Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 11:26 AM EST

PDB ID	:	5TAY
EMDB ID	:	EMD-8389
Title	:	Structure of rabbit RyR1 (ryanodine dataset, class 2)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.60 Å(reported)

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

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

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

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

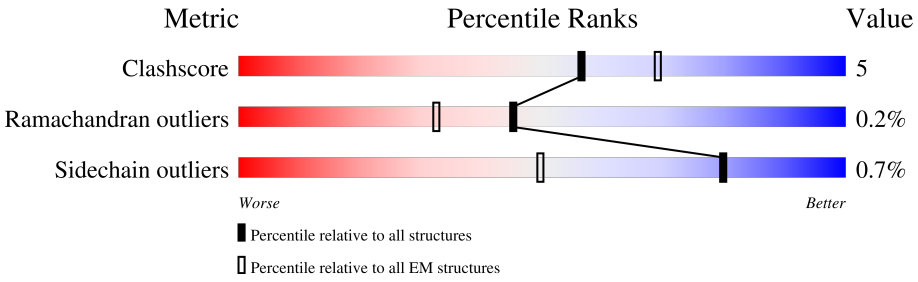
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	108	22% 89% 10%
1	F	108	22% 86% 13%
1	H	108	22% 87% 12%
1	J	108	22% 86% 13%
2	B	4416	34% 84% 10% 5%
2	E	4416	36% 84% 10% 5%
2	G	4416	34% 84% 10% 5%
2	I	4416	36% 85% 10% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 121276 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

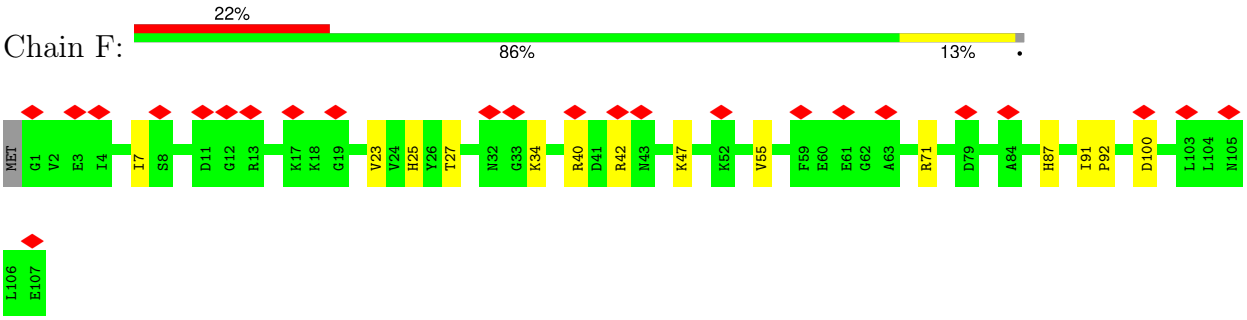
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Ca 1 1	0
4	G	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0

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.

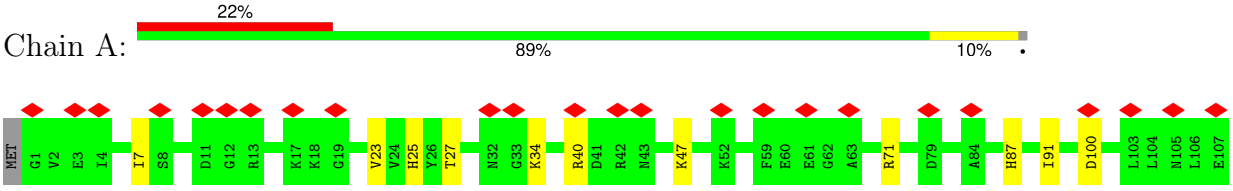
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



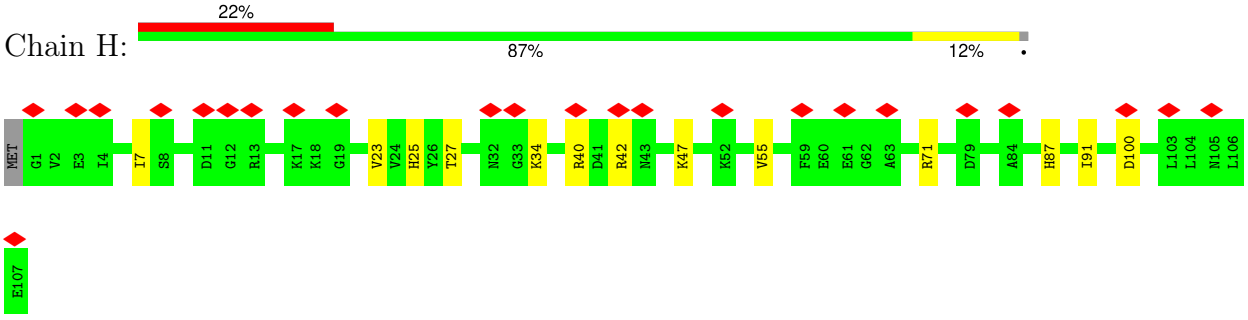
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



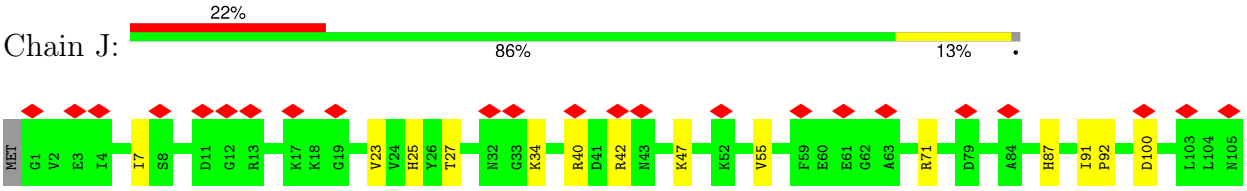
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



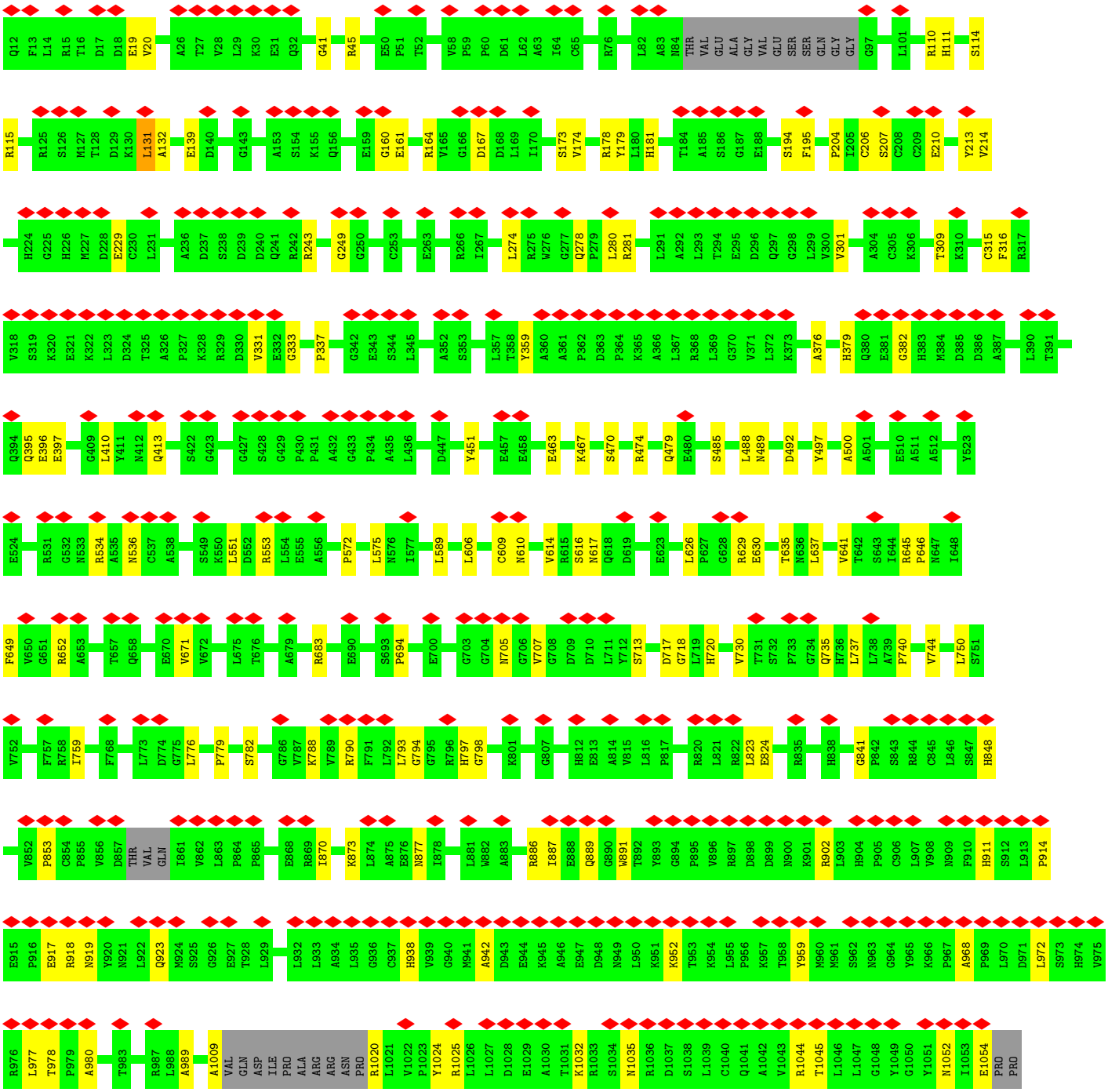
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

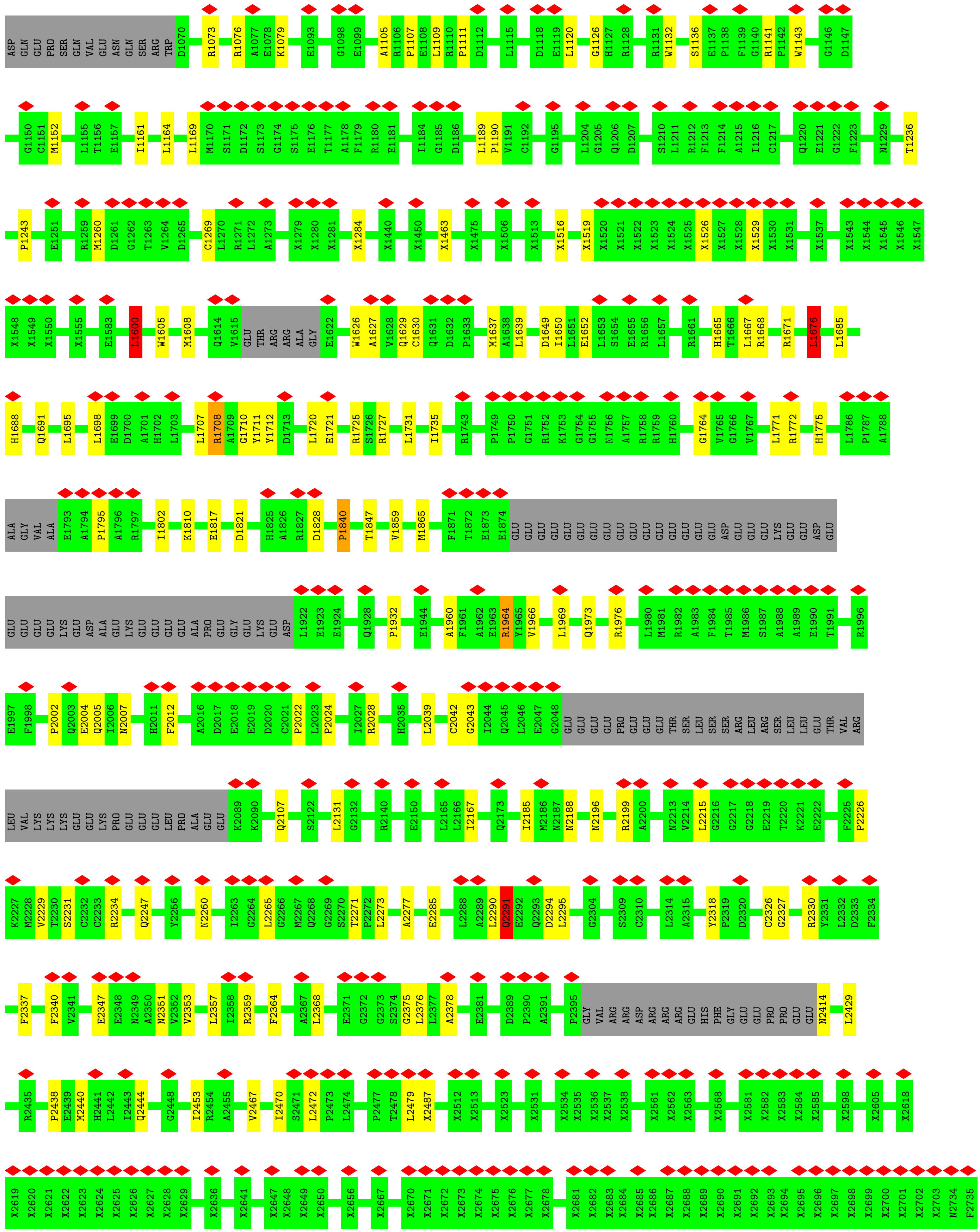
Chain J:

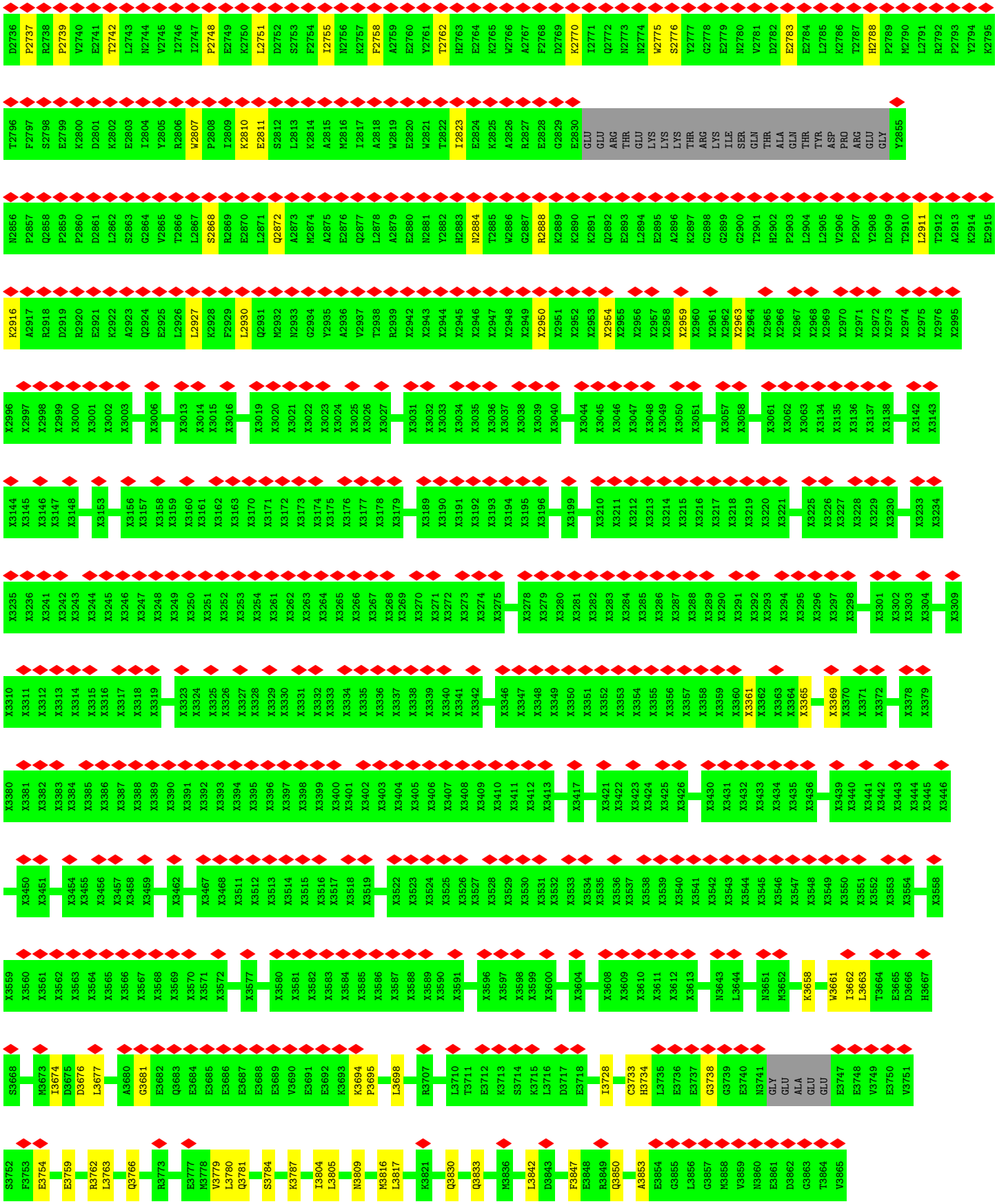


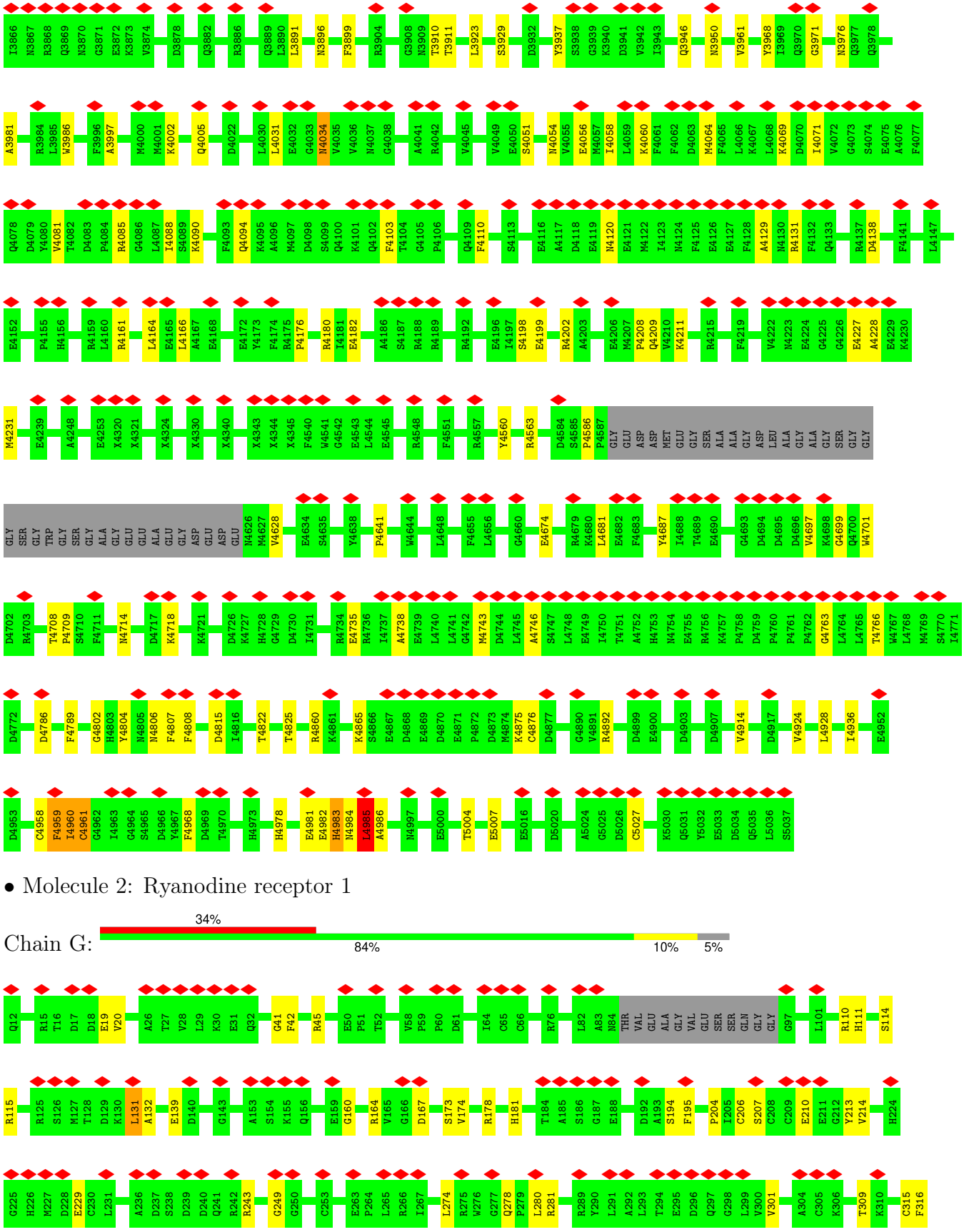
• Molecule 2: Ryanodine receptor 1

Chain B:



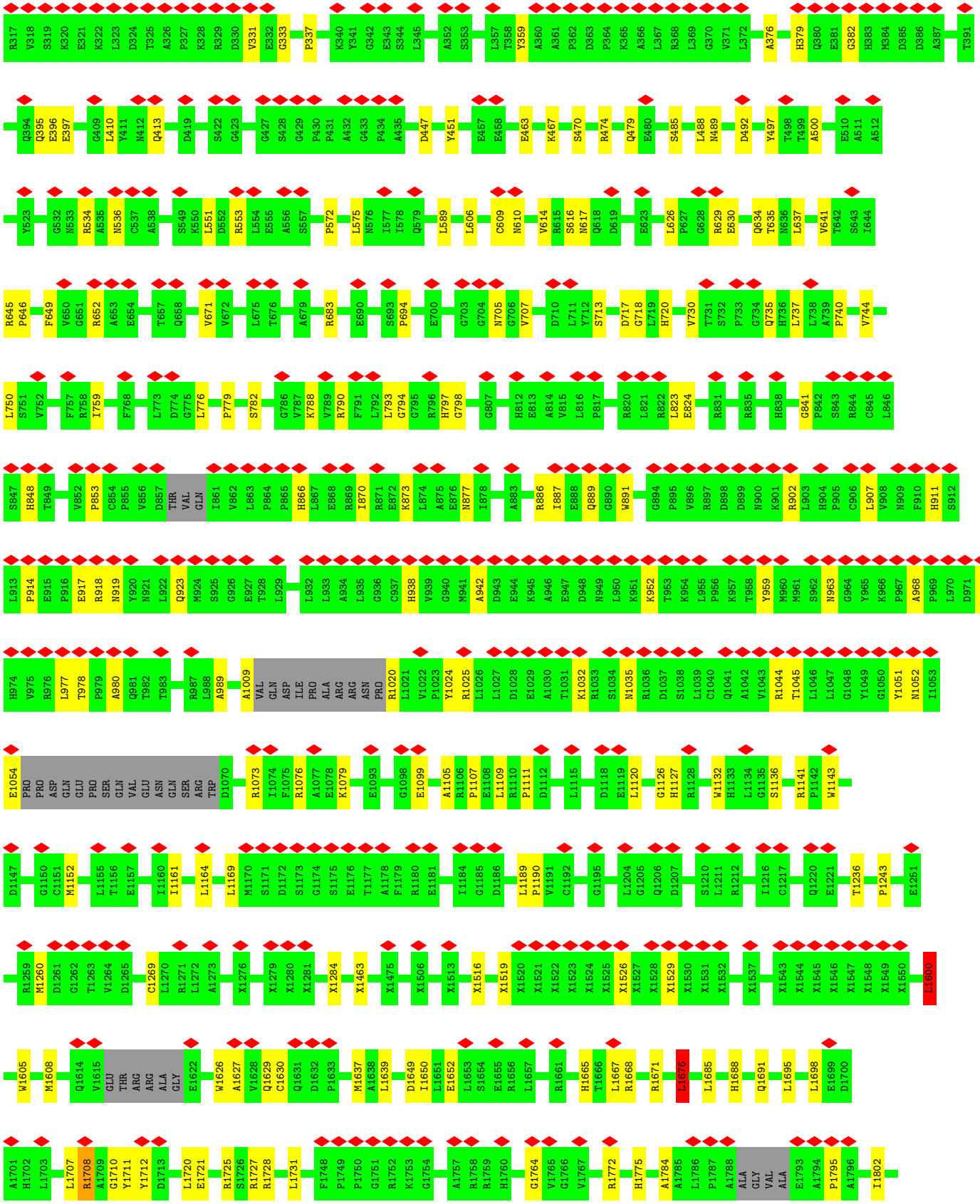

ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1073 R1076 A1077 E1078 K1079 E1093 G1098 E1099 A1105 R1106 P1107 E1108 L1109 R1110 P1111 D1112 L1115 D1118 E1119 L1120 G1126 H1127 R1128 R1131 W1132 S1136 E1137 P1138 F1139 G1140 R1141 P1142 W1143 G1146 D1147
G1150 C1151 M1152 L1155 T1156 E1157 I1161 L1164 L1169 M1170 S1171 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179 R1180 E1181 I1184 G1185 D1186 L1189 P1190 V1191 C1192 G1195 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 F1213 F1214 A1215 I1216 C1217 Q1220 E1221 G1222 F1223 N1229 T1236
P1243 E1251 R1259 M1260 D1261 G1262 T1263 V1264 D1265 C1269 L1270 R1271 L1272 A1273 X1279 X1280 X1281 X1284 X1440 X1450 X1463 X1475 X1506 X1513 X1516 X1519 X1520 X1521 X1522 X1523 X1524 X1525 X1526 X1527 X1528 X1529 X1530 X1531 X1537 X1543 X1544 X1545 X1546 X1547
X1548 X1549 X1550 X1555 E1583 L1600 W1605 M1608 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 D1649 I1650 L1651 E1652 L1653 S1654 E1655 R1656 L1657 R1661 H1665 T1666 L1667 R1668 R1671 L1676 L1685
H1688 Q1691 L1695 L1698 E1699 D1700 A1701 H1702 L1703 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 L1720 E1721 R1725 S1726 R1727 L1731 I1735 R1743 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 H1760 G1764 V1765 G1766 V1767 L1771 R1772 H1775 L1786 P1787 A1788
ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 I1802 K1810 E1817 D1821 H1825 A1826 R1827 D1828 P1840 T1847 V1859 M1865 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU GLU LYS GLU GLU ASP GLU
GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 Q1928 P1932 E1944 A1960 F1961 A1962 E1963 R1964 Y1965 V1966 L1969 Q1973 R1976 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 R1996
E1997 F1998 P2002 Q2003 E2004 Q2005 I2006 N2007 H2011 F2012 A2016 D2017 E2018 E2019 D2020 C2021 P2022 L2023 P2024 I2027 R2028 H2035 L2039 C2042 G2043 I2044 Q2045 L2046 E2047 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG
LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 K2090 Q2107 S2122 L2131 G2132 R2140 E2150 L2165 L2166 I2167 Q2173 I2185 M2186 N2187 N2188 N2196 R2199 A2200 N2213 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 F2225 P2226
K2227 M2228 V2229 T2230 S2231 C2232 C2233 R2234 Q2247 Y2256 N2260 I2263 G2264 L2265 G2266 M2267 Q2268 G2269 S2270 T2271 P2272 L2273 A2277 E2285 L2288 A2289 L2290 Q2291 E2292 Q2293 D2294 L2295 G2304 S2309 C2310 L2314 A2315 Y2318 P2319 D2320 C2326 G2327 R2330 Y2331 L2332 D2333 F2334
F2337 F2340 V2341 E2347 E2348 N2349 A2350 N2351 V2352 V2353 L2357 I2358 R2359 F2364 A2367 L2368 E2371 G2372 G2373 S2374 G2375 L2376 L2377 A2378 E2381 D2389 P2390 A2391 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 L2429
R2435 P2438 E2439 M2440 H2441 L2442 I2443 Q2444 G2448 I2453 R2454 A2455 V2467 I2470 S2471 L2472 P2473 L2474 P2477 T2478 L2479 X2487 X2512 X2513 X2523 X2531 X2534 X2535 X2536 X2537 X2538 X2561 X2562 X2563 X2568 X2581 X2582 X2583 X2584 X2585 X2598 X2605 X2618
X2619 X2620 X2621 X2622 X2623 X2624 X2625 X2626 X2627 X2628 X2629 X2636 X2641 X2647 X2648 X2649 X2650 X2656 X2667 X2670 X2671 X2672 X2673 X2674 X2675 X2676 X2677 X2678 X2681 X2682 X2683 X2684 X2685 X2686 X2687 X2688 X2689 X2690 X2691 X2692 X2693 X2694 X2695 X2696 X2697 X2698 X2699 X2700 X2701 X2702 X2703 N2734 F2735

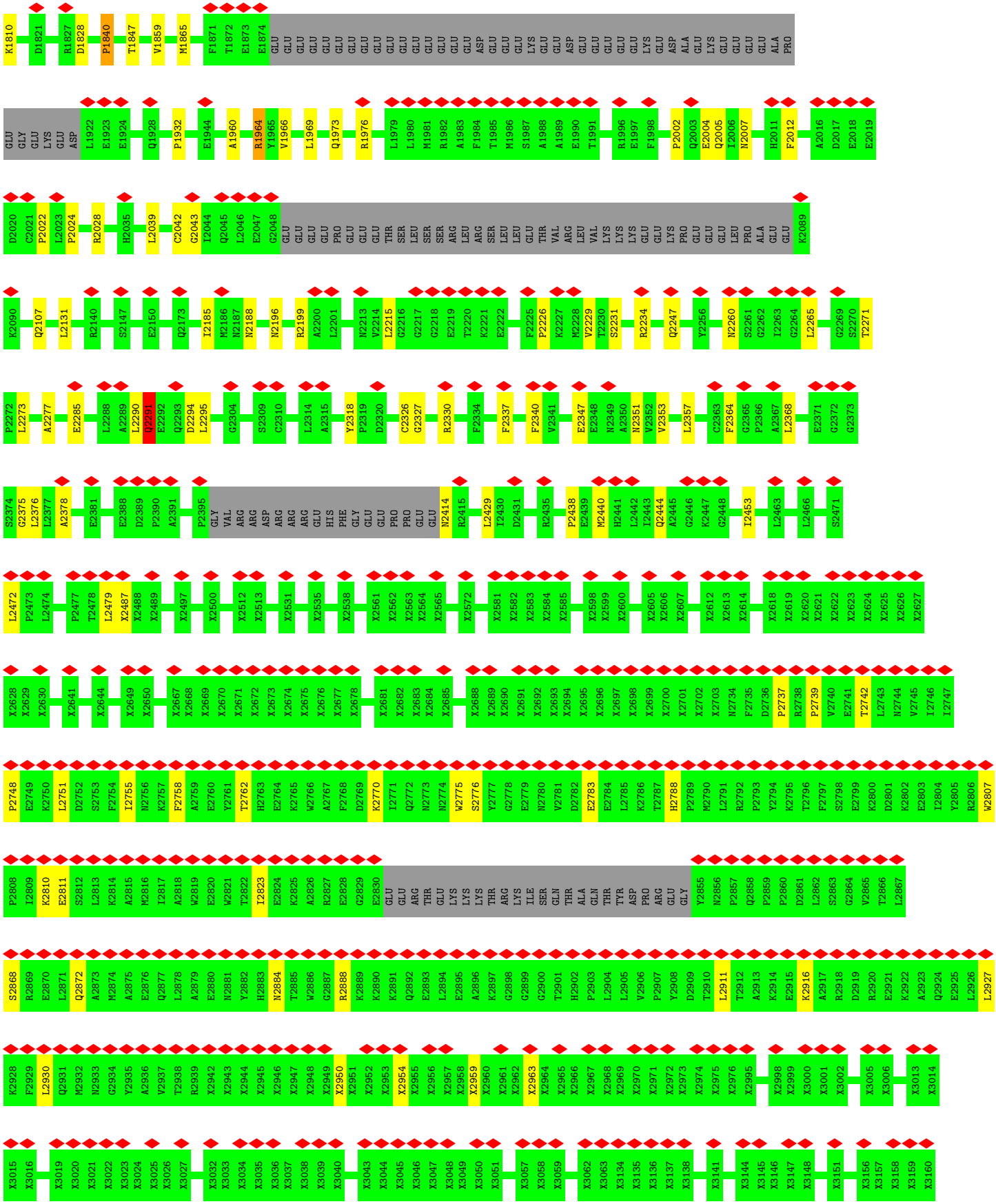

D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 P2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795
T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855
N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915
K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2949 X2950 X2951 X2952 X2953 X2954 X2955 X2956 X2957 X2958 X2959 X2960 X2961 X2962 X2963 X2964 X2965 X2966 X2967 X2968 X2969 X2970 X2971 X2972 X2973 X2974 X2975 X2976 X2995
X2996 X2997 X2998 X2999 X3000 X3001 X3002 X3003 X3006 X3013 X3014 X3015 X3016 X3019 X3020 X3021 X3022 X3023 X3024 X3025 X3026 X3027 X3031 X3032 X3033 X3034 X3035 X3036 X3037 X3038 X3039 X3040 X3044 X3045 X3046 X3047 X3048 X3049 X3050 X3051 X3057 X3058 X3061 X3062 X3063 X3134 X3135 X3136 X3137 X3138 X3142 X3143
X3144 X3145 X3146 X3147 X3148 X3153 X3156 X3157 X3158 X3159 X3160 X3161 X3162 X3163 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3189 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3199 X3210 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3225 X3226 X3227 X3228 X3229 X3230 X3233 X3234
X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3292 X3293 X3294 X3295 X3296 X3297 X3298 X3301 X3302 X3303 X3304 X3309
X3310 X3311 X3312 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3323 X3324 X3325 X3326 X3327 X3328 X3329 X3330 X3331 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3346 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3369 X3370 X3371 X3372 X3378 X3379
X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407 X3408 X3409 X3410 X3411 X3412 X3413 X3417 X3421 X3422 X3423 X3424 X3425 X3426 X3430 X3431 X3432 X3433 X3434 X3435 X3436 X3439 X3440 X3441 X3442 X3443 X3444 X3445 X3446
X3450 X3451 X3454 X3455 X3456 X3457 X3458 X3459 X3462 X3467 X3468 X3511 X3512 X3513 X3514 X3515 X3516 X3517 X3518 X3519 X3522 X3523 X3524 X3525 X3526 X3527 X3528 X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3536 X3537 X3538 X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3554 X3558
X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3569 X3570 X3571 X3572 X3577 X3580 X3581 X3582 X3583 X3584 X3585 X3586 X3587 X3588 X3589 X3590 X3591 X3596 X3597 X3598 X3599 X3600 X3604 X3608 X3609 X3610 X3611 X3612 X3613 N3643 L3644 N3651 M3652 K3658 W3661 I3662 L3663 T3664 E3665 D3666 H3667
S3668 M3673 I3674 D3675 D3676 L3677 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 K3694 P3695 L3698 R3707 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 E3718 I3728 C3733 H3734 L3735 E3736 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751
S3752 F3753 E3754 E3759 R3762 L3763 Q3766 R3773 E3777 M3778 V3779 L3780 Q3781 S3784 K3787 I3804 L3805 N3809 M3816 L3817 K3821 Q3830 Q3833 M3836 L3842 D3843 F3847 E3848 R3849 Q3850 A3853 E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865

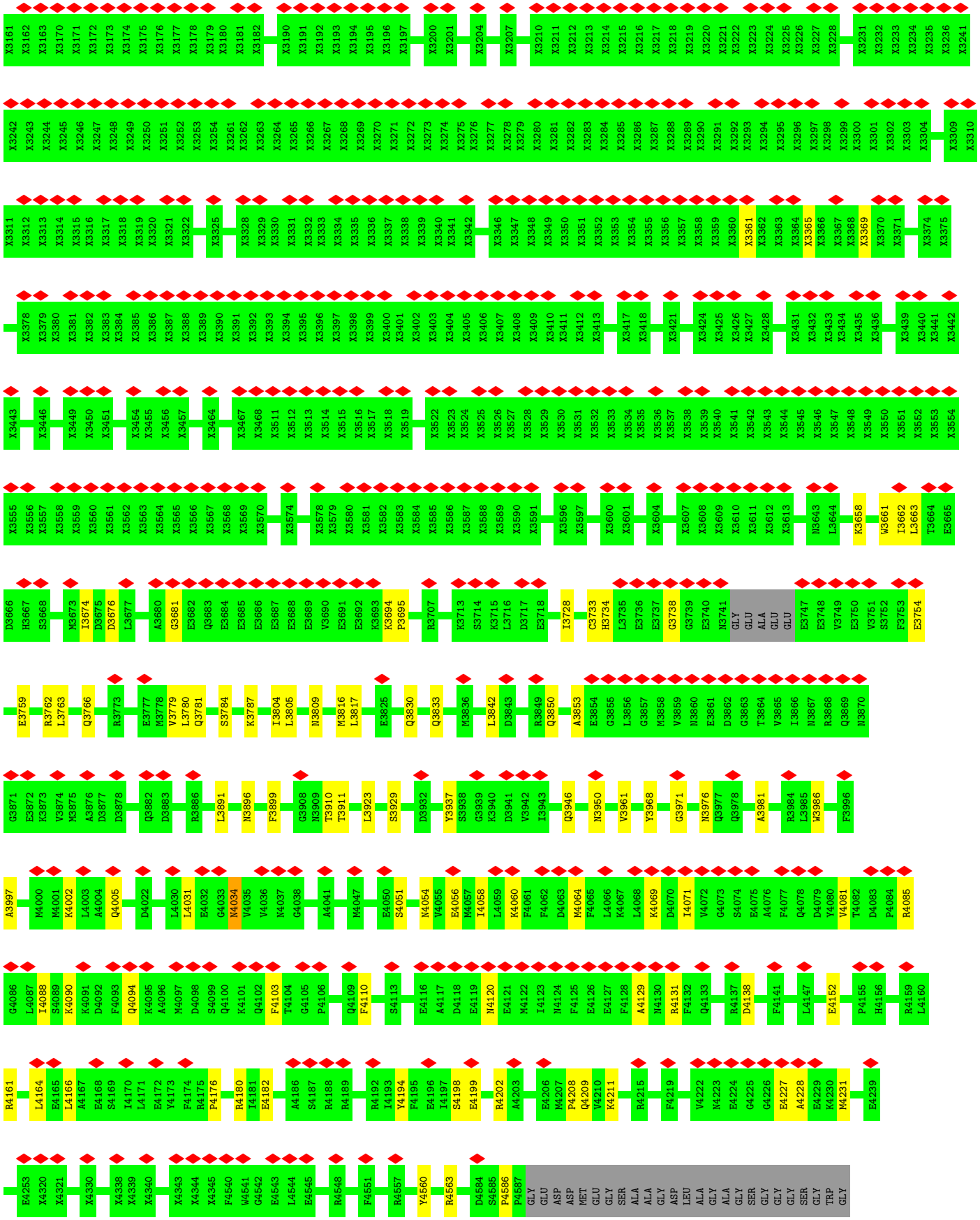


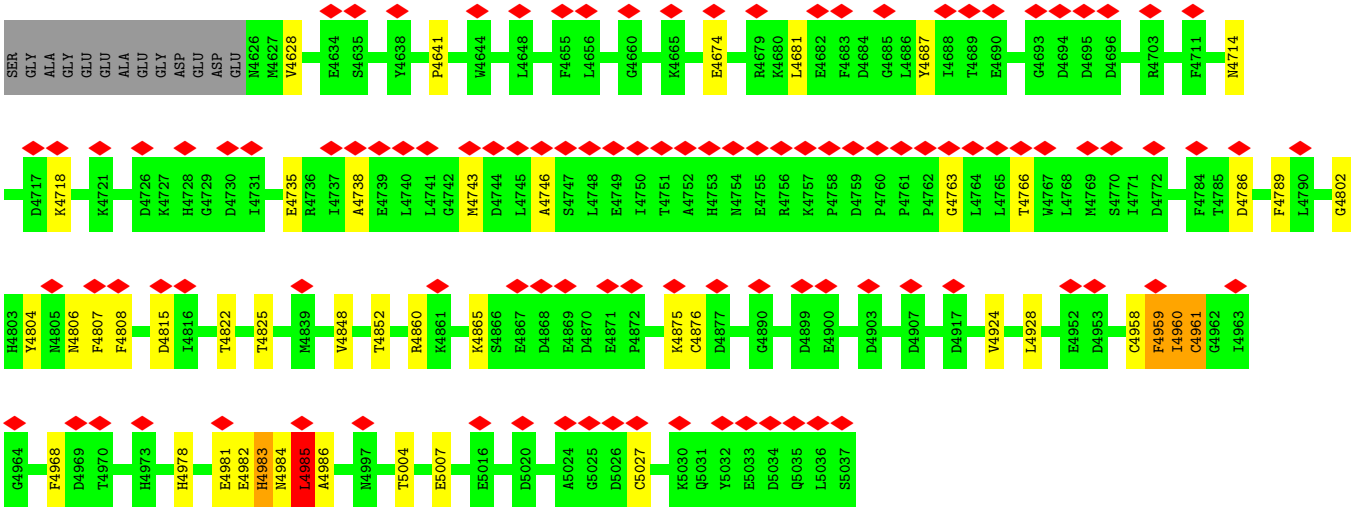
• Molecule 2: Ryanodine receptor 1

Chain G:


R317 V318 S319 K320 E321 K322 L323 D324 T325 A326 P327 K328 R329 D330 Y331 E332 G333 P337 K340 Y341 G342 E343 S344 L345 A352 S353 L357 T358 Y359 A360 A361 P362 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 A376 H379 Q380 E381 G382 H383 M384 D385 D386 A387 T391
Q394 Q395 E396 E397 G409 L410 Y411 N412 Q413 D419 S422 G423 G427 S428 G429 P430 P431 A432 G433 P434 A435 D447 Y451 E457 E458 E463 K467 S470 R474 Q479 E480 S485 L488 N489 D492 Y497 T498 T499 A500 E510 A511 A512
Y523 G532 N533 R534 A535 N536 C537 A538 S549 K550 L551 D552 R553 L554 E555 A556 S557 P572 L575 N576 I577 I578 Q579 L589 L606 C609 N610 V614 H615 S616 N617 Q618 D619 E623 L626 F627 G628 R629 E630 Q634 T635 N636 L637 V641 T642 S643 I644
R645 P646 F649 V650 G651 R652 A653 E654 T657 Q658 V671 V672 L675 T676 A679 R683 E690 S693 P694 E700 G703 G704 N705 G706 V707 D710 L711 Y712 S713 D717 G718 L719 H720 V730 T731 S732 P733 G734 Q735 H736 L737 L738 A739 P740 V744
L750 S751 V752 F757 R758 I759 F768 L773 D774 G775 L776 P779 S782 G786 V787 K788 V789 R790 F791 L792 L793 G794 G795 R796 H797 G798 G807 H812 E813 A814 V815 L816 P817 R820 L821 R822 L823 E824 R831 R835 H838 G841 P842 S843 R844 C845 L846
S847 H848 T849 V852 P853 C854 P855 V856 D857 THR VAL GLN I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 A883 R886 I887 E888 Q889 G890 W891 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912
L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 N924 S925 G926 E927 T928 L929 L932 L933 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973
H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 R987 I988 A989 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 V1022 P1023 Y1024 R1025 L1026 L1027 D1028 E1029 A1030 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053
E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1073 I1074 F1075 R1076 A1077 E1078 K1079 E1093 G1098 E1099 A1105 R1106 P1107 E1108 L1109 R1110 P1111 D1112 L1115 D1118 E1119 L1120 G1126 H1127 R1128 W1132 H1133 L1134 G1135 S1136 R1141 P1142 W1143
D1147 G1150 C1151 M1152 L1155 T1156 E1157 I1160 I1161 L1164 L1169 M1170 S1171 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179 R1180 E1181 I1184 G1185 D1186 L1189 P1190 V1191 C1192 G1195 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 T1216 C1217 Q1220 E1221 T1236 P1243 E1251
R1259 M1260 D1261 G1262 T1263 V1264 D1265 C1269 L1270 R1271 L1272 A1273 X1276 X1279 X1280 X1281 X1284 X1463 X1475 X1506 X1513 X1516 X1519 X1520 X1521 X1522 X1523 X1524 X1525 X1526 X1527 X1528 X1529 X1530 X1531 X1532 X1537 X1543 X1544 X1545 X1546 X1547 X1548 X1549 X1550 L1600
W1605 M1608 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 D1649 I1650 L1651 E1652 L1653 S1654 E1655 R1656 L1657 R1661 H1665 T1666 L1667 R1668 R1671 L1676 L1685 H1688 Q1691 L1695 L1698 E1699 D1700
A1701 H1702 L1703 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 L1720 E1721 R1725 S1726 R1727 R1728 L1731 F1748 P1749 P1750 G1751 R1752 K1753 G1754 A1757 R1758 R1759 H1760 G1764 V1765 G1766 V1767 R1772 H1775 A1784 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 I1802

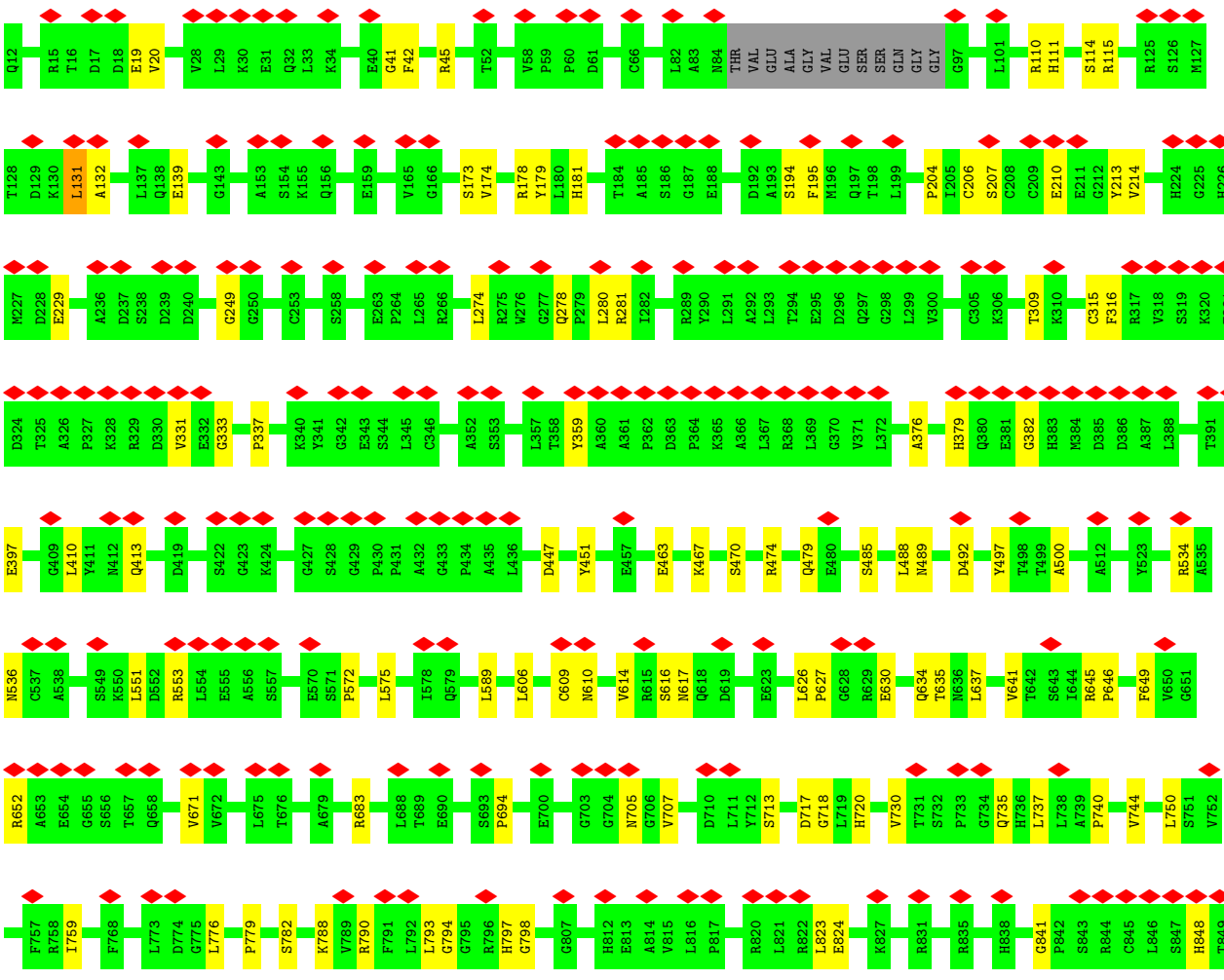

K1810 D1821 R1827 D1828 P1840 T1847 V1859 M1865 F1871 T1872 E1873 E1874 GLU
GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 Q1928 P1932 E1944 A1960 R1964 Y1965 V1966 L1969 Q1973 R1976 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 R1996 E1997 F1998 P2002 Q2003 E2004 Q2005 I2006 N2007 H2011 F2012 A2016 D2017 E2018 E2019
D2020 C2021 P2022 L2023 P2024 R2028 H2035 L2039 C2042 G2043 I2044 Q2045 L2046 E2047 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089
K2090 Q2107 L2131 R2140 S2147 E2150 Q2173 I2185 M2186 N2187 N2188 N2196 R2199 A2200 L2201 N2213 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 F2225 P2226 K2227 M2228 V2229 T2230 S2231 R2234 Q2247 Y2256 N2260 S2261 G2262 I2263 G2264 L2265 G2269 S2270 T2271
P2272 L2273 A2277 E2285 L2288 A2289 L2290 Q2291 E2292 Q2293 D2294 L2295 G2304 S2309 C2310 L2314 A2315 Y2318 P2319 D2320 C2326 G2327 R2330 F2334 F2337 F2340 V2341 E2347 E2348 N2349 A2350 N2351 V2352 V2353 L2357 C2363 F2364 G2365 P2366 A2367 L2368 E2371 G2372 G2373
S2374 G2375 L2376 L2377 A2378 E2381 E2388 D2389 P2390 A2391 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2415 L2429 I2430 D2431 R2435 P2438 E2439 M2440 H2441 L2442 I2443 Q2444 A2445 G2446 K2447 G2448 I2453 L2463 L2466 S2471
L2472 P2473 L2474 P2477 T2478 L2479 X2487 X2488 X2489 X2497 X2500 X2512 X2513 X2531 X2535 X2538 X2561 X2562 X2563 X2564 X2565 X2572 X2581 X2582 X2583 X2584 X2585 X2598 X2599 X2600 X2605 X2606 X2607 X2612 X2613 X2614 X2618 X2619 X2620 X2621 X2622 X2623 X2624 X2625 X2626 X2627
X2628 X2629 X2630 X2641 X2644 X2649 X2650 X2667 X2668 X2669 X2670 X2671 X2672 X2673 X2674 X2675 X2676 X2677 X2678 X2681 X2682 X2683 X2684 X2685 X2688 X2689 X2690 X2691 X2692 X2693 X2694 X2695 X2696 X2697 X2698 X2699 X2700 X2701 X2702 X2703 N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747
P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807
P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867
S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927
K2928 P2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 K2942 K2943 K2944 K2945 K2946 K2947 K2948 K2949 K2950 K2951 K2952 K2953 K2954 K2955 K2956 K2957 K2958 K2959 K2960 K2961 K2962 K2963 K2964 K2965 K2966 K2967 K2968 K2969 K2970 K2971 K2972 K2973 K2974 K2975 K2976 K2995 K2998 K2999 K3000 K3001 K3002 K3005 K3006 K3013 K3014
X3015 X3016 X3019 X3020 X3021 X3022 X3023 X3024 X3025 X3026 X3027 X3032 X3033 X3034 X3035 X3036 X3037 X3038 X3039 X3040 X3043 X3044 X3045 X3046 X3047 X3048 X3049 X3050 X3051 X3057 X3058 X3059 X3062 X3063 X3134 X3135 X3136 X3137 X3138 X3141 X3144 X3145 X3146 X3147 X3148 X3151 X3156 X3157 X3158 X3159 X3160

