Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 10:51 PM EST

PDB ID	:	7TDI
EMDB ID	:	EMD-25830
Title	:	Rabbit RyR1 with AMP-PCP and high Ca2+ embedded in nanodisc in closed-inactivated conformation class 2 (Dataset-A)
Authors	:	Nayak, A.R.; Samso, M.
Deposited on	:	2021-12-31
Resolution	:	3.30 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:

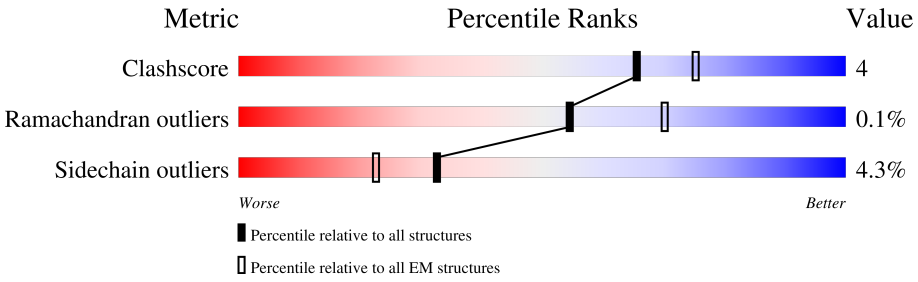
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	5037	20% 73% 9% 18%
1	B	5037	18% 73% 9% 18%
1	C	5037	19% 73% 8% 18%
1	D	5037	18% 73% 8% • 18%

2 Entry composition

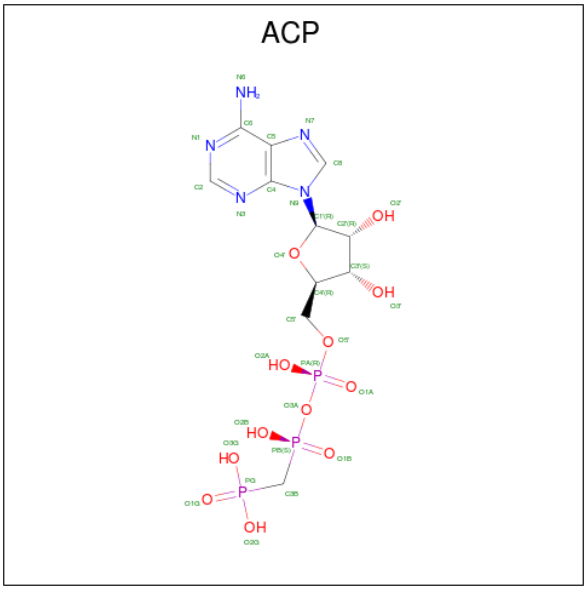
There are 4 unique types of molecules in this entry. The entry contains 117132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1,Ryanodine receptor 1,RyR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	4134	Total	C	N	O	S	0	0
			29249	18516	5181	5395	157		
1	C	4134	Total	C	N	O	S	0	0
			29249	18516	5181	5395	157		
1	D	4134	Total	C	N	O	S	0	0
			29249	18516	5181	5395	157		
1	A	4134	Total	C	N	O	S	0	0
			29249	18516	5181	5395	157		

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	C	1	Total	C	N	O	P	0
			31	11	5	12	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	A	1	Total	C	N	O	P	0
			31	11	5	12	3	

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

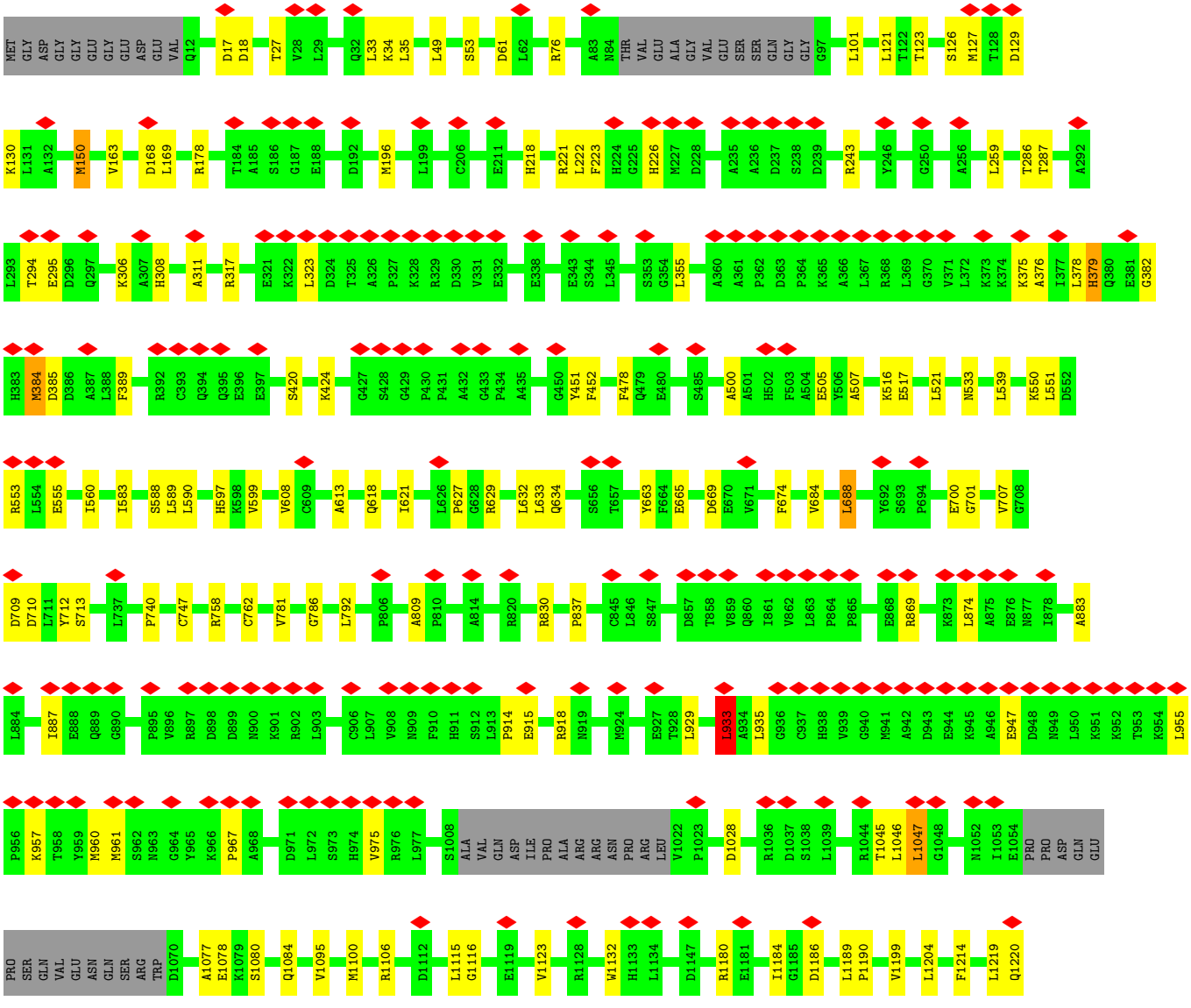
Mol	Chain	Residues	Atoms		AltConf
4	B	2	Total	Ca	0
			2	2	
4	C	2	Total	Ca	0
			2	2	
4	D	2	Total	Ca	0
			2	2	
4	A	2	Total	Ca	0
			2	2	

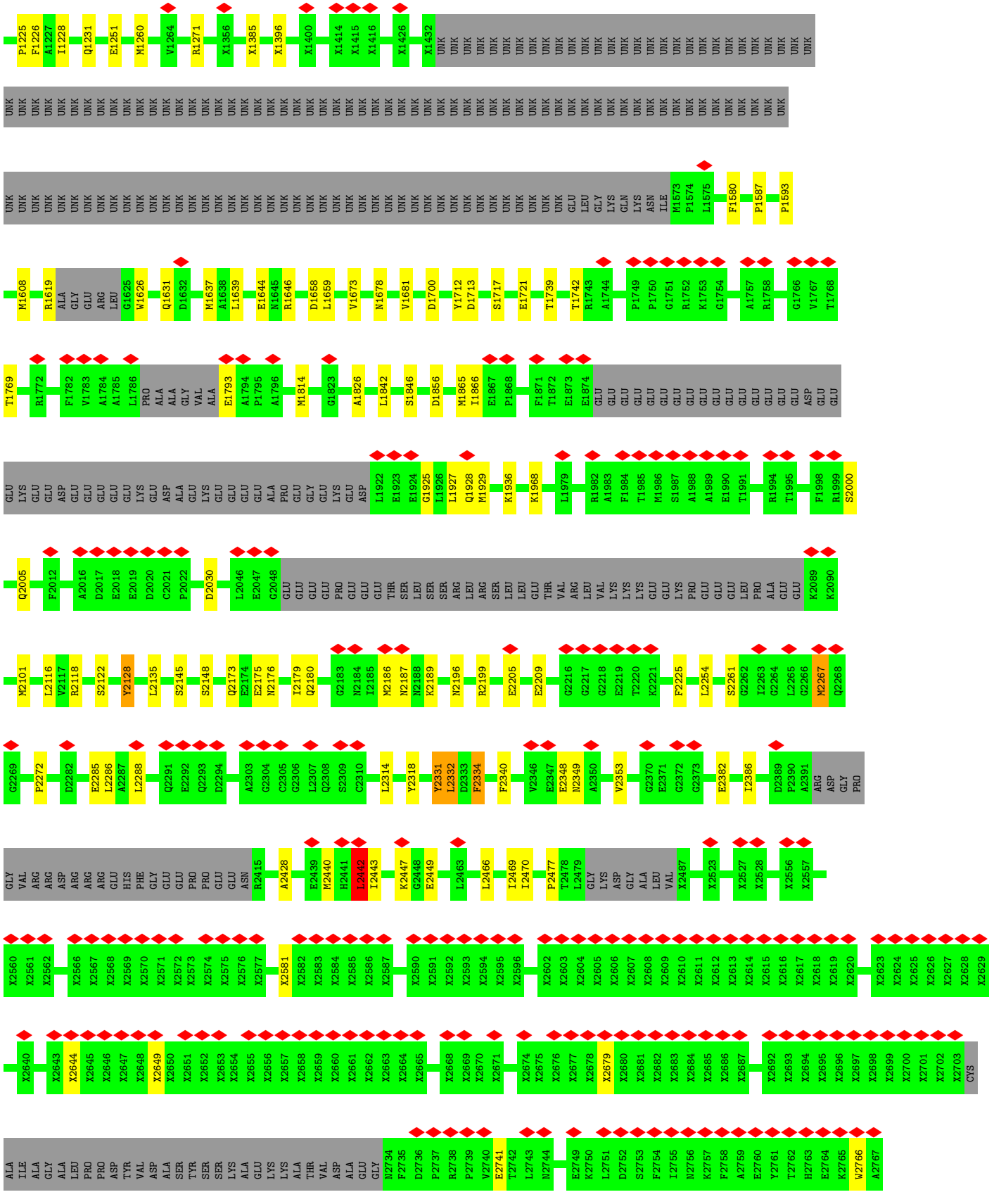
3 Residue-property plots (i)

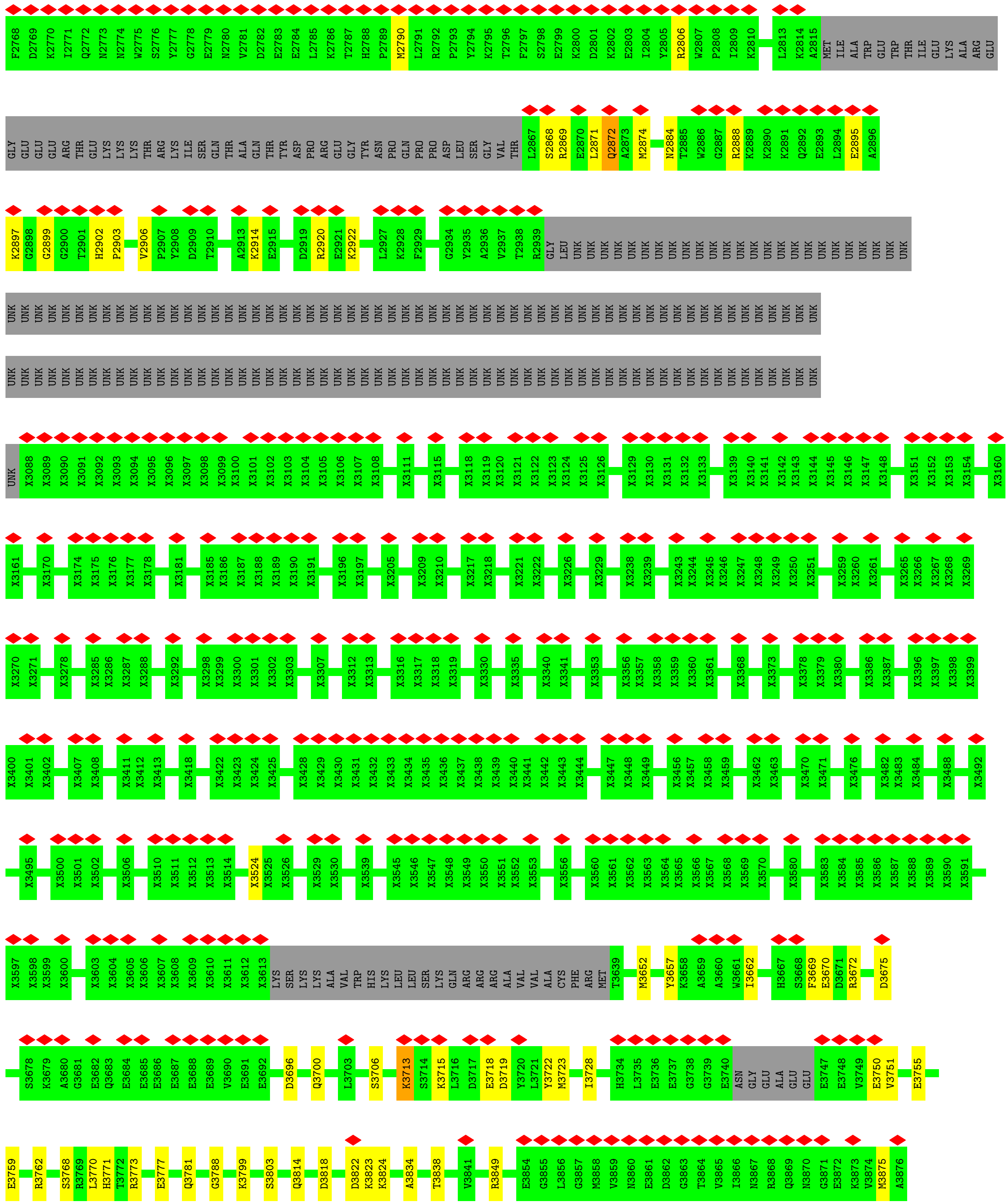
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

