230	SER

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Mol	Chain	Res	Type
1	C	2230	SER
1	D	2230	SER
1	A	468	GLU
1	A	1947	MET
1	A	2676	PRO
1	B	468	GLU
1	B	1947	MET
1	B	2676	PRO
1	C	468	GLU
1	C	1947	MET
1	C	2676	PRO
1	D	468	GLU
1	D	1947	MET
1	D	2676	PRO
1	A	1781	PRO
1	B	1781	PRO
1	C	1781	PRO
1	D	1781	PRO
1	A	1262	PRO
1	A	2231	PRO
1	B	1262	PRO
1	B	2231	PRO
1	C	1262	PRO
1	C	2231	PRO
1	D	1262	PRO
1	D	2231	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3178/4355 (73%)	3164 (100%)	14 (0%)	91 94
1	B	3178/4355 (73%)	3164 (100%)	14 (0%)	91 94
1	C	3178/4355 (73%)	3164 (100%)	14 (0%)	91 94
1	D	3178/4355 (73%)	3164 (100%)	14 (0%)	91 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	88/88 (100%)	87 (99%)	1 (1%)	73	85
2	F	88/88 (100%)	87 (99%)	1 (1%)	73	85
2	G	88/88 (100%)	87 (99%)	1 (1%)	73	85
2	H	88/88 (100%)	87 (99%)	1 (1%)	73	85
All	All	13064/17772 (74%)	13004 (100%)	60 (0%)	89	93

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	ARG
1	A	542	ARG
1	A	640	ARG
1	A	941	LYS
1	A	987	LYS
1	A	2017	ASP
1	A	2072	SER
1	A	2203	CYS
1	A	2335	ARG
1	A	2405	MET
1	A	2744	GLU
1	A	2779	LYS
1	A	3653	GLU
1	A	3654	ASP
1	B	343	ARG
1	B	542	ARG
1	B	640	ARG
1	B	941	LYS
1	B	987	LYS
1	B	2017	ASP
1	B	2072	SER
1	B	2203	CYS
1	B	2335	ARG
1	B	2405	MET
1	B	2744	GLU
1	B	2779	LYS
1	B	3653	GLU
1	B	3654	ASP
1	C	343	ARG
1	C	542	ARG
1	C	640	ARG
1	C	941	LYS

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Mol	Chain	Res	Type
1	C	987	LYS
1	C	2017	ASP
1	C	2072	SER
1	C	2203	CYS
1	C	2335	ARG
1	C	2405	MET
1	C	2744	GLU
1	C	2779	LYS
1	C	3653	GLU
1	C	3654	ASP
1	D	343	ARG
1	D	542	ARG
1	D	640	ARG
1	D	941	LYS
1	D	987	LYS
1	D	2017	ASP
1	D	2072	SER
1	D	2203	CYS
1	D	2335	ARG
1	D	2405	MET
1	D	2744	GLU
1	D	2779	LYS
1	D	3653	GLU
1	D	3654	ASP
2	E	49	ARG
2	F	49	ARG
2	G	49	ARG
2	H	49	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	240	HIS
1	A	781	ASN
1	A	1157	GLN
1	A	1287	GLN
1	A	1944	ASN
1	A	2150	ASN
1	A	2176	ASN
1	A	2210	GLN
1	A	2249	ASN

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Mol	Chain	Res	Type
1	A	2317	ASN
1	A	2578	GLN
1	A	2691	GLN
1	A	2846	ASN
1	A	4557	HIS
1	A	4635	ASN
1	A	4878	GLN
1	B	168	GLN
1	B	240	HIS
1	B	781	ASN
1	B	1157	GLN
1	B	1287	GLN
1	B	1944	ASN
1	B	2150	ASN
1	B	2176	ASN
1	B	2210	GLN
1	B	2249	ASN
1	B	2317	ASN
1	B	2578	GLN
1	B	2691	GLN
1	B	2846	ASN
1	B	4557	HIS
1	B	4635	ASN
1	B	4878	GLN
1	C	168	GLN
1	C	240	HIS
1	C	781	ASN
1	C	1157	GLN
1	C	1944	ASN
1	C	2150	ASN
1	C	2176	ASN
1	C	2249	ASN
1	C	2317	ASN
1	C	2578	GLN
1	C	2691	GLN
1	C	2846	ASN
1	C	4557	HIS
1	C	4628	GLN
1	C	4635	ASN
1	C	4878	GLN
1	D	168	GLN
1	D	240	HIS

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Mol	Chain	Res	Type
1	D	781	ASN
1	D	1157	GLN
1	D	1944	ASN
1	D	2150	ASN
1	D	2176	ASN
1	D	2210	GLN
1	D	2249	ASN
1	D	2317	ASN
1	D	2578	GLN
1	D	2691	GLN
1	D	2846	ASN
1	D	4557	HIS
1	D	4635	ASN
1	D	4878	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

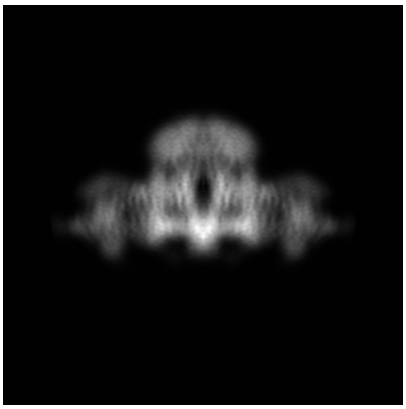
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21862. These allow visual inspection of the internal detail of the map and identification of artifacts.