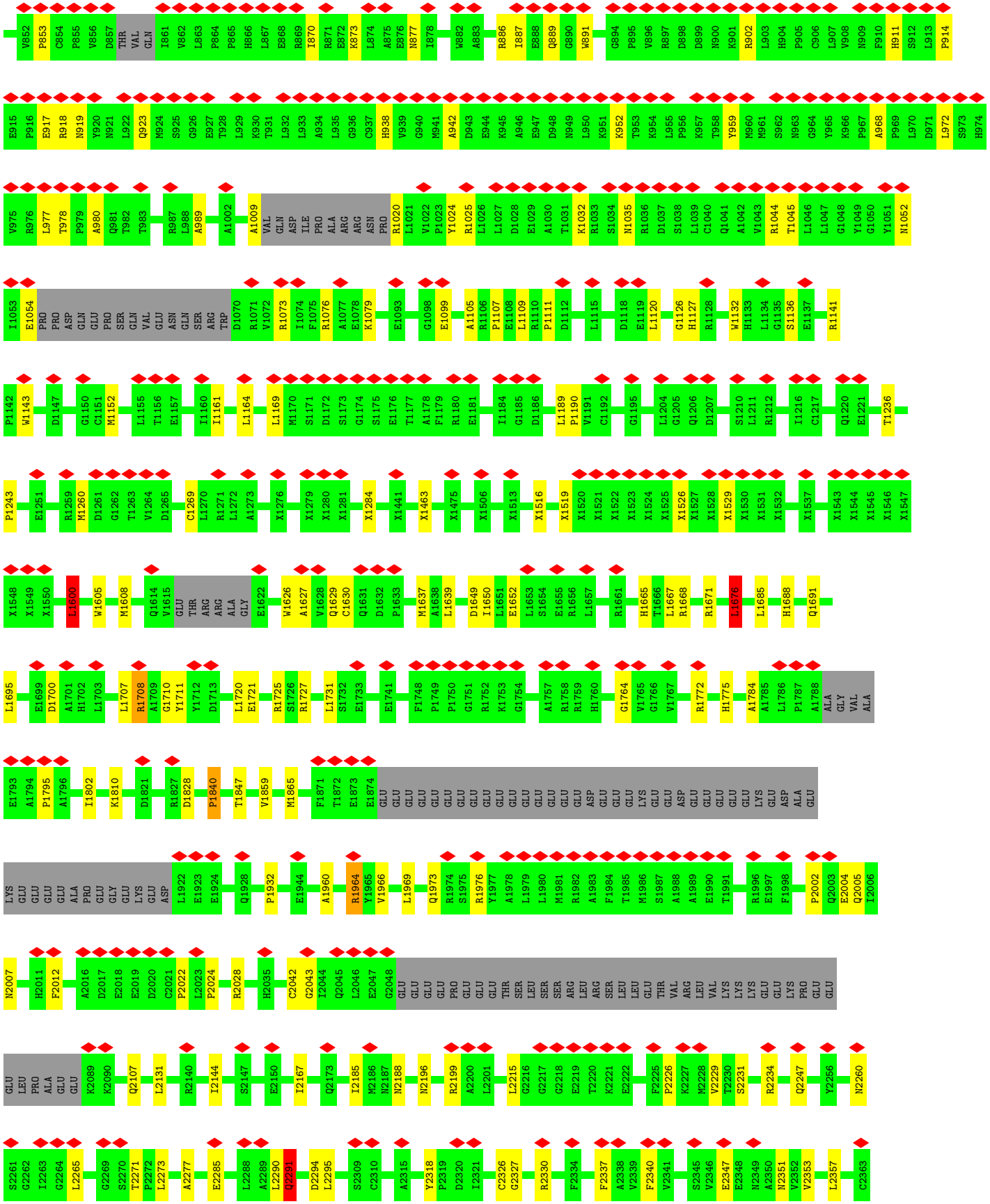

X3161 X3162 X3163 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3180 X3181 X3182 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3200 X3201 X3204 X3207 X3210 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222 X3223 X3224 X3225 X3226 X3227 X3228 X3231 X3232 X3233 X3234 X3235 X3236 X3241
X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3276 X3277 X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3292 X3293 X3294 X3295 X3296 X3297 X3298 X3299 X3300 X3301 X3302 X3303 X3304 X3309 X3310
X3311 X3312 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3320 X3321 X3322 X3325 X3328 X3329 X3330 X3331 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3346 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3367 X3368 X3369 X3370 X3371 X3374 X3375
X3378 X3379 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407 X3408 X3409 X3410 X3411 X3412 X3413 X3417 X3418 X3421 X3424 X3425 X3426 X3427 X3428 X3431 X3432 X3433 X3434 X3435 X3436 X3439 X3440 X3441 X3442
X3443 X3446 X3449 X3450 X3451 X3454 X3455 X3456 X3457 X3464 X3467 X3468 X3511 X3512 X3513 X3514 X3515 X3516 X3517 X3518 X3519 X3522 X3523 X3524 X3525 X3526 X3527 X3528 X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3536 X3537 X3538 X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3554
X3555 X3556 X3557 X3558 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3569 X3570 X3574 X3578 X3579 X3580 X3581 X3582 X3583 X3584 X3585 X3586 X3587 X3588 X3589 X3590 X3591 X3596 X3597 X3600 X3601 X3604 X3607 X3608 X3609 X3610 X3611 X3612 X3613 N3643 L3644 K3658 W3661 I3662 L3663 T3664 E3665
D3666 H3667 S3668 M3673 I3674 D3675 D3676 L3677 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 K3694 P3695 R3707 K3713 S3714 K3715 L3716 D3717 E3718 I3728 C3733 H3734 L3735 E3736 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 S3752 F3753 E3754
E3759 R3762 L3763 Q3766 R3773 E3777 M3778 V3779 L3780 Q3781 S3784 K3787 I3804 L3805 N3809 M3816 L3817 E3825 Q3830 Q3833 M3836 L3842 D3843 R3849 Q3850 A3853 E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870
G3871 E3872 K3873 V3874 M3875 A3876 D3877 D3878 Q3882 D3883 R3886 L3891 N3896 F3899 G3908 N3909 T3910 T3911 L3923 S3929 D3932 Y3937 S3938 G3939 K3940 D3941 V3942 I3943 Q3946 N3950 V3961 Y3968 G3971 N3976 Q3977 Q3978 A3981 R3984 L3985 W3986 F3996
A3997 M4000 M4001 K4002 L4003 A4004 Q4005 D4022 L4030 L4031 E4032 G4033 N4034 V4035 V4036 N4037 G4038 A4041 M4047 E4050 S4051 N4054 V4055 E4056 M4057 I4058 L4059 K4060 F4061 F4062 D4063 M4064 F4065 L4066 K4067 L4068 K4069 D4070 I4071 V4072 G4073 S4074 E4075 A4076 F4077 Q4078 D4079 Y4080 V4081 T4082 D4083 P4084 R4085
G4086 L4087 I4088 S4089 K4090 K4091 D4092 F4093 Q4094 K4095 A4096 M4097 D4098 S4099 Q4100 K4101 Q4102 F4103 T4104 G4105 P4106 Q4109 F4110 S4113 E4116 A4117 D4118 E4119 N4120 E4121 M4122 I4123 N4124 F4125 E4126 E4127 F4128 A4129 N4130 R4131 F4132 Q4133 R4137 D4138 F4141 L4147 E4152 P4155 H4156 R4159 L4160
R4161 L4164 E4165 L4166 A4167 E4168 S4169 I4170 L4171 E4172 Y4173 F4174 R4175 P4176 R4180 I4181 E4182 A4186 S4187 R4188 R4189 R4192 I4193 Y4194 F4195 E4196 I4197 S4198 E4199 R4202 A4203 E4206 M4207 P4208 Q4209 V4210 K4211 R4215 F4219 V4222 N4223 E4224 G4225 G4226 E4227 A4228 E4229 K4230 M4231 E4239
E4253 X4320 X4321 X4330 X4338 X4339 X4340 X4343 X4344 X4345 F4540 W4541 G4542 E4543 L4544 E4545 R4548 F4551 R4557 Y4560 R4563 D4584 S4585 P4586 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY

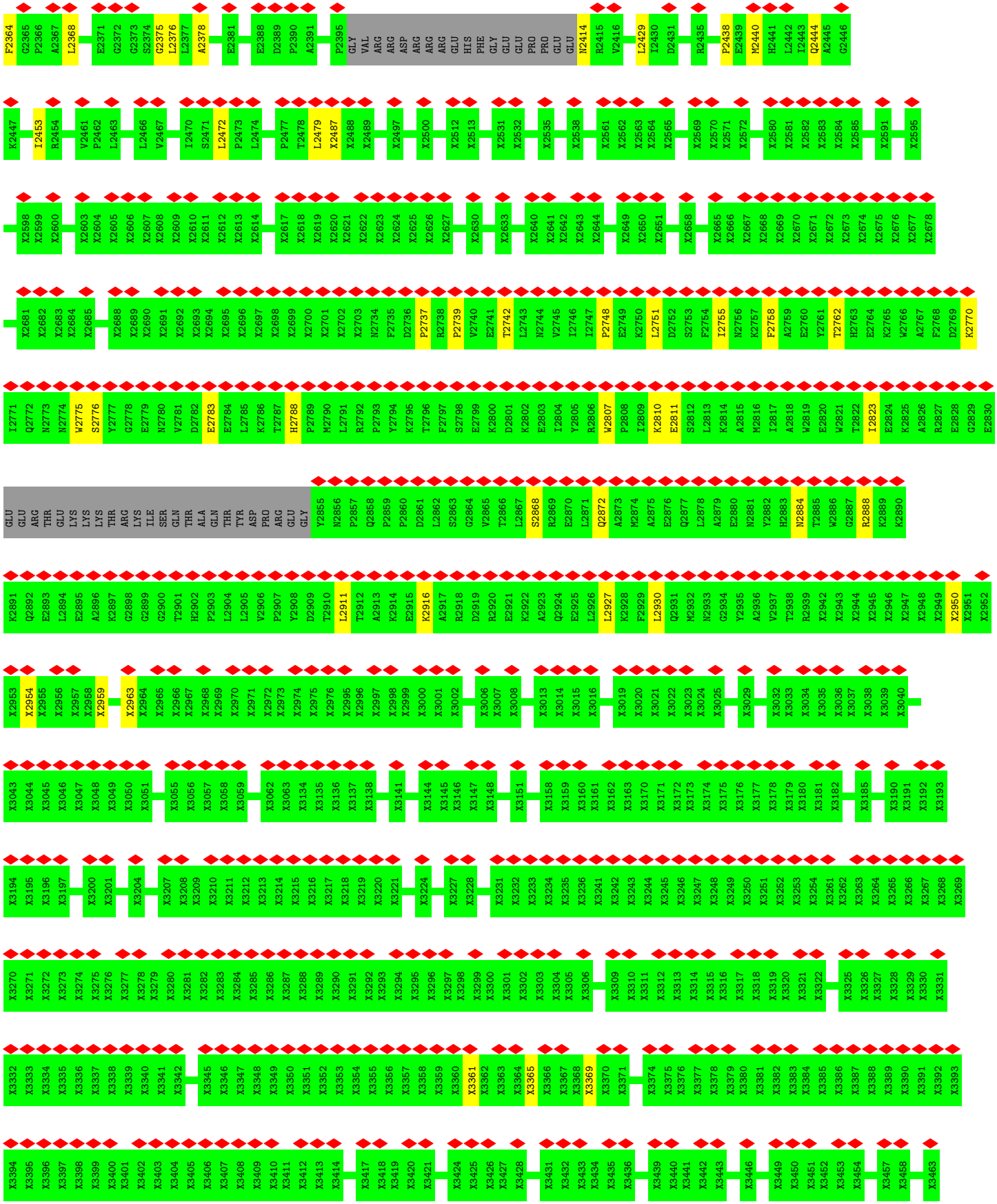


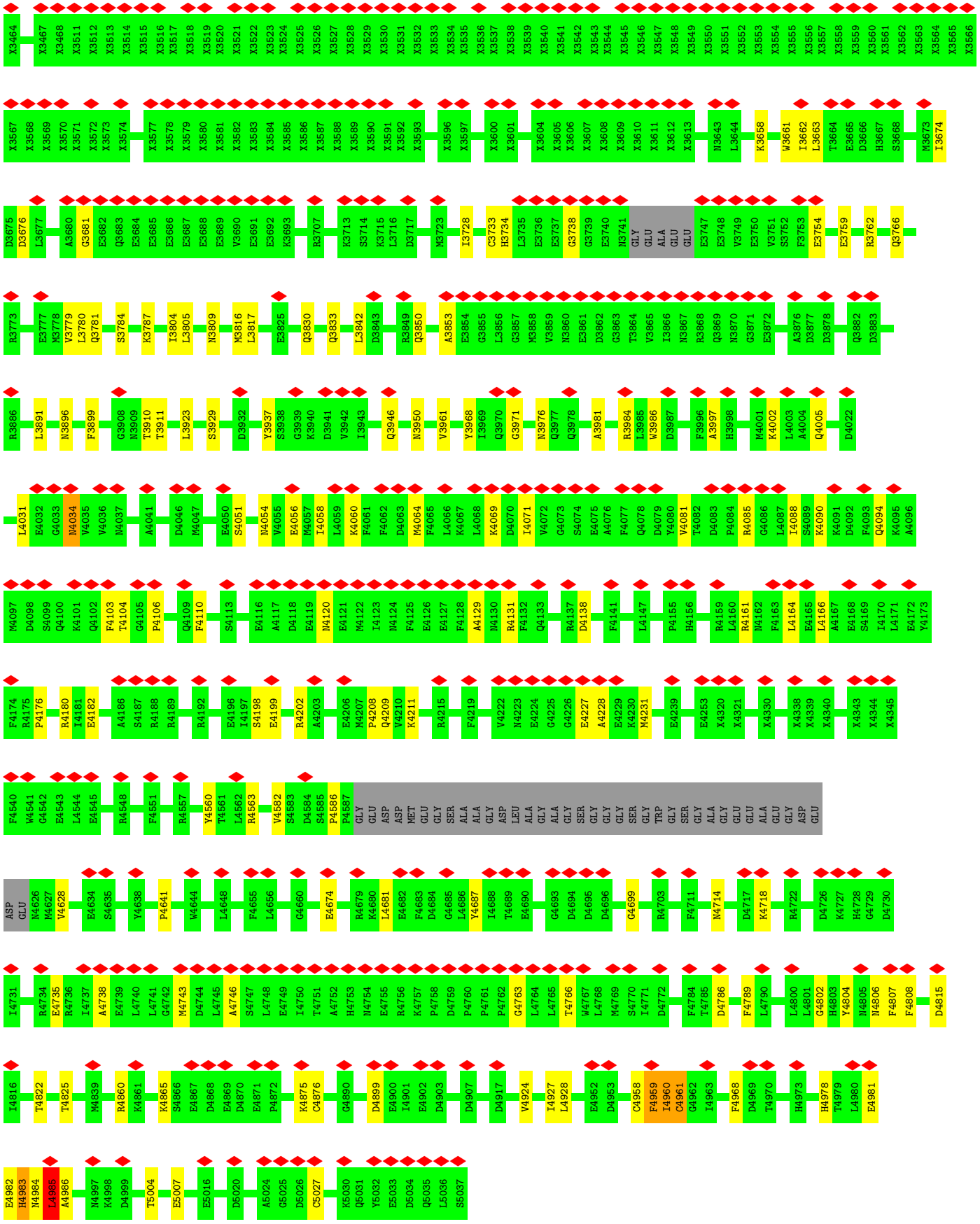
• Molecule 2: Ryanodine receptor 1

Chain I:



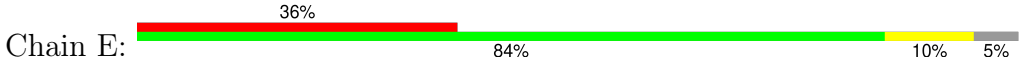


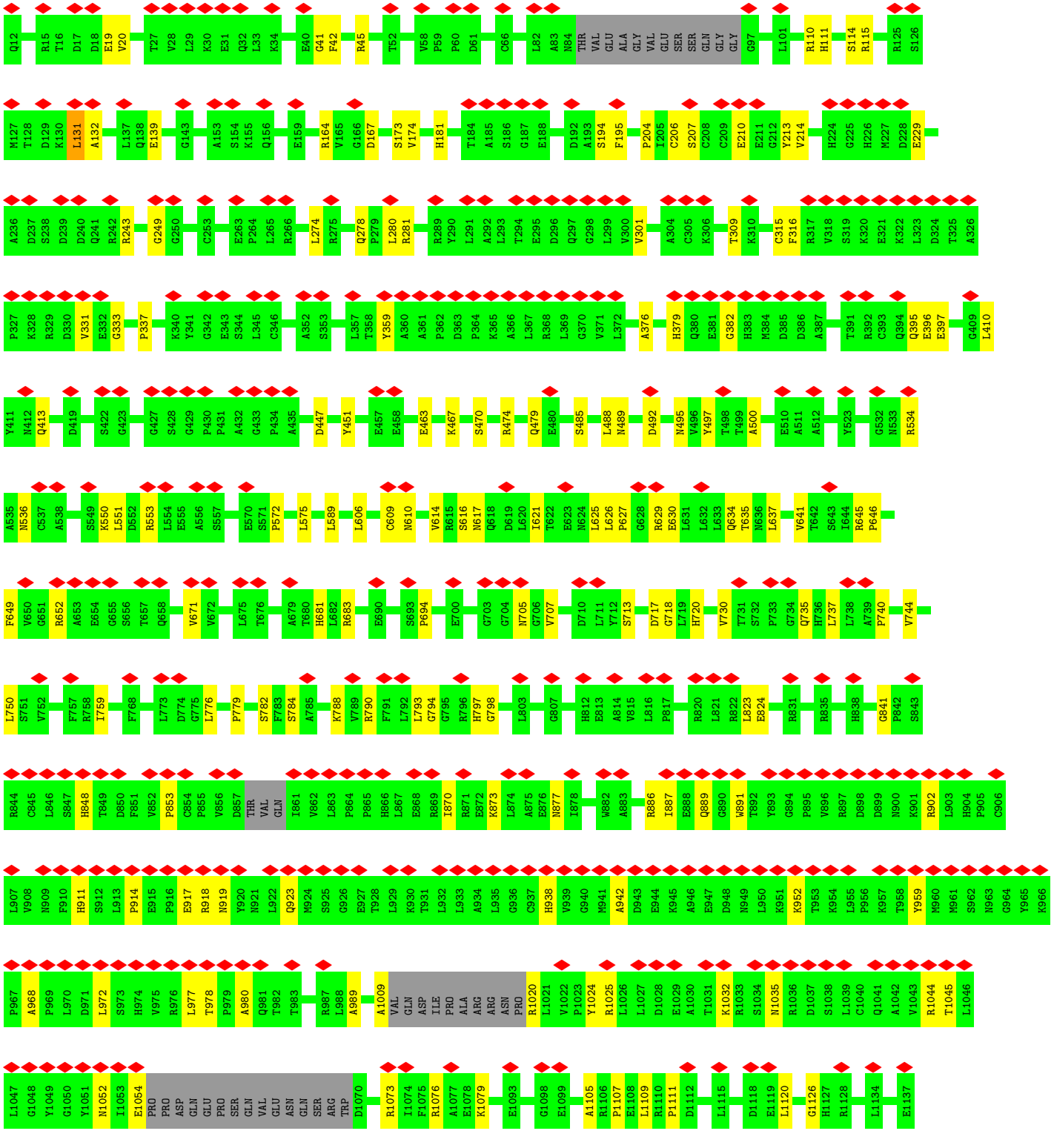

F2364 G2365 P2366 A2367 L2368 E2371 G2372 G2373 S2374 G2375 L2376 L2377 A2378 E2381 E2388 D2389 P2390 A2391 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2415 V2416 L2429 I2430 D2431 R2435 P2438 E2439 M2440 H2441 L2442 I2443 Q2444 A2445 G2446
K2447 I2453 R2454 V2461 P2462 L2463 L2466 V2467 I2470 S2471 L2472 P2473 L2474 P2477 T2478 L2479 X2487 X2488 X2489 X2497 X2500 X2512 X2513 X2531 X2532 X2535 X2538 X2561 X2562 X2563 X2564 X2565 X2569 X2570 X2571 X2572 X2580 X2581 X2582 X2583 X2584 X2585 X2591 X2595
X2598 X2599 X2600 X2603 X2604 X2605 X2606 X2607 X2608 X2609 X2610 X2611 X2612 X2613 X2614 X2617 X2618 X2619 X2620 X2621 X2622 X2623 X2624 X2625 X2626 X2627 X2630 X2633 X2640 X2641 X2642 X2643 X2644 X2649 X2650 X2651 X2658 X2665 X2666 X2667 X2668 X2669 X2670 X2671 X2672 X2673 X2674 X2675 X2676 X2677 X2678
X2681 X2682 X2683 X2684 X2685 X2688 X2689 X2690 X2691 X2692 X2693 X2694 X2695 X2696 X2697 X2698 X2699 X2700 X2701 X2702 X2703 N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770
I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830
GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890
K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2949 X2950 X2951 X2952
X2953 X2954 X2955 X2956 X2957 X2958 X2959 X2963 X2964 X2965 X2966 X2967 X2968 X2969 X2970 X2971 X2972 X2973 X2974 X2975 X2976 X2995 X2996 X2997 X2998 X2999 X3000 X3001 X3002 X3006 X3007 X3008 X3013 X3014 X3015 X3016 X3019 X3020 X3021 X3022 X3023 X3024 X3025 X3029 X3032 X3033 X3034 X3035 X3036 X3037 X3038 X3039 X3040
X3043 X3044 X3045 X3046 X3047 X3048 X3049 X3050 X3051 X3055 X3056 X3057 X3058 X3059 X3062 X3063 X3134 X3135 X3136 X3137 X3138 X3141 X3144 X3145 X3146 X3147 X3148 X3151 X3158 X3159 X3160 X3161 X3162 X3163 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3180 X3181 X3182 X3185 X3190 X3191 X3192 X3193
X3194 X3195 X3196 X3197 X3200 X3201 X3204 X3207 X3208 X3209 X3210 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3224 X3227 X3228 X3231 X3232 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269
X3270 X3271 X3272 X3273 X3274 X3275 X3276 X3277 X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3292 X3293 X3294 X3295 X3296 X3297 X3298 X3299 X3300 X3301 X3302 X3303 X3304 X3305 X3306 X3309 X3310 X3311 X3312 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3320 X3321 X3322 X3325 X3326 X3327 X3328 X3329 X3330 X3331
X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3345 X3346 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3367 X3368 X3369 X3370 X3371 X3374 X3375 X3376 X3377 X3378 X3379 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393
X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407 X3408 X3409 X3410 X3411 X3412 X3413 X3414 X3417 X3418 X3419 X3420 X3421 X3424 X3425 X3426 X3427 X3428 X3431 X3432 X3433 X3434 X3435 X3436 X3439 X3440 X3441 X3442 X3443 X3446 X3449 X3450 X3451 X3452 X3453 X3454 X3457 X3458 X3463