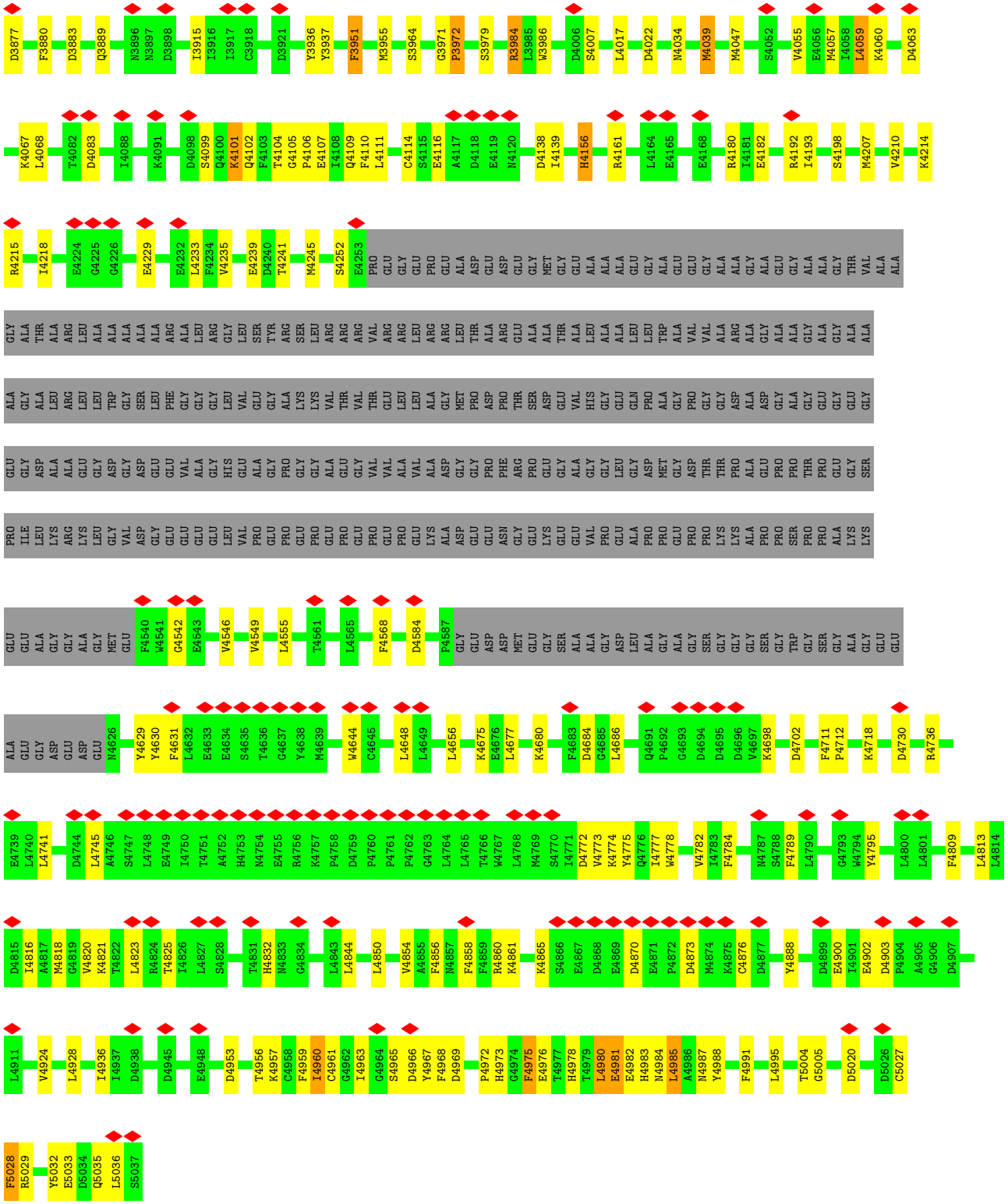
- Molecule 1: Ryanodine receptor 1,Ryanodine receptor 1,RyR1

Chain B:



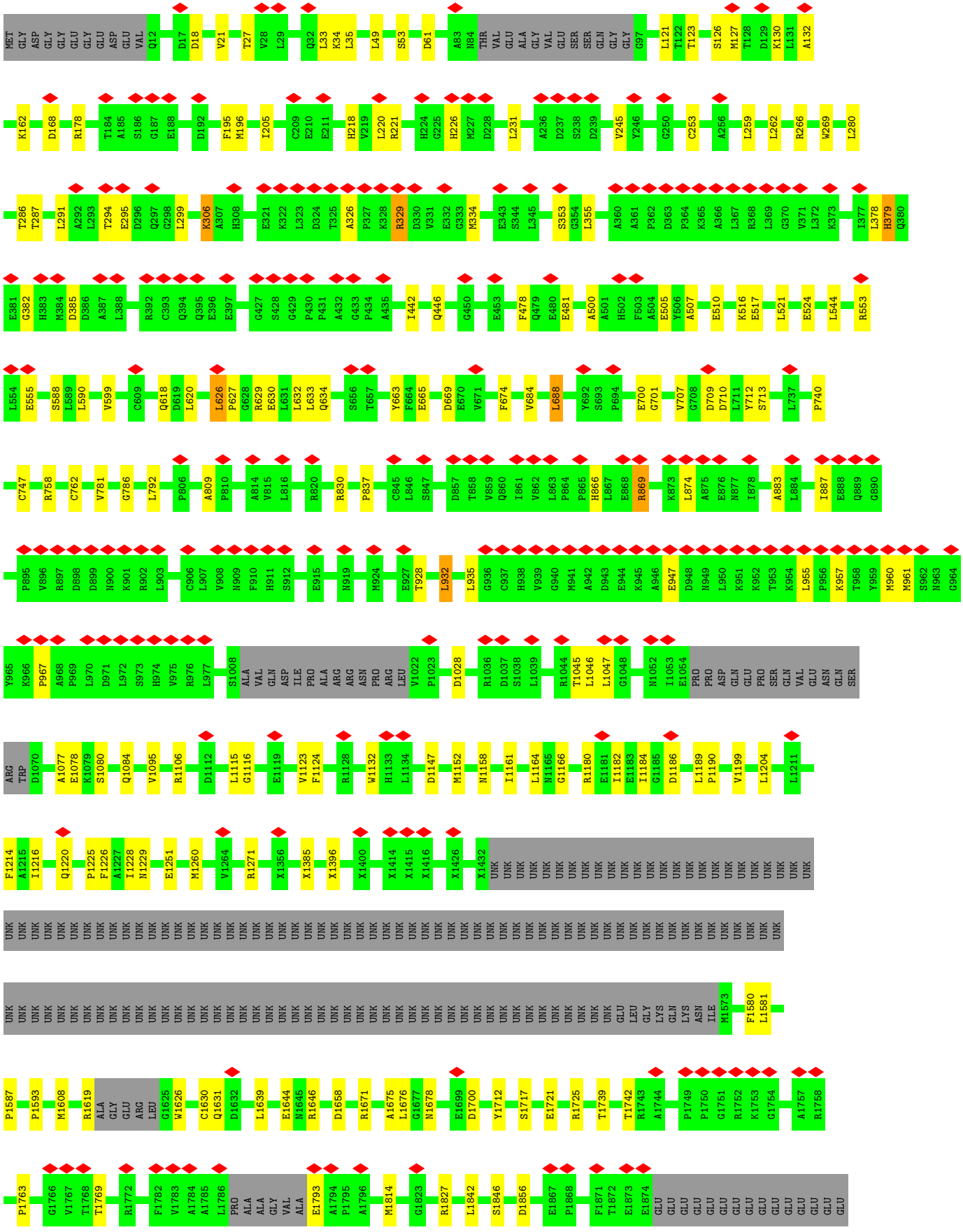

P1225 F1226 A1227 I1228 Q1231 E1251 M1260 V1264 R1271 X1356 X1385 X1396 X1400 X1414 X1415 X1416 X1426 X1432 UNK
M1573 P1574 L1575 F1580 P1587 P1593
M1608 R1619 ALA GLY GLU ARG LEU G1625 W1626 Q1631 D1632 M1637 A1638 L1639 E1644 N1645 R1646 D1658 L1659 V1673 N1678 V1681 D1700 Y1712 D1713 S1717 E1721 T1739 T1742 R1743 A1744 P1749 P1750 G1751 R1752 K1753 G1754 A1757 R1758 G1766 V1767 T1768
T1769 R1772 F1782 V1783 A1784 A1785 L1786 PRO ALA ALA GLY VAL ALA E1793 A1794 P1795 A1796 M1814 G1823 A1826 L1842 S1846 D1856 M1865 I1866 E1867 P1868 F1871 T1872 E1873 E1874 GLU ASP
L1922 E1923 E1924 G1925 L1926 L1927 Q1928 M1929 K1936 K1968 L1979 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 R1994 T1995 F1998 R1999 S2000
Q2005 F2012 A2016 D2017 E2018 E2019 D2020 C2021 P2022 D2030 L2046 E2047 G2048 K2089 K2090
M2101 L2116 V2117 R2118 S2122 Y2128 L2135 S2145 S2148 Q2173 E2174 E2175 N2176 I2179 Q2180 G2183 N2184 I2185 M2186 N2187 N2188 K2189 N2196 R2199 E2205 E2209 G2216 G2217 G2218 E2219 T2220 K2221 F2225 L2254 S2261 G2262 I2263 G2264 L2265 G2266 M2267 Q2268
G2269 P2272 D2282 E2285 L2286 A2287 L2288 Q2291 E2292 Q2293 D2294 A2303 G2304 C2305 G2306 L2307 Q2308 S2309 C2310 L2314 Y2318 Y2331 L2332 D2333 F2334 F2340 V2346 E2347 E2348 N2349 A2350 V2353 G2370 E2371 G2372 G2373 E2382 I2386 D2389 P2390 A2391 ARG ASP GLY PRO
R2415 A2428 E2439 M2440 H2441 L2442 I2443 K2447 G2448 E2449 L2463 L2466 I2469 I2470 P2477 T2478 L2479 GLY LYS ASP GLY ALA LEU VAL X2487 X2523 X2527 X2528 X2556 X2557
X2560 X2561 X2562 X2566 X2567 X2568 X2569 X2570 X2571 X2572 X2573 X2574 X2575 X2576 X2577 X2581 X2582 X2583 X2584 X2585 X2586 X2587 X2590 X2591 X2592 X2593 X2594 X2595 X2596 X2602 X2603 X2604 X2605 X2606 X2607 X2608 X2609 X2610 X2611 X2612 X2613 X2614 X2615 X2616 X2617 X2618 X2619 X2620 X2623 X2624 X2625 X2626 X2627 X2628 X2629
X2640 X2643 X2644 X2645 X2646 X2647 X2648 X2649 X2650 X2651 X2652 X2653 X2654 X2655 X2656 X2657 X2658 X2659 X2660 X2661 X2662 X2663 X2664 X2665 X2668 X2669 X2670 X2671 X2674 X2675 X2676 X2677 X2678 X2679 X2680 X2681 X2682 X2683 X2684 X2685 X2686 X2687 X2692 X2693 X2694 X2695 X2696 X2697 X2698 X2699 X2700 X2701 X2702 X2703 CYS
ALA ILE ALA GLY ALA LEU PRO PRO ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767

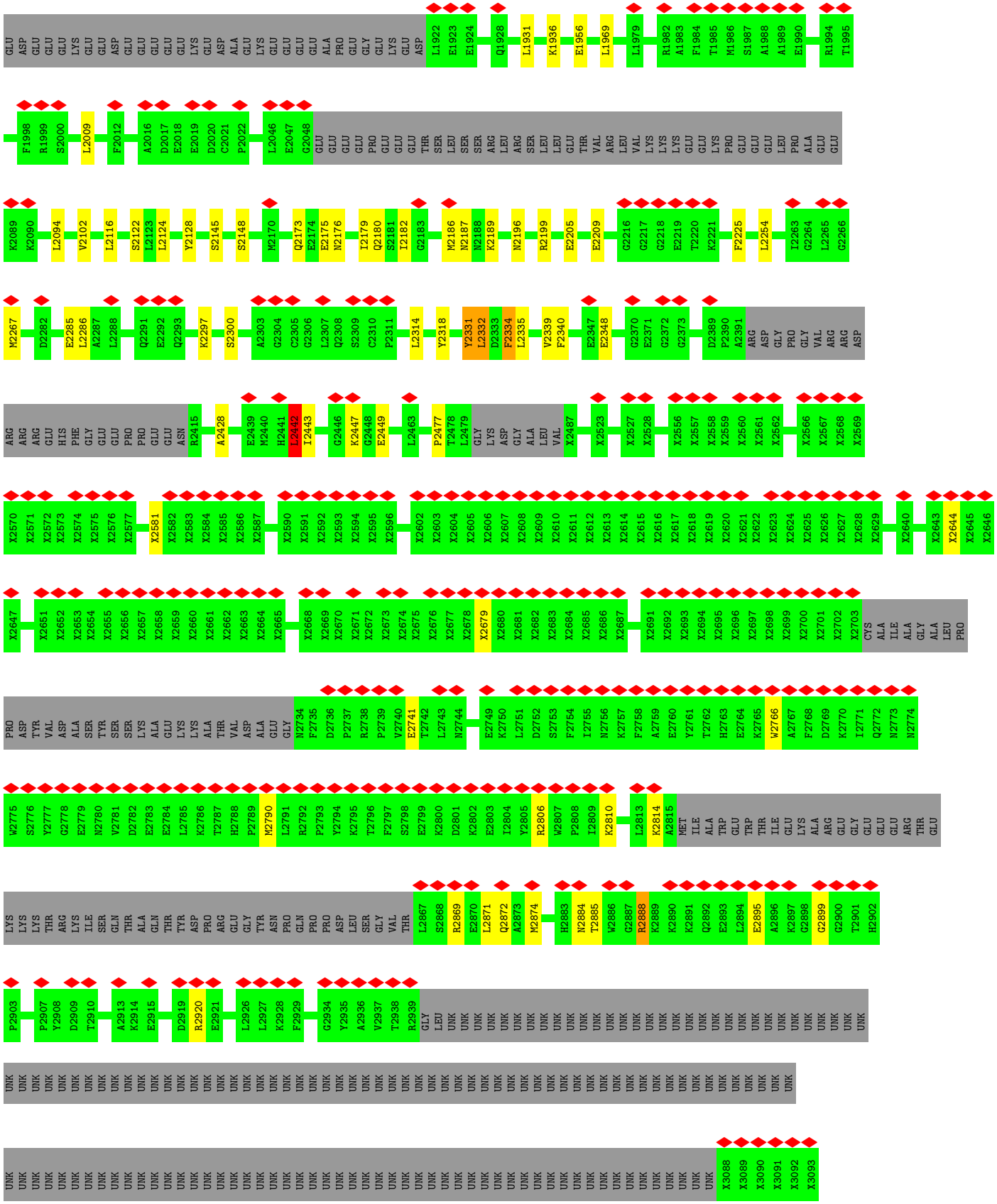

F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 L2813 K2814 A2815 MET ILE ALA TRP GLU TRP THR ILE GLU LYS ALA ARG GLU
GLY GLU GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY TYR ASN PRO GLN PRO PRO ASP LEU SER GLY VAL THR L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896
K2897 G2898 G2899 G2900 T2901 H2902 P2903 V2906 P2907 Y2908 D2909 T2910 A2913 K2914 E2915 D2919 R2920 E2921 K2922 L2927 K2928 F2929 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
UNK X3088 X3089 X3090 X3091 X3092 X3093 X3094 X3095 X3096 X3097 X3098 X3099 X3100 X3101 X3102 X3103 X3104 X3105 X3106 X3107 X3108 X3111 X3115 X3118 X3119 X3120 X3121 X3122 X3123 X3124 X3125 X3126 X3129 X3130 X3131 X3132 X3133 X3139 X3140 X3141 X3142 X3143 X3144 X3145 X3146 X3147 X3148 X3151 X3152 X3153 X3154 X3160
X3161 X3170 X3174 X3175 X3176 X3177 X3178 X3181 X3185 X3186 X3187 X3188 X3189 X3190 X3191 X3196 X3197 X3205 X3209 X3210 X3217 X3218 X3221 X3222 X3226 X3229 X3238 X3239 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3259 X3260 X3261 X3265 X3266 X3267 X3268 X3269
X3270 X3271 X3278 X3285 X3286 X3287 X3288 X3292 X3298 X3299 X3300 X3301 X3302 X3303 X3307 X3312 X3313 X3316 X3317 X3318 X3319 X3330 X3335 X3340 X3341 X3353 X3356 X3357 X3358 X3359 X3360 X3361 X3368 X3373 X3378 X3379 X3380 X3386 X3387 X3396 X3397 X3398 X3399
X3400 X3401 X3402 X3407 X3408 X3411 X3412 X3413 X3418 X3422 X3423 X3424 X3425 X3428 X3429 X3430 X3431 X3432 X3433 X3434 X3435 X3436 X3437 X3438 X3439 X3440 X3441 X3442 X3443 X3444 X3447 X3448 X3449 X3456 X3457 X3458 X3459 X3462 X3463 X3470 X3471 X3476 X3482 X3483 X3484 X3488 X3492
X3495 X3500 X3501 X3502 X3506 X3510 X3511 X3512 X3513 X3514 X3524 X3525 X3526 X3529 X3530 X3539 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3556 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3569 X3570 X3580 X3583 X3584 X3585 X3586 X3587 X3588 X3589 X3590 X3591
X3597 X3598 X3599 X3600 X3603 X3604 X3605 X3606 X3607 X3608 X3609 X3610 X3611 X3612 X3613 LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA ALA VAL VAL ALA CYS PHE ARG MET T3639 M3652 Y3657 K3658 A3659 A3660 W3661 I3662 H3667 S3668 F3669 E3670 D3671 R3672 D3675
S3678 K3679 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 D3696 Q3700 L3703 S3706 K3713 S3714 K3715 L3716 D3717 E3718 D3719 Y3720 L3721 Y3722 M3723 I3728 H3734 L3735 E3736 E3737 G3738 G3739 E3740 ASN GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 E3755
E3759 R3762 S3768 R3769 L3770 H3771 T3772 R3773 E3777 Q3781 G3788 K3799 S3803 Q3814 D3818 D3822 K3823 K3824 A3834 T3838 V3841 R3849 E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 V3874 M3875 A3876