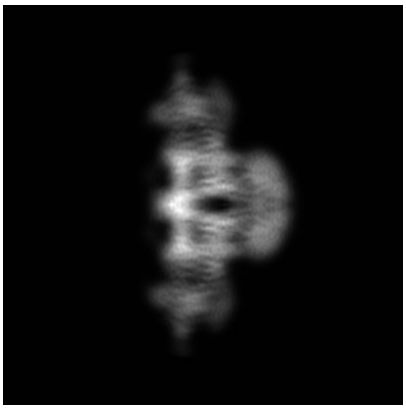
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

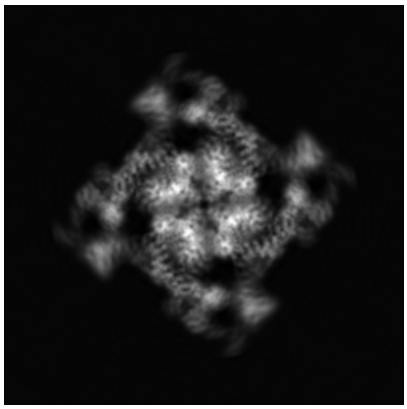
6.1.1 Primary map



X

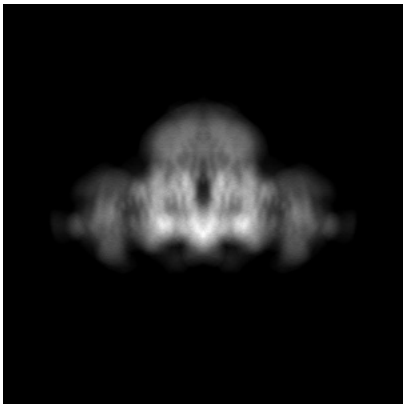


Y

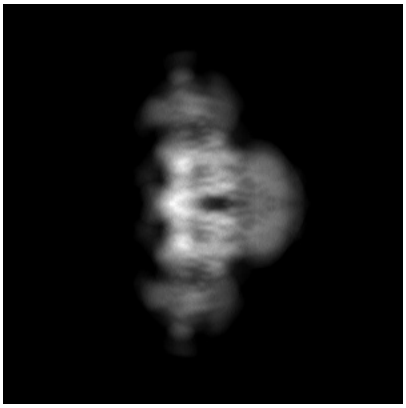


Z

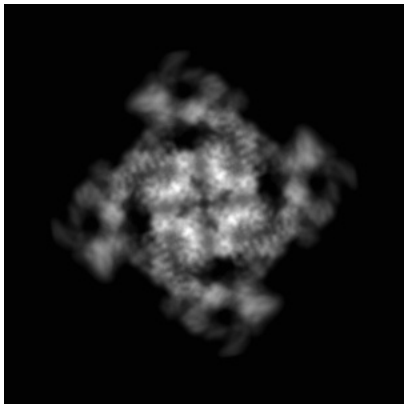
6.1.2 Raw map



X



Y

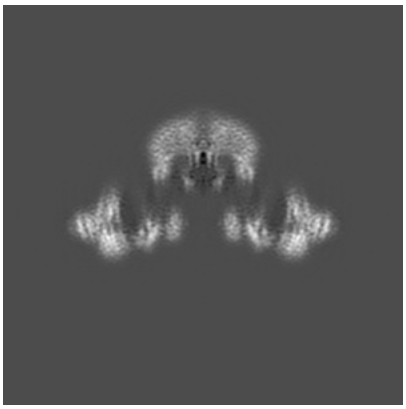


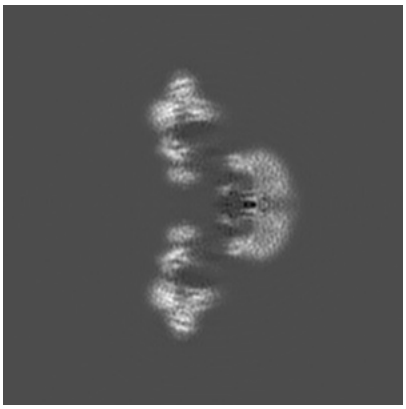
Z

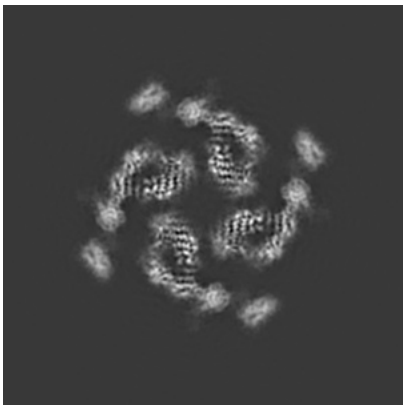
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