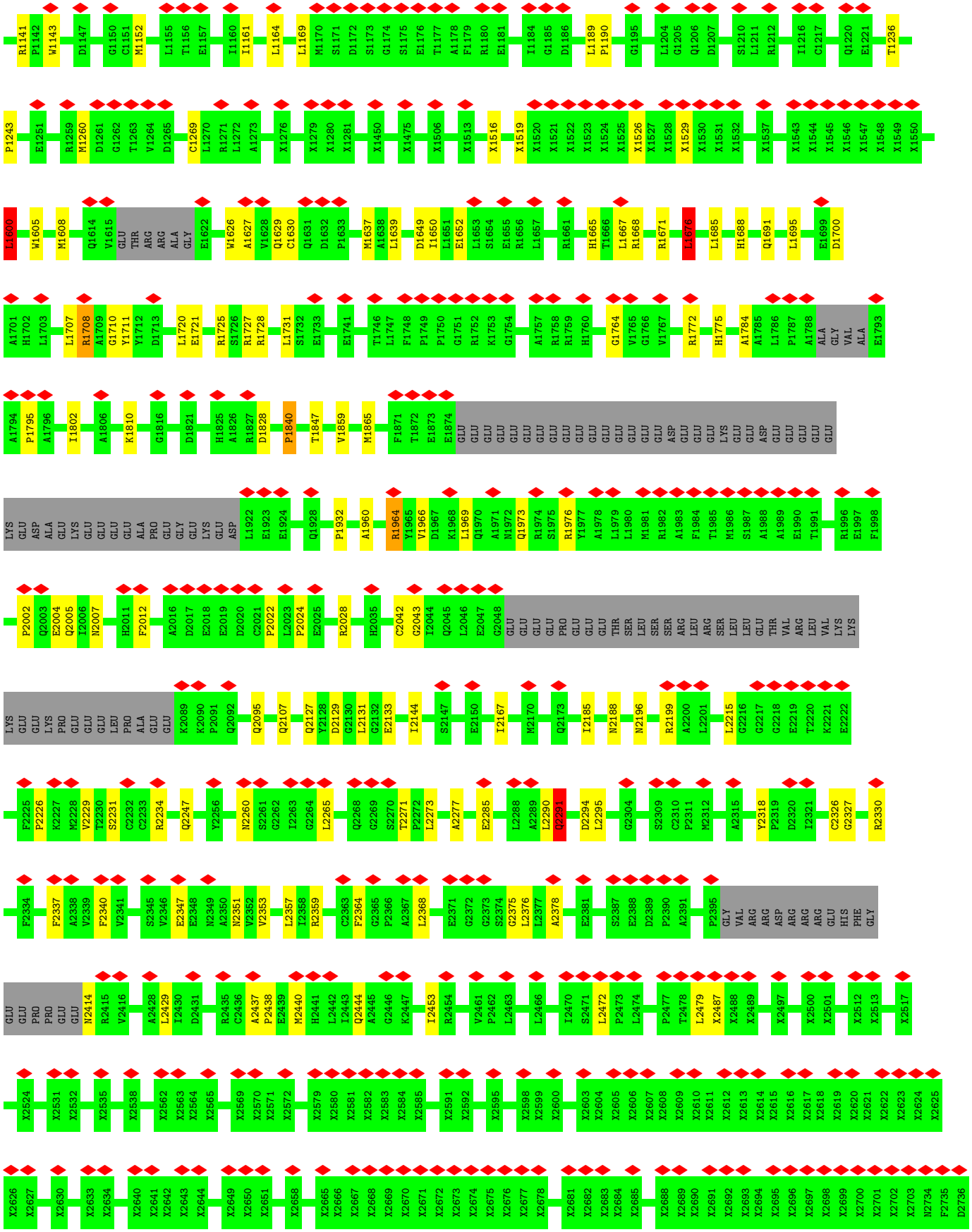

X3464 X3467 X3468 X3511 X3512 X3513 X3514 X3515 X3516 X3517 X3518 X3519 X3520 X3521 X3522 X3523 X3524 X3525 X3526 X3527 X3528 X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3536 X3537 X3538 X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3554 X3555 X3556 X3557 X3558 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566
X3567 X3568 X3569 X3570 X3571 X3572 X3573 X3574 X3577 X3578 X3579 X3580 X3581 X3582 X3583 X3584 X3585 X3586 X3587 X3588 X3589 X3590 X3591 X3592 X3593 X3596 X3597 X3600 X3601 X3604 X3605 X3606 X3607 X3608 X3609 X3610 X3611 X3612 X3613 N3643 L3644 K3658 W3661 I3662 L3663 T3664 E3665 D3666 H3667 S3668 M3673 I3674
D3675 D3676 L3677 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 R3707 K3713 S3714 K3715 L3716 D3717 M3723 I3728 C3733 H3734 L3735 E3736 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 S3752 F3753 E3754 E3759 R3762 Q3766
R3773 E3777 M3778 V3779 L3780 Q3781 S3784 K3787 I3804 L3805 N3809 M3816 L3817 E3825 Q3830 Q3833 L3842 D3843 R3849 Q3850 A3853 E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 A3876 D3877 D3878 Q3882 D3883
R3886 L3891 N3896 F3899 G3908 N3909 T3910 T3911 L3923 S3929 D3932 Y3937 S3938 G3939 K3940 D3941 V3942 I3943 Q3946 N3950 V3961 Y3968 I3969 Q3970 G3971 N3976 Q3977 Q3978 A3981 R3984 L3985 W3986 D3987 F3996 A3997 H3998 M4001 K4002 L4003 A4004 Q4005 D4022
L4031 E4032 G4033 N4034 V4035 V4036 N4037 A4041 D4046 M4047 E4050 S4051 N4054 V4055 E4056 M4057 I4058 L4059 K4060 F4061 P4062 D4063 M4064 F4065 L4066 K4067 L4068 K4069 Q3970 D4070 I4071 V4072 G4073 S4074 E4075 A4076 F4077 Q4078 D4079 Y4080 V4081 T4082 D4083 P4084 R4085 G4086 L4087 I4088 S4089 K4090 K4091 D4092 F4093 Q4094 K4095 A4096
M4097 D4098 S4099 Q4100 K4101 Q4102 F4103 T4104 G4105 P4106 Q4109 F4110 S4113 E4116 A4117 D4118 E4119 N4120 E4121 M4122 I4123 N4124 F4125 E4126 E4127 F4128 A4129 N4130 R4131 F4132 Q4133 R4137 D4138 F4141 L4147 P4155 H4156 R4159 L4160 R4161 M4162 F4163 L4164 E4165 L4166 A4167 E4168 S4169 I4170 L4171 E4172 Y4173
F4174 R4175 P4176 R4180 I4181 E4182 A4186 S4187 R4188 R4189 R4192 E4196 I4197 S4198 E4199 R4202 A4203 E4206 M4207 P4208 Q4209 Y4210 K4211 R4215 F4219 V4222 N4223 E4224 G4225 G4226 E4227 A4228 E4229 K4230 M4231 E4239 E4253 X4320 X4321 X4330 X4338 X4339 X4340 X4343 X4344 X4345
F4540 W4541 G4542 E4543 L4544 E4545 R4548 F4551 R4557 Y4560 T4561 L4562 R4563 V4582 S4583 D4584 S4585 P4586 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU
ASP GLU N4626 M4627 V4628 E4634 S4635 Y4638 P4641 W4644 L4648 F4655 L4656 G4660 E4674 R4679 K4680 L4681 E4682 F4683 D4684 G4685 L4686 Y4687 I4688 T4689 E4690 G4693 D4694 D4695 D4696 G4699 R4703 F4711 N4714 D4717 K4718 R4722 D4726 K4727 H4728 G4729 D4730
I4731 R4734 E4735 R4736 I4737 A4738 E4739 L4740 L4741 G4742 M4743 D4744 L4745 A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 T4766 W4767 L4768 M4769 S4770 I4771 D4772 F4784 T4785 D4786 F4789 L4790 L4800 L4801 G4802 H4803 Y4804 N4805 N4806 F4807 F4808 D4815
I4816 T4822 T4825 M4839 R4860 K4861 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872 K4875 C4876 G4890 D4899 E4900 I4901 E4902 D4903 D4907 D4917 V4924 I4927 L4928 E4952 D4953 C4958 F4959 I4960 C4961 G4962 I4963 F4968 D4969 T4970 H4973 H4978 T4979 L4980 E4981
E4982 H4983 N4984 L4985 A4986 N4997 K4998 D4999 T5004 E5007 E5016 D5020 A5024 G5025 D5026 C5027 K5030 Q5031 Y5032 E5033 D5034 Q5035 L5036 S5037

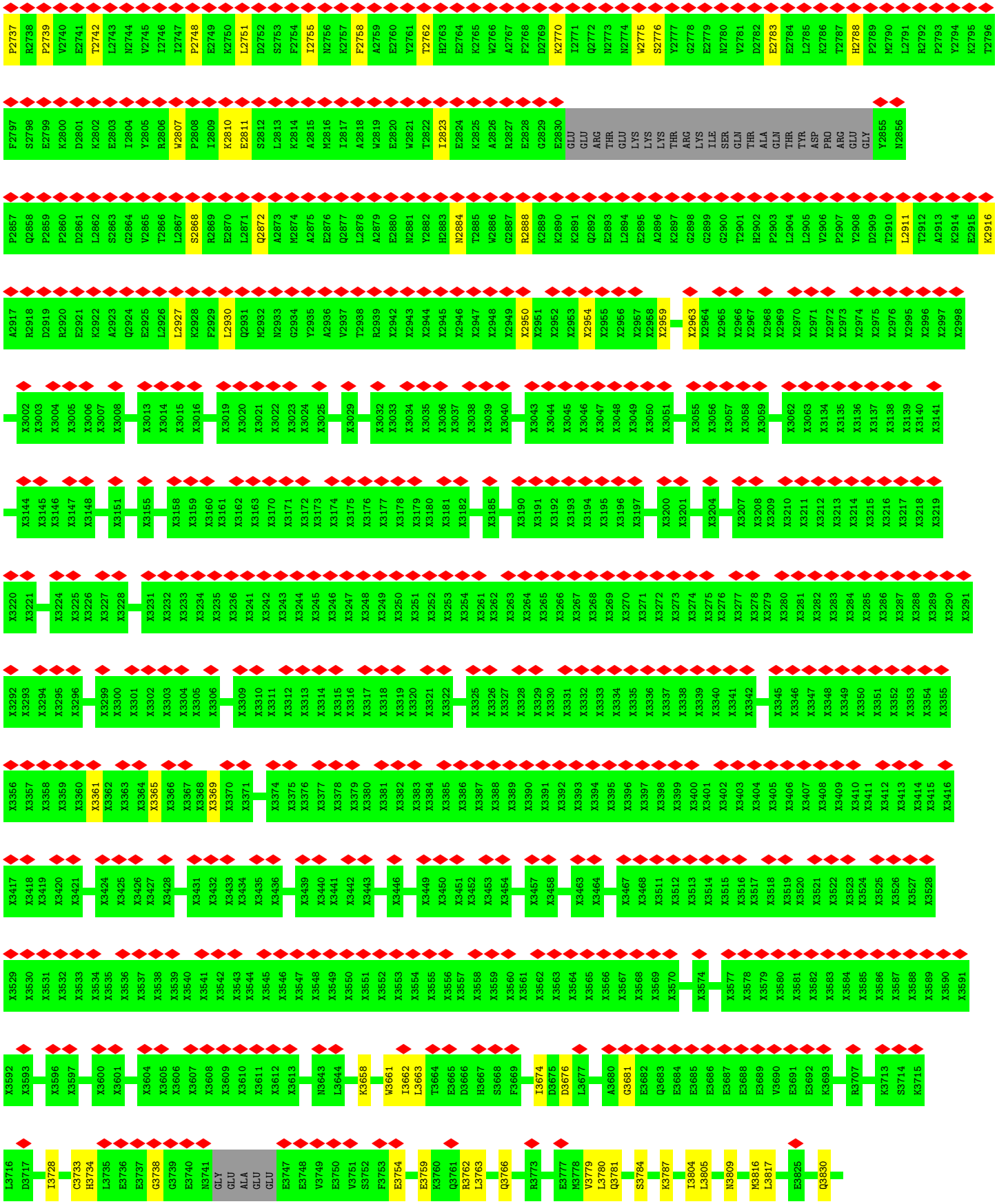
• Molecule 2: Ryanodine receptor 1

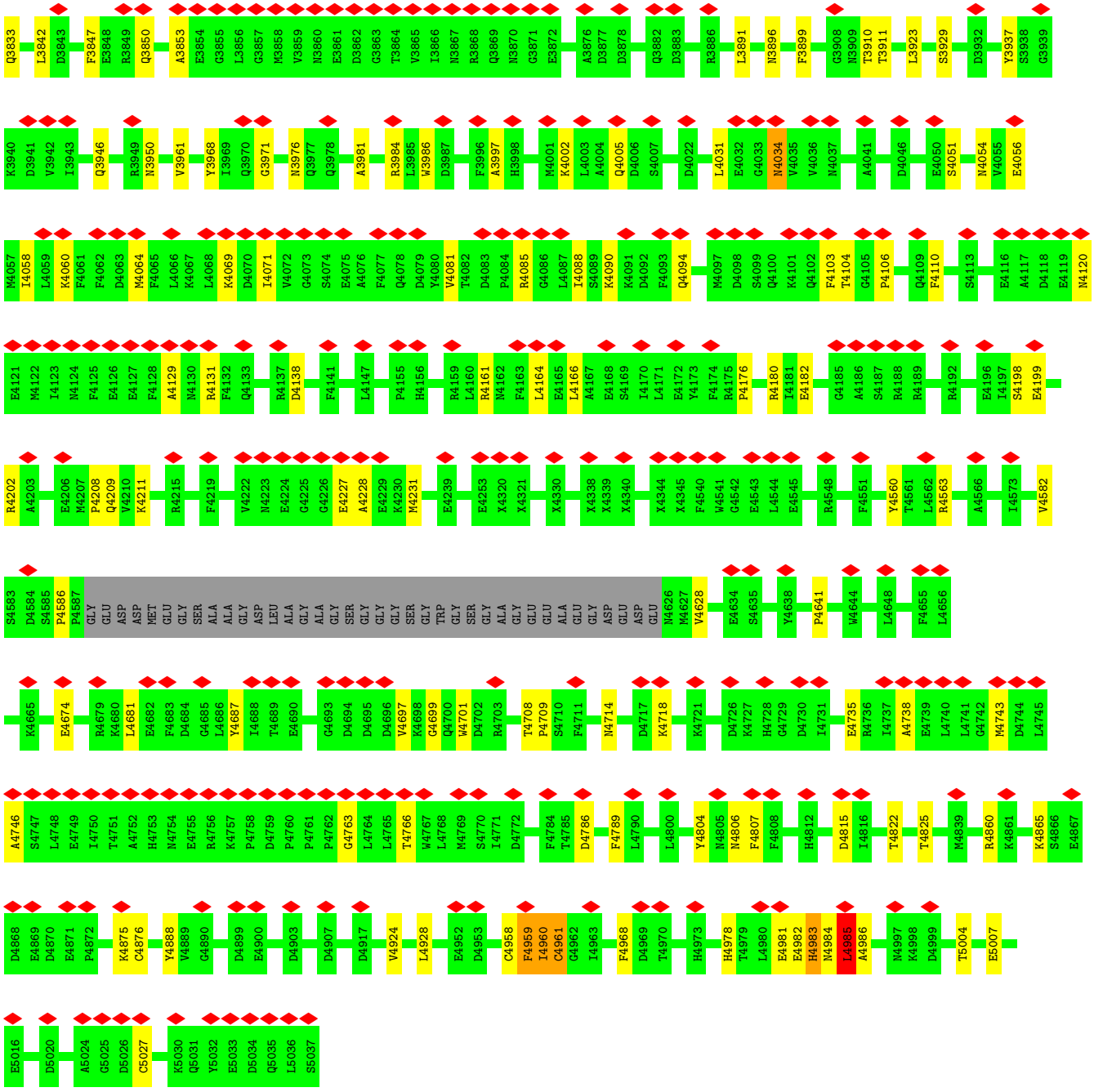
Chain E:








P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796
F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856
P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916
A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2949 X2950 X2951 X2952 X2953 X2954 X2955 X2956 X2957 X2958 X2959 X2963 X2964 X2965 X2966 X2967 X2968 X2969 X2970 X2971 X2972 X2973 X2974 X2975 X2976 X2995 X2996 X2997 X2998
X3002 X3003 X3004 X3005 X3006 X3007 X3008 X3013 X3014 X3015 X3016 X3019 X3020 X3021 X3022 X3023 X3024 X3025 X3029 X3032 X3033 X3034 X3035 X3036 X3037 X3038 X3039 X3040 X3043 X3044 X3045 X3046 X3047 X3048 X3049 X3050 X3051 X3055 X3056 X3057 X3058 X3059 X3062 X3063 X3134 X3135 X3136 X3137 X3138 X3139 X3140 X3141
X3144 X3145 X3146 X3147 X3148 X3151 X3155 X3158 X3159 X3160 X3161 X3162 X3163 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3180 X3181 X3182 X3185 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3200 X3201 X3204 X3207 X3208 X3209 X3210 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219
X3220 X3221 X3224 X3225 X3226 X3227 X3228 X3231 X3232 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3276 X3277 X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291
X3292 X3293 X3294 X3295 X3296 X3299 X3300 X3301 X3302 X3303 X3304 X3305 X3306 X3309 X3310 X3311 X3312 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3320 X3321 X3322 X3325 X3326 X3327 X3328 X3329 X3330 X3331 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3345 X3346 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355
X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3367 X3368 X3369 X3370 X3371 X3374 X3375 X3376 X3377 X3378 X3379 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407 X3408 X3409 X3410 X3411 X3412 X3413 X3414 X3415 X3416
X3417 X3418 X3419 X3420 X3421 X3424 X3425 X3426 X3427 X3428 X3431 X3432 X3433 X3434 X3435 X3436 X3439 X3440 X3441 X3442 X3443 X3446 X3449 X3450 X3451 X3452 X3453 X3454 X3457 X3458 X3463 X3464 X3467 X3468 X3511 X3512 X3513 X3514 X3515 X3516 X3517 X3518 X3519 X3520 X3521 X3522 X3523 X3524 X3525 X3526 X3527 X3528
X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3536 X3537 X3538 X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3554 X3555 X3556 X3557 X3558 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3569 X3570 X3574 X3577 X3578 X3579 X3580 X3581 X3582 X3583 X3584 X3585 X3586 X3587 X3588 X3589 X3590 X3591
X3592 X3593 X3596 X3597 X3600 X3601 X3604 X3605 X3606 X3607 X3608 X3609 X3610 X3611 X3612 X3613 N3643 L3644 K3658 W3661 I3662 L3663 T3664 E3665 D3666 H3667 S3668 F3669 I3674 D3675 D3676 L3677 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 R3707 K3713 S3714 K3715
L3716 D3717 I3728 C3733 H3734 L3735 E3736 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 S3752 F3753 E3754 E3759 K3760 Q3761 R3762 L3763 Q3766 R3773 E3777 M3778 V3779 L3780 Q3781 S3784 K3787 I3804 L3805 N3809 M3816 L3817 E3825 Q3830


Q3833 L3842 D3843 F3847 E3848 R3849 Q3850 A3853 E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 A3876 D3877 D3878 Q3882 D3883 R3886 L3891 N3896 F3899 G3908 N3909 T3910 T3911 L3923 S3929 D3932 Y3937 S3938 G3939
K3940 D3941 V3942 I3943 Q3946 R3949 N3950 V3961 Y3968 I3969 Q3970 G3971 N3976 Q3977 Q3978 A3981 R3984 L3985 W3986 D3987 F3996 A3997 H3998 M4001 K4002 L4003 A4004 Q4005 D4006 S4007 D4022 L4031 E4032 G4033 N4034 V4035 V4036 N4037 A4041 D4046 E4050 S4051 N4054 V4055 E4056
M4057 I4058 L4059 K4060 F4061 F4062 D4063 M4064 F4065 L4066 K4067 L4068 K4069 D4070 I4071 V4072 G4073 S4074 A4075 A4076 F4077 Q4078 D4079 Y4080 V4081 T4082 D4083 P4084 R4085 G4086 L4087 I4088 S4089 K4090 K4091 D4092 F4093 Q4094 M4097 D4098 S4099 Q4100 K4101 Q4102 F4103 T4104 G4105 P4106 Q4109 F4110 S4113 E4116 A4117 D4118 E4119 N4120
E4121 M4122 I4123 N4124 F4125 E4126 E4127 F4128 A4129 N4130 R4131 F4132 Q4133 R4137 D4138 F4141 L4147 P4155 H4156 R4159 L4160 R4161 N4162 F4163 L4164 E4165 L4166 A4167 E4168 S4169 I4170 L4171 E4172 Y4173 F4174 R4175 P4176 R4180 I4181 E4182 G4185 A4186 S4187 R4188 R4189 R4192 E4196 I4197 S4198 E4199
R4202 A4203 E4206 M4207 P4208 Q4209 V4210 K4211 R4215 F4219 V4222 N4223 E4224 G4225 G4226 E4227 A4228 E4229 K4230 M4231 E4239 E4253 X4320 X4321 X4330 X4338 X4339 X4340 X4344 X4345 F4540 W4541 G4542 E4543 L4544 E4545 R4548 F4551 Y4560 T4561 L4562 R4563 A4566 I4573 V4582
S4583 D4584 S4585 P4586 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY GLY SER GLY TRP GLY SER GLY ALA ALA GLY GLU GLU ALA GLU GLY GLY ASP GLU ASP GLU N4626 M4627 V4628 E4634 S4635 Y4638 P4641 W4644 L4648 F4655 L4656
K4665 E4674 R4679 K4680 L4681 E4682 F4683 D4684 G4685 L4686 Y4687 I4688 T4689 E4690 G4693 D4694 D4695 D4696 V4697 K4698 G4699 Q4700 W4701 D4702 R4703 T4708 P4709 S4710 F4711 N4714 D4717 K4718 K4721 D4726 K4727 H4728 G4729 D4730 I4731 E4735 R4736 I4737 A4738 E4739 L4740 L4741 G4742 M4743 D4744 L4745
A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 T4766 W4767 L4768 M4769 S4770 I4771 D4772 F4784 T4785 D4786 F4789 L4790 L4800 Y4804 N4805 N4806 F4807 F4808 H4812 D4815 I4816 T4822 T4825 M4839 R4860 K4861 K4865 S4866 E4867
D4868 E4869 D4870 E4871 P4872 K4875 C4876 Y4888 V4889 G4890 D4899 E4900 D4903 D4907 D4917 V4924 L4928 E4952 D4953 C4958 F4959 I4960 C4961 G4962 I4963 F4968 D4969 T4970 H4973 H4978 T4979 L4980 E4981 E4982 H4983 N4984 L4985 A4986 N4997 K4998 D4999 T5004 E5007
E5016 D5020 A5024 G5025 D5026 C5027 K5030 Q5031 Y5032 E5033 D5034 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.133	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	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, CA