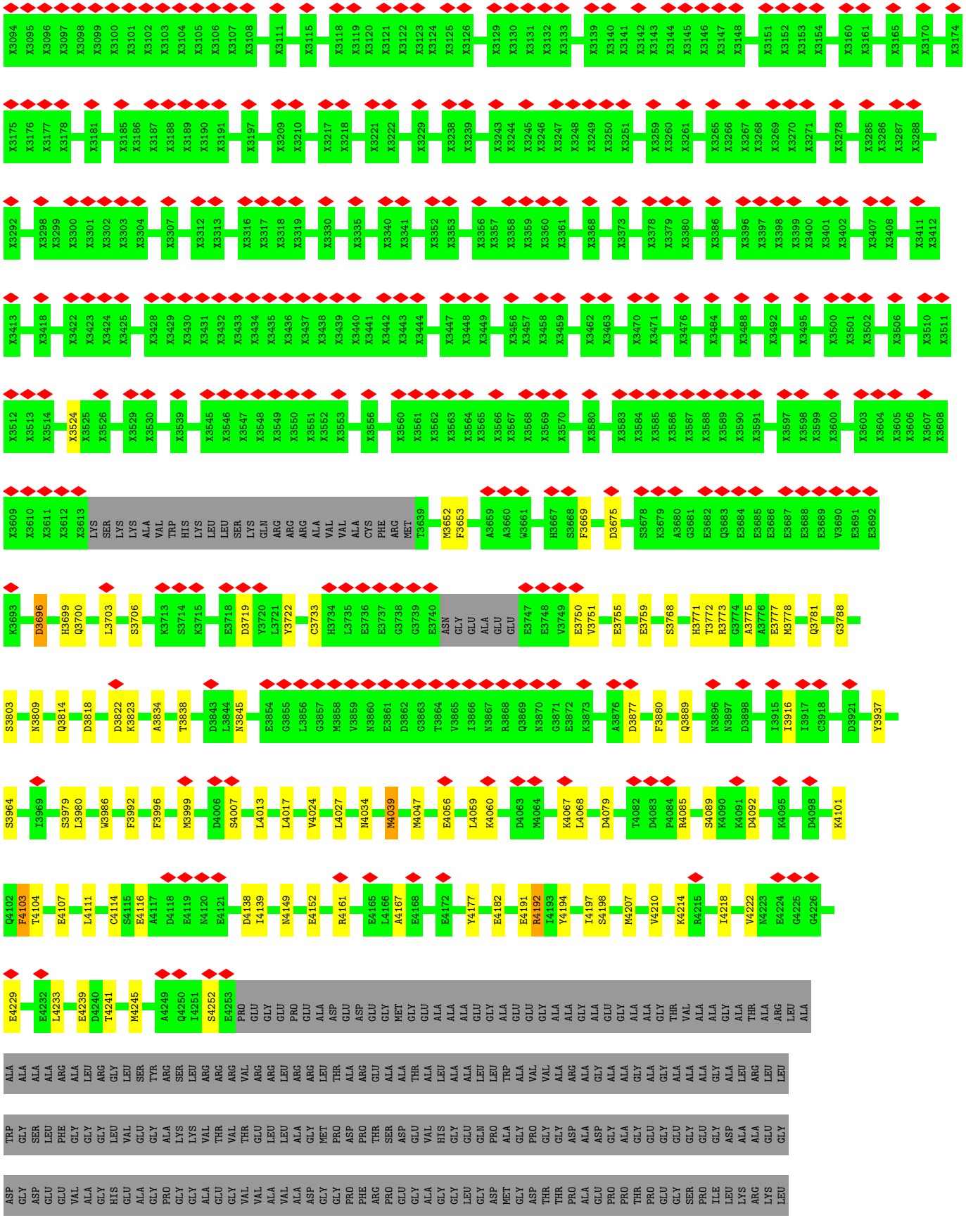


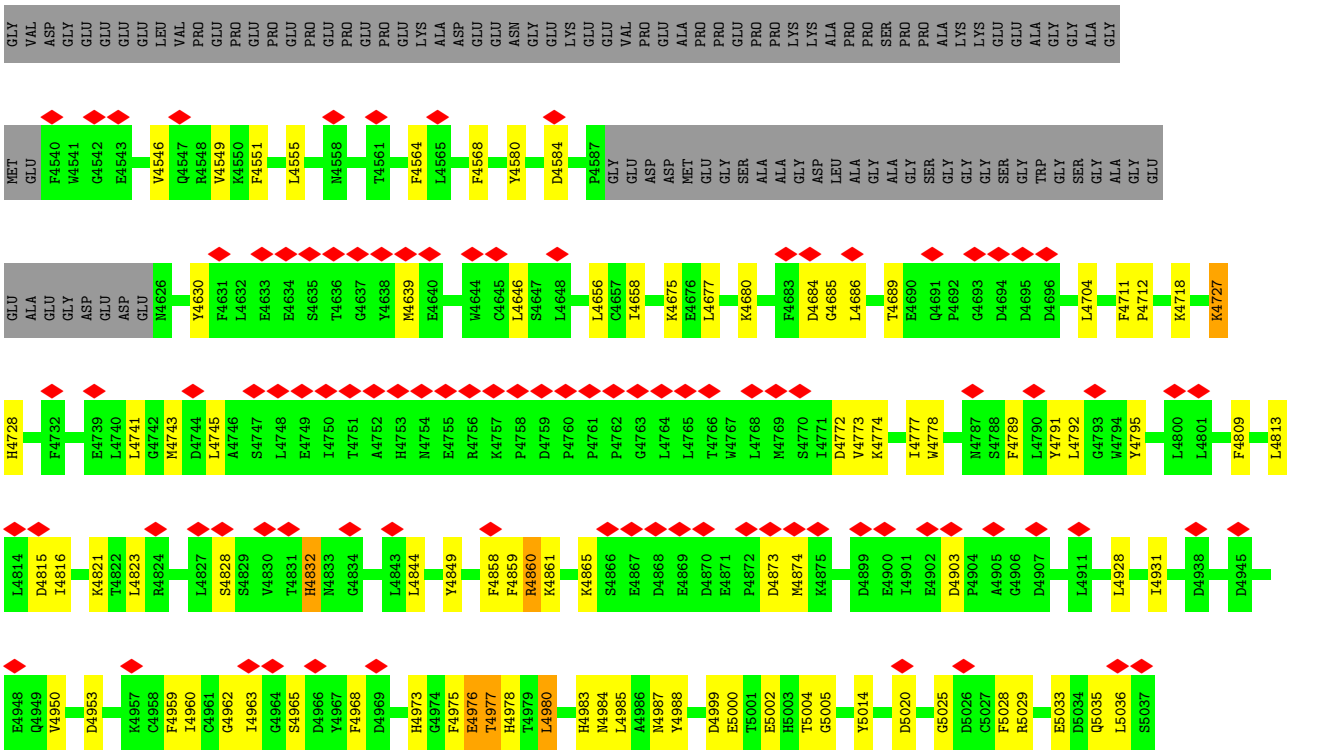
• Molecule 1: Ryanodine receptor 1,Ryanodine receptor 1,RyR1

Chain C:



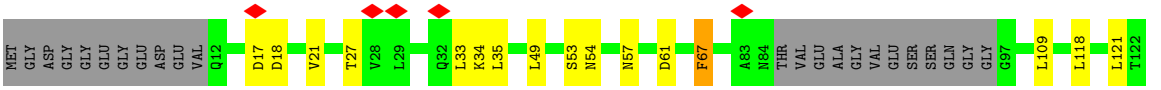


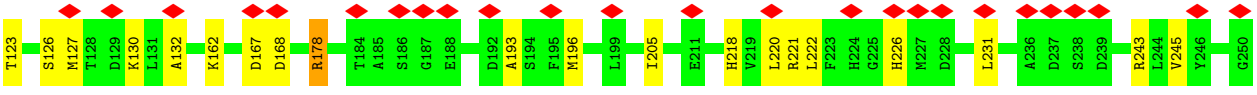

X3094 X3095 X3096 X3097 X3098 X3099 X3100 X3101 X3102 X3103 X3104 X3105 X3106 X3107 X3108 X3111 X3115 X3118 X3119 X3120 X3121 X3122 X3123 X3124 X3125 X3126 X3129 X3130 X3131 X3132 X3133 X3139 X3140 X3141 X3142 X3143 X3144 X3145 X3146 X3147 X3148 X3151 X3152 X3153 X3154 X3160 X3161 X3165 X3170 X3174
X3175 X3176 X3177 X3178 X3181 X3185 X3186 X3187 X3188 X3189 X3190 X3191 X3197 X3209 X3210 X3217 X3218 X3221 X3222 X3229 X3238 X3239 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3259 X3260 X3261 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3278 X3285 X3286 X3287 X3288
X3292 X3298 X3299 X3300 X3301 X3302 X3303 X3304 X3307 X3312 X3313 X3316 X3317 X3318 X3319 X3330 X3335 X3340 X3341 X3352 X3353 X3356 X3357 X3358 X3359 X3360 X3361 X3368 X3373 X3378 X3379 X3380 X3386 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3407 X3408 X3411 X3412
X3413 X3418 X3422 X3423 X3424 X3425 X3428 X3429 X3430 X3431 X3432 X3433 X3434 X3435 X3436 X3437 X3438 X3439 X3440 X3441 X3442 X3443 X3444 X3447 X3448 X3449 X3456 X3457 X3458 X3459 X3462 X3463 X3470 X3471 X3476 X3484 X3488 X3492 X3495 X3500 X3501 X3502 X3506 X3510 X3511
X3512 X3513 X3514 X3524 X3525 X3526 X3529 X3530 X3539 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3556 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3569 X3570 X3580 X3583 X3584 X3585 X3586 X3587 X3588 X3589 X3590 X3591 X3597 X3598 X3599 X3600 X3603 X3604 X3605 X3606 X3607 X3608
X3609 X3610 X3611 X3612 X3613 LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET T3639 M3652 F3653 A3659 A3660 W3661 H3667 S3668 F3669 D3675 S3678 K3679 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692
K3693 D3696 H3699 Q3700 L3703 S3706 K3713 S3714 K3715 E3718 D3719 Y3720 L3721 Y3722 C3733 H3734 L3735 E3736 E3737 G3738 G3739 E3740 ASN GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 E3755 E3759 S3768 H3771 T3772 R3773 G3774 A3775 A3776 E3777 M3778 Q3781 G3788
S3803 N3809 Q3814 D3818 D3822 K3823 A3834 T3838 D3843 L3844 N3845 E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 A3876 D3877 F3880 Q3889 N3896 N3897 D3898 I3915 I3916 I3917 C3918 D3921 Y3937
S3964 I3969 S3979 L3980 W3986 F3992 F3996 M3999 D4006 S4007 L4013 L4017 V4024 L4027 N4034 M4039 M4047 E4056 L4059 K4060 D4063 M4064 K4067 L4068 D4079 T4082 D4083 P4084 R4085 S4089 K4090 K4091 D4092 K4095 D4098 K4101
Q4102 F4103 T4104 E4107 L4111 C4114 S4115 E4116 A4117 D4118 E4119 N4120 E4121 D4138 I4139 N4149 E4152 R4161 E4165 L4166 A4167 E4168 E4172 Y4177 E4182 E4191 R4192 I4193 Y4194 I4197 S4198 M4207 V4210 K4214 R4215 I4218 V4222 N4223 E4224 G4225 G4226
E4229 E4232 L4233 E4239 D4240 T4241 M4245 A4249 Q4250 I4251 S4252 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA ALA GLY ALA LEU ARG LEU ALA
ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG ARG LEU ARG ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA ALA GLY ALA ALA ALA GLY ALA ALA GLY ALA ALA GLY ALA ALA GLY THR ALA ALA ALA ALA GLY ALA LEU ARG LEU LEU
TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU GLY VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLU GLU GLY GLU GLY GLU GLY GLU GLY ALA LEU GLY ASP ALA ALA GLU GLY
ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU

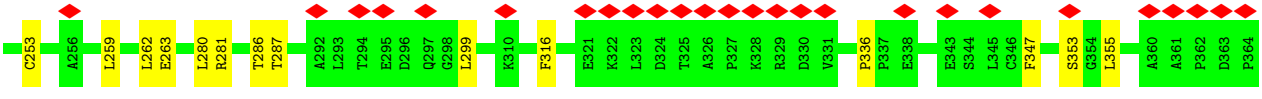


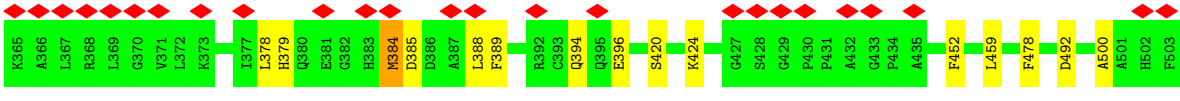
• Molecule 1: Ryanodine receptor 1,Ryanodine receptor 1,RyR1

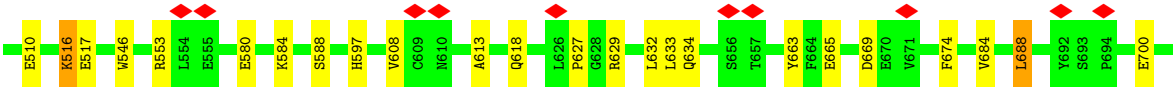
Chain D:

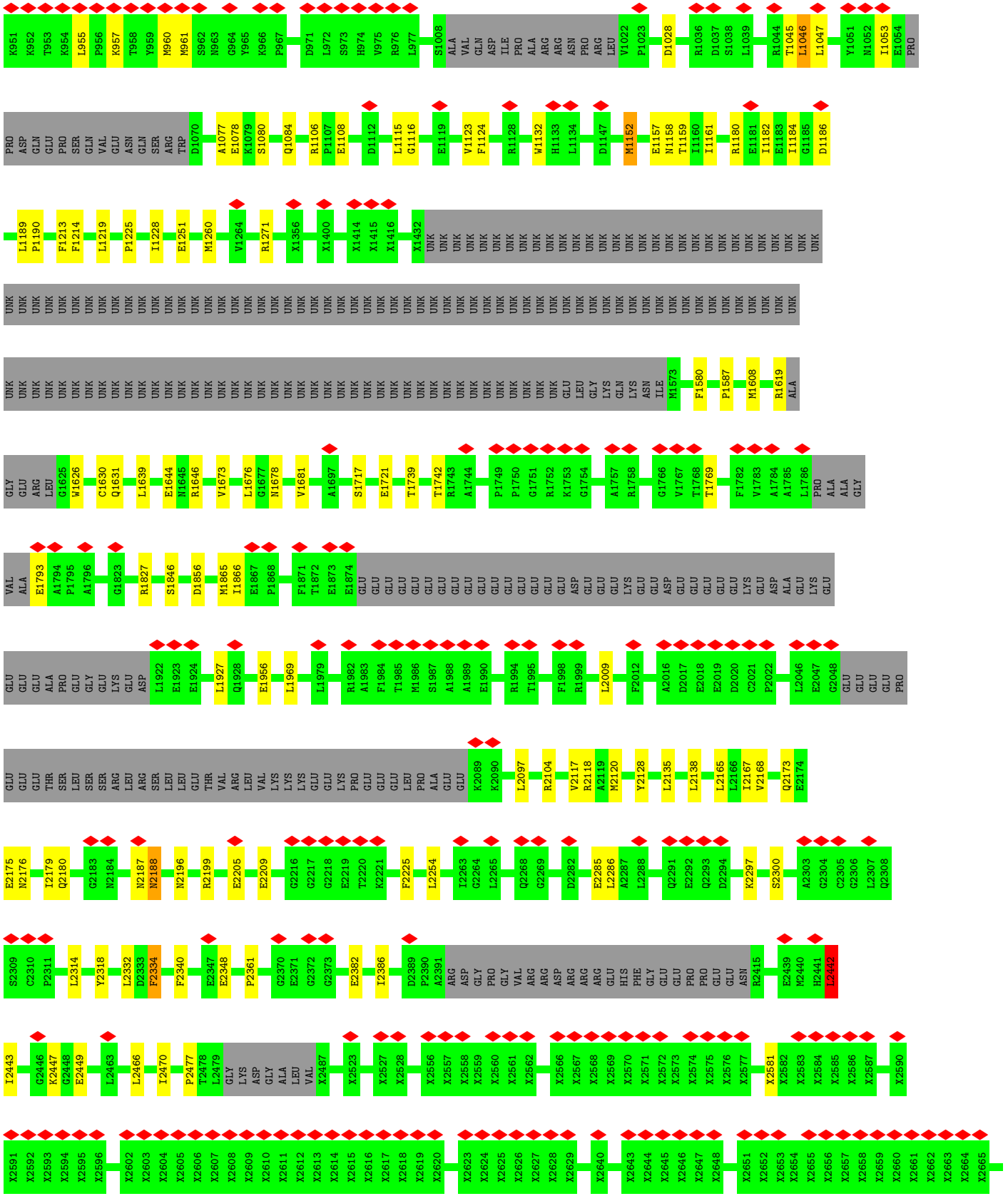


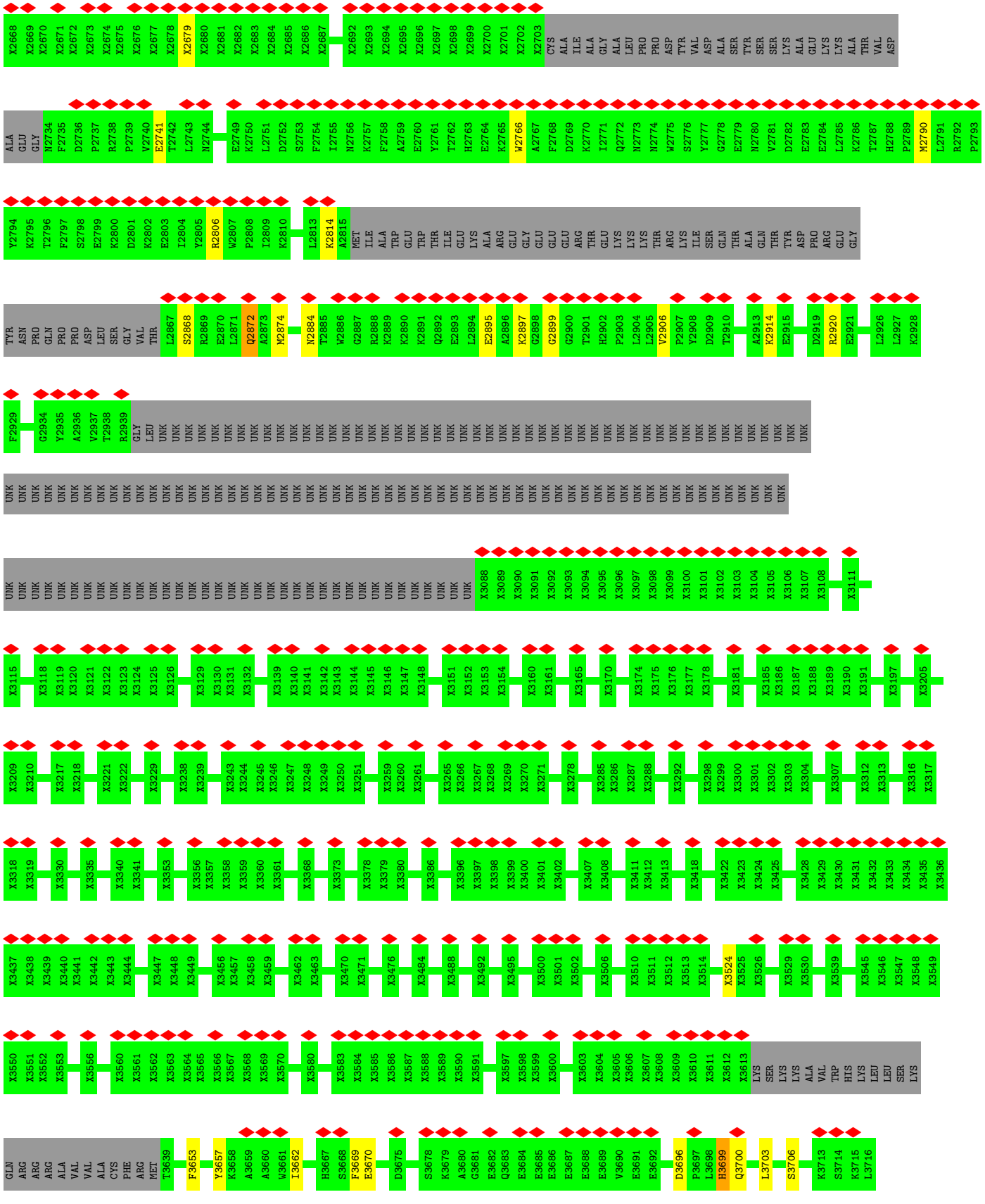


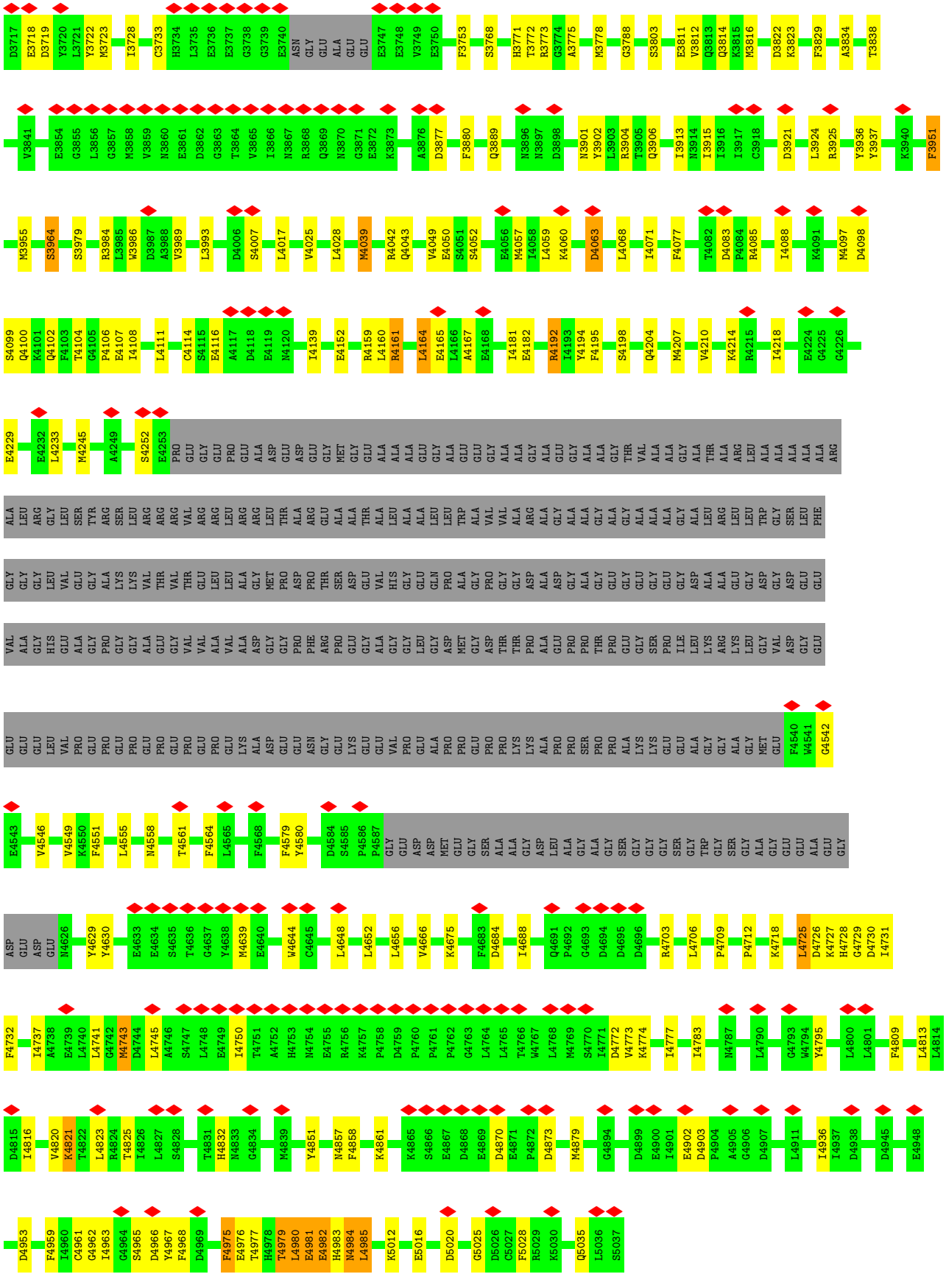






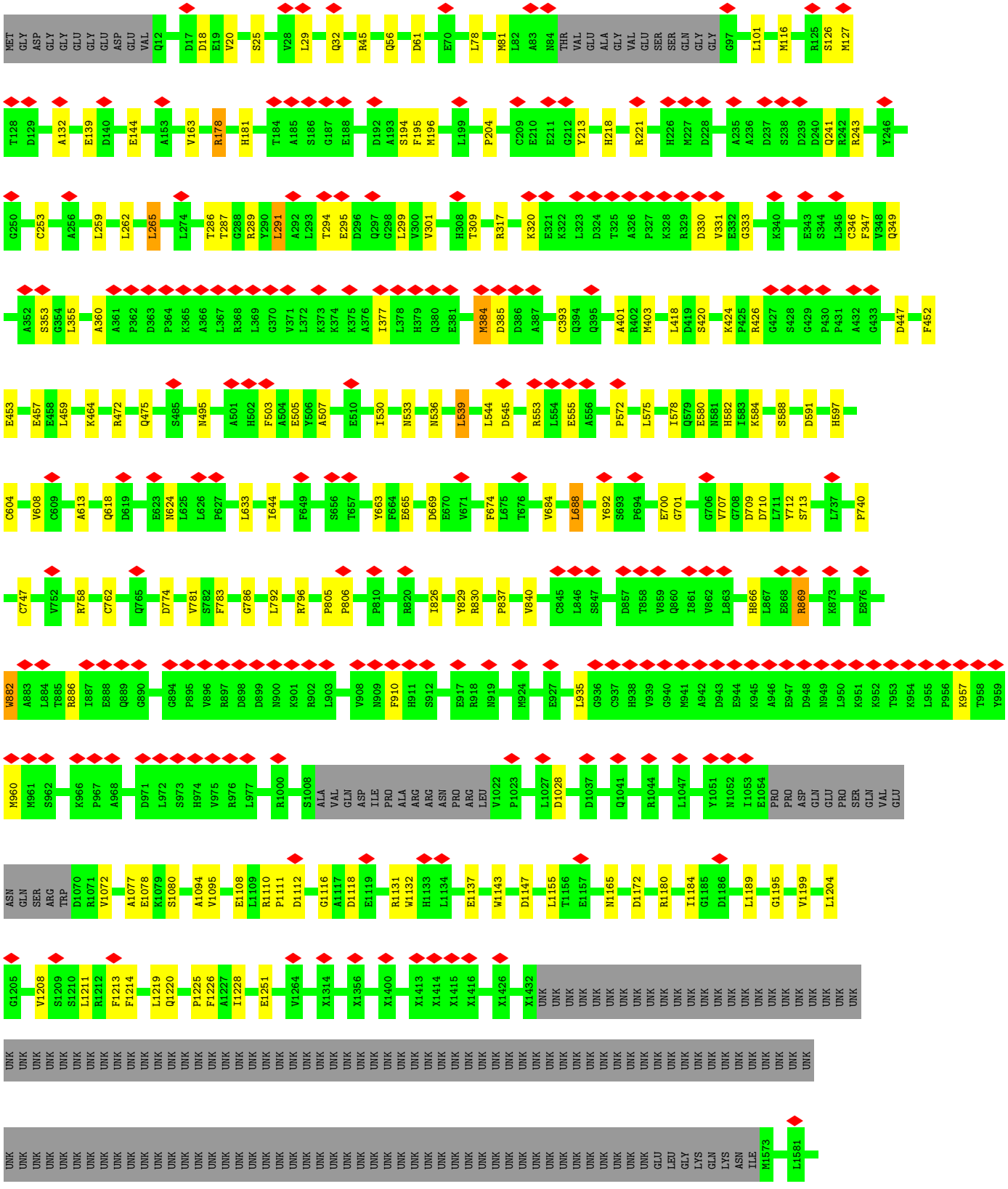


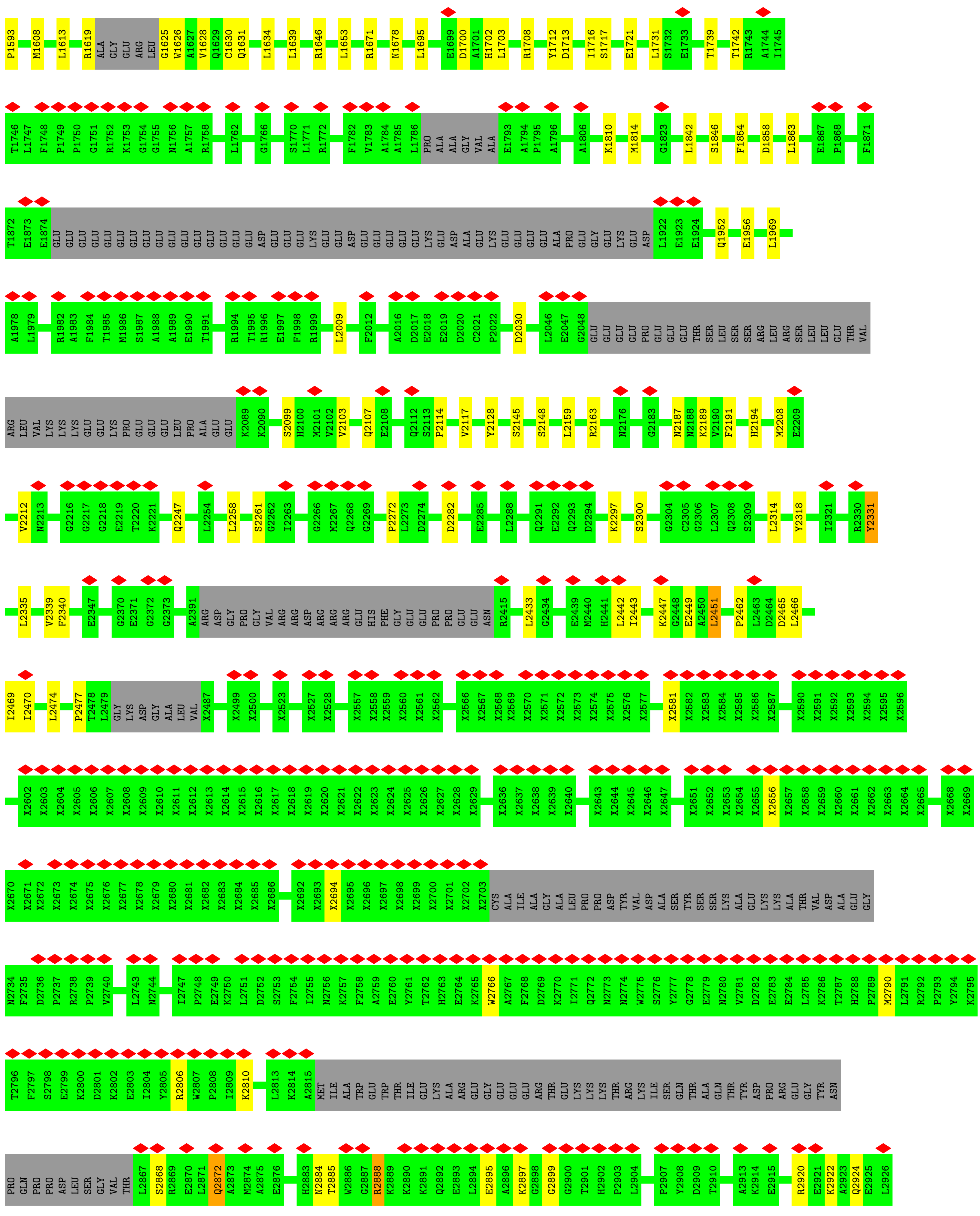

X2668 X2669 X2670 X2671 X2672 X2673 X2674 X2675 X2676 X2677 X2678 X2679 X2680 X2681 X2682 X2683 X2684 X2685 X2686 X2687 X2692 X2693 X2694 X2695 X2696 X2697 X2698 X2699 X2700 X2701 X2702 X2703
CYS ALA ILE ALA GLY ALA LEU PRO PRO ASP TYR VAL ASP ALA SER TYR SER LYS ALA GLU LYS LYS ALA THR VAL ASP
ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 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 L2813 K2814 A2815
MET ILE ALA TRP GLU TRP THR ILE GLU LYS ALA ARG GLU GLY GLU GLU GLU ARG THR GLU LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY
TYR ASN PRO GLN PRO PRO ASP LEU SER GLY VAL THR L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 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 A2913 K2914 E2915 D2919 R2920 E2921 L2926 L2927 K2928
F2929 G2934 Y2935 A2936 V2937 T2938 R2939
GLY LEU UNK UNK UNK