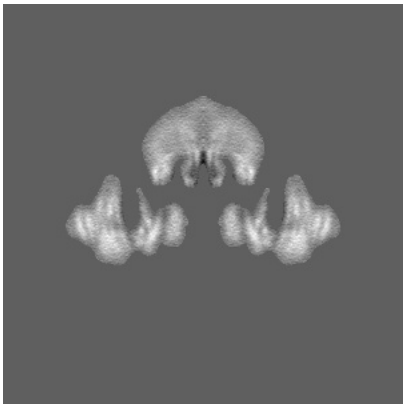
6.2.1 Primary map

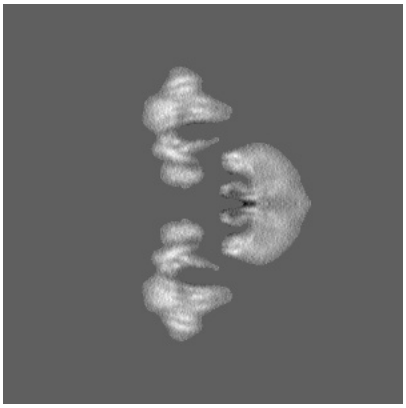

X Index: 176

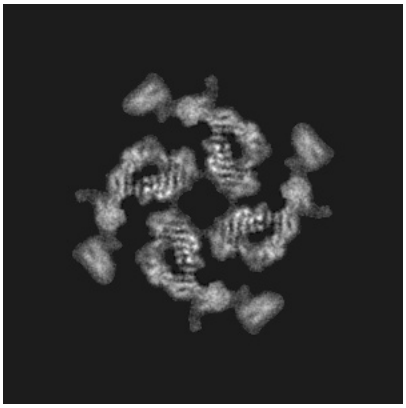

Y Index: 176


Z Index: 176

6.2.2 Raw map


X Index: 352

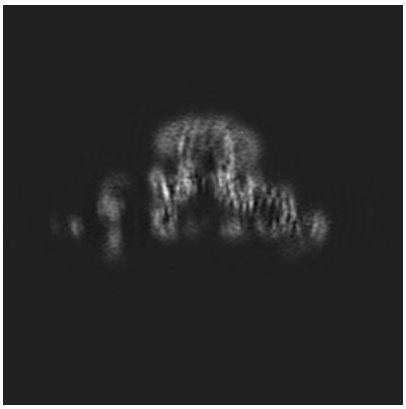

Y Index: 352


Z Index: 352

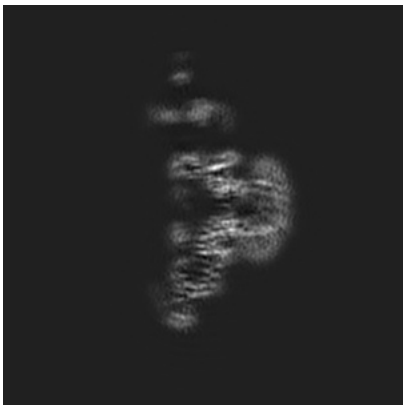
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

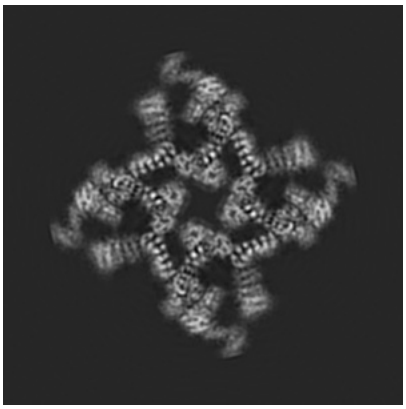
6.3.1 Primary map



X Index: 191

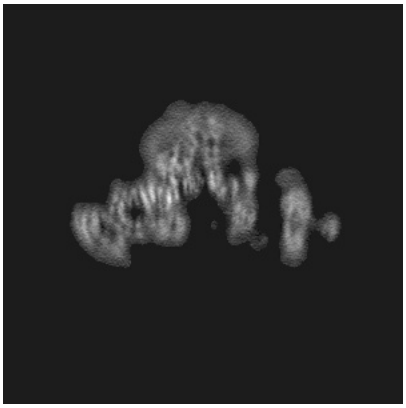


Y Index: 191



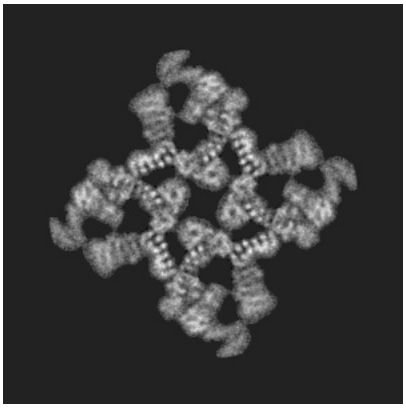
Z Index: 159

6.3.2 Raw map



X Index: 330

Y Index: 330

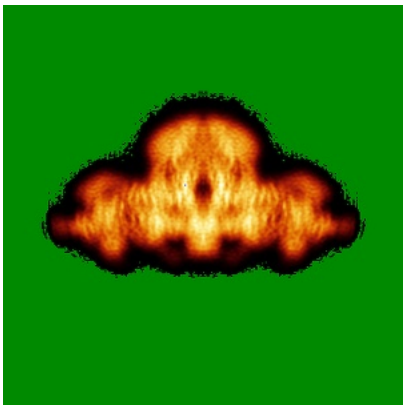


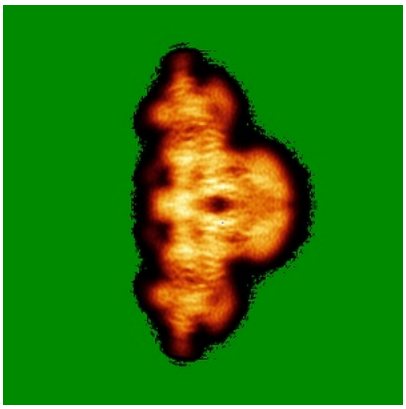
Z Index: 318

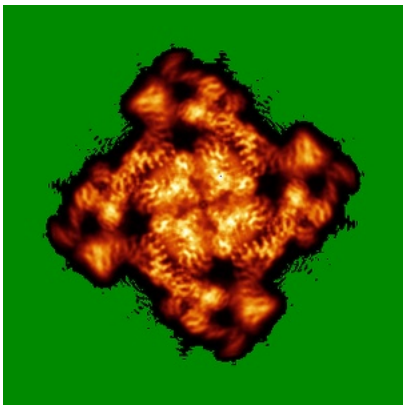
The images above show the largest variance slices of the map in three orthogonal directions.