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	0.30	0/834	0.53	0/1123
1	F	0.30	0/834	0.53	0/1123
1	H	0.30	0/834	0.53	0/1123
1	J	0.30	0/834	0.53	0/1123
2	B	0.30	0/25428	0.54	6/34534 (0.0%)
2	E	0.30	0/25428	0.54	6/34534 (0.0%)
2	G	0.30	0/25428	0.54	6/34534 (0.0%)
2	I	0.30	0/25428	0.54	6/34534 (0.0%)
All	All	0.30	0/105048	0.54	24/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	131	LEU	CA-CB-CG	7.94	133.56	115.30
2	I	131	LEU	CA-CB-CG	7.93	133.53	115.30
2	B	131	LEU	CA-CB-CG	7.92	133.53	115.30
2	G	131	LEU	CA-CB-CG	7.91	133.49	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1676	LEU	CA-CB-CG	6.62	130.52	115.30
2	I	1676	LEU	CA-CB-CG	6.61	130.50	115.30
2	B	1676	LEU	CA-CB-CG	6.60	130.49	115.30
2	G	1676	LEU	CA-CB-CG	6.59	130.46	115.30
2	G	1600	LEU	CA-CB-CG	6.37	129.94	115.30
2	E	1600	LEU	CA-CB-CG	6.35	129.91	115.30
2	B	1600	LEU	CA-CB-CG	6.34	129.88	115.30
2	I	1600	LEU	CA-CB-CG	6.33	129.86	115.30
2	B	4985	LEU	CA-CB-CG	5.79	128.63	115.30
2	I	4985	LEU	CA-CB-CG	5.79	128.62	115.30
2	G	4985	LEU	CA-CB-CG	5.79	128.61	115.30
2	E	4985	LEU	CA-CB-CG	5.77	128.58	115.30
2	E	977	LEU	CA-CB-CG	5.20	127.27	115.30
2	G	977	LEU	CA-CB-CG	5.20	127.25	115.30
2	I	977	LEU	CA-CB-CG	5.19	127.24	115.30
2	B	977	LEU	CA-CB-CG	5.19	127.24	115.30
2	G	2290	LEU	CA-CB-CG	5.17	127.19	115.30
2	E	2290	LEU	CA-CB-CG	5.17	127.18	115.30
2	B	2290	LEU	CA-CB-CG	5.16	127.16	115.30
2	I	2290	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	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	818	0	824	6	0
1	F	818	0	824	10	0
1	H	818	0	824	9	0
1	J	818	0	824	9	0
2	B	29499	0	24750	264	0
2	E	29499	0	24750	264	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	29499	0	24750	256	0
2	I	29499	0	24750	256	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102296	1050	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 (1050) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4968:PHE:HE2	2:B:4978:HIS:CE1	1.29	1.49
2:I:4968:PHE:HE2	2:I:4978:HIS:CE1	1.29	1.48
2:E:4968:PHE:HE2	2:E:4978:HIS:CE1	1.29	1.48
2:G:4968:PHE:HE2	2:G:4978:HIS:CE1	1.29	1.48
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.09	1.41
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.09	1.39
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.09	1.39
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.09	1.39
2:G:4968:PHE:CE2	2:G:4978:HIS:HE1	1.56	1.16
2:E:4968:PHE:CE2	2:E:4978:HIS:HE1	1.56	1.05
2:I:4968:PHE:CE2	2:I:4978:HIS:HE1	1.56	1.02
2:B:4968:PHE:CE2	2:B:4978:HIS:HE1	1.56	1.02
2:G:4968:PHE:CD2	2:G:4978:HIS:ND1	2.30	1.00
2:I:4968:PHE:CD2	2:I:4978:HIS:ND1	2.30	1.00
2:B:4968:PHE:CD2	2:B:4978:HIS:ND1	2.30	0.99
2:E:4968:PHE:CD2	2:E:4978:HIS:ND1	2.30	0.98
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.35	0.94
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.35	0.94
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.35	0.93
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.35	0.93
2:G:4968:PHE:CD2	2:G:4978:HIS:CE1	2.72	0.77
2:B:4231:MET:SD	2:B:4960:ILE:HD12	2.32	0.70
2:G:4231:MET:SD	2:G:4960:ILE:HD12	2.32	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4231:MET:SD	2:I:4960:ILE:HD12	2.32	0.69
2:E:4231:MET:SD	2:E:4960:ILE:HD12	2.32	0.69
2:B:379:HIS:HD2	2:B:382:GLY:H	1.42	0.68
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.92	0.68
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.92	0.68
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.92	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.42	0.67
2:I:379:HIS:HD2	2:I:382:GLY:H	1.42	0.67
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.92	0.67
2:I:4968:PHE:CD2	2:I:4978:HIS:CE1	2.72	0.67
2:B:626:LEU:HD23	2:B:630:GLU:H	1.60	0.67
2:I:626:LEU:HD23	2:I:630:GLU:H	1.60	0.66
2:G:379:HIS:HD2	2:G:382:GLY:H	1.42	0.66
2:E:4968:PHE:HD2	2:E:4978:HIS:ND1	1.90	0.66
2:G:626:LEU:HD23	2:G:630:GLU:H	1.60	0.66
2:E:626:LEU:HD23	2:E:630:GLU:H	1.60	0.66
2:G:111:HIS:HD2	2:G:114:SER:H	1.42	0.66
2:B:111:HIS:HD2	2:B:114:SER:H	1.42	0.66
2:I:111:HIS:HD2	2:I:114:SER:H	1.42	0.66
2:G:4968:PHE:HD2	2:G:4978:HIS:ND1	1.90	0.65
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.30	0.65
2:I:4968:PHE:HD2	2:I:4978:HIS:ND1	1.90	0.65
2:E:4968:PHE:CD2	2:E:4978:HIS:CE1	2.72	0.64
2:E:111:HIS:HD2	2:E:114:SER:H	1.42	0.64
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.30	0.64
2:B:179:TYR:OH	2:E:2359:ARG:NH1	2.31	0.63
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.30	0.63
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.30	0.63
2:B:4968:PHE:HD2	2:B:4978:HIS:ND1	1.90	0.63
2:E:4968:PHE:HE2	2:E:4978:HIS:HE1	0.67	0.62
2:I:132:ALA:HA	2:I:194:SER:HB2	1.82	0.62
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.65	0.62
2:G:132:ALA:HA	2:G:194:SER:HB2	1.82	0.62
2:B:132:ALA:HA	2:B:194:SER:HB2	1.82	0.61
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.65	0.61
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.65	0.61
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.83	0.61
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.34	0.61
2:E:132:ALA:HA	2:E:194:SER:HB2	1.82	0.61
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.65	0.61
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.34	0.61
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.61
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.83	0.61
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.34	0.61
2:G:4182:GLU:OE2	2:G:4983:HIS:CE1	2.54	0.61
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.83	0.60
2:B:4182:GLU:OE2	2:B:4983:HIS:CE1	2.54	0.60
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.83	0.60
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.34	0.60
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.84	0.60
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.60
2:E:4982:GLU:HG3	2:E:5027:CYS:SG	2.42	0.60
2:E:4182:GLU:OE2	2:E:4983:HIS:CE1	2.54	0.60
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.83	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.60
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.84	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.84	0.60
2:G:4982:GLU:HG3	2:G:5027:CYS:SG	2.42	0.60
2:I:4182:GLU:OE2	2:I:4983:HIS:CE1	2.54	0.60
2:B:4968:PHE:HE2	2:B:4978:HIS:HE1	0.67	0.59
2:B:4982:GLU:HG3	2:B:5027:CYS:SG	2.42	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.35	0.59
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.35	0.59
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.83	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.85	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.85	0.59
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.83	0.59
2:I:4982:GLU:HG3	2:I:5027:CYS:SG	2.42	0.59
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.85	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.85	0.58
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.35	0.58
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.84	0.58
2:B:4968:PHE:CD2	2:B:4978:HIS:CE1	2.72	0.58
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.86	0.58
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.36	0.58
2:I:4968:PHE:HE2	2:I:4978:HIS:HE1	0.67	0.58
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.69	0.58
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.21	0.58
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.69	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.86	0.58
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.86	0.58
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.21	0.58
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.36	0.58
2:B:2359:ARG:NH1	2:I:179:TYR:OH	2.36	0.58
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.69	0.58
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.86	0.57
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.36	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.57
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.36	0.57
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.37	0.57
2:B:4056:GLU:HG3	2:B:4166:LEU:HD21	1.87	0.57
2:G:4056:GLU:HG3	2:G:4166:LEU:HD21	1.87	0.57
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.86	0.57
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.38	0.57
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.21	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.57
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.69	0.57
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.87	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.69	0.57
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.35	0.57
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.69	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.57
2:I:4056:GLU:HG3	2:I:4166:LEU:HD21	1.87	0.57
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.87	0.57
2:G:2107:GLN:HG3	2:G:3681:GLY:HA2	1.87	0.57
2:G:4968:PHE:HE2	2:G:4978:HIS:HE1	0.67	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.69	0.57
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.87	0.57
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.86	0.57
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.38	0.56
2:I:4180:ARG:HH22	2:I:4981:GLU:HA	1.70	0.56
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.88	0.56
2:E:4056:GLU:HG3	2:E:4166:LEU:HD21	1.87	0.56
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.38	0.56
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.38	0.56
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.87	0.56
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.87	0.56
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.86	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.69	0.56
2:I:2107:GLN:HG3	2:I:3681:GLY:HA2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.38	0.56
2:E:3734:HIS:O	2:E:3738:GLY:N	2.39	0.56
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.56
2:B:4180:ARG:HH22	2:B:4981:GLU:HA	1.70	0.56
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.38	0.56
2:I:744:VAL:HG22	2:I:759:ILE:HG12	1.88	0.56
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.71	0.56
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.87	0.56
2:G:3734:HIS:O	2:G:3738:GLY:N	2.39	0.56
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.87	0.56
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.38	0.56
2:G:4180:ARG:HH22	2:G:4981:GLU:HA	1.70	0.56
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.88	0.56
2:E:359:TYR:HA	2:E:376:ALA:HA	1.88	0.56
2:E:2107:GLN:HG3	2:E:3681:GLY:HA2	1.87	0.56
2:G:359:TYR:HA	2:G:376:ALA:HA	1.88	0.56
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.87	0.56
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.87	0.56
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.38	0.56
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.71	0.56
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.38	0.56
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.87	0.56
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.38	0.56
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.38	0.56
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.87	0.56
2:B:395:GLN:HG3	2:B:397:GLU:H	1.71	0.56
2:B:744:VAL:HG22	2:B:759:ILE:HG12	1.88	0.56
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.56
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.21	0.56
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.71	0.55
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.71	0.55
2:G:744:VAL:HG22	2:G:759:ILE:HG12	1.88	0.55
2:G:395:GLN:HG3	2:G:397:GLU:H	1.71	0.55
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.87	0.55
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.71	0.55
2:I:395:GLN:HG3	2:I:397:GLU:H	1.71	0.55
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.71	0.55
2:E:609:CYS:SG	2:E:610:ASN:N	2.80	0.55
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.87	0.55
2:B:1009:ALA:O	2:B:1020:ARG:N	2.40	0.55
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.87	0.55
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.55
2:B:2107:GLN:HG3	2:B:3681:GLY:HA2	1.87	0.55
2:E:744:VAL:HG22	2:E:759:ILE:HG12	1.88	0.55
2:G:4161:ARG:HD3	2:G:4164:LEU:HD12	1.89	0.55
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.89	0.55
2:B:4982:GLU:OE1	2:B:4982:GLU:HA	2.07	0.55
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.87	0.55
2:I:359:TYR:HA	2:I:376:ALA:HA	1.88	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.80	0.55
2:I:1009:ALA:O	2:I:1020:ARG:N	2.40	0.55
2:I:4982:GLU:OE1	2:I:4982:GLU:HA	2.07	0.55
2:E:4180:ARG:HH22	2:E:4981:GLU:HA	1.70	0.55
2:B:359:TYR:HA	2:B:376:ALA:HA	1.88	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:I:730:VAL:O	2:I:735:GLN:NE2	2.40	0.54
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.90	0.54
2:E:1009:ALA:O	2:E:1020:ARG:N	2.40	0.54
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.54
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.40	0.54
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.40	0.54
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.54
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.89	0.54
2:B:315:CYS:SG	2:B:316:PHE:N	2.81	0.54
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.90	0.54
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.89	0.54
2:G:609:CYS:SG	2:G:610:ASN:N	2.80	0.54
2:I:4161:ARG:HD3	2:I:4164:LEU:HD12	1.89	0.54
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.90	0.54
2:B:609:CYS:SG	2:B:610:ASN:N	2.80	0.54
2:G:730:VAL:O	2:G:735:GLN:NE2	2.40	0.54
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.41	0.54
2:E:730:VAL:O	2:E:735:GLN:NE2	2.40	0.54
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.71	0.54
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.90	0.54
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.41	0.54
2:G:315:CYS:SG	2:G:316:PHE:N	2.81	0.54
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.41	0.54
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.90	0.54
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.41	0.54
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.89	0.54
2:E:4982:GLU:OE1	2:E:4982:GLU:HA	2.07	0.54
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.90	0.54
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.54
2:B:730:VAL:O	2:B:735:GLN:NE2	2.40	0.54
2:B:4161:ARG:HD3	2:B:4164:LEU:HD12	1.89	0.54
2:I:315:CYS:SG	2:I:316:PHE:N	2.81	0.54
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.90	0.54
2:E:395:GLN:HG3	2:E:397:GLU:H	1.71	0.54
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.37	0.54
2:B:614:VAL:HG22	2:B:616:SER:H	1.73	0.54
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.71	0.54
2:G:1009:ALA:O	2:G:1020:ARG:N	2.40	0.54
2:G:4982:GLU:OE1	2:G:4982:GLU:HA	2.07	0.54
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.41	0.54
2:E:315:CYS:SG	2:E:316:PHE:N	2.81	0.54
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.72	0.54
2:B:853:PRO:HB3	2:B:1024:TYR:H	1.72	0.54
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.90	0.54
2:G:853:PRO:HB3	2:G:1024:TYR:H	1.72	0.54
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.89	0.54
2:E:2479:LEU:O	2:E:2487:UNK:N	2.41	0.54
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.41	0.53
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.90	0.53
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.37	0.53
2:I:2479:LEU:O	2:I:2487:UNK:N	2.41	0.53
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.53
2:E:4031:LEU:HB3	2:E:4034:ASN:HB2	1.90	0.53
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.90	0.53
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.73	0.53
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.81	0.53
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.90	0.53
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.89	0.53
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.40	0.53
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.40	0.53
2:E:614:VAL:HG22	2:E:616:SER:H	1.73	0.53
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.90	0.53
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.89	0.53
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.90	0.53
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.90	0.53
2:E:4161:ARG:HD3	2:E:4164:LEU:HD12	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4031:LEU:HB3	2:G:4034:ASN:HB2	1.90	0.53
2:I:4031:LEU:HB3	2:I:4034:ASN:HB2	1.90	0.53
2:E:2347:GLU:O	2:E:2351:ASN:N	2.41	0.53
2:B:4031:LEU:HB3	2:B:4034:ASN:HB2	1.90	0.53
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.41	0.53
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.41	0.53
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.74	0.53
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.74	0.53
2:B:2479:LEU:O	2:B:2487:UNK:N	2.41	0.53
2:I:3733:CYS:HA	2:I:3766:GLN:HG2	1.91	0.53
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.81	0.53
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.72	0.53
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.73	0.53
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.90	0.53
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.74	0.53
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.73	0.52
2:B:3734:HIS:O	2:B:3738:GLY:N	2.39	0.52
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.91	0.52
2:I:614:VAL:HG22	2:I:616:SER:H	1.73	0.52
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.42	0.52
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.89	0.52
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.91	0.52
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.91	0.52
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.92	0.52
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.74	0.52
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	1.92	0.52
2:E:1516:UNK:N	2:E:1529:UNK:O	2.43	0.52
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.91	0.52
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.37	0.52
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.42	0.52
2:B:3733:CYS:HA	2:B:3766:GLN:HG2	1.91	0.52
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	1.92	0.52
2:G:1516:UNK:N	2:G:1529:UNK:O	2.42	0.52
2:I:1516:UNK:N	2:I:1529:UNK:O	2.42	0.52
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	1.92	0.52
2:B:1516:UNK:N	2:B:1529:UNK:O	2.42	0.52
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.92	0.52
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.73	0.52
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	1.92	0.52
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.91	0.52
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.92	0.52
2:G:2479:LEU:O	2:G:2487:UNK:N	2.41	0.52
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.91	0.52
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.91	0.52
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.92	0.52
2:E:3733:CYS:HA	2:E:3766:GLN:HG2	1.91	0.52
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.75	0.52
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.92	0.52
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.92	0.52
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.91	0.52
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.92	0.52
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.91	0.52
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.74	0.52
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.91	0.52
2:B:3968:TYR:O	2:B:3976:ASN:ND2	2.43	0.52
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.92	0.52
2:I:3734:HIS:O	2:I:3738:GLY:N	2.39	0.52
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.74	0.52
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.75	0.51
1:J:34:LYS:HE3	2:I:634:GLN:HB3	1.93	0.51
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.93	0.51
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.93	0.51
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.92	0.51
2:G:331:VAL:HG12	2:G:333:GLY:H	1.76	0.51
2:I:331:VAL:HG12	2:I:333:GLY:H	1.76	0.51
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.74	0.51
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.74	0.51
2:G:614:VAL:HG22	2:G:616:SER:H	1.73	0.51
2:G:3968:TYR:O	2:G:3976:ASN:ND2	2.43	0.51
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.93	0.51
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.93	0.51
2:G:3733:CYS:HA	2:G:3766:GLN:HG2	1.91	0.51
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.81	0.51
2:G:160:GLY:O	2:I:3984:ARG:NH2	2.39	0.51
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.81	0.51
2:I:3968:TYR:O	2:I:3976:ASN:ND2	2.43	0.51
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.76	0.51
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.93	0.51
2:B:2353:VAL:O	2:B:2357:LEU:N	2.44	0.51
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.75	0.51
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.75	0.51
2:I:2353:VAL:O	2:I:2357:LEU:N	2.44	0.51
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.44	0.51
1:A:27:THR:HB	1:A:100:ASP:HB3	1.94	0.51
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.44	0.51
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.93	0.51
2:E:331:VAL:HG12	2:E:333:GLY:H	1.76	0.51
2:E:2353:VAL:O	2:E:2357:LEU:N	2.44	0.51
2:E:3968:TYR:O	2:E:3976:ASN:ND2	2.43	0.51
2:B:331:VAL:HG12	2:B:333:GLY:H	1.76	0.50
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.37	0.50
2:G:2347:GLU:O	2:G:2351:ASN:N	2.41	0.50
2:G:2353:VAL:O	2:G:2357:LEU:N	2.44	0.50
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	1.93	0.50
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.44	0.50
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.93	0.50
2:I:41:GLY:O	2:I:45:ARG:NH1	2.45	0.50
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.76	0.50
1:F:27:THR:HB	1:F:100:ASP:HB3	1.93	0.50
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.42	0.50
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.44	0.50
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	1.93	0.50
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.91	0.50
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.94	0.50
2:E:41:GLY:O	2:E:45:ARG:NH1	2.45	0.50
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.44	0.50
2:B:41:GLY:O	2:B:45:ARG:NH1	2.45	0.50
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.94	0.50
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.91	0.50
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.92	0.50
2:I:2347:GLU:O	2:I:2351:ASN:N	2.41	0.50
2:B:160:GLY:O	2:E:3984:ARG:NH2	2.43	0.50
1:J:27:THR:HB	1:J:100:ASP:HB3	1.93	0.50
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.77	0.50
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.94	0.50
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.77	0.50
2:G:41:GLY:O	2:G:45:ARG:NH1	2.45	0.49
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.44	0.49
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	1.93	0.49
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.77	0.49
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.76	0.49
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.94	0.49
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.77	0.49
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.77	0.49
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.77	0.49
2:B:4090:LYS:O	2:B:4094:GLN:N	2.46	0.49
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.94	0.49
2:E:776:LEU:HG	2:E:848:HIS:HA	1.95	0.49
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.78	0.49
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.78	0.49
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.77	0.49
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.95	0.49
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.95	0.49
1:H:27:THR:HB	1:H:100:ASP:HB3	1.93	0.49
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.95	0.49
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.95	0.49
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.95	0.49
2:G:3997:ALA:HA	2:G:4058:ILE:HD11	1.95	0.49
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.29	0.49
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.95	0.49
2:I:2868:SER:O	2:I:2872:GLN:N	2.45	0.49
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.77	0.49
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.78	0.49
2:B:776:LEU:HG	2:B:848:HIS:HA	1.95	0.49
2:B:4822:THR:O	2:B:4825:THR:OG1	2.30	0.49
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.95	0.49
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.95	0.49
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.78	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.41	0.49
2:G:794:GLY:H	2:G:798:GLY:HA3	1.78	0.49
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.95	0.49
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.95	0.48
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.94	0.48
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.78	0.48
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	1.93	0.48
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.95	0.48
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.94	0.48
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.96	0.48
2:I:794:GLY:H	2:I:798:GLY:HA3	1.78	0.48
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.96	0.48
2:B:794:GLY:H	2:B:798:GLY:HA3	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3997:ALA:HA	2:B:4058:ILE:HD11	1.95	0.48
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.96	0.48
2:G:776:LEU:HG	2:G:848:HIS:HA	1.95	0.48
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.76	0.48
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.44	0.48
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.94	0.48
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.42	0.48
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.96	0.48
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.94	0.48
2:I:3997:ALA:HA	2:I:4058:ILE:HD11	1.95	0.48
2:E:794:GLY:H	2:E:798:GLY:HA3	1.78	0.48
2:E:2868:SER:O	2:E:2872:GLN:N	2.45	0.48
2:E:4090:LYS:O	2:E:4094:GLN:N	2.46	0.48
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.96	0.48
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.95	0.48
2:G:396:GLU:OE2	2:G:451:TYR:OH	2.29	0.48
2:G:4090:LYS:O	2:G:4094:GLN:N	2.46	0.48
2:I:776:LEU:HG	2:I:848:HIS:HA	1.95	0.48
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.96	0.48
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.48
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.94	0.48
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.96	0.48
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.78	0.48
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.96	0.48
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.96	0.48
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.95	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.29	0.48
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.95	0.48
2:E:4822:THR:O	2:E:4825:THR:OG1	2.30	0.48
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.96	0.48
2:B:1650:ILE:HG13	2:B:1707:LEU:HD21	1.96	0.48
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.95	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.95	0.48
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.78	0.48
2:B:978:THR:HB	2:B:980:ALA:H	1.80	0.47
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.96	0.47
2:G:4822:THR:O	2:G:4825:THR:OG1	2.30	0.47
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.94	0.47
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.95	0.47
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.95	0.47
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:396:GLU:OE2	2:E:451:TYR:OH	2.29	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.95	0.47
2:E:3997:ALA:HA	2:E:4058:ILE:HD11	1.95	0.47
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.78	0.47
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.97	0.47
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.79	0.47
2:I:4090:LYS:O	2:I:4094:GLN:N	2.46	0.47
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.46	0.47
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.96	0.47
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.96	0.47
2:E:1650:ILE:HG13	2:E:1707:LEU:HD21	1.96	0.47
2:E:2375:GLY:HA3	2:E:2378:ALA:HB3	1.97	0.47
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.95	0.47
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.96	0.47
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.96	0.47
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.47
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.96	0.47
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.97	0.47
2:G:2868:SER:O	2:G:2872:GLN:N	2.45	0.47
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.97	0.47
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.97	0.47