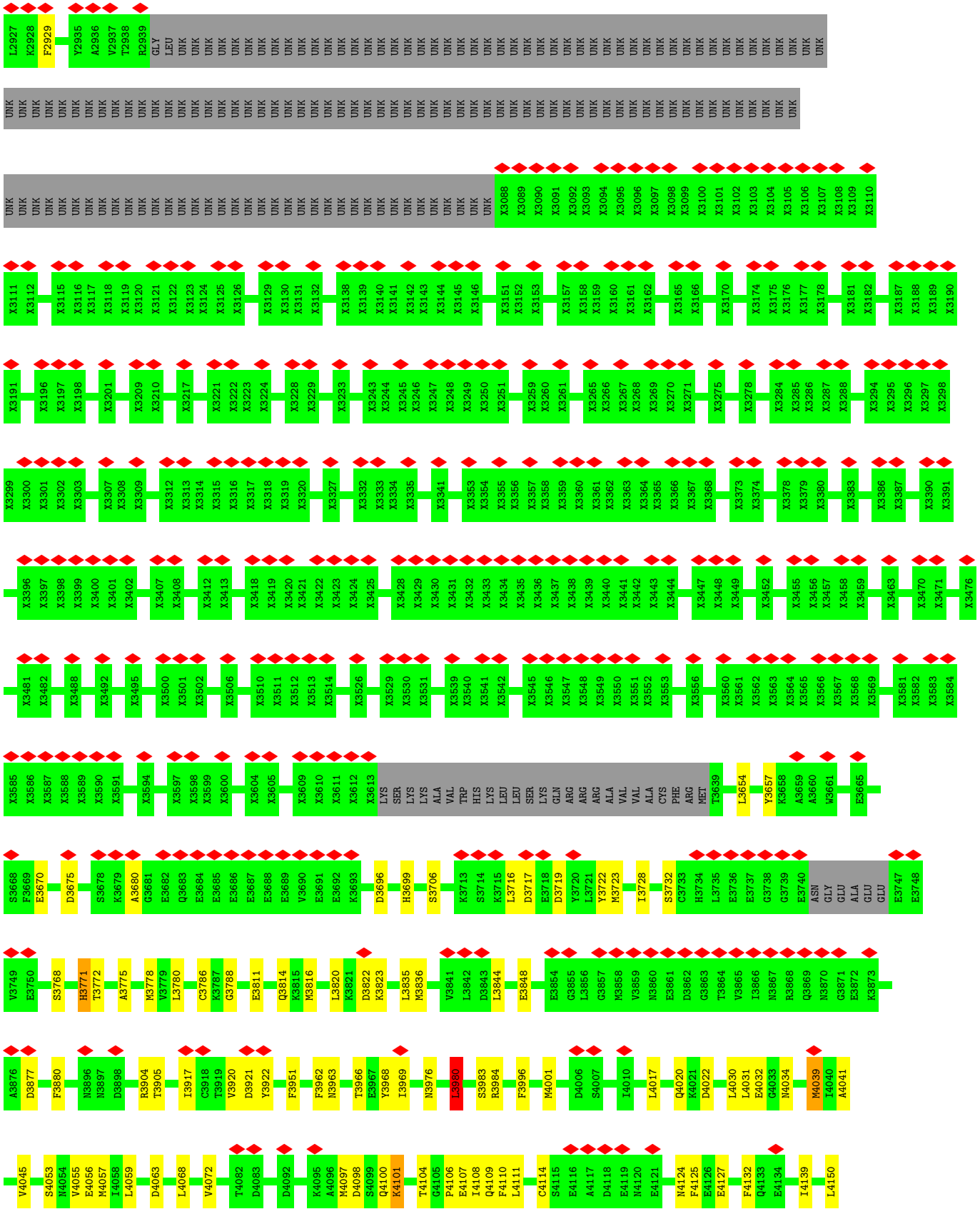


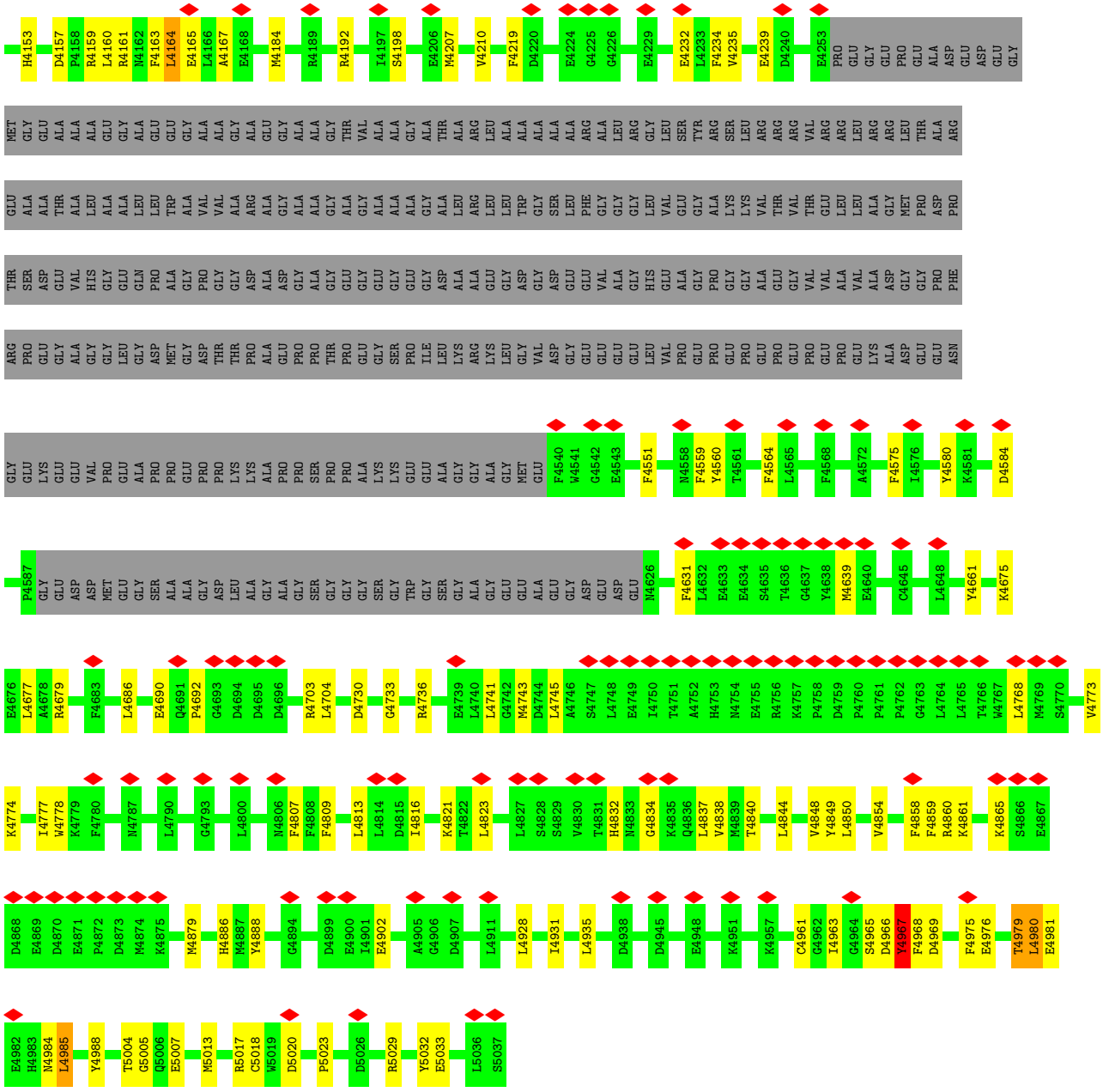
• Molecule 1: Ryanodine receptor 1,Ryanodine receptor 1,RyR1

Chain A:




P1593 M1608 L1613 R1619 ALA GLY GLU ARG LEU G1625 W1626 A1627 V1628 Q1629 C1630 Q1631 L1634 L1639 R1646 L1653 R1671 N1678 L1695 E1699 D1700 A1701 H1702 L1703 R1708 Y1712 D1713 I1716 S1717 E1721 L1731 S1732 E1733 T1739 T1742 R1743 A1744 I1745
T1746 L1747 F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 L1762 G1766 S1770 L1771 R1772 F1782 V1783 A1784 A1785 L1786 PRO ALA ALA GLY VAL ALA E1793 A1794 P1795 A1796 A1806 K1810 M1814 G1823 L1842 S1846 F1854 D1858 L1863 E1867 P1868 F1871
T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP 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 Q1952 E1956 L1969
A1978 L1979 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 R1994 T1995 R1996 E1997 F1998 R1999 L2009 F2012 A2016 D2017 E2018 E2019 D2020 C2021 P2022 D2030 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 S2099 H2100 M2101 V2102 V2103 Q2107 E2108 Q2112 S2113 P2114 V2117 Y2128 S2145 S2148 L2159 R2163 N2176 G2183 N2187 N2188 K2189 V2190 F2191 H2194 M2208 E2209
V2212 N2213 G2216 G2217 G2218 E2219 T2220 K2221 Q2247 L2254 L2258 S2261 G2262 I2263 G2266 M2267 Q2268 G2269 P2272 L2273 D2274 D2282 E2285 L2288 Q2291 E2292 Q2293 D2294 K2297 S2300 G2304 C2305 G2306 L2307 Q2308 S2309 L2314 Y2318 I2321 R2330 Y2331
L2335 V2339 F2340 E2347 G2370 E2371 G2372 G2373 A2391 ARG ASP GLY PRO GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU ASN R2415 L2433 G2434 E2439 M2440 H2441 L2442 I2443 K2447 G2448 E2449 A2450 L2451 P2462 L2463 D2464 D2465 L2466
I2469 I2470 L2474 P2477 T2478 L2479 GLY LYS ASP GLY ALA LEU VAL X2487 X2499 X2500 X2523 X2527 X2528 X2557 X2558 X2559 X2560 X2561 X2562 X2566 X2567 X2568 X2569 X2570 X2571 X2572 X2573 X2574 X2575 X2576 X2577 X2581 X2582 X2583 X2584 X2585 X2586 X2587 X2590 X2591 X2592 X2593 X2594 X2595 X2596
X2602 X2603 X2604 X2605 X2606 X2607 X2608 X2609 X2610 X2611 X2612 X2613 X2614 X2615 X2616 X2617 X2618 X2619 X2620 X2621 X2622 X2623 X2624 X2625 X2626 X2627 X2628 X2629 X2636 X2637 X2638 X2639 X2640 X2643 X2644 X2645 X2646 X2647 X2651 X2652 X2653 X2654 X2655 X2656 X2657 X2658 X2659 X2660 X2661 X2662 X2663 X2664 X2665 X2668 X2669
X2670 X2671 X2672 X2673 X2674 X2675 X2676 X2677 X2678 X2679 X2680 X2681 X2682 X2683 X2684 X2685 X2686 X2692 X2693 X2694 X2695 X2696 X2697 X2698 X2699 X2700 X2701 X2702 X2703 CYS ALA ILE ALA GLY ALA LEU PRO PRO ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY
N2734 F2735 D2736 P2737 R2738 P2739 V2740 L2743 N2744 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 L2813 K2814 A2815 MET ILE ALA TRP GLU TRP THR ILE GLU LYS ALA ARG GLU GLY GLU GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY TYR ASN
PRO GLN PRO PRO ASP LEU SER GLY VAL THR L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 P2907 Y2908 D2909 T2910 A2913 K2914 E2915 R2920 E2921 K2922 A2923 Q2924 E2925 L2926


L2927 K2928 F2929 Y2935 A2936 V2937 T2938 R2939 GLY LEU UNK
UNK
X3088 X3089 X3090 X3091 X3092 X3093 X3094 X3095 X3096 X3097 X3098 X3099 X3100 X3101 X3102 X3103 X3104 X3105 X3106 X3107 X3108 X3109 X3110
X3111 X3112 X3115 X3116 X3117 X3118 X3119 X3120 X3121 X3122 X3123 X3124 X3125 X3126 X3129 X3130 X3131 X3132 X3138 X3139 X3140 X3141 X3142 X3143 X3144 X3145 X3146 X3151 X3152 X3153 X3157 X3158 X3159 X3160 X3161 X3162 X3165 X3166 X3170 X3174 X3175 X3176 X3177 X3178 X3181 X3182 X3187 X3188 X3189 X3190
X3191 X3196 X3197 X3198 X3201 X3209 X3210 X3217 X3221 X3222 X3223 X3224 X3228 X3229 X3233 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3259 X3260 X3261 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3275 X3278 X3284 X3285 X3286 X3287 X3288 X3294 X3295 X3296 X3297 X3298
X3299 X3300 X3301 X3302 X3303 X3307 X3308 X3309 X3312 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3320 X3327 X3332 X3333 X3334 X3335 X3341 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3367 X3368 X3373 X3374 X3378 X3379 X3380 X3383 X3386 X3387 X3390 X3391
X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3407 X3408 X3412 X3413 X3418 X3419 X3420 X3421 X3422 X3423 X3424 X3425 X3428 X3429 X3430 X3431 X3432 X3433 X3434 X3435 X3436 X3437 X3438 X3439 X3440 X3441 X3442 X3443 X3444 X3447 X3448 X3449 X3452 X3455 X3456 X3457 X3458 X3459 X3463 X3470 X3471 X3476
X3481 X3482 X3488 X3492 X3495 X3500 X3501 X3502 X3506 X3510 X3511 X3512 X3513 X3514 X3526 X3529 X3530 X3531 X3539 X3540 X3541 X3542 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3556 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3569 X3581 X3582 X3583 X3584
X3585 X3586 X3587 X3588 X3589 X3590 X3591 X3594 X3597 X3598 X3599 X3600 X3604 X3605 X3609 X3610 X3611 X3612 X3613 LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET T3639 L3654 Y3657 K3658 A3659 A3660 W3661 E3665
S3668 F3669 E3670 D3675 S3678 K3679 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 D3696 H3699 S3706 K3713 S3714 K3715 L3716 D3717 E3718 D3719 Y3720 L3721 Y3722 M3723 I3728 S3732 C3733 H3734 L3735 E3736 E3737 G3738 G3739 E3740 ASN GLY GLU ALA GLU GLU E3747 E3748
Y3749 E3750 S3768 H3771 T3772 A3775 M3778 V3779 L3780 C3786 K3787 G3788 E3811 Q3814 K3815 M3816 L3820 K3821 D3822 K3823 L3835 M3836 V3841 L3842 D3843 L3844 E3848 E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873
A3876 D3877 F3880 N3896 N3897 D3898 R3904 T3905 I3917 C3918 T3919 V3920 D3921 Y3922 F3951 F3962 N3963 T3966 E3967 Y3968 I3969 N3976 L3980 S3983 R3984 F3996 M4001 D4006 S4007 I4010 L4017 Q4020 K4021 D4022 L4030 L4031 E4032 G4033 N4034 M4039 I4040 A4041
V4045 S4053 N4054 V4055 E4056 M4057 I4058 L4059 D4063 L4068 V4072 T4082 D4083 D4092 K4095 A4096 M4097 D4098 S4099 Q4100 K4101 T4104 G4105 P4106 E4107 I4108 Q4109 F4110 L4111 C4114 S4115 E4116 A4117 D4118 E4119 N4120 E4121 N4124 F4125 E4126 E4127 F4132 Q4133 E4134 I4139 L4150