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

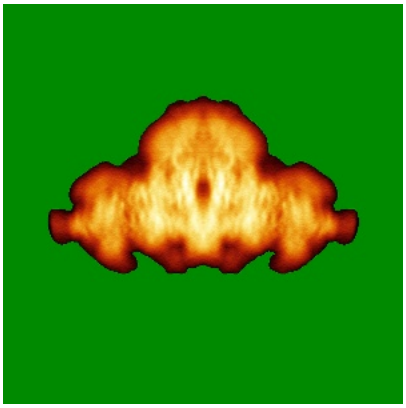
6.4.1 Primary map

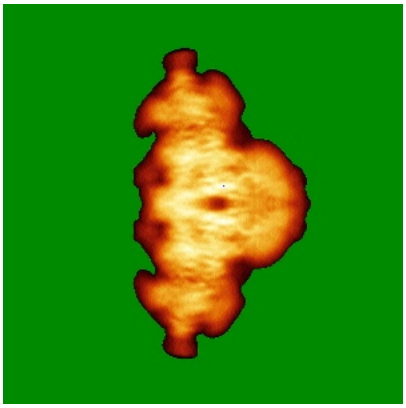

X

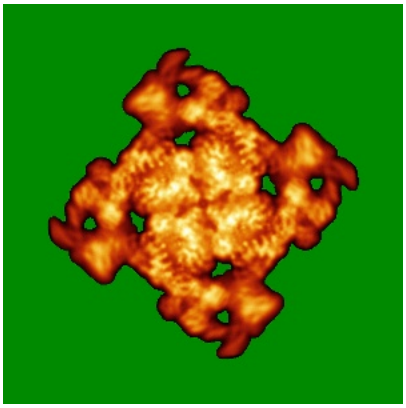

Y


Z

6.4.2 Raw 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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

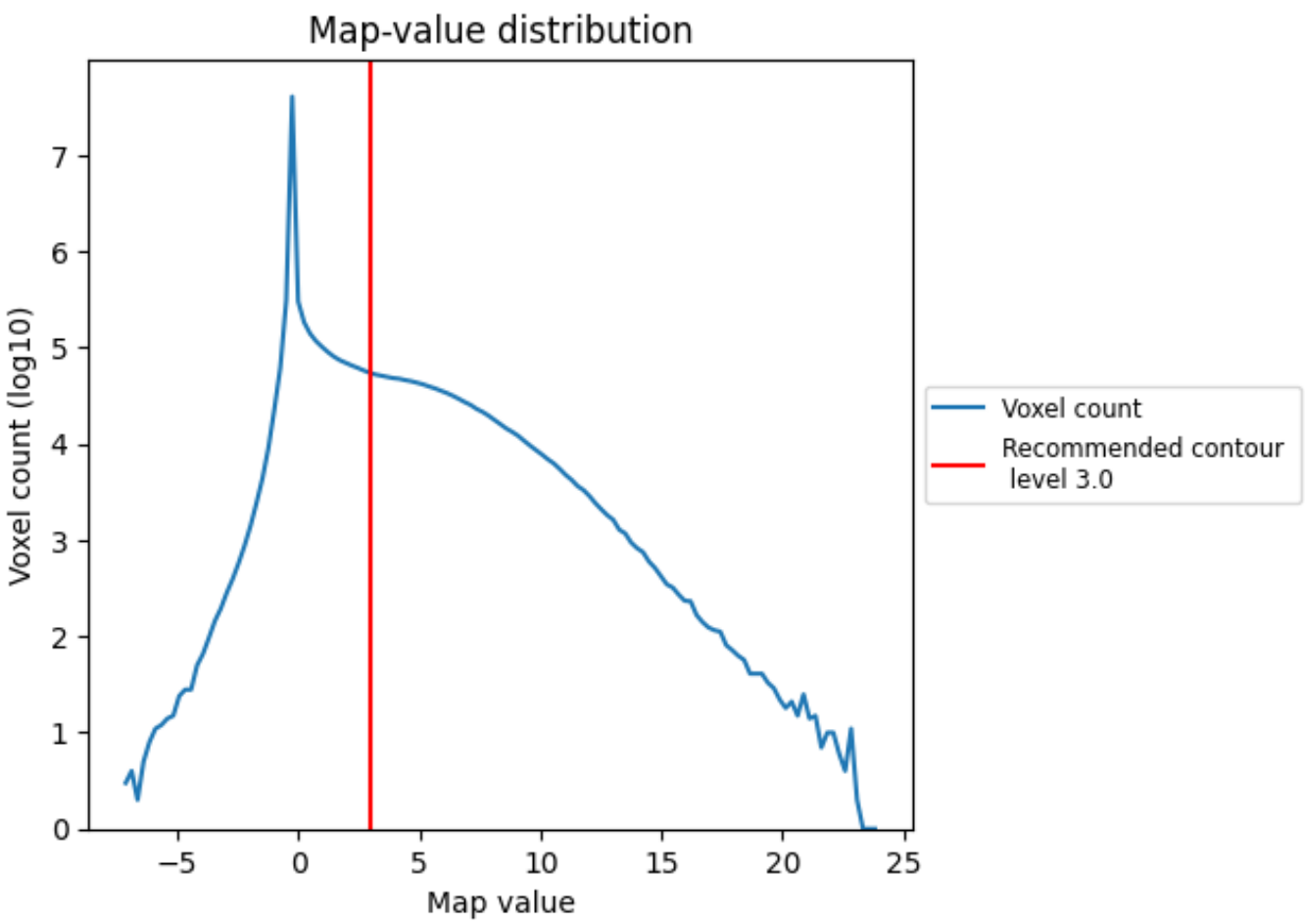
6.6 Mask visualisation (i)