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.95	0.47
2:B:2375:GLY:HA3	2:B:2378:ALA:HB3	1.97	0.47
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.49	0.47
2:I:978:THR:HB	2:I:980:ALA:H	1.80	0.47
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.97	0.47
2:E:978:THR:HB	2:E:980:ALA:H	1.80	0.47
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.96	0.47
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.43	0.47
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.96	0.47
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.49	0.47
2:I:1650:ILE:HG13	2:I:1707:LEU:HD21	1.96	0.47
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.97	0.47
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.49	0.47
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.48	0.47
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.96	0.47
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.79	0.47
2:E:645:ARG:N	2:E:824:GLU:O	2.42	0.47
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.97	0.47
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.49	0.47
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:HIS:CD2	2:B:114:SER:H	2.29	0.46
2:B:4865:LYS:HG3	2:B:4875:LYS:HZ3	1.79	0.46
2:G:485:SER:HA	2:G:488:LEU:HB2	1.96	0.46
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.79	0.46
2:I:2375:GLY:HA3	2:I:2378:ALA:HB3	1.97	0.46
2:E:1865:MET:SD	2:E:1865:MET:N	2.89	0.46
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.98	0.46
2:B:1865:MET:SD	2:B:1865:MET:N	2.88	0.46
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.46	0.46
2:G:2375:GLY:HA3	2:G:2378:ALA:HB3	1.97	0.46
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.96	0.46
2:E:485:SER:HA	2:E:488:LEU:HB2	1.96	0.46
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.98	0.46
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.48	0.46
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.96	0.46
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.98	0.46
2:I:2364:PHE:HD1	2:I:2429:LEU:HD21	1.81	0.46
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.48	0.46
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.96	0.46
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.97	0.46
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.48	0.46
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.81	0.46
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.48	0.46
2:E:2364:PHE:HD1	2:E:2429:LEU:HD21	1.81	0.46
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.79	0.46
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.84	0.46
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.97	0.46
2:B:2868:SER:O	2:B:2872:GLN:N	2.45	0.46
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.81	0.46
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.84	0.46
2:G:1650:ILE:HG13	2:G:1707:LEU:HD21	1.96	0.46
2:G:1865:MET:SD	2:G:1865:MET:N	2.88	0.46
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.97	0.46
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.96	0.46
2:B:485:SER:HA	2:B:488:LEU:HB2	1.96	0.46
2:B:2364:PHE:HD1	2:B:2429:LEU:HD21	1.81	0.46
2:G:978:THR:HB	2:G:980:ALA:H	1.79	0.46
2:G:2364:PHE:HD1	2:G:2429:LEU:HD21	1.80	0.46
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.84	0.46
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.34	0.46
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:485:SER:HA	2:I:488:LEU:HB2	1.96	0.46
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.97	0.45
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.98	0.45
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.34	0.45
2:I:1865:MET:SD	2:I:1865:MET:N	2.88	0.45
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.81	0.45
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.47	0.45
2:B:4958:CYS:HB2	2:B:4961:CYS:H	1.82	0.45
2:G:2291:GLN:HE21	2:G:2294:ASP:H	1.65	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.48	0.45
2:E:2291:GLN:HE21	2:E:2294:ASP:H	1.64	0.45
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.97	0.45
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.98	0.45
2:B:4069:LYS:HG3	2:B:4129:ALA:HB1	1.99	0.45
2:G:4069:LYS:HG3	2:G:4129:ALA:HB1	1.99	0.45
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.14	0.45
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.99	0.45
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.34	0.45
2:I:4005:GLN:HE21	2:I:4110:PHE:HE1	1.63	0.45
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.97	0.45
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.97	0.45
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.99	0.45
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.98	0.45
2:E:4005:GLN:HE21	2:E:4110:PHE:HE1	1.63	0.45
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.14	0.45
2:B:4005:GLN:HE21	2:B:4110:PHE:HE1	1.63	0.45
2:G:278:GLN:N	2:G:315:CYS:SG	2.90	0.45
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.75	0.45
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.81	0.45
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.46	0.45
2:I:213:TYR:CG	2:I:337:PRO:HB2	2.52	0.45
2:I:4069:LYS:HG3	2:I:4129:ALA:HB1	1.99	0.45
2:I:4958:CYS:HB2	2:I:4961:CYS:H	1.82	0.45
2:E:4069:LYS:HG3	2:E:4129:ALA:HB1	1.99	0.45
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.99	0.45
2:B:164:ARG:N	2:B:167:ASP:OD2	2.43	0.45
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.98	0.45
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	1.99	0.45
2:I:206:CYS:SG	2:I:207:SER:N	2.90	0.45
2:I:2291:GLN:HE21	2:I:2294:ASP:H	1.65	0.45
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.97	0.45
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.98	0.45
2:B:2291:GLN:HE21	2:B:2294:ASP:H	1.64	0.45
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.48	0.45
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.97	0.45
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.47	0.45
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.99	0.45
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	1.99	0.45
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.84	0.45
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.97	0.45
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.46	0.45
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.75	0.45
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.81	0.45
2:G:213:TYR:CG	2:G:337:PRO:HB2	2.52	0.45
2:G:4005:GLN:HE21	2:G:4110:PHE:HE1	1.63	0.45
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.99	0.45
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.30	0.45
2:B:213:TYR:CG	2:B:337:PRO:HB2	2.52	0.45
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.30	0.45
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.30	0.45
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.99	0.45
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.81	0.45
2:E:4958:CYS:HB2	2:E:4961:CYS:H	1.82	0.45
2:B:4959:PHE:O	2:B:4959:PHE:CD1	2.71	0.44
2:B:4960:ILE:HG12	2:B:4985:LEU:HD23	2.00	0.44
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.99	0.44
2:E:2959:UNK:O	2:E:2963:UNK:N	2.50	0.44
2:I:652:ARG:HB2	2:I:750:LEU:HD13	1.99	0.44
2:I:4960:ILE:HG12	2:I:4985:LEU:HD23	2.00	0.44
2:E:206:CYS:SG	2:E:207:SER:N	2.90	0.44
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.99	0.44
2:B:278:GLN:N	2:B:315:CYS:SG	2.90	0.44
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.34	0.44
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	1.99	0.44
2:G:2959:UNK:O	2:G:2963:UNK:N	2.50	0.44
2:G:3759:GLU:O	2:G:3763:LEU:N	2.48	0.44
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.81	0.44
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.14	0.44
2:B:645:ARG:N	2:B:824:GLU:O	2.42	0.44
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.99	0.44
2:G:206:CYS:SG	2:G:207:SER:N	2.90	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.14	0.44
2:G:652:ARG:HB2	2:G:750:LEU:HD13	2.00	0.44
2:G:4960:ILE:HG12	2:G:4985:LEU:HD23	2.00	0.44
2:I:278:GLN:N	2:I:315:CYS:SG	2.90	0.44
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.75	0.44
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.99	0.44
2:E:3759:GLU:O	2:E:3763:LEU:N	2.48	0.44
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.99	0.44
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.34	0.44
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.99	0.44
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.98	0.44
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	1.99	0.44
2:I:551:LEU:HD21	2:I:589:LEU:HD13	2.00	0.44
2:E:551:LEU:HD21	2:E:589:LEU:HD13	2.00	0.44
2:E:606:LEU:O	2:E:617:ASN:ND2	2.51	0.44
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	1.99	0.44
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.70	0.44
2:B:606:LEU:O	2:B:617:ASN:ND2	2.51	0.44
2:B:652:ARG:HB2	2:B:750:LEU:HD13	1.99	0.44
2:G:551:LEU:HD21	2:G:589:LEU:HD13	2.00	0.44
2:G:1720:LEU:HD12	2:G:1847:THR:HG23	1.99	0.44
2:I:4822:THR:O	2:I:4825:THR:OG1	2.30	0.44
2:E:213:TYR:CG	2:E:337:PRO:HB2	2.52	0.44
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.98	0.44
2:E:793:LEU:HB2	2:E:797:HIS:H	1.83	0.44
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.99	0.44
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.75	0.44
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.30	0.44
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.91	0.44
2:B:2959:UNK:O	2:B:2963:UNK:N	2.50	0.44
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.51	0.44
2:G:4959:PHE:O	2:G:4959:PHE:CD1	2.71	0.44
2:I:641:VAL:HG21	2:I:705:ASN:HA	2.00	0.44
2:I:911:HIS:O	2:I:918:ARG:NH2	2.48	0.44
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.48	0.44
2:I:2959:UNK:O	2:I:2963:UNK:N	2.50	0.44
2:I:4984:ASN:C	2:I:4986:ALA:H	2.21	0.44
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.99	0.44
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	2.00	0.44
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.00	0.44
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.91	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.51	0.44
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	2.00	0.44
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.51	0.44
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.46	0.44
2:E:4960:ILE:HG12	2:E:4985:LEU:HD23	2.00	0.44
1:F:34:LYS:HE3	2:E:634:GLN:HB3	2.00	0.43
2:B:1695:LEU:HB3	2:B:1810:LYS:HZ2	1.83	0.43
2:I:606:LEU:O	2:I:617:ASN:ND2	2.51	0.43
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.70	0.43
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.82	0.43
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.91	0.43
1:F:23:VAL:HG22	1:F:47:LYS:HG2	2.00	0.43
2:G:606:LEU:O	2:G:617:ASN:ND2	2.51	0.43
2:G:1132:TRP:HE1	2:G:1136:SER:HG	1.61	0.43
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.48	0.43
2:B:243:ARG:NH1	2:B:301:VAL:O	2.49	0.43
2:B:793:LEU:HB2	2:B:797:HIS:H	1.83	0.43
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.99	0.43
2:B:4209:GLN:HE22	2:B:4560:TYR:HE2	1.66	0.43
2:B:4984:ASN:C	2:B:4986:ALA:H	2.21	0.43
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.91	0.43
2:G:4209:GLN:HE22	2:G:4560:TYR:HE2	1.66	0.43
2:I:4209:GLN:HE22	2:I:4560:TYR:HE2	1.66	0.43
1:J:23:VAL:HG22	1:J:47:LYS:HG2	2.01	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.90	0.43
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.00	0.43
2:B:4563:ARG:NH1	2:B:4815:ASP:OD1	2.52	0.43
2:B:4968:PHE:HD2	2:B:4978:HIS:HD1	1.47	0.43
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.99	0.43
2:G:4958:CYS:HB2	2:G:4961:CYS:H	1.82	0.43
2:I:1720:LEU:HD12	2:I:1847:THR:HG23	1.99	0.43
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.00	0.43
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.99	0.43
2:E:652:ARG:HB2	2:E:750:LEU:HD13	1.99	0.43
2:E:4586:PRO:HB3	2:E:4628:VAL:HG21	2.01	0.43
2:B:551:LEU:HD21	2:B:589:LEU:HD13	2.00	0.43
2:G:889:GLN:O	2:G:902:ARG:NH1	2.52	0.43
2:G:914:PRO:HD2	2:G:917:GLU:HB2	2.00	0.43
2:G:2775:TRP:HZ3	2:G:2783:GLU:HA	1.84	0.43
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.00	0.43
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1132:TRP:HE1	2:I:1136:SER:HG	1.65	0.43
2:I:4563:ARG:NH1	2:I:4815:ASP:OD1	2.52	0.43
2:E:914:PRO:HD2	2:E:917:GLU:HB2	2.00	0.43
2:E:919:ASN:O	2:E:923:GLN:N	2.52	0.43
2:E:1720:LEU:HD12	2:E:1847:THR:HG23	1.99	0.43
2:E:4209:GLN:HE22	2:E:4560:TYR:HE2	1.67	0.43
1:H:23:VAL:HG22	1:H:47:LYS:HG2	2.01	0.43
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.84	0.43
2:B:889:GLN:O	2:B:902:ARG:NH1	2.52	0.43
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.99	0.43
2:G:641:VAL:HG21	2:G:705:ASN:HA	2.00	0.43
2:E:2775:TRP:HZ3	2:E:2783:GLU:HA	1.84	0.43
2:E:4984:ASN:C	2:E:4986:ALA:H	2.21	0.43
2:B:2440:MET:O	2:B:2444:GLN:N	2.51	0.43
2:G:4563:ARG:NH1	2:G:4815:ASP:OD1	2.52	0.43
2:E:889:GLN:O	2:E:902:ARG:NH1	2.52	0.43
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.51	0.43
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.34	0.43
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.00	0.43
2:G:4198:SER:OG	2:G:4199:GLU:N	2.52	0.43
2:G:4984:ASN:C	2:G:4986:ALA:H	2.21	0.43
2:I:4071:ILE:HG13	2:I:4103:PHE:HZ	1.84	0.43
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.84	0.43
1:J:55:VAL:HA	2:I:1784:ALA:HA	2.00	0.43
2:B:870:ILE:HD12	2:B:873:LYS:HB2	2.01	0.43
2:B:911:HIS:O	2:B:918:ARG:NH2	2.48	0.43
2:B:1966:VAL:HA	2:B:1969:LEU:HB3	2.01	0.43
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.00	0.43
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.84	0.43
2:G:1695:LEU:HB3	2:G:1810:LYS:HZ2	1.83	0.43
2:G:1966:VAL:HA	2:G:1969:LEU:HB3	2.01	0.43
2:G:4586:PRO:HB3	2:G:4628:VAL:HG21	2.01	0.43
2:I:793:LEU:HB2	2:I:797:HIS:H	1.83	0.43
2:I:2440:MET:O	2:I:2444:GLN:N	2.51	0.43
2:I:4198:SER:OG	2:I:4199:GLU:N	2.52	0.43
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.30	0.43
2:E:243:ARG:NH1	2:E:301:VAL:O	2.49	0.43
2:E:870:ILE:HD12	2:E:873:LYS:HB2	2.01	0.43
1:A:23:VAL:HG22	1:A:47:LYS:HG2	2.01	0.43
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.52	0.43
2:B:4936:ILE:HG21	2:I:4927:ILE:HG12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:790:ARG:HG2	2:G:1627:ALA:HA	2.01	0.43
2:G:793:LEU:HB2	2:G:797:HIS:H	1.83	0.43
2:G:2440:MET:O	2:G:2444:GLN:N	2.51	0.43
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.54	0.43
2:I:1695:LEU:HB3	2:I:1810:LYS:HZ2	1.83	0.43
2:E:1966:VAL:HA	2:E:1969:LEU:HB3	2.01	0.43
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	2.01	0.43
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	2.00	0.43
2:B:919:ASN:O	2:B:923:GLN:N	2.52	0.42
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	2.01	0.42
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	2.01	0.42
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.01	0.42
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.44	0.42
2:I:790:ARG:HG2	2:I:1627:ALA:HA	2.01	0.42
2:I:2758:PHE:O	2:I:2762:THR:N	2.46	0.42
2:E:1708:ARG:HG2	2:E:1711:TYR:CD2	2.54	0.42
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.01	0.42
2:E:4563:ARG:NH1	2:E:4815:ASP:OD1	2.52	0.42
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.99	0.42
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.54	0.42
2:B:4071:ILE:HG13	2:B:4103:PHE:HZ	1.84	0.42
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	2.01	0.42
2:I:1966:VAL:HA	2:I:1969:LEU:HB3	2.01	0.42
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	2.01	0.42
2:E:649:PHE:HB3	2:E:776:LEU:HD13	2.01	0.42
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.00	0.42
2:E:4198:SER:OG	2:E:4199:GLU:N	2.52	0.42
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.29	0.42
2:B:914:PRO:HD2	2:B:917:GLU:HB2	2.00	0.42
2:G:20:VAL:HG12	2:G:204:PRO:HA	2.01	0.42
2:G:919:ASN:O	2:G:923:GLN:N	2.52	0.42
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.85	0.42
2:G:4071:ILE:HG13	2:G:4103:PHE:HZ	1.84	0.42
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.27	0.42
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.84	0.42
2:I:919:ASN:O	2:I:923:GLN:N	2.52	0.42
2:I:2775:TRP:HZ3	2:I:2783:GLU:HA	1.84	0.42
2:I:3754:GLU:HG3	2:I:4718:LYS:HD2	2.01	0.42
2:E:2144:ILE:H	2:E:2144:ILE:HG13	1.79	0.42
2:E:2742:THR:OG1	2:E:2811:GLU:OE1	2.34	0.42
2:E:3754:GLU:HG3	2:E:4718:LYS:HD2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:ASN:HA	2:B:492:ASP:HB2	2.01	0.42
2:B:649:PHE:HB3	2:B:776:LEU:HD13	2.02	0.42
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.93	0.42
2:B:4051:SER:OG	2:B:4054:ASN:OD1	2.37	0.42
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.00	0.42
2:G:4051:SER:OG	2:G:4054:ASN:OD1	2.37	0.42
2:I:20:VAL:HG12	2:I:204:PRO:HA	2.01	0.42
2:I:889:GLN:O	2:I:902:ARG:NH1	2.52	0.42
2:I:914:PRO:HD2	2:I:917:GLU:HB2	2.00	0.42
2:I:4051:SER:OG	2:I:4054:ASN:OD1	2.37	0.42
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.47	0.42
2:E:2440:MET:O	2:E:2444:GLN:N	2.51	0.42
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.54	0.42
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.85	0.42
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.52	0.42
2:G:649:PHE:HB3	2:G:776:LEU:HD13	2.01	0.42
2:I:649:PHE:HB3	2:I:776:LEU:HD13	2.01	0.42
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.54	0.42
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.84	0.42
2:E:1695:LEU:HB3	2:E:1810:LYS:HZ2	1.83	0.42
2:E:2776:SER:O	2:E:2788:HIS:N	2.52	0.42
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.52	0.42
2:E:4071:ILE:HG13	2:E:4103:PHE:HZ	1.84	0.42
1:H:34:LYS:HE3	2:G:634:GLN:HB3	2.02	0.42
2:B:790:ARG:HG2	2:B:1627:ALA:HA	2.01	0.42
2:B:3754:GLU:HG3	2:B:4718:LYS:HD2	2.01	0.42
2:B:4586:PRO:HB3	2:B:4628:VAL:HG21	2.01	0.42
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.84	0.42
2:G:645:ARG:N	2:G:824:GLU:O	2.42	0.42
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.93	0.42
2:E:280:LEU:HD21	2:E:316:PHE:HE2	1.85	0.42
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.01	0.42
2:B:2215:LEU:HD23	2:B:2260:ASN:HB3	2.02	0.42
2:B:2775:TRP:HZ3	2:B:2783:GLU:HA	1.84	0.42
2:B:4198:SER:OG	2:B:4199:GLU:N	2.52	0.42
2:B:4708:THR:HA	2:B:4709:PRO:HD3	1.94	0.42
2:G:489:ASN:HA	2:G:492:ASP:HB2	2.01	0.42
2:G:2012:PHE:CG	2:G:2022:PRO:HD3	2.55	0.42
2:G:2776:SER:O	2:G:2788:HIS:N	2.52	0.42
2:I:181:HIS:CE1	2:I:195:PHE:HB2	2.55	0.42
2:E:181:HIS:CE1	2:E:195:PHE:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.00	0.42
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.93	0.42
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	2.01	0.42
2:B:181:HIS:CE1	2:B:195:PHE:HB2	2.55	0.42
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.55	0.42
2:I:1708:ARG:HG2	2:I:1711:TYR:CD2	2.54	0.42
2:I:3842:LEU:O	2:I:3929:SER:OG	2.38	0.42
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	2.02	0.42
2:E:20:VAL:HG12	2:E:204:PRO:HA	2.01	0.42
2:E:788:LYS:HG2	2:E:1629:GLN:HA	2.02	0.42
2:E:2012:PHE:CG	2:E:2022:PRO:HD3	2.55	0.42
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.55	0.42
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.02	0.42
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.55	0.42
2:B:3842:LEU:O	2:B:3929:SER:OG	2.38	0.42
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.02	0.42
2:G:870:ILE:HD12	2:G:873:LYS:HB2	2.01	0.42
2:G:1708:ARG:HG2	2:G:1711:TYR:CD2	2.54	0.42
2:G:3754:GLU:HG3	2:G:4718:LYS:HD2	2.01	0.42
2:G:3842:LEU:O	2:G:3929:SER:OG	2.38	0.42
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.52	0.42
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.85	0.42
2:I:4586:PRO:HB3	2:I:4628:VAL:HG21	2.01	0.42
1:F:25:HIS:HB3	1:F:40:ARG:HD3	2.02	0.42
1:F:87:HIS:H	1:F:91:ILE:HB	1.85	0.42
2:B:20:VAL:HG12	2:B:204:PRO:HA	2.01	0.42
2:B:1189:LEU:HD12	2:B:1190:PRO:HD2	2.02	0.42
2:B:2950:UNK:O	2:B:2954:UNK:N	2.53	0.42
2:B:4804:TYR:HB3	2:B:4806:ASN:HD22	1.85	0.42
2:G:243:ARG:NH1	2:G:301:VAL:O	2.49	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.85	0.42
2:G:3759:GLU:HA	2:G:3762:ARG:HB2	2.02	0.42
2:I:870:ILE:HD12	2:I:873:LYS:HB2	2.01	0.42
2:I:2012:PHE:CG	2:I:2022:PRO:HD3	2.55	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.42
2:E:2215:LEU:HD23	2:E:2260:ASN:HB3	2.02	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:E:4708:THR:HA	2:E:4709:PRO:HD3	1.94	0.42
1:H:25:HIS:HB3	1:H:40:ARG:HD3	2.02	0.41
1:J:25:HIS:HB3	1:J:40:ARG:HD3	2.02	0.41
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1132:TRP:HE1	2:B:1136:SER:HG	1.68	0.41
2:B:1284:UNK:HA	2:B:1463:UNK:HA	2.02	0.41
2:G:181:HIS:CE1	2:G:195:PHE:HB2	2.55	0.41
2:G:788:LYS:HG2	2:G:1629:GLN:HA	2.02	0.41
2:G:2185:ILE:HA	2:G:2188:ASN:ND2	2.35	0.41
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.01	0.41
2:G:2950:UNK:O	2:G:2954:UNK:N	2.53	0.41
2:E:3759:GLU:HA	2:E:3762:ARG:HB2	2.02	0.41
2:E:4960:ILE:HD13	2:E:4960:ILE:HA	1.83	0.41
1:H:87:HIS:H	1:H:91:ILE:HB	1.85	0.41
2:B:3365:UNK:O	2:B:3369:UNK:N	2.53	0.41
2:B:4231:MET:CE	2:B:4960:ILE:HD12	2.51	0.41
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.41
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.02	0.41
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	2.01	0.41
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.01	0.41
2:E:278:GLN:N	2:E:315:CYS:SG	2.90	0.41
2:E:489:ASN:HA	2:E:492:ASP:HB2	2.01	0.41
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	2.02	0.41
2:B:4735:GLU:HA	2:B:4738:ALA:HB3	2.02	0.41
2:G:4231:MET:CE	2:G:4960:ILE:HD12	2.50	0.41
2:I:2742:THR:OG1	2:I:2811:GLU:OE1	2.34	0.41
2:I:2950:UNK:O	2:I:2954:UNK:N	2.53	0.41
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.01	0.41
2:E:2185:ILE:HA	2:E:2188:ASN:HD21	1.85	0.41
2:B:2776:SER:O	2:B:2788:HIS:N	2.52	0.41
2:G:164:ARG:N	2:G:167:ASP:OD2	2.43	0.41
2:G:173:SER:HB3	2:G:178:ARG:H	1.85	0.41
2:G:280:LEU:HD21	2:G:316:PHE:HE2	1.85	0.41
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	2.03	0.41
2:G:5004:THR:H	2:G:5007:GLU:HB2	1.86	0.41
2:I:173:SER:HB3	2:I:178:ARG:H	1.85	0.41
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.93	0.41
2:I:2185:ILE:HA	2:I:2188:ASN:ND2	2.35	0.41
2:I:3759:GLU:HA	2:I:3762:ARG:HB2	2.02	0.41
2:E:173:SER:OG	2:E:174:VAL:N	2.54	0.41
2:E:2950:UNK:O	2:E:2954:UNK:N	2.53	0.41
2:E:4804:TYR:HB3	2:E:4806:ASN:HD22	1.85	0.41
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	2.03	0.41
2:B:3759:GLU:O	2:B:3763:LEU:N	2.48	0.41
2:B:5004:THR:H	2:B:5007:GLU:HB2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:280:LEU:HD21	2:I:316:PHE:HE2	1.85	0.41
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.44	0.41
2:I:1189:LEU:HD12	2:I:1190:PRO:HD2	2.02	0.41
2:I:2215:LEU:HD23	2:I:2260:ASN:HB3	2.02	0.41
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.84	0.41
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.55	0.41
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	2.03	0.41
2:I:4804:TYR:HB3	2:I:4806:ASN:HD22	1.85	0.41
2:I:4928:LEU:HD13	2:I:4928:LEU:HA	1.91	0.41
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.52	0.41
2:B:173:SER:HB3	2:B:178:ARG:H	1.85	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CD2	2.54	0.41
2:B:4697:VAL:O	2:B:4701:TRP:N	2.52	0.41
2:B:4914:VAL:HG23	2:E:4888:TYR:CD1	2.55	0.41
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	2.01	0.41
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.41
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.52	0.41
2:I:4231:MET:CE	2:I:4960:ILE:HD12	2.51	0.41
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	2.03	0.41
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.84	0.41
2:E:3842:LEU:O	2:E:3929:SER:OG	2.38	0.41
2:E:4231:MET:CE	2:E:4960:ILE:HD12	2.51	0.41
1:F:92:PRO:HD3	2:E:627:PRO:HB2	2.02	0.41
2:B:173:SER:OG	2:B:174:VAL:N	2.54	0.41
2:B:788:LYS:HG2	2:B:1629:GLN:HA	2.02	0.41
2:G:911:HIS:O	2:G:918:ARG:NH2	2.48	0.41
2:I:2185:ILE:HA	2:I:2188:ASN:HD21	1.85	0.41
2:I:2776:SER:O	2:I:2788:HIS:N	2.52	0.41
2:I:3361:UNK:O	2:I:3365:UNK:N	2.54	0.41
2:E:2437:ALA:HA	2:E:2438:PRO:HD3	1.94	0.41
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.02	0.41
2:B:1817:GLU:O	2:B:1821:ASP:N	2.50	0.41
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.84	0.41
2:G:1189:LEU:HD12	2:G:1190:PRO:HD2	2.02	0.41
2:G:2039:LEU:HA	2:G:2042:CYS:HB3	2.03	0.41
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	2.02	0.41
2:G:3361:UNK:O	2:G:3365:UNK:N	2.54	0.41
2:G:4060:LYS:NZ	2:G:4064:MET:SD	2.94	0.41
2:I:173:SER:OG	2:I:174:VAL:N	2.54	0.41
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.85	0.41
1:A:25:HIS:HB3	1:A:40:ARG:HD3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:H	1:A:91:ILE:HB	1.85	0.41
1:J:87:HIS:H	1:J:91:ILE:HB	1.85	0.41
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.03	0.41
2:B:2039:LEU:HA	2:B:2042:CYS:HB3	2.03	0.41
2:B:2185:ILE:HA	2:B:2188:ASN:HD21	1.85	0.41
2:B:3361:UNK:O	2:B:3365:UNK:N	2.54	0.41
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	2.02	0.41
2:G:173:SER:OG	2:G:174:VAL:N	2.54	0.41
2:G:1284:UNK:HA	2:G:1463:UNK:HA	2.02	0.41
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.03	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.93	0.41
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	2.03	0.41
2:I:489:ASN:HA	2:I:492:ASP:HB2	2.01	0.41
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	2.03	0.41
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.54	0.41
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	2.02	0.41
2:I:3676:ASP:N	2:I:3676:ASP:OD1	2.52	0.41
2:I:4060:LYS:NZ	2:I:4064:MET:SD	2.94	0.41
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	2.03	0.41
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.30	0.41
2:I:4735:GLU:HA	2:I:4738:ALA:HB3	2.02	0.41
2:E:2129:ASP:O	2:E:2133:GLU:N	2.49	0.41
2:E:4051:SER:OG	2:E:4054:ASN:OD1	2.37	0.41
2:E:4060:LYS:NZ	2:E:4064:MET:SD	2.94	0.41
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	2.02	0.41
2:E:4697:VAL:O	2:E:4701:TRP:N	2.52	0.41
2:E:5004:THR:H	2:E:5007:GLU:HB2	1.86	0.41
2:B:2012:PHE:CG	2:B:2022:PRO:HD3	2.55	0.41
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	2.02	0.41
2:B:3677:LEU:O	2:B:3698:LEU:N	2.54	0.41
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	2.03	0.41
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	2.03	0.41
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.02	0.41
2:G:2185:ILE:HA	2:G:2188:ASN:HD21	1.85	0.41
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	2.02	0.41
2:I:788:LYS:HG2	2:I:1629:GLN:HA	2.02	0.41
2:I:2144:ILE:H	2:I:2144:ILE:HG13	1.79	0.41
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.54	0.41
1:A:34:LYS:HD3	2:B:629:ARG:HD2	2.03	0.40
2:B:280:LEU:HD21	2:B:316:PHE:HE2	1.85	0.40
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.87	0.40
2:G:866:HIS:O	2:G:1051:TYR:OH	2.28	0.40
2:G:2215:LEU:HD23	2:G:2260:ASN:HB3	2.02	0.40
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.40
2:E:911:HIS:O	2:E:918:ARG:NH2	2.48	0.40
2:E:1189:LEU:HD12	2:E:1190:PRO:HD2	2.02	0.40
2:E:3658:LYS:HA	2:E:3661:TRP:CE2	2.56	0.40
2:E:4735:GLU:HA	2:E:4738:ALA:HB3	2.02	0.40
2:B:3658:LYS:HA	2:B:3661:TRP:CE2	2.56	0.40
2:G:907:LEU:O	2:G:963:ASN:ND2	2.42	0.40
2:I:1284:UNK:HA	2:I:1463:UNK:HA	2.02	0.40
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.02	0.40
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.87	0.40
2:E:164:ARG:N	2:E:167:ASP:OD2	2.43	0.40
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.02	0.40
2:E:495:ASN:HD21	2:E:550:LYS:HE3	1.87	0.40
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	2.03	0.40
1:H:55:VAL:HA	2:G:1784:ALA:HA	2.04	0.40
2:B:3694:LYS:HA	2:B:3695:PRO:HD3	1.93	0.40
2:B:3847:PHE:HA	2:B:3850:GLN:HG2	2.04	0.40
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.55	0.40
2:G:4735:GLU:HA	2:G:4738:ALA:HB3	2.02	0.40
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.03	0.40
2:E:2185:ILE:HA	2:E:2188:ASN:ND2	2.35	0.40
2:E:3361:UNK:O	2:E:3365:UNK:N	2.54	0.40
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.55	0.40
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	2.04	0.40
2:B:2185:ILE:HA	2:B:2188:ASN:ND2	2.35	0.40
2:B:3759:GLU:HA	2:B:3762:ARG:HB2	2.02	0.40
2:G:3676:ASP:N	2:G:3676:ASP:OD1	2.52	0.40
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.40	0.40
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.03	0.40
2:I:5004:THR:H	2:I:5007:GLU:HB2	1.86	0.40
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.04	0.40
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.02	0.40
2:E:3847:PHE:HA	2:E:3850:GLN:HG2	2.04	0.40
2:B:2467:VAL:HA	2:B:2470:ILE:HD12	2.03	0.40
2:B:4060:LYS:NZ	2:B:4064:MET:SD	2.94	0.40
2:G:4804:TYR:HB3	2:G:4806:ASN:HD22	1.85	0.40
2:I:645:ARG:N	2:I:824:GLU:O	2.42	0.40
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:621:ILE:O	2:E:625:LEU:N	2.52	0.40
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	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	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2892 (89%)	337 (10%)	6 (0%)	44	78
2	E	3235/4416 (73%)	2894 (90%)	335 (10%)	6 (0%)	44	78
2	G	3235/4416 (73%)	2895 (90%)	334 (10%)	6 (0%)	44	78
2	I	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	44	78
All	All	13360/18096 (74%)	11944 (89%)	1392 (10%)	24 (0%)	45	78