H4153 D4157 P4158 R4159 L4160 R4161 W4162 F4163 L4164 E4165 L4166 A4167 E4168 M4184 R4189 R4192 I4197 S4198 E4206 M4207 V4210 F4219 D4220 E4224 G4225 G4226 E4229 E4232 L4233 F4234 V4235 E4239 D4240 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY
MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA ALA GLY GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU ARG THR ALA ARG
GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA ALA GLY ALA ALA LEU ARG LEU LEU TRP GLY ALA ALA SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU LEU ALA GLY MET PRO ASP PRO
THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ALA ASP GLY ALA GLY GLU GLY GLU GLY GLY SER PRO GLU GLU GLY ASP ALA GLY VAL ALA GLY HIS GLU ALA ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE
ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY GLY SER PRO ILE LEU LYS ARG LYS LYS ALA ALA GLU GLY GLU GLU GLU GLU LEU VAL PRO GLU GLY PRO GLU PRO GLU PRO GLU PRO GLU GLY VAL PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN
GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 W4541 G4542 E4543 F4551 N4558 F4559 Y4560 T4561 F4564 L4565 F4568 A4572 F4575 I4576 Y4580 K4581 D4584
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 GLU ALA GLU GLY ASP GLU ASP GLU N4626 F4631 L4632 E4633 E4634 S4635 T4636 G4637 Y4638 M4639 E4640 C4645 L4648 Y4661 K4675
E4676 L4677 A4678 R4679 F4683 L4686 E4690 Q4691 P4692 G4693 D4694 D4695 D4696 R4703 L4704 D4730 G4733 R4736 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 V4773
K4774 I4777 W4778 K4779 F4780 N4787 L4790 G4793 L4800 N4806 F4807 F4808 F4809 L4813 L4814 D4815 I4816 K4821 T4822 L4823 L4827 S4828 S4829 V4830 T4831 H4832 N4833 G4834 K4835 Q4836 L4837 V4838 M4839 T4840 L4844 V4848 Y4849 L4850 V4854 F4858 F4859 R4860 K4861 K4865 S4866 E4867
D4868 E4869 D4870 E4871 P4872 D4873 M4874 K4875 N4879 H4886 M4887 Y4888 G4894 D4899 E4900 I4901 E4902 A4905 G4906 D4907 L4911 L4928 I4931 L4935 D4938 D4945 E4948 K4961 K4957 C4961 G4962 I4963 G4964 S4965 D4966 Y4967 F4968 D4969 F4975 E4976 T4979 L4980 E4981
E4982 H4983 N4984 L4985 Y4988 T5004 G5005 Q5006 E5007 M5013 R5017 C5018 W5019 D5020 P5023 D5026 R5029 Y5032 E5033 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	159444	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.090	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	477.36002, 477.36002, 477.36002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.105, 1.105, 1.105	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: ACP, CA, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/25301	0.56	19/34345 (0.1%)
1	B	0.27	0/25301	0.55	18/34345 (0.1%)
1	C	0.27	0/25301	0.55	18/34345 (0.1%)
1	D	0.29	2/25301 (0.0%)	0.57	21/34345 (0.1%)
All	All	0.28	2/101204 (0.0%)	0.56	76/137380 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4709	PRO	CG-CD	-16.10	0.97	1.50
1	D	4709	PRO	N-CD	7.50	1.58	1.47

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	4709	PRO	N-CD-CG	-15.58	79.83	103.20
1	D	4709	PRO	CA-N-CD	-10.61	96.65	111.50
1	A	2462	PRO	CA-N-CD	-10.00	97.50	111.50
1	B	967	PRO	CA-N-CD	-9.79	97.80	111.50
1	C	967	PRO	CA-N-CD	-9.50	98.20	111.50
1	C	4745	LEU	CA-CB-CG	9.25	136.58	115.30
1	B	1587	PRO	CA-N-CD	-8.82	99.16	111.50
1	D	4709	PRO	CA-CB-CG	-8.60	87.67	104.00
1	A	2477	PRO	CA-N-CD	-8.39	99.75	111.50
1	D	688	LEU	CA-CB-CG	7.93	133.55	115.30
1	C	688	LEU	CA-CB-CG	7.72	133.06	115.30
1	B	3972	PRO	CA-N-CD	-7.72	100.69	111.50
1	D	1587	PRO	CA-N-CD	-7.64	100.80	111.50
1	C	1587	PRO	CA-N-CD	-7.61	100.85	111.50
1	B	688	LEU	CA-CB-CG	7.60	132.79	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	4985	LEU	CA-CB-CG	7.51	132.58	115.30
1	B	4063	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	688	LEU	CA-CB-CG	7.45	132.42	115.30
1	D	874	LEU	CA-CB-CG	7.42	132.36	115.30
1	D	4063	ASP	CB-CG-OD1	7.39	124.95	118.30
1	D	2477	PRO	CA-N-CD	-7.38	101.17	111.50
1	C	2477	PRO	CA-N-CD	-7.29	101.29	111.50
1	B	2477	PRO	CA-N-CD	-7.26	101.33	111.50
1	C	932	LEU	CA-CB-CG	7.16	131.77	115.30
1	B	933	LEU	CA-CB-CG	7.15	131.75	115.30
1	B	2332	LEU	CA-CB-CG	6.94	131.27	115.30
1	D	510	GLU	CA-CB-CG	6.88	128.54	113.40
1	B	4745	LEU	CA-CB-CG	6.85	131.06	115.30
1	D	4745	LEU	CA-CB-CG	6.79	130.92	115.30
1	A	4745	LEU	CA-CB-CG	6.76	130.84	115.30
1	B	874	LEU	CA-CB-CG	6.74	130.79	115.30
1	B	4059	LEU	CA-CB-CG	6.59	130.46	115.30
1	C	2332	LEU	CA-CB-CG	6.53	130.32	115.30
1	A	4639	MET	CA-CB-CG	6.53	124.40	113.30
1	D	4953	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	4063	ASP	CB-CG-OD1	6.48	124.13	118.30
1	C	874	LEU	CA-CB-CG	6.45	130.13	115.30
1	D	935	LEU	CA-CB-CG	6.33	129.87	115.30
1	B	4953	ASP	CB-CG-OD1	6.28	123.95	118.30
1	C	4953	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	935	LEU	CA-CB-CG	6.16	129.48	115.30
1	A	3822	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	510	GLU	CA-CB-CG	6.02	126.65	113.40
1	B	129	ASP	CB-CG-OD1	5.91	123.62	118.30
1	D	2332	LEU	CA-CB-CG	5.91	128.89	115.30
1	D	3822	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	935	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	3822	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	935	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	591	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	3822	ASP	CB-CG-OD1	5.57	123.32	118.30
1	A	4639	MET	CB-CG-SD	5.51	128.95	112.40
1	A	2451	LEU	CA-CB-CG	5.50	127.95	115.30
1	C	620	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	3980	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	127	MET	CB-CG-SD	5.45	128.74	112.40
1	D	4639	MET	CB-CG-SD	5.39	128.58	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4001	MET	CB-CG-SD	5.33	128.38	112.40
1	D	127	MET	CB-CG-SD	5.29	128.27	112.40
1	A	241	GLN	CA-CB-CG	5.29	125.03	113.40
1	D	4639	MET	CA-CB-CG	5.29	122.29	113.30
1	C	127	MET	CB-CG-SD	5.26	128.18	112.40
1	A	2258	LEU	CA-CB-CG	5.26	127.39	115.30
1	C	2186	MET	CB-CG-SD	5.22	128.06	112.40
1	D	2097	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	2186	MET	CB-CG-SD	5.15	127.84	112.40
1	C	2442	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	127	MET	CB-CG-SD	5.14	127.81	112.40
1	D	4709	PRO	N-CA-CB	-5.12	96.97	102.60
1	D	2442	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	291	LEU	CA-CB-CG	5.03	126.87	115.30
1	C	626	LEU	CA-CB-CG	5.02	126.85	115.30
1	C	1658	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	1111	PRO	CA-N-CD	-5.01	104.48	111.50
1	B	2442	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	1653	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

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	29249	0	24792	232	0
1	B	29249	0	24790	229	0
1	C	29249	0	24795	213	0
1	D	29249	0	24791	224	0
2	A	31	0	13	0	0
2	B	31	0	13	4	0
2	C	31	0	13	0	0
2	D	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
All	All	117132	0	99220	884	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 4.