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

7 Map analysis (i)

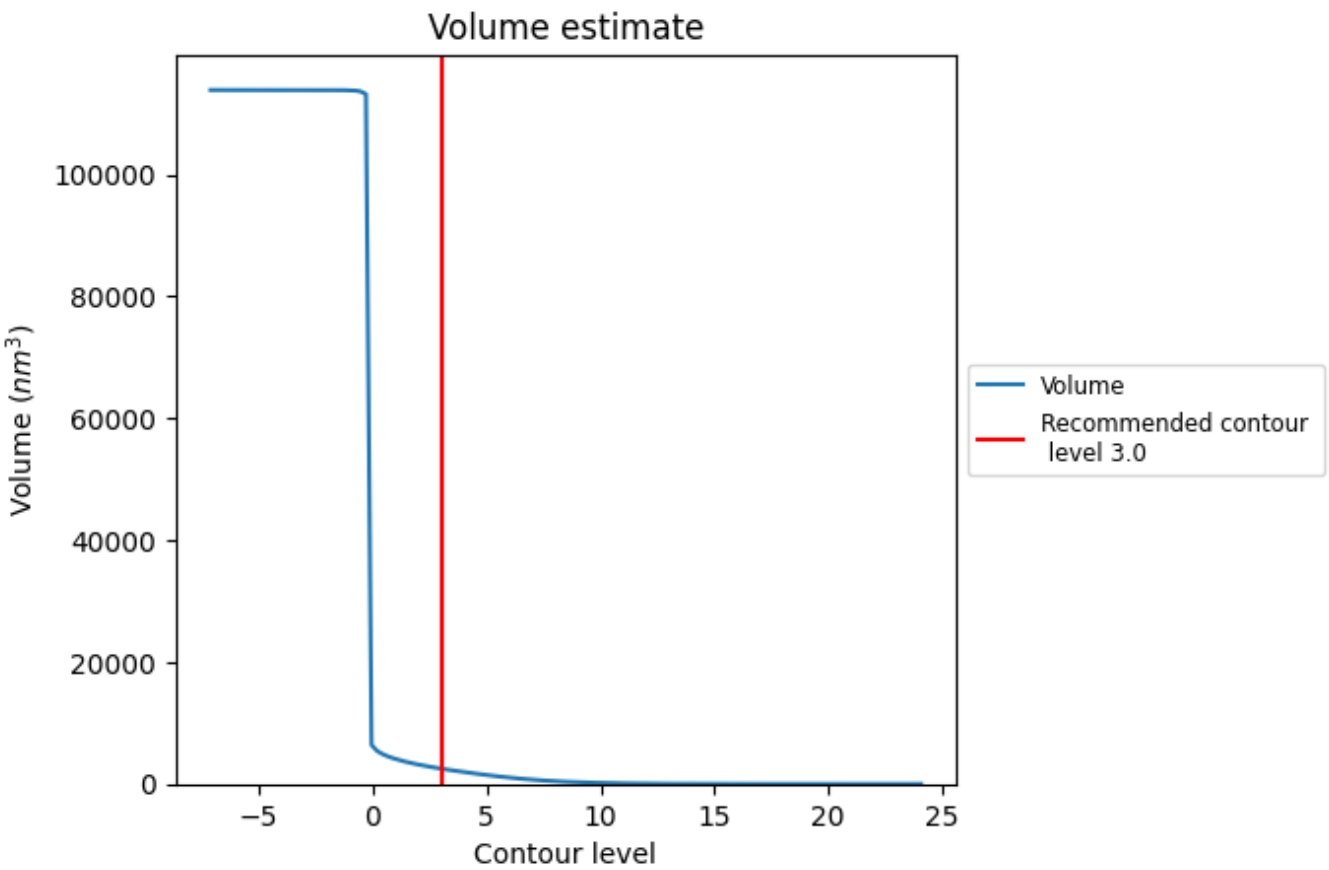
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