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	E	4985	LEU
2	B	1840	PRO
2	B	4985	LEU
2	G	1840	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	4985	LEU
2	I	1840	PRO
2	I	4985	LEU
2	E	1840	PRO
2	B	1932	PRO
2	B	2291	GLN
2	B	4641	PRO
2	G	1932	PRO
2	G	2291	GLN
2	G	4641	PRO
2	I	1932	PRO
2	I	2291	GLN
2	I	4641	PRO
2	E	1932	PRO
2	E	2291	GLN
2	E	4641	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	88/89 (99%)	88 (100%)	0	100 100
1	F	88/89 (99%)	88 (100%)	0	100 100
1	H	88/89 (99%)	88 (100%)	0	100 100
1	J	88/89 (99%)	88 (100%)	0	100 100
2	B	2493/3022 (82%)	2474 (99%)	19 (1%)	79 84
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	79 84
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	79 84
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	79 84
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	80 87

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

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3663	LEU
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4959	PHE
2	B	4960	ILE
2	B	4961	CYS
2	B	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3663	LEU
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4959	PHE
2	G	4960	ILE
2	G	4961	CYS
2	G	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3663	LEU
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4959	PHE
2	I	4960	ILE
2	I	4961	CYS
2	I	4983	HIS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3663	LEU
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4959	PHE
2	E	4960	ILE
2	E	4961	CYS
2	E	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	71	GLN
2	B	113	HIS
2	B	224	HIS
2	B	379	HIS
2	B	383	HIS
2	B	413	GLN
2	B	479	GLN
2	B	797	HIS
2	B	921	ASN
2	B	1041	GLN
2	B	1598	GLN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	2041	HIS
2	B	2127	GLN
2	B	2291	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	3994	HIS
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4142	ASN
2	B	4209	GLN
2	B	4806	ASN
2	G	57	ASN
2	G	71	GLN
2	G	111	HIS
2	G	113	HIS
2	G	224	HIS
2	G	379	HIS
2	G	383	HIS
2	G	413	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	479	GLN
2	G	797	HIS
2	G	921	ASN
2	G	1041	GLN
2	G	1598	GLN
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	1973	GLN
2	G	2041	HIS
2	G	2127	GLN
2	G	2291	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	3994	HIS
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4142	ASN
2	G	4209	GLN
2	G	4806	ASN
2	I	57	ASN
2	I	71	GLN
2	I	111	HIS
2	I	113	HIS
2	I	224	HIS
2	I	379	HIS
2	I	383	HIS
2	I	413	GLN
2	I	479	GLN
2	I	797	HIS
2	I	921	ASN
2	I	1041	GLN
2	I	1158	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1598	GLN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	2041	HIS
2	I	2127	GLN
2	I	2291	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	3994	HIS
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4209	GLN
2	I	4806	ASN
2	E	57	ASN
2	E	71	GLN
2	E	111	HIS
2	E	113	HIS
2	E	224	HIS
2	E	379	HIS
2	E	383	HIS
2	E	413	GLN
2	E	479	GLN
2	E	797	HIS
2	E	921	ASN
2	E	1041	GLN
2	E	1598	GLN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1760	HIS
2	E	1775	HIS
2	E	2041	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	2127	GLN
2	E	2291	GLN
2	E	3809	ASN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	3994	HIS
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4130	ASN
2	E	4142	ASN
2	E	4209	GLN
2	E	4806	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	G	14
2	I	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.85
1	G	4345:UNK	C	4540:PHE	N	73.85
1	I	4345:UNK	C	4540:PHE	N	73.85
1	E	4345:UNK	C	4540:PHE	N	73.85
1	B	3613:UNK	C	3639:THR	N	45.57
1	G	3613:UNK	C	3639:THR	N	45.57
1	I	3613:UNK	C	3639:THR	N	45.57
1	E	3613:UNK	C	3639:THR	N	45.57
1	B	4253:GLU	C	4320:UNK	N	29.50
1	G	4253:GLU	C	4320:UNK	N	29.50
1	I	4253:GLU	C	4320:UNK	N	29.50
1	E	4253:GLU	C	4320:UNK	N	29.50
1	B	3163:UNK	C	3170:UNK	N	15.85
1	G	3163:UNK	C	3170:UNK	N	15.85
1	I	3163:UNK	C	3170:UNK	N	15.85
1	E	3163:UNK	C	3170:UNK	N	15.85
1	B	3063:UNK	C	3134:UNK	N	15.15
1	G	3063:UNK	C	3134:UNK	N	15.15
1	I	3063:UNK	C	3134:UNK	N	15.15
1	E	3063:UNK	C	3134:UNK	N	15.15
1	B	3468:UNK	C	3511:UNK	N	14.46
1	G	3468:UNK	C	3511:UNK	N	14.46
1	I	3468:UNK	C	3511:UNK	N	14.46
1	E	3468:UNK	C	3511:UNK	N	14.46

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2703:UNK	C	2734:ASN	N	13.26
1	G	2703:UNK	C	2734:ASN	N	13.26
1	I	2703:UNK	C	2734:ASN	N	13.26
1	E	2703:UNK	C	2734:ASN	N	13.26
1	B	3236:UNK	C	3241:UNK	N	13.11
1	G	3236:UNK	C	3241:UNK	N	13.11
1	I	3236:UNK	C	3241:UNK	N	13.11
1	E	3236:UNK	C	3241:UNK	N	13.11
1	B	1564:UNK	C	1573:MET	N	12.51
1	G	1564:UNK	C	1573:MET	N	12.51
1	I	1564:UNK	C	1573:MET	N	12.51
1	E	1564:UNK	C	1573:MET	N	12.51
1	B	2976:UNK	C	2995:UNK	N	12.28
1	G	2976:UNK	C	2995:UNK	N	12.28
1	I	2976:UNK	C	2995:UNK	N	12.28
1	E	2976:UNK	C	2995:UNK	N	12.28
1	B	3254:UNK	C	3261:UNK	N	8.55
1	G	3254:UNK	C	3261:UNK	N	8.55
1	I	3254:UNK	C	3261:UNK	N	8.55
1	E	3254:UNK	C	3261:UNK	N	8.55
1	B	1297:UNK	C	1430:UNK	N	5.58
1	G	1297:UNK	C	1430:UNK	N	5.58
1	I	1297:UNK	C	1430:UNK	N	5.58
1	E	1297:UNK	C	1430:UNK	N	5.58
1	B	2479:LEU	C	2487:UNK	N	3.51
1	G	2479:LEU	C	2487:UNK	N	3.51
1	I	2479:LEU	C	2487:UNK	N	3.51
1	E	2479:LEU	C	2487:UNK	N	3.51
1	B	2939:ARG	C	2942:UNK	N	3.39
1	G	2939:ARG	C	2942:UNK	N	3.39
1	I	2939:ARG	C	2942:UNK	N	3.39
1	E	2939:ARG	C	2942:UNK	N	3.39

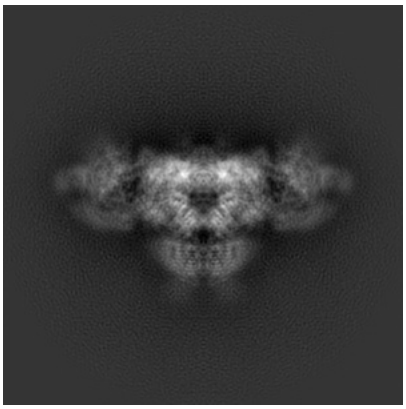
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8389. These allow visual inspection of the internal detail of the map and identification of artifacts.

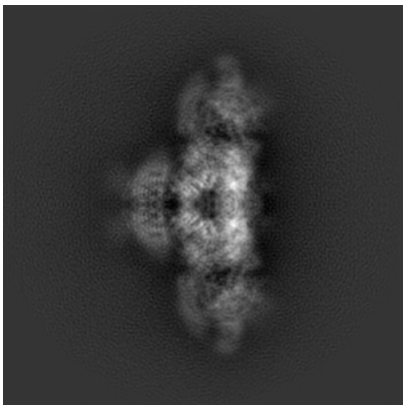
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

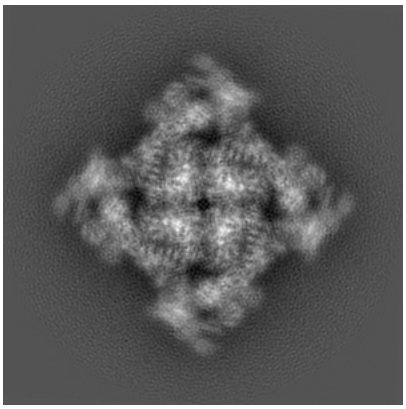
6.1.1 Primary map



X

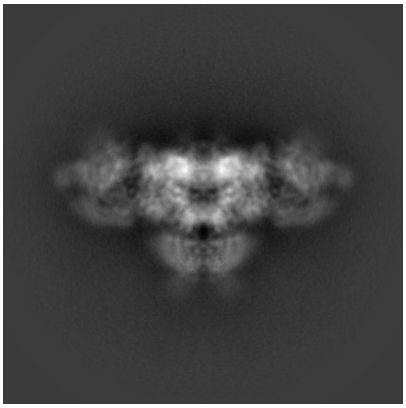


Y

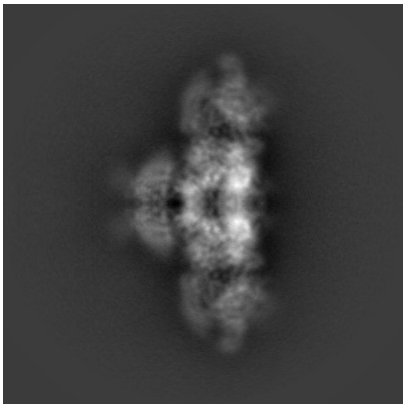


Z

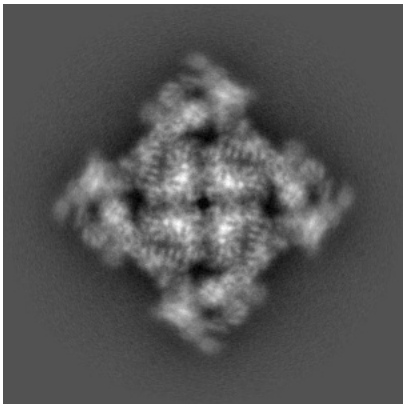
6.1.2 Raw map



X



Y

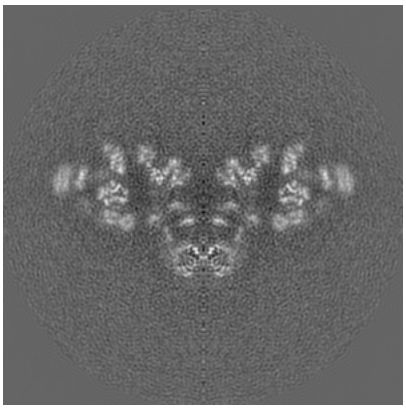


Z

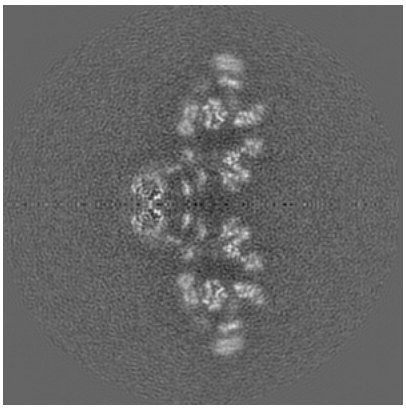
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

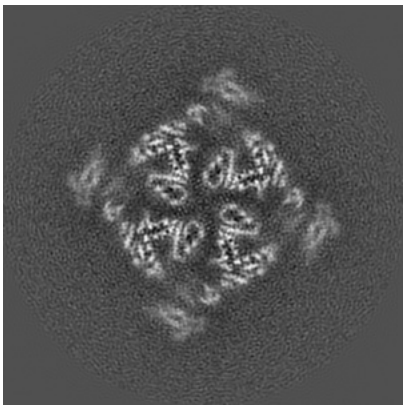
6.2.1 Primary map



X Index: 200

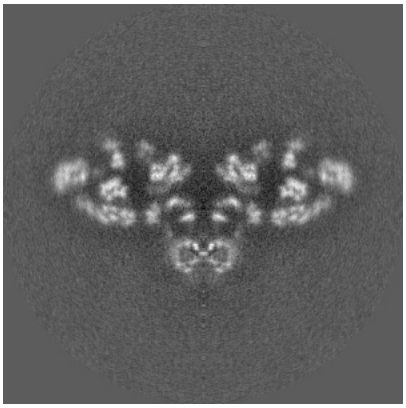


Y Index: 200

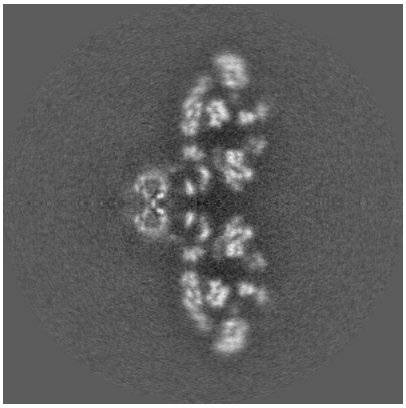


Z Index: 200

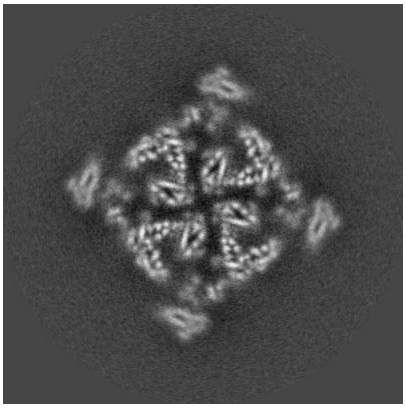
6.2.2 Raw map



X Index: 200



Y Index: 200

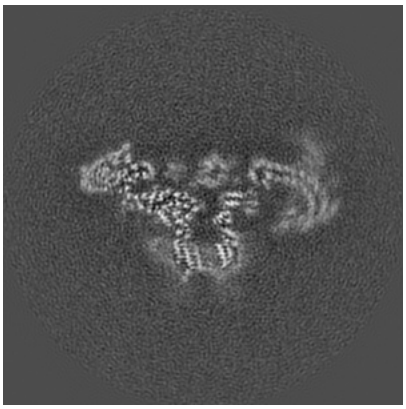


Z Index: 200

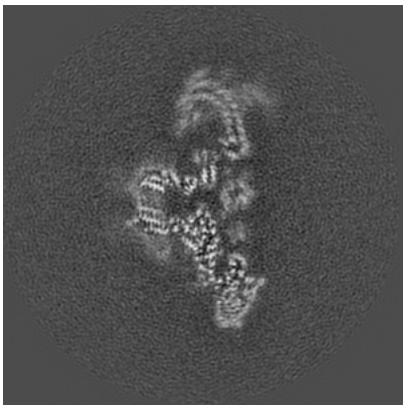
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

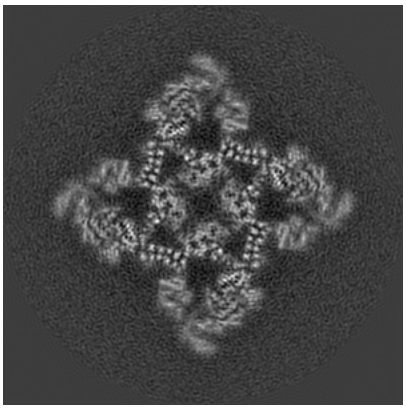
6.3.1 Primary map



X Index: 225

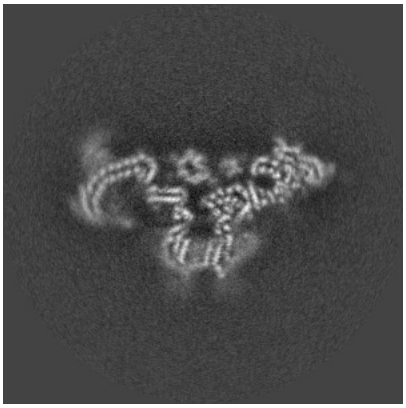


Y Index: 175

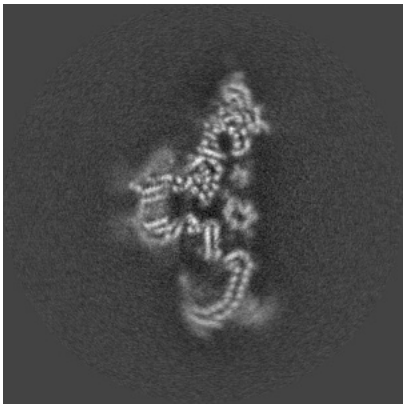


Z Index: 226

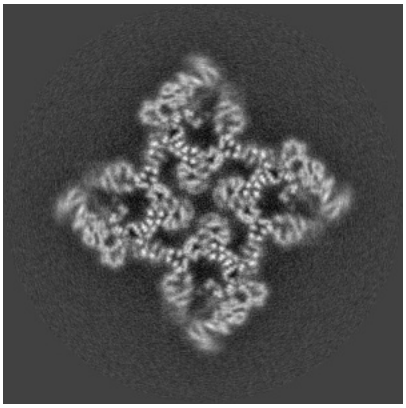
6.3.2 Raw map



X Index: 175



Y Index: 225

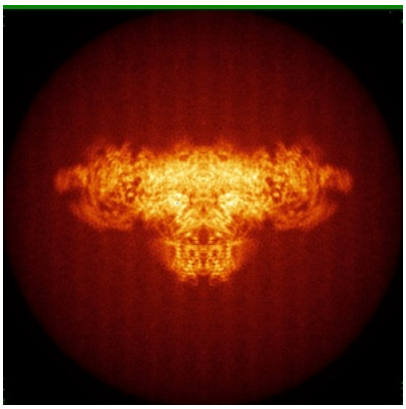


Z Index: 234

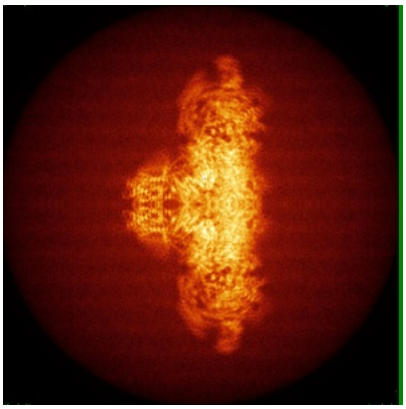
The images above show the largest variance slices of the map in three orthogonal directions.

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

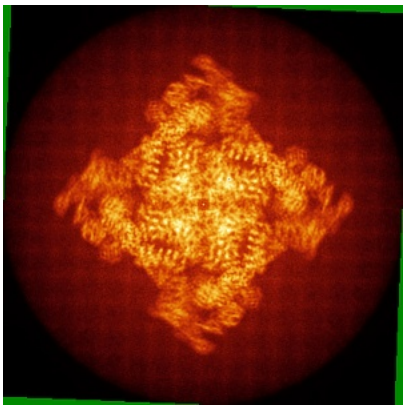
6.4.1 Primary map



X

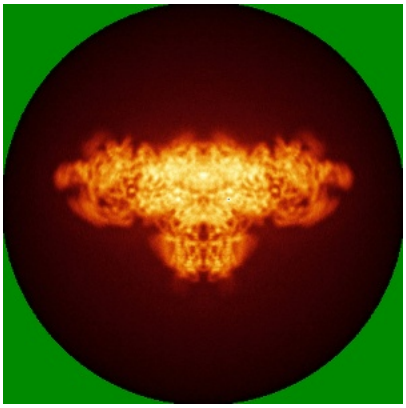


Y

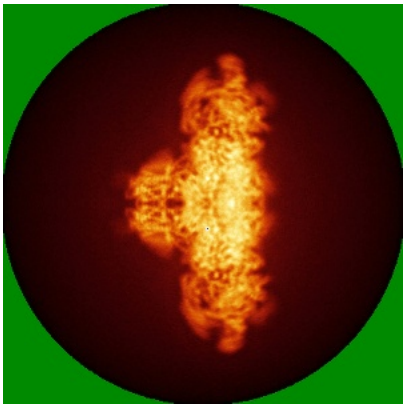


Z

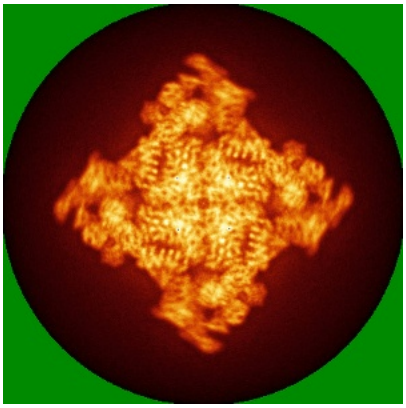
6.4.2 Raw map



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 0.04. 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.