All (884) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4961:CYS:SG	1:A:4963:ILE:HG22	1.54	1.48
1:A:4961:CYS:SG	1:A:4963:ILE:CG2	2.16	1.33
1:D:4980:LEU:HA	1:D:4984:ASN:HD21	1.34	0.92
1:A:5029:ARG:O	1:A:5033:GLU:HB3	1.73	0.88
1:B:4960:ILE:HG13	1:B:4983:HIS:HB3	1.60	0.83
1:D:4975:PHE:O	1:D:4979:THR:HG22	1.80	0.81
1:C:5029:ARG:O	1:C:5033:GLU:HB3	1.85	0.77
1:A:4975:PHE:O	1:A:4979:THR:HG22	1.85	0.77
1:A:4961:CYS:SG	1:A:4963:ILE:HG21	2.26	0.72
1:B:4104:THR:HB	1:B:4107:GLU:OE2	1.90	0.72
1:B:384:MET:N	1:B:384:MET:SD	2.66	0.69
1:D:384:MET:SD	1:D:384:MET:N	2.66	0.68
1:A:384:MET:SD	1:A:384:MET:N	2.67	0.68
1:C:4977:THR:HA	1:C:4980:LEU:HD23	1.76	0.68
1:D:4104:THR:HB	1:D:4107:GLU:OE2	1.94	0.67
1:D:4182:GLU:HG2	1:D:4192:ARG:HG3	1.76	0.67
1:B:786:GLY:H	1:B:1631:GLN:HA	1.59	0.67
1:C:786:GLY:H	1:C:1631:GLN:HA	1.59	0.67
1:A:20:VAL:HG22	1:A:204:PRO:HA	1.77	0.67
1:D:786:GLY:H	1:D:1631:GLN:HA	1.61	0.66
1:A:4975:PHE:O	1:A:4979:THR:CG2	2.43	0.66
1:A:533:ASN:HB3	1:A:536:ASN:HB2	1.79	0.65
1:D:3921:ASP:HA	1:D:3924:LEU:HD12	1.78	0.65
1:A:644:ILE:HG13	1:A:1628:VAL:HG21	1.78	0.65
1:B:4104:THR:HG22	1:B:4106:PRO:HD2	1.78	0.64
1:A:4017:LEU:HD22	1:A:4139:ILE:HG21	1.79	0.64
1:C:1936:LYS:HB2	1:C:2116:LEU:HD11	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2885:THR:OG1	1:C:2888:ARG:NH2	2.29	0.64
1:A:786:GLY:H	1:A:1631:GLN:HA	1.62	0.64
1:D:4976:GLU:O	1:D:4979:THR:HG23	1.98	0.64
1:C:4960:ILE:HD11	1:C:4985:LEU:HD21	1.78	0.64
1:B:1078:GLU:HG3	1:B:1080:SER:H	1.64	0.63
1:C:1078:GLU:HG3	1:C:1080:SER:H	1.63	0.63
1:B:1936:LYS:HB2	1:B:2116:LEU:HD11	1.82	0.62
1:B:3713:LYS:NZ	1:B:3715:LYS:O	2.33	0.62
1:A:181:HIS:HD1	1:A:194:SER:HG	1.42	0.62
1:C:517:GLU:OE1	1:C:517:GLU:N	2.32	0.62
1:D:3733:CYS:HG	1:D:3803:SER:HG	1.47	0.61
1:A:1078:GLU:HG3	1:A:1080:SER:H	1.64	0.61
1:B:3814:GLN:NE2	1:B:3818:ASP:OD2	2.33	0.61
1:A:4902:GLU:N	1:A:4902:GLU:OE1	2.33	0.61
1:A:4980:LEU:HG	1:A:4981:GLU:N	2.15	0.61
1:D:1078:GLU:HG3	1:D:1080:SER:H	1.64	0.61
1:D:1225:PRO:HG2	1:D:1228:ILE:HB	1.82	0.60
1:D:3696:ASP:OD2	1:D:3773:ARG:NH2	2.34	0.60
1:A:840:VAL:HG12	1:A:1199:VAL:HG22	1.83	0.60
1:B:4960:ILE:HD12	1:B:4988:TYR:HE2	1.67	0.60
1:A:1077:ALA:HB3	1:A:1189:LEU:HB2	1.83	0.60
1:C:2766:TRP:HD1	1:C:2790:MET:HB3	1.65	0.60
1:C:4059:LEU:HD13	1:C:4167:ALA:HB2	1.83	0.60
1:D:2117:VAL:HA	1:D:2120:MET:HG2	1.83	0.59
1:D:2766:TRP:HD1	1:D:2790:MET:HB3	1.67	0.59
1:A:2107:GLN:NE2	1:A:3680:ALA:O	2.35	0.59
1:B:4680:LYS:HD2	1:B:4686:LEU:HD22	1.84	0.59
1:B:2766:TRP:HD1	1:B:2790:MET:HB3	1.68	0.59
1:D:4181:ILE:HG12	1:D:4195:PHE:HE1	1.67	0.59
1:A:4235:VAL:HG11	1:A:5017:ARG:HH12	1.67	0.59
1:C:3772:THR:HG22	1:C:3773:ARG:HG3	1.84	0.59
1:D:4059:LEU:HD13	1:D:4167:ALA:HB2	1.83	0.59
1:B:663:TYR:HD1	1:B:747:CYS:HB3	1.68	0.59
1:A:1671:ARG:NH1	1:A:1713:ASP:OD2	2.36	0.59
1:B:2868:SER:O	1:B:2872:GLN:NE2	2.35	0.58
1:C:4104:THR:HB	1:C:4107:GLU:OE2	2.03	0.58
1:D:2118:ARG:NH2	1:D:3719:ASP:OD1	2.36	0.58
1:A:4059:LEU:HD13	1:A:4167:ALA:HB2	1.84	0.58
1:D:34:LYS:H	1:D:53:SER:HB3	1.67	0.58
1:B:4960:ILE:HD11	2:B:5101:ACP:HN62	1.68	0.58
1:D:3719:ASP:HB3	1:D:3722:TYR:HB3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4068:LEU:HD22	1:D:4111:LEU:HD11	1.86	0.58
1:C:663:TYR:HD1	1:C:747:CYS:HB3	1.68	0.58
1:C:1115:LEU:HB3	1:C:1123:VAL:HG11	1.86	0.58
1:D:663:TYR:HD1	1:D:747:CYS:HB3	1.69	0.58
1:A:4844:LEU:HD13	1:A:4928:LEU:HG	1.84	0.57
1:B:955:LEU:HD22	1:B:960:MET:HG2	1.84	0.57
1:A:4039:MET:SD	1:A:4039:MET:N	2.70	0.57
1:B:4039:MET:SD	1:B:4039:MET:N	2.71	0.57
1:B:4976:GLU:O	1:B:4980:LEU:HB2	2.04	0.57
1:C:4685:GLY:HA3	1:C:4689:THR:HB	1.85	0.57
1:D:221:ARG:NH1	1:D:253:CYS:O	2.38	0.57
1:C:2314:LEU:HA	1:C:2318:TYR:HB2	1.86	0.57
1:D:3768:SER:O	1:D:3772:THR:OG1	2.21	0.57
1:C:262:LEU:HB2	1:C:280:LEU:HD13	1.86	0.57
1:D:4688:ILE:HD11	1:D:4732:PHE:HD2	1.70	0.57
1:A:2766:TRP:HD1	1:A:2790:MET:HB3	1.69	0.57
1:A:5007:GLU:N	1:A:5007:GLU:OE1	2.38	0.57
1:B:627:PRO:O	1:B:629:ARG:NH1	2.38	0.57
1:A:663:TYR:HD1	1:A:747:CYS:HB3	1.70	0.57
1:B:3799:LYS:NZ	1:B:3883:ASP:OD2	2.37	0.57
1:A:2247:GLN:NE2	1:A:2282:ASP:O	2.37	0.57
1:B:4936:ILE:HG21	1:A:4931:ILE:HG22	1.86	0.57
1:C:3719:ASP:HB3	1:C:3722:TYR:HB3	1.86	0.57
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.38	0.57
1:B:34:LYS:H	1:B:53:SER:HB3	1.70	0.56
1:C:4039:MET:SD	1:C:4039:MET:N	2.70	0.56
1:B:2314:LEU:HA	1:B:2318:TYR:HB2	1.86	0.56
1:D:262:LEU:HB2	1:D:280:LEU:HD13	1.87	0.56
1:D:627:PRO:O	1:D:629:ARG:NH1	2.38	0.56
1:A:505:GLU:HG3	1:A:507:ALA:H	1.70	0.56
1:A:665:GLU:HB2	1:A:792:LEU:HD12	1.88	0.56
1:D:2314:LEU:HA	1:D:2318:TYR:HB2	1.87	0.56
1:D:2447:LYS:HG3	1:D:2449:GLU:H	1.71	0.56
1:A:3719:ASP:HB3	1:A:3722:TYR:HB3	1.87	0.56
1:A:1137:GLU:OE1	1:A:1137:GLU:N	2.39	0.56
1:A:1854:PHE:HB3	1:A:1858:ASP:HB2	1.86	0.56
1:A:4068:LEU:HD22	1:A:4111:LEU:HD11	1.88	0.56
1:B:5004:THR:OG1	1:B:5005:GLY:N	2.39	0.56
1:B:4983:HIS:HA	1:B:4988:TYR:OH	2.06	0.56
1:A:495:ASN:ND2	1:A:555:GLU:OE1	2.39	0.56
1:A:4966:ASP:C	1:A:4968:PHE:H	2.09	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1045:THR:HG23	1:D:1046:LEU:HD23	1.87	0.55
1:A:2868:SER:O	1:A:2872:GLN:NE2	2.39	0.55
1:A:4184:MET:HG2	1:A:5023:PRO:HA	1.88	0.55
1:B:1115:LEU:HB3	1:B:1123:VAL:HG11	1.88	0.55
1:B:3759:GLU:OE1	1:B:3762:ARG:NH2	2.39	0.55
1:D:505:GLU:HG3	1:D:507:ALA:H	1.72	0.55
1:A:669:ASP:OD1	1:A:669:ASP:N	2.40	0.55
1:B:4180:ARG:HB2	1:B:4192:ARG:HD2	1.89	0.55
1:C:126:SER:HB3	1:C:132:ALA:HB2	1.88	0.55
1:A:882:TRP:HD1	1:A:886:ARG:HD3	1.71	0.55
1:B:1739:THR:HG23	1:B:1742:THR:H	1.72	0.55
1:C:2447:LYS:HG3	1:C:2449:GLU:H	1.72	0.55
1:D:1619:ARG:HA	1:D:1626:TRP:H	1.71	0.55
1:D:4071:ILE:HD12	1:D:4100:GLN:HG3	1.89	0.55
1:B:2466:LEU:O	1:B:2470:ILE:HD12	2.07	0.55
1:D:167:ASP:N	1:D:167:ASP:OD1	2.35	0.55
1:A:4239:GLU:OE2	1:A:4679:ARG:NH2	2.39	0.55
1:A:1739:THR:HG23	1:A:1742:THR:H	1.71	0.55
1:C:2581:UNK:N	1:C:2899:GLY:O	2.40	0.55
1:A:3877:ASP:HB2	1:A:3880:PHE:HB3	1.89	0.55
1:D:4962:GLY:H	1:D:5025:GLY:HA2	1.72	0.55
1:B:4985:LEU:HA	1:B:4988:TYR:HD2	1.72	0.55
1:C:830:ARG:HH21	1:C:837:PRO:HB3	1.71	0.55
1:C:2331:TYR:HD1	1:C:2332:LEU:H	1.53	0.55
1:D:633:LEU:HD23	1:D:1639:LEU:HD11	1.89	0.55
1:B:308:HIS:CE1	1:B:311:ALA:H	2.23	0.54
1:C:1251:GLU:OE1	1:C:1251:GLU:N	2.39	0.54
1:D:54:ASN:OD1	1:D:57:ASN:ND2	2.40	0.54
1:D:830:ARG:HH21	1:D:837:PRO:HB3	1.72	0.54
1:C:4860:ARG:NH2	1:D:4629:TYR:OH	2.40	0.54
1:D:517:GLU:OE2	1:D:517:GLU:N	2.39	0.54
1:A:420:SER:O	1:A:424:LYS:NZ	2.41	0.54
1:A:2581:UNK:N	1:A:2899:GLY:O	2.40	0.54
1:D:1251:GLU:OE1	1:D:1251:GLU:N	2.40	0.54
1:D:4097:MET:HB3	1:D:4108:ILE:HD13	1.89	0.54
1:A:830:ARG:HH21	1:A:837:PRO:HB3	1.72	0.54
1:A:1712:TYR:OH	1:A:1814:MET:SD	2.66	0.54
1:C:1225:PRO:HG2	1:C:1228:ILE:HB	1.89	0.54
1:B:3719:ASP:HB3	1:B:3722:TYR:HB3	1.89	0.54
1:B:4229:GLU:OE1	1:B:4229:GLU:N	2.41	0.54
1:C:1229:ASN:H	1:C:1827:ARG:HH21	1.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:669:ASP:N	1:D:669:ASP:OD1	2.40	0.54
1:B:669:ASP:N	1:B:669:ASP:OD1	2.40	0.54
1:A:221:ARG:HH21	1:A:259:LEU:HD21	1.73	0.54
1:A:291:LEU:HD12	1:A:299:LEU:HD11	1.90	0.54
1:A:4584:ASP:N	1:A:4584:ASP:OD1	2.41	0.54
1:B:2581:UNK:N	1:B:2899:GLY:O	2.41	0.54
1:D:1739:THR:HG23	1:D:1742:THR:H	1.72	0.54
1:A:1703:LEU:HD23	1:A:1708:ARG:HB2	1.90	0.54
1:B:1251:GLU:OE1	1:B:1251:GLU:N	2.41	0.54
1:C:1739:THR:HG23	1:C:1742:THR:H	1.72	0.54
1:D:2135:LEU:HD13	1:D:3662:ILE:HD13	1.89	0.54
1:B:505:GLU:HG3	1:B:507:ALA:H	1.73	0.53
1:B:4959:PHE:HD2	1:B:4960:ILE:HD13	1.74	0.53
1:D:4060:LYS:HA	1:D:4063:ASP:HB3	1.90	0.53
1:B:196:MET:SD	1:B:196:MET:N	2.82	0.53
1:D:61:ASP:OD1	1:D:61:ASP:N	2.41	0.53
1:C:669:ASP:OD1	1:C:669:ASP:N	2.40	0.53
1:A:317:ARG:NH1	1:A:349:GLN:OE1	2.41	0.53
1:C:4727:LYS:HD2	1:C:4728:HIS:CD2	2.44	0.53
1:B:1644:GLU:OE1	1:B:1646:ARG:NH1	2.42	0.53
1:C:1045:THR:HG23	1:C:1046:LEU:HD23	1.90	0.53
1:A:2447:LYS:HG3	1:A:2449:GLU:H	1.73	0.53
1:B:955:LEU:HD13	1:B:960:MET:HE3	1.90	0.53
1:B:2135:LEU:HD13	1:B:3662:ILE:HD13	1.90	0.53
1:A:3670:GLU:HB3	1:A:3728:ILE:HG23	1.90	0.53
1:A:4963:ILE:HD11	1:A:4967:TYR:HD2	1.73	0.53
1:B:2447:LYS:HG3	1:B:2449:GLU:H	1.73	0.53
1:C:627:PRO:O	1:C:629:ARG:NH1	2.42	0.53
1:D:4039:MET:SD	1:D:4039:MET:N	2.69	0.53
1:B:4978:HIS:CE1	1:B:5027:CYS:SG	3.01	0.53
1:A:2885:THR:HA	1:A:2888:ARG:HE	1.71	0.53
1:B:420:SER:O	1:B:424:LYS:NZ	2.42	0.53
1:C:505:GLU:HG3	1:C:507:ALA:H	1.73	0.53
1:D:947:GLU:N	1:D:947:GLU:OE1	2.42	0.53
1:B:375:LYS:NZ	1:B:376:ALA:O	2.41	0.52
1:C:4068:LEU:HD22	1:C:4111:LEU:HD11	1.91	0.52
1:D:4773:VAL:O	1:D:4777:ILE:HG12	2.09	0.52
1:A:426:ARG:HH22	1:A:503:PHE:HA	1.74	0.52
1:B:5027:CYS:C	1:B:5029:ARG:H	2.13	0.52
1:C:955:LEU:HD22	1:C:960:MET:HG2	1.91	0.52
1:D:420:SER:O	1:D:424:LYS:NZ	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3902:TYR:O	1:D:3906:GLN:NE2	2.42	0.52
1:A:1172:ASP:OD1	1:A:1172:ASP:N	2.37	0.52
1:C:1619:ARG:HA	1:C:1626:TRP:H	1.73	0.52
1:D:2466:LEU:O	1:D:2470:ILE:HD12	2.10	0.52
1:D:353:SER:HB3	1:D:355:LEU:HD22	1.91	0.52
1:D:221:ARG:HH21	1:D:259:LEU:HD21	1.75	0.52
1:D:3768:SER:HA	1:D:3771:HIS:CE1	2.44	0.52
1:B:1619:ARG:HA	1:B:1626:TRP:H	1.74	0.52
1:D:2581:UNK:N	1:D:2899:GLY:O	2.42	0.52
1:D:3889:GLN:HB2	1:D:3964:SER:HA	1.91	0.52
1:B:4985:LEU:HA	1:B:4988:TYR:CD2	2.45	0.52
1:C:34:LYS:H	1:C:53:SER:HB3	1.75	0.52
1:C:5004:THR:OG1	1:C:5005:GLY:N	2.43	0.52
1:D:347:PHE:HA	1:D:388:LEU:HD12	1.92	0.52
1:A:1225:PRO:HG2	1:A:1228:ILE:HB	1.92	0.52
1:D:2188:ASN:C	1:D:2188:ASN:HD22	2.07	0.52
1:A:3768:SER:O	1:A:3772:THR:OG1	2.25	0.52
1:B:4068:LEU:HD22	1:B:4111:LEU:HD11	1.91	0.52
1:C:3777:GLU:O	1:C:3781:GLN:HG3	2.09	0.52
1:D:4902:GLU:OE1	1:D:4902:GLU:N	2.38	0.52
1:A:331:VAL:HG22	1:A:333:GLY:H	1.74	0.52
1:A:4097:MET:HB3	1:A:4108:ILE:HD13	1.92	0.52
1:B:4182:GLU:OE1	1:B:4983:HIS:CD2	2.64	0.51
1:C:1077:ALA:HB3	1:C:1189:LEU:HB3	1.92	0.51
1:A:45:ARG:NH1	1:A:447:ASP:OD2	2.42	0.51
1:C:326:ALA:O	1:C:329:ARG:NH1	2.43	0.51
1:C:4978:HIS:HE1	1:C:4983:HIS:CE1	2.28	0.51
1:D:1115:LEU:HB3	1:D:1123:VAL:HG11	1.92	0.51
1:A:584:LYS:NZ	1:A:624:ASN:OD1	2.42	0.51
1:B:1077:ALA:HB3	1:B:1189:LEU:HB3	1.92	0.51
1:B:4007:SER:OG	1:B:4116:GLU:OE2	2.27	0.51
1:A:4104:THR:HB	1:A:4107:GLU:OE2	2.11	0.51
1:B:4241:THR:O	1:B:4245:MET:HG2	2.10	0.51
1:D:1077:ALA:HB3	1:D:1189:LEU:HB3	1.92	0.51
1:C:4241:THR:O	1:C:4245:MET:HG2	2.10	0.51
1:B:4844:LEU:HD11	1:B:4924:VAL:HG13	1.91	0.51
1:B:4963:ILE:H	1:B:4963:ILE:HD12	1.76	0.51
1:C:1793:GLU:N	1:C:2173:GLN:O	2.44	0.51
1:D:1260:MET:SD	1:D:1271:ARG:NH2	2.84	0.51
1:A:346:CYS:SG	1:A:347:PHE:N	2.83	0.51
1:A:584:LYS:HG2	1:A:624:ASN:HD21	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1644:GLU:OE1	1:D:1646:ARG:NH1	2.43	0.51
1:A:3976:ASN:O	1:A:3980:LEU:HD12	2.11	0.51
1:B:516:LYS:NZ	1:B:555:GLU:O	2.44	0.51
1:B:1028:ASP:N	1:B:1028:ASP:OD1	2.44	0.51
1:B:1793:GLU:N	1:B:2173:GLN:O	2.43	0.51
1:B:2349:ASN:O	1:B:2353:VAL:HG23	2.11	0.51
1:C:4773:VAL:O	1:C:4777:ILE:HG12	2.11	0.51
1:A:4160:LEU:HA	1:A:4163:PHE:HD2	1.76	0.51
1:D:4104:THR:HG22	1:D:4106:PRO:HD2	1.93	0.51
1:D:4976:GLU:O	1:D:4980:LEU:HG	2.11	0.51
1:B:1260:MET:SD	1:B:1271:ARG:NH2	2.85	0.50
1:A:688:LEU:HB3	1:A:712:TYR:HB3	1.92	0.50
1:B:4860:ARG:NH2	1:B:4876:CYS:O	2.43	0.50
1:C:516:LYS:NZ	1:C:555:GLU:O	2.43	0.50
1:A:196:MET:SD	1:A:196:MET:N	2.84	0.50
1:A:960:MET:SD	1:A:960:MET:N	2.84	0.50
1:B:2331:TYR:HD1	1:B:2332:LEU:H	1.59	0.50
1:A:4053:SER:O	1:A:4056:GLU:HG3	2.10	0.50
1:B:4736:ARG:NH1	1:C:4079:ASP:OD2	2.43	0.50