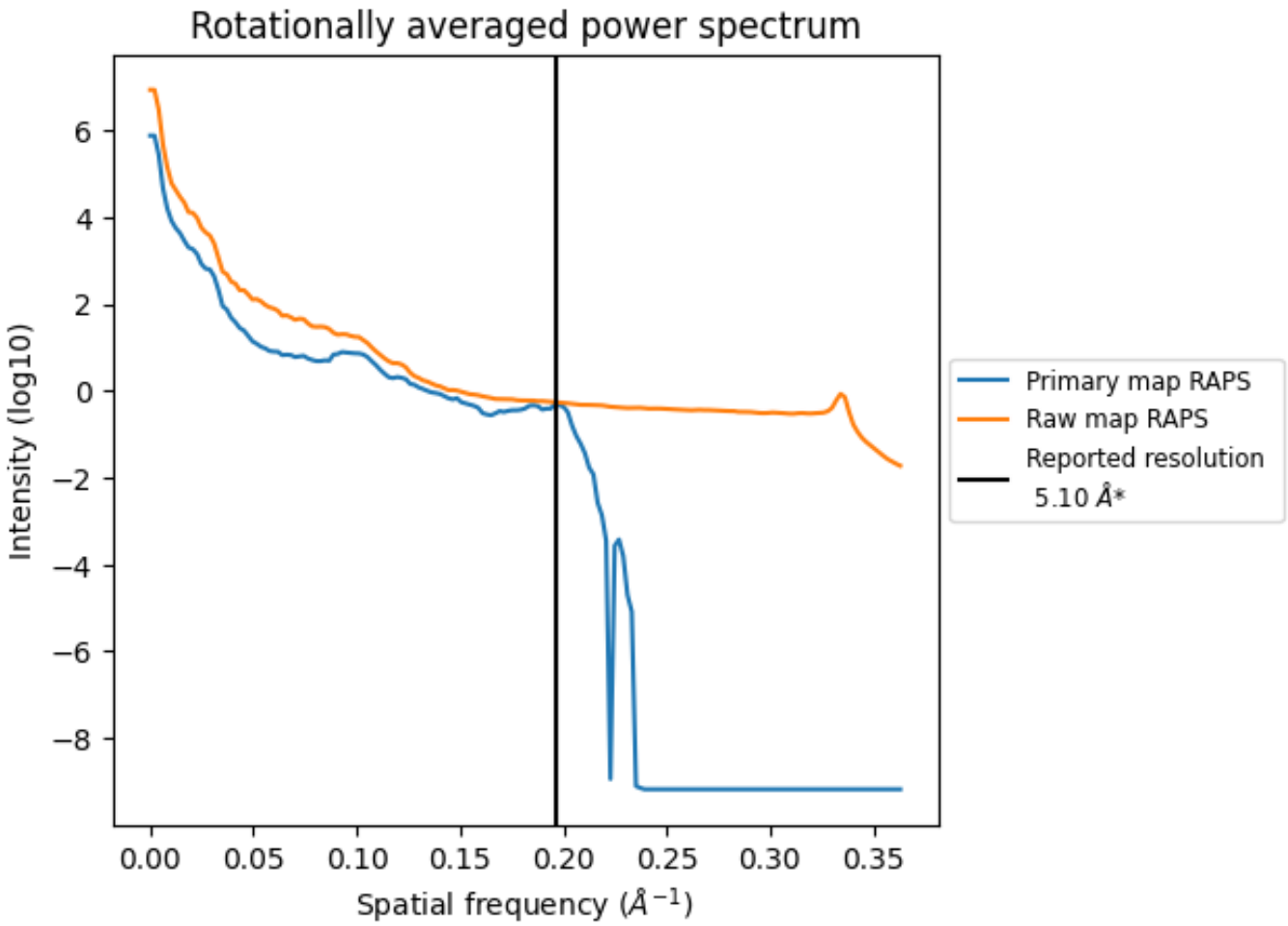
7.2 Volume estimate (i)



The volume at the recommended contour level is 2507 nm^3; this corresponds to an approximate mass of 2265 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)