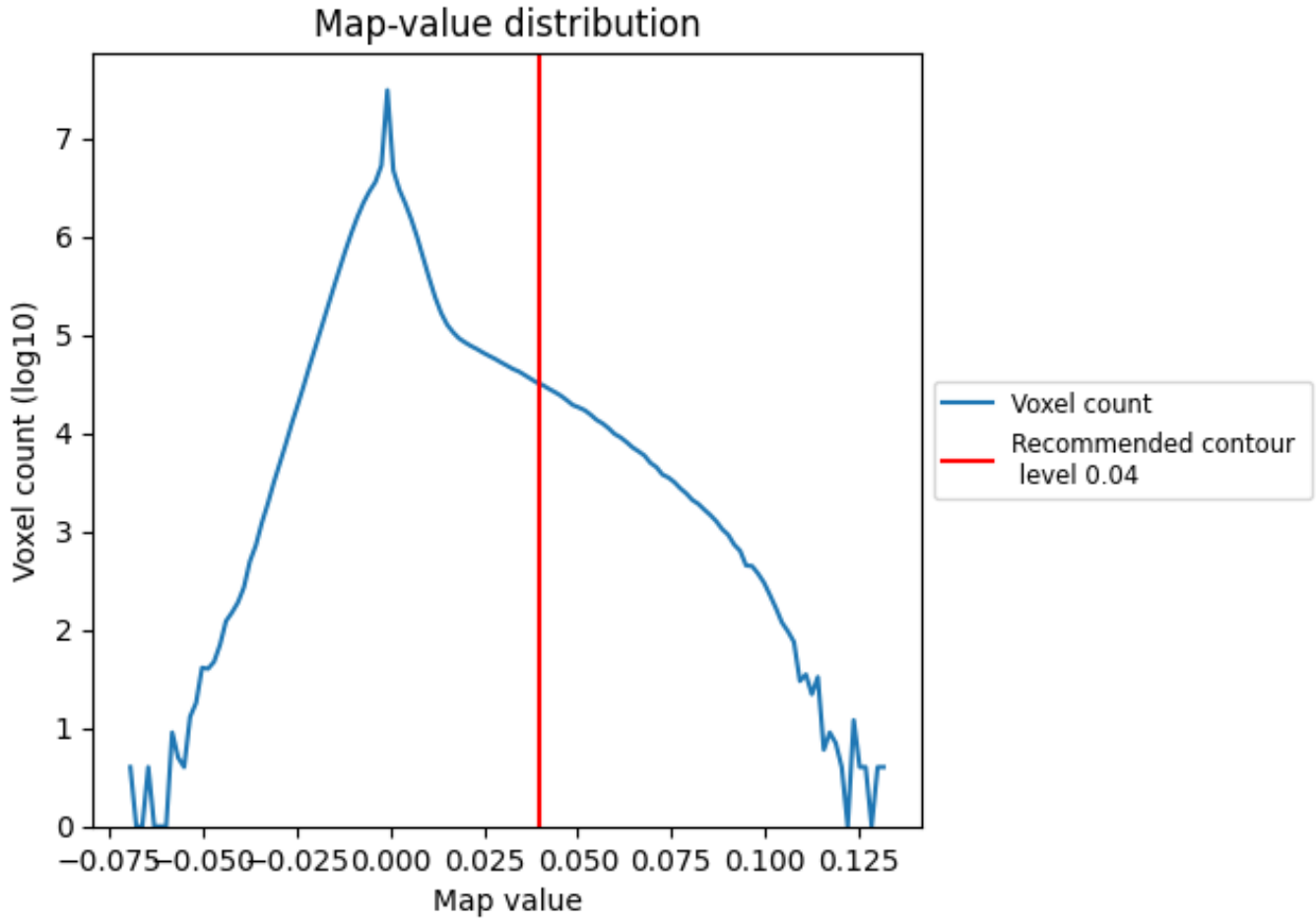
6.6 Mask visualisation (i)

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

7 Map analysis

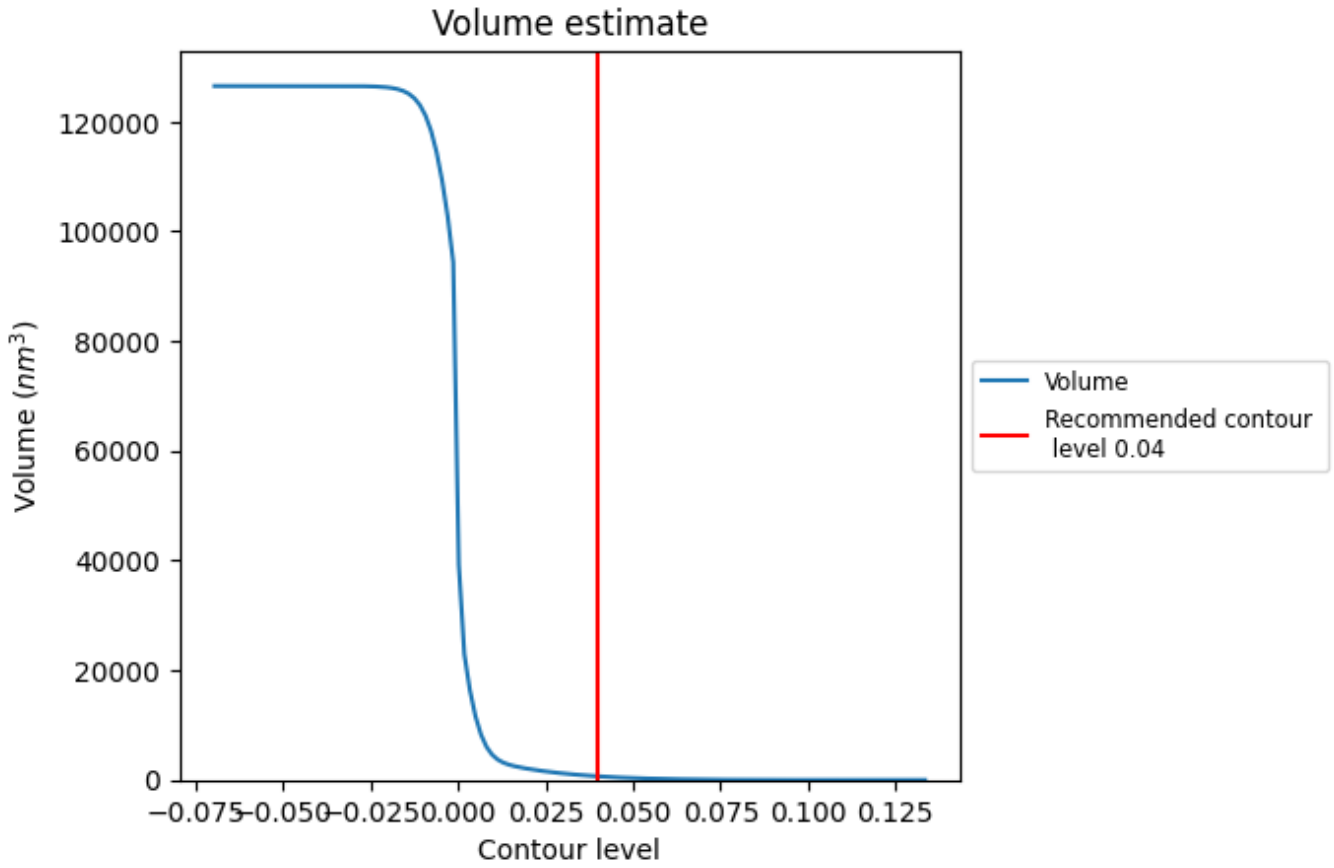
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

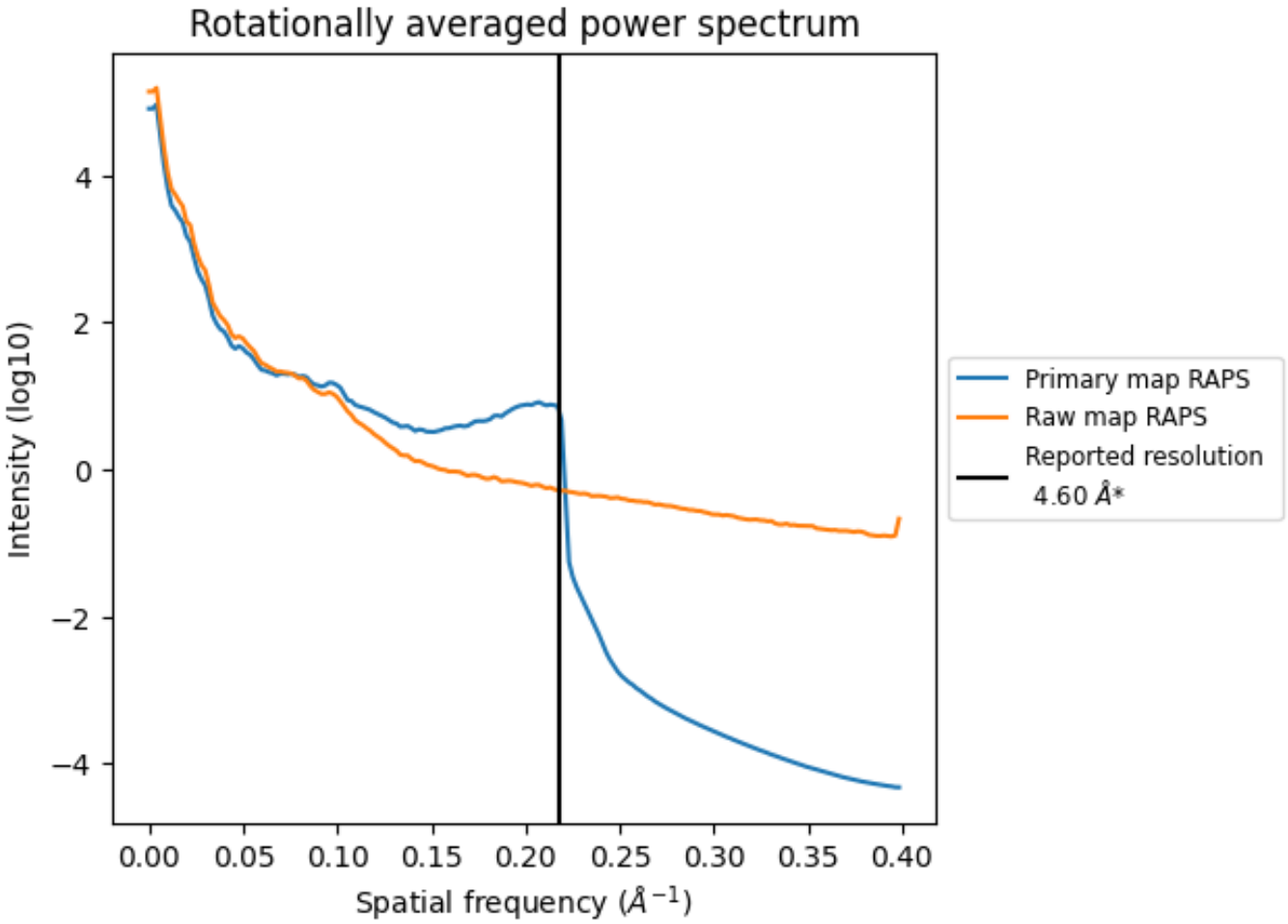
7.2 Volume estimate



The volume at the recommended contour level is 666 nm^3; this corresponds to an approximate mass of 601 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)

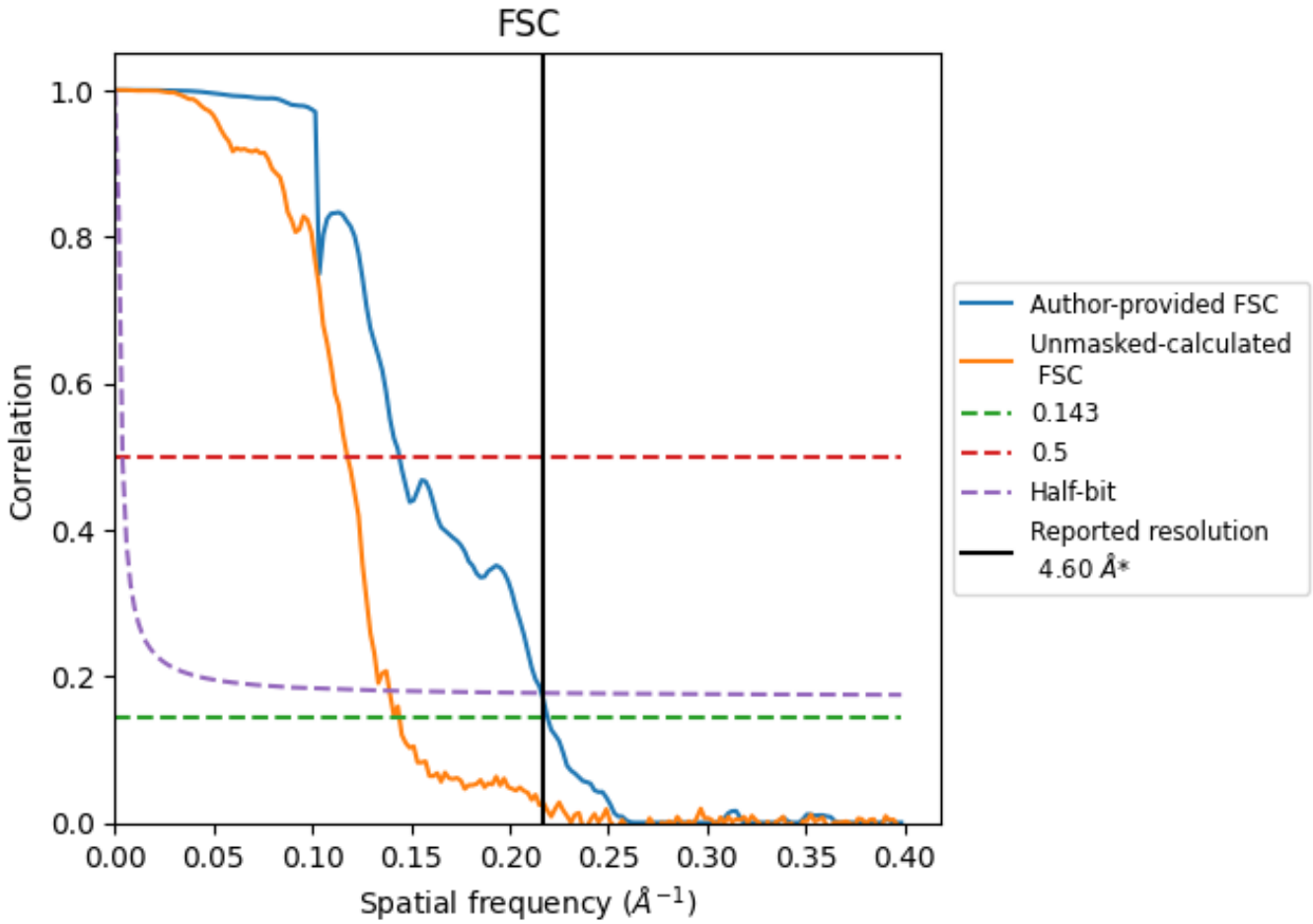


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8.2 Resolution estimates (i)

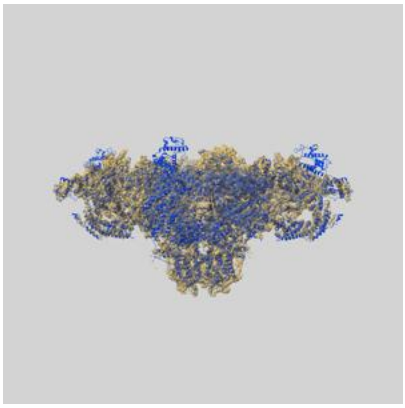
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.56	6.94	4.63
Unmasked-calculated*	6.93	8.49	7.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.93 differs from the reported value 4.6 by more than 10 %

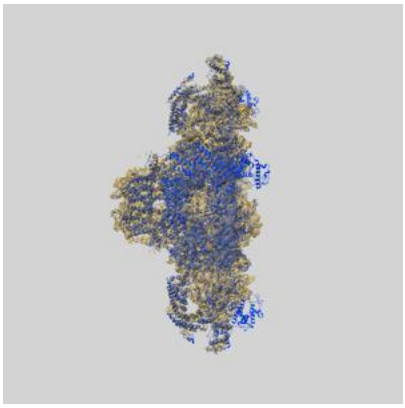
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8389 and PDB model 5TAY. Per-residue inclusion information can be found in section 3 on page 5.

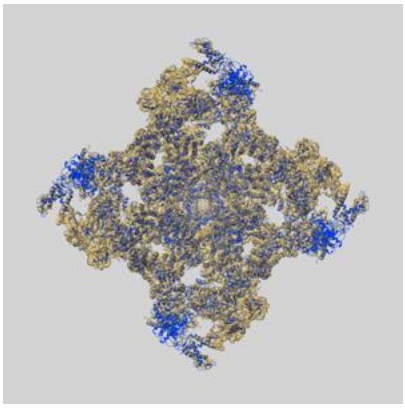
9.1 Map-model overlay



X



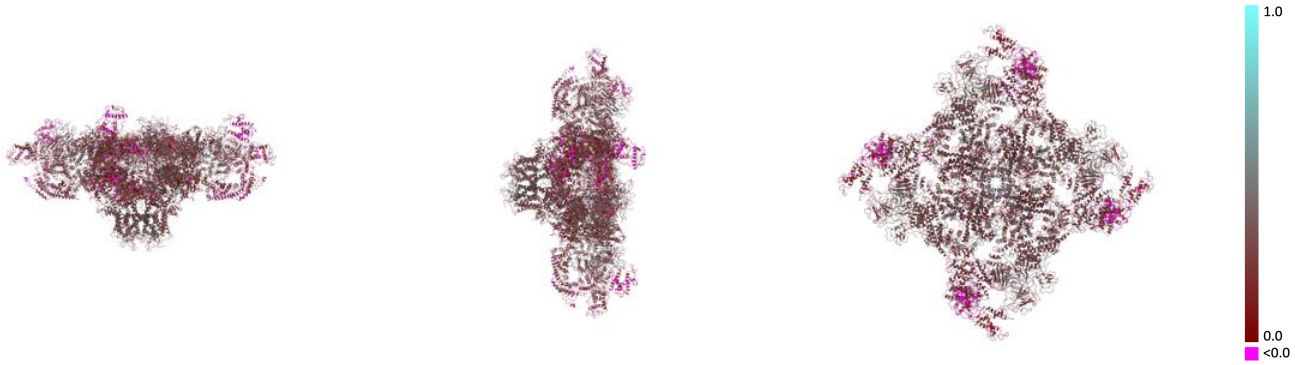
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

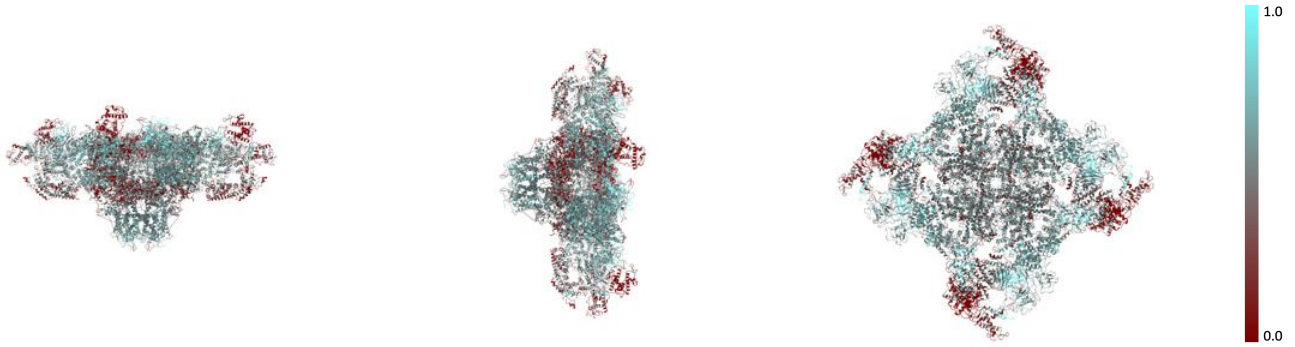
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

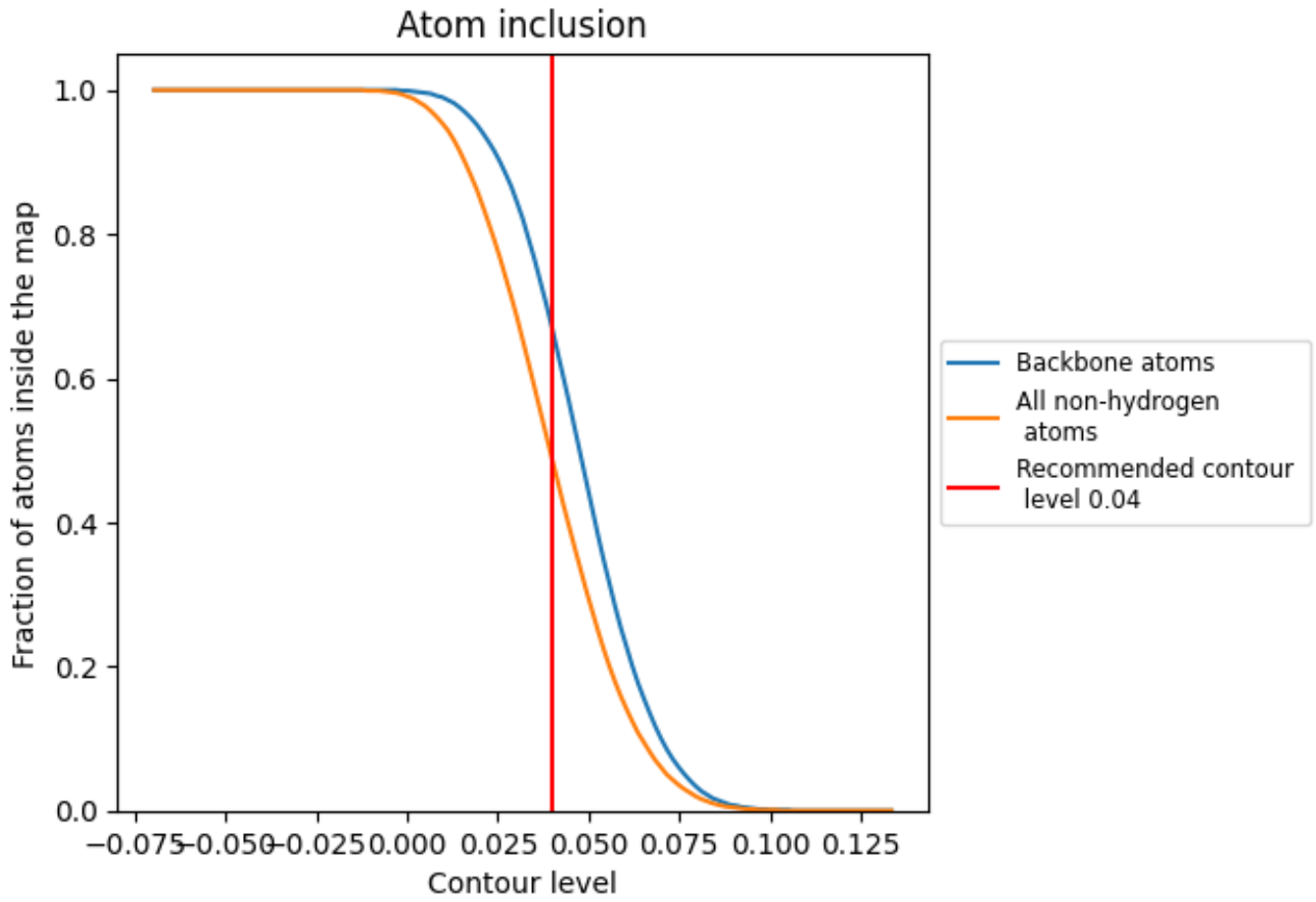
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4870	0.2640
A	0.5660	0.3270
B	0.4910	0.2670
E	0.4800	0.2570
F	0.5670	0.3310
G	0.4890	0.2650
H	0.5670	0.3300
I	0.4810	0.2590
J	0.5650	0.3280