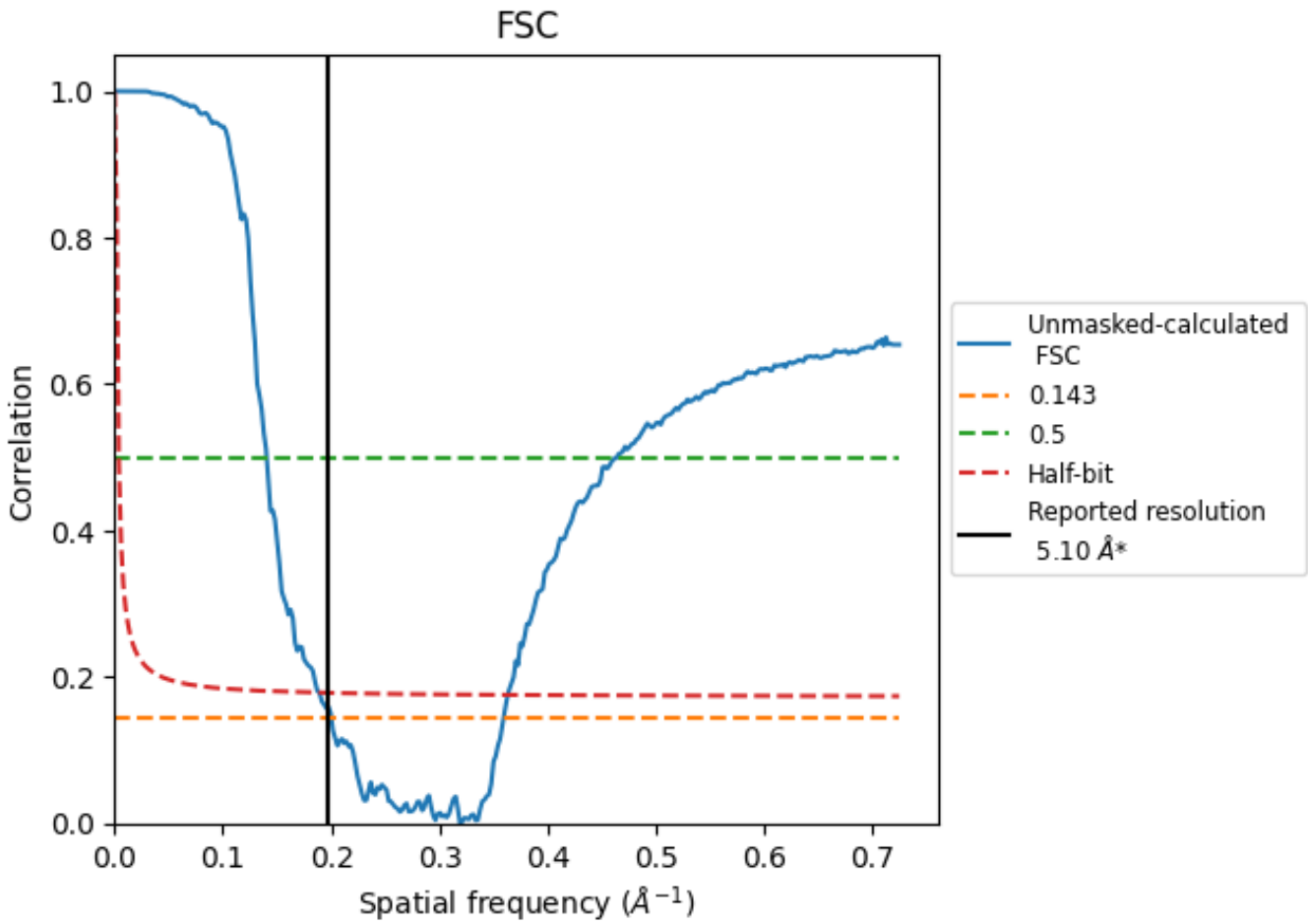


*Reported resolution corresponds to spatial frequency of 0.196 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.196 Å^{-1}

8.2 Resolution estimates (i)

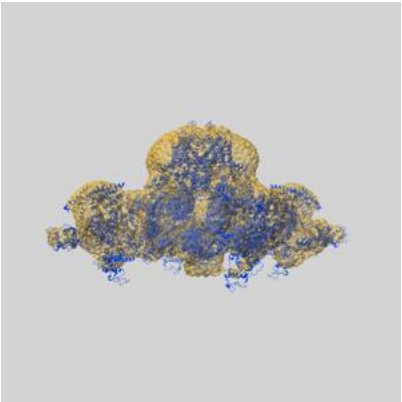
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.99	7.12	5.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

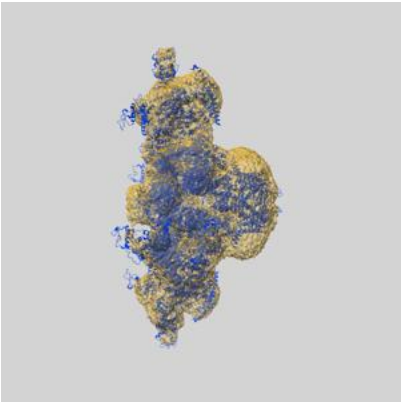
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21862 and PDB model 6WOV. Per-residue inclusion information can be found in section 3 on page 4.

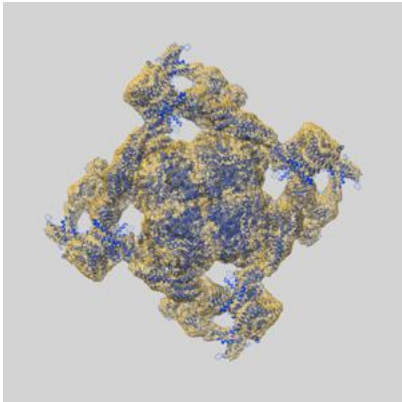
9.1 Map-model overlay (i)



X



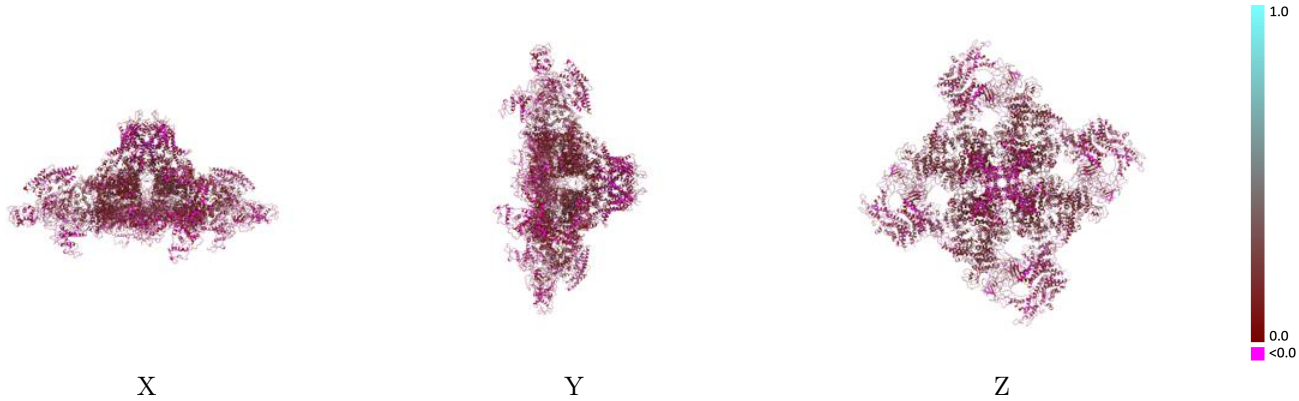
Y



Z

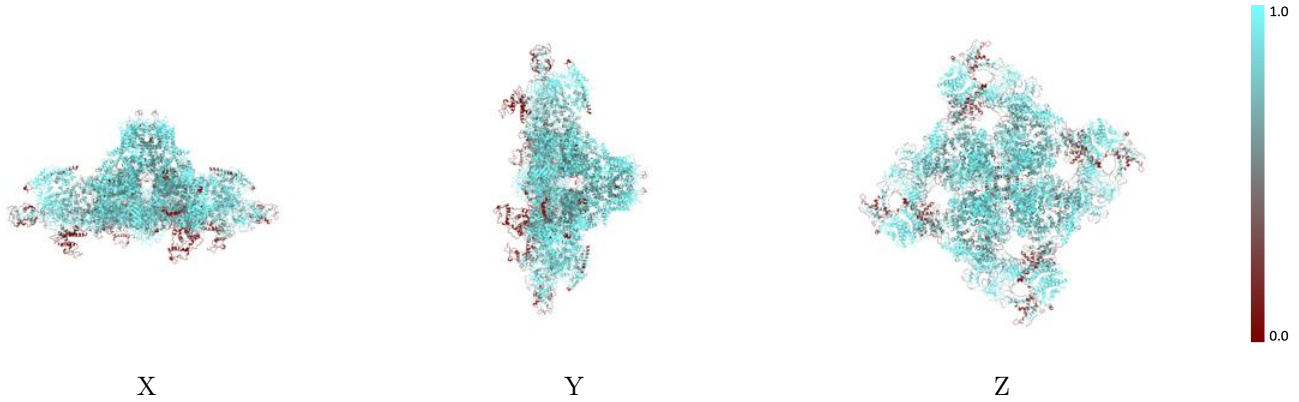
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



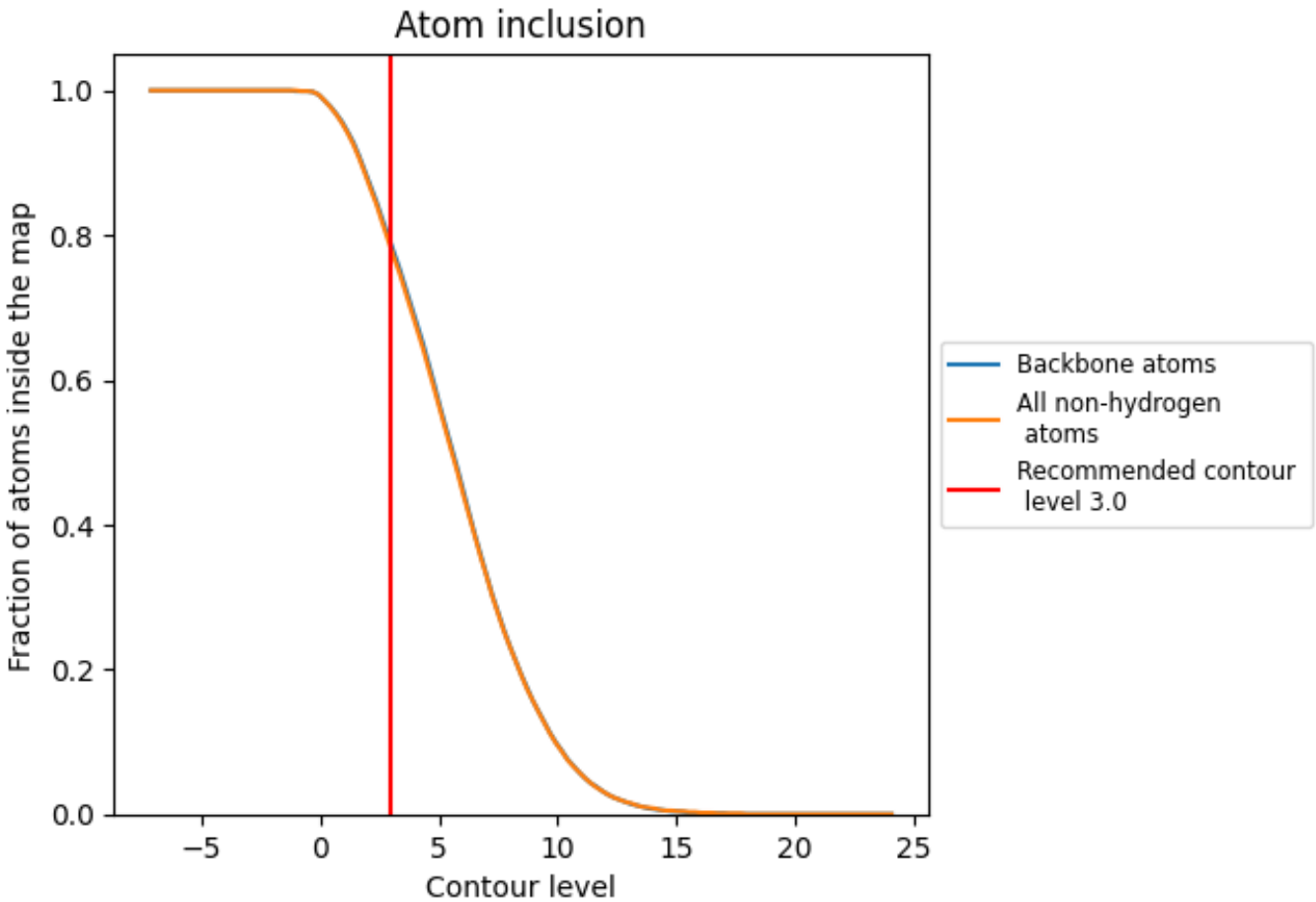
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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 (3.0).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7800	0.1330
A	0.7820	0.1330
B	0.7810	0.1330
C	0.7820	0.1330
D	0.7820	0.1330
E	0.7670	0.1520
F	0.7720	0.1540
G	0.7640	0.1470
H	0.7640	0.1430