1:C:1644:GLU:OE1	1:C:1646:ARG:NH1	2.42	0.50
1:C:2102:VAL:HG11	1:C:2124:LEU:HD13	1.92	0.50
1:C:2644:UNK:N	1:C:2871:LEU:O	2.44	0.50
1:C:5000:GLU:OE1	1:C:5000:GLU:N	2.37	0.50
1:D:4983:HIS:C	1:D:4985:LEU:H	2.15	0.50
1:A:243:ARG:HD3	1:A:301:VAL:HG23	1.93	0.50
1:B:688:LEU:HB3	1:B:712:TYR:HB3	1.93	0.50
1:C:162:LYS:HG3	1:D:3984:ARG:HH21	1.77	0.50
1:D:4728:HIS:HB3	1:D:4732:PHE:CD2	2.46	0.50
1:D:4977:THR:O	1:D:4981:GLU:HB2	2.11	0.50
1:A:144:GLU:OE1	1:A:144:GLU:N	2.40	0.50
1:B:4968:PHE:HB3	1:B:4975:PHE:N	2.27	0.50
1:A:3904:ARG:HG2	1:A:3905:THR:HG23	1.94	0.50
1:B:1045:THR:HG23	1:B:1046:LEU:HD23	1.92	0.50
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.93	0.50
1:C:633:LEU:HD23	1:C:1639:LEU:HD11	1.93	0.50
1:A:221:ARG:NH1	1:A:253:CYS:O	2.44	0.50
1:A:1108:GLU:N	1:A:1108:GLU:OE2	2.45	0.50
1:B:830:ARG:HH21	1:B:837:PRO:HB3	1.76	0.50
1:B:3768:SER:HA	1:B:3771:HIS:CE1	2.47	0.50
1:D:1084:GLN:NE2	1:D:1186:ASP:O	2.45	0.50
1:D:1152:MET:HG3	1:D:1161:ILE:HB	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:ASP:OD1	1:A:1028:ASP:N	2.44	0.50
1:D:2165:LEU:HD12	1:D:2168:VAL:HB	1.94	0.50
1:A:3969:ILE:HD12	1:A:4030:LEU:HD13	1.93	0.50
1:B:61:ASP:OD1	1:B:61:ASP:N	2.41	0.49
1:C:4017:LEU:HD22	1:C:4139:ILE:HG21	1.93	0.49
1:D:955:LEU:HD22	1:D:960:MET:HG2	1.93	0.49
1:B:101:LEU:HD23	1:B:163:VAL:HG21	1.94	0.49
1:B:3777:GLU:O	1:B:3781:GLN:HG3	2.12	0.49
1:C:947:GLU:N	1:C:947:GLU:OE1	2.45	0.49
1:D:126:SER:HB3	1:D:132:ALA:HB2	1.95	0.49
1:D:4057:MET:HA	1:D:4060:LYS:HG2	1.93	0.49
1:D:4963:ILE:HD12	1:D:4963:ILE:H	1.77	0.49
1:A:4161:ARG:O	1:A:4165:GLU:HG2	2.12	0.49
1:D:4017:LEU:HD22	1:D:4139:ILE:HG21	1.94	0.49
1:D:4546:VAL:HA	1:D:4549:VAL:HG22	1.94	0.49
1:A:684:VAL:HG12	1:A:781:VAL:HG22	1.94	0.49
1:C:3916:ILE:HG21	1:C:3980:LEU:HD11	1.95	0.49
1:D:4820:VAL:HB	1:D:4823:LEU:HB2	1.94	0.49
1:A:4837:LEU:O	1:A:4840:THR:OG1	2.23	0.49
1:C:1700:ASP:OD1	1:C:1700:ASP:N	2.46	0.49
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.31	0.49
1:A:669:ASP:HA	1:A:740:PRO:HA	1.94	0.49
1:A:1204:LEU:HD12	1:A:1226:PHE:HB3	1.95	0.49
1:A:2208:MET:O	1:A:2212:VAL:HG23	2.12	0.49
1:A:3780:LEU:HD11	1:A:3816:MET:HG3	1.94	0.49
1:B:3889:GLN:HB2	1:B:3964:SER:HA	1.95	0.49
1:D:4049:VAL:HG21	1:D:4159:ARG:HD2	1.94	0.49
1:B:2897:LYS:O	1:B:2897:LYS:NZ	2.45	0.49
1:D:3829:PHE:HB2	1:D:3913:ILE:HD13	1.95	0.49
1:A:126:SER:HB3	1:A:132:ALA:HB2	1.95	0.49
1:C:2187:ASN:OD1	1:C:2187:ASN:N	2.46	0.49
1:D:632:LEU:O	1:D:634:GLN:NE2	2.45	0.49
1:D:4982:GLU:O	1:D:4983:HIS:HB2	2.12	0.49
1:A:4966:ASP:C	1:A:4968:PHE:N	2.65	0.49
1:B:1220:GLN:HG3	1:C:3524:UNK:HA	1.95	0.49
1:B:4773:VAL:O	1:B:4777:ILE:HG12	2.13	0.49
1:C:1095:VAL:HB	1:C:1199:VAL:HB	1.95	0.49
1:C:1260:MET:SD	1:C:1271:ARG:NH2	2.86	0.49
1:C:4089:SER:OG	1:C:4092:ASP:OD1	2.31	0.49
1:D:355:LEU:HD11	1:D:378:LEU:HB3	1.94	0.49
1:B:4055:VAL:O	1:B:4059:LEU:HD12	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1147:ASP:HB3	1:C:1164:LEU:HD11	1.95	0.48
1:C:2267:MET:SD	1:C:2267:MET:N	2.86	0.48
1:C:4984:ASN:OD1	1:C:4987:ASN:HB2	2.13	0.48
1:B:1865:MET:HG3	1:B:1866:ILE:HG12	1.94	0.48
1:C:1220:GLN:HG3	1:D:3524:UNK:HA	1.94	0.48
1:A:633:LEU:HD23	1:A:1639:LEU:HD11	1.95	0.48
1:A:1208:VAL:HA	1:A:1211:LEU:HD12	1.95	0.48
1:A:3717:ASP:OD1	1:A:3717:ASP:N	2.41	0.48
1:D:669:ASP:HA	1:D:740:PRO:HA	1.95	0.48
1:A:5004:THR:OG1	1:A:5005:GLY:N	2.45	0.48
1:B:4960:ILE:HD12	1:B:4988:TYR:CE2	2.48	0.48
1:D:4097:MET:HG3	1:D:4108:ILE:HG23	1.95	0.48
1:B:1700:ASP:N	1:B:1700:ASP:OD1	2.46	0.48
1:B:2649:UNK:H	1:B:2869:ARG:HE	1.61	0.48
1:B:4057:MET:HA	1:B:4060:LYS:HG2	1.96	0.48
1:B:4546:VAL:HA	1:B:4549:VAL:HG22	1.94	0.48
1:C:928:THR:O	1:C:932:LEU:HD12	2.14	0.48
1:C:3733:CYS:SG	1:C:3803:SER:OG	2.68	0.48
1:B:5028:PHE:CE1	1:B:5032:TYR:HB2	2.48	0.48
1:A:572:PRO:HA	1:A:575:LEU:HD13	1.96	0.48
1:C:618:GLN:OE1	1:C:1678:ASN:ND2	2.43	0.48
1:C:1028:ASP:OD1	1:C:1028:ASP:N	2.44	0.48
1:D:1028:ASP:OD1	1:D:1028:ASP:N	2.44	0.48
1:A:330:ASP:N	1:A:330:ASP:OD1	2.46	0.48
1:A:2314:LEU:HA	1:A:2318:TYR:HB2	1.95	0.48
1:B:3524:UNK:HA	1:A:1220:GLN:HG3	1.96	0.48
1:C:669:ASP:HA	1:C:740:PRO:HA	1.96	0.48
1:C:4546:VAL:HA	1:C:4549:VAL:HG22	1.95	0.48
1:D:162:LYS:HG3	1:A:3984:ARG:HH12	1.78	0.48
1:B:2118:ARG:NH2	1:B:3719:ASP:OD1	2.43	0.48
1:D:2196:ASN:OD1	1:D:2199:ARG:NH2	2.46	0.48
1:A:1695:LEU:HD22	1:A:1810:LYS:HE2	1.94	0.48
1:A:2187:ASN:OD1	1:A:2187:ASN:N	2.46	0.48
1:A:4976:GLU:H	1:A:4976:GLU:CD	2.16	0.48
1:B:4985:LEU:H	1:B:4985:LEU:HG	1.40	0.48
1:C:221:ARG:NH1	1:C:253:CYS:O	2.47	0.48
1:C:1084:GLN:NE2	1:C:1186:ASP:O	2.47	0.48
1:B:669:ASP:HA	1:B:740:PRO:HA	1.95	0.47
1:B:1084:GLN:NE2	1:B:1186:ASP:O	2.47	0.47
1:C:35:LEU:HB3	1:C:49:LEU:HB3	1.95	0.47
1:A:4124:ASN:HB3	1:A:4127:GLU:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASP:N	1:B:18:ASP:OD1	2.47	0.47
1:B:2922:LYS:HB3	1:B:2922:LYS:HE3	1.65	0.47
1:A:101:LEU:HD23	1:A:163:VAL:HG21	1.96	0.47
1:B:2581:UNK:HA	1:B:2895:GLU:HG3	1.96	0.47
1:C:4222:VAL:HG21	1:C:4950:VAL:HG23	1.95	0.47
1:D:18:ASP:N	1:D:18:ASP:OD1	2.47	0.47
1:B:633:LEU:HD23	1:B:1639:LEU:HD11	1.96	0.47
1:B:4813:LEU:HA	1:B:4816:ILE:HG22	1.97	0.47
1:A:1700:ASP:OD1	1:A:1700:ASP:N	2.45	0.47
1:B:1927:LEU:HD13	1:B:2101:MET:HG3	1.96	0.47
1:C:1717:SER:HA	1:C:1721:GLU:HB2	1.97	0.47
1:C:4931:ILE:HG22	1:D:4936:ILE:HG21	1.96	0.47
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.95	0.47
1:D:4152:GLU:OE2	1:D:4194:TYR:OH	2.32	0.47
1:A:78:LEU:HA	1:A:81:MET:HG2	1.96	0.47
1:A:1619:ARG:HA	1:A:1626:TRP:H	1.79	0.47
1:C:700:GLU:HG2	1:C:709:ASP:HB3	1.96	0.47
1:D:665:GLU:HB2	1:D:792:LEU:HD12	1.97	0.47
1:D:935:LEU:HD11	1:D:1053:ILE:HG13	1.96	0.47
1:D:2187:ASN:OD1	1:D:2187:ASN:N	2.46	0.47
1:D:4813:LEU:HA	1:D:4816:ILE:HG22	1.94	0.47
1:A:4985:LEU:O	1:A:4988:TYR:HB2	2.15	0.47
1:B:35:LEU:HB3	1:B:49:LEU:HB3	1.95	0.47
1:B:700:GLU:HG2	1:B:709:ASP:HB3	1.97	0.47
1:B:2644:UNK:N	1:B:2871:LEU:O	2.39	0.47
1:C:21:VAL:HB	1:C:205:ILE:HD11	1.96	0.47
1:C:1158:ASN:HB3	1:C:1182:ILE:HG22	1.96	0.47
1:D:874:LEU:HD21	1:D:929:LEU:HD11	1.96	0.47
1:D:2442:LEU:HD23	1:D:2443:ILE:H	1.79	0.47
1:D:4728:HIS:HB2	1:D:4737:ILE:HD11	1.95	0.47
1:D:4983:HIS:C	1:D:4985:LEU:N	2.68	0.47
1:A:578:ILE:HD12	1:A:578:ILE:H	1.78	0.47
1:A:4675:LYS:HB3	1:A:4675:LYS:HE3	1.78	0.47
1:C:517:GLU:O	1:C:521:LEU:HG	2.15	0.47
1:C:3751:VAL:HG13	1:C:3755:GLU:HB2	1.95	0.47
1:C:4984:ASN:O	1:C:4985:LEU:HB2	2.15	0.47
1:D:35:LEU:HB3	1:D:49:LEU:HB3	1.97	0.47
1:B:2267:MET:HE2	1:B:2267:MET:H	1.80	0.47
1:D:688:LEU:HB3	1:D:712:TYR:HB3	1.96	0.47
1:D:1793:GLU:N	1:D:2173:GLN:O	2.47	0.47
1:D:4555:LEU:HD11	1:D:4656:LEU:HD22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:GLU:HG2	1:A:709:ASP:HB3	1.96	0.47
1:B:2332:LEU:HD11	1:B:2428:ALA:HB1	1.97	0.47
1:B:3713:LYS:HZ3	1:B:3715:LYS:H	1.63	0.47
1:B:3751:VAL:HG13	1:B:3755:GLU:HB2	1.96	0.47
1:B:2196:ASN:OD1	1:B:2199:ARG:NH2	2.48	0.46
1:B:2288:LEU:HD23	1:B:3849:ARG:HB3	1.97	0.46
1:C:701:GLY:HA2	1:C:1646:ARG:HA	1.97	0.46
1:C:4828:SER:O	1:C:4832:HIS:HB2	2.15	0.46
1:C:4963:ILE:HD12	1:C:4963:ILE:H	1.79	0.46
1:B:4778:TRP:O	1:B:4782:VAL:HG23	2.15	0.46
1:C:355:LEU:HD11	1:C:378:LEU:HB3	1.96	0.46
1:C:684:VAL:HG12	1:C:781:VAL:HG22	1.97	0.46
1:C:3733:CYS:HG	1:C:3803:SER:HG	1.58	0.46
1:D:4558:ASN:O	1:D:4561:THR:OG1	2.32	0.46
1:A:18:ASP:OD1	1:A:18:ASP:N	2.48	0.46
1:A:4692:PRO:HD2	1:A:4703:ARG:HH22	1.79	0.46
1:B:665:GLU:HB2	1:B:792:LEU:HD12	1.97	0.46
1:B:701:GLY:HA2	1:B:1646:ARG:HA	1.97	0.46
1:B:4774:LYS:HE2	1:B:4774:LYS:HB3	1.74	0.46
1:B:4902:GLU:OE1	1:B:4902:GLU:N	2.42	0.46
1:C:18:ASP:OD1	1:C:18:ASP:N	2.47	0.46
1:C:2442:LEU:HD23	1:C:2443:ILE:H	1.80	0.46
1:C:4727:LYS:HE2	1:C:4727:LYS:HB3	1.43	0.46
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.97	0.46
1:C:4704:LEU:HD11	1:C:4778:TRP:HB2	1.98	0.46
1:D:4712:PRO:HB2	1:D:4718:LYS:HD2	1.96	0.46
1:A:1110:ARG:HG2	1:A:1110:ARG:HH11	1.80	0.46
1:B:632:LEU:O	1:B:634:GLN:NE2	2.48	0.46
1:C:663:TYR:HB3	1:C:809:ALA:HB2	1.98	0.46
1:C:4976:GLU:HG3	1:C:4977:THR:N	2.31	0.46
1:D:4204:GLN:HB2	1:D:4245:MET:HE1	1.98	0.46
1:A:2114:PRO:HA	1:A:2117:VAL:HG12	1.98	0.46
1:A:4055:VAL:O	1:A:4059:LEU:HG	2.16	0.46
1:B:2442:LEU:HD23	1:B:2443:ILE:H	1.81	0.46
1:C:2679:UNK:HA	1:C:2741:GLU:HA	1.98	0.46
1:C:4007:SER:OG	1:C:4116:GLU:OE2	2.33	0.46
1:D:126:SER:OG	1:D:130:LYS:O	2.33	0.46
1:D:3989:VAL:O	1:D:3993:LEU:HG	2.15	0.46
1:B:618:GLN:OE1	1:B:1678:ASN:ND2	2.44	0.46
1:B:1106:ARG:NH1	1:B:1184:ILE:O	2.48	0.46
1:B:1717:SER:HA	1:B:1721:GLU:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:618:GLN:OE1	1:D:1678:ASN:ND2	2.46	0.46
1:A:1147:ASP:OD1	1:A:1165:ASN:ND2	2.42	0.46
1:A:3775:ALA:HA	1:A:3778:MET:HG3	1.97	0.46
1:A:3844:LEU:O	1:A:3848:GLU:HG2	2.15	0.46
1:B:517:GLU:O	1:B:521:LEU:HG	2.16	0.46
1:B:4629:TYR:OH	1:A:4860:ARG:NH2	2.44	0.46
1:B:4856:PHE:HA	1:B:4860:ARG:HB2	1.98	0.46
1:D:1157:GLU:OE1	1:D:1159:THR:OG1	2.29	0.46
1:D:2581:UNK:HA	1:D:2895:GLU:HG3	1.96	0.46
1:A:701:GLY:HA2	1:A:1646:ARG:HA	1.97	0.46
1:A:3811:GLU:HA	1:A:3814:GLN:HG3	1.98	0.46
1:A:4733:GLY:H	1:A:4736:ARG:HD3	1.81	0.46
1:C:665:GLU:HB2	1:C:792:LEU:HD12	1.98	0.46
1:D:4961:CYS:HB2	1:D:4963:ILE:HD12	1.98	0.46
1:A:4976:GLU:HB2	1:A:4980:LEU:HD23	1.98	0.46
1:B:4961:CYS:HB2	1:B:4963:ILE:HD12	1.97	0.46
1:B:5029:ARG:O	1:B:5033:GLU:HB3	2.16	0.46
1:D:608:VAL:HG22	1:D:613:ALA:HB2	1.98	0.46
1:D:955:LEU:HD13	1:D:960:MET:HE3	1.98	0.46
1:D:1865:MET:HG3	1:D:1866:ILE:HG12	1.97	0.46
1:A:61:ASP:OD1	1:A:61:ASP:N	2.43	0.46
1:B:4067:LYS:HD2	1:B:4102:GLN:HB3	1.98	0.45
1:C:4056:GLU:HA	1:C:4059:LEU:HG	1.97	0.45
1:C:4658:ILE:HD12	1:C:4792:LEU:HD12	1.97	0.45
1:C:4774:LYS:HE2	1:C:4774:LYS:HB3	1.74	0.45
1:D:1856:ASP:OD1	1:D:1856:ASP:N	2.49	0.45
1:B:4060:LYS:HE2	1:B:4060:LYS:HB2	1.86	0.45
1:B:4712:PRO:HB2	1:B:4718:LYS:HD2	1.98	0.45
1:C:4813:LEU:HA	1:C:4816:ILE:HG22	1.98	0.45
1:D:700:GLU:HG2	1:D:709:ASP:HB3	1.97	0.45
1:B:27:THR:HB	1:B:33:LEU:HB2	1.98	0.45
1:B:3951:PHE:O	1:B:3955:MET:HG3	2.16	0.45
1:C:3877:ASP:HB2	1:C:3880:PHE:HB3	1.98	0.45
1:C:4191:GLU:OE2	1:C:4191:GLU:N	2.49	0.45
1:D:4980:LEU:HG	1:D:4980:LEU:H	1.59	0.45
1:A:4053:SER:O	1:A:4057:MET:HG2	2.15	0.45
1:B:221:ARG:HH21	1:B:259:LEU:HD21	1.81	0.45
1:C:3823:LYS:HA	1:C:3823:LYS:HD3	1.63	0.45
1:A:5013:MET:HG3	1:A:5018:CYS:HB3	1.98	0.45
1:B:4903:ASP:OD1	1:B:4903:ASP:N	2.47	0.45
1:C:286:THR:HG23	1:C:287:THR:HG23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2285:GLU:HG2	1:D:2286:LEU:HG	1.98	0.45
1:A:472:ARG:NH1	1:A:475:GLN:OE1	2.47	0.45
1:A:3716:LEU:HD12	1:A:3716:LEU:H	1.81	0.45
1:B:286:THR:HG23	1:B:287:THR:HG23	1.99	0.45
1:C:707:VAL:HG13	1:C:713:SER:HB3	1.99	0.45
1:C:1385:UNK:HA	1:C:1396:UNK:HA	1.99	0.45
1:C:1769:THR:HG23	1:C:1956:GLU:HG2	1.99	0.45
1:D:286:THR:HG23	1:D:287:THR:HG23	1.97	0.45
1:D:957:LYS:HA	1:D:960:MET:HB2	1.98	0.45
1:D:4007:SER:OG	1:D:4116:GLU:OE2	2.34	0.45
1:A:2581:UNK:HA	1:A:2895:GLU:HG3	1.97	0.45
1:B:4980:LEU:HB3	1:B:4981:GLU:CD	2.37	0.45
1:C:61:ASP:OD1	1:C:61:ASP:N	2.41	0.45
1:C:4214:LYS:O	1:C:4218:ILE:HG13	2.16	0.45
1:C:4239:GLU:OE1	1:C:5014:TYR:OH	2.35	0.45
1:C:4903:ASP:OD1	1:C:4903:ASP:N	2.48	0.45
1:D:3719:ASP:O	1:D:3723:MET:HG2	2.16	0.45
1:B:2285:GLU:HG2	1:B:2286:LEU:HG	1.97	0.45
1:B:3823:LYS:HA	1:B:3823:LYS:HD3	1.63	0.45
1:C:442:ILE:O	1:C:446:GLN:HG2	2.17	0.45
1:C:866:HIS:O	1:C:869:ARG:NH1	2.46	0.45
1:D:663:TYR:HB3	1:D:809:ALA:HB2	1.99	0.45
1:D:4730:ASP:OD1	1:A:4101:LYS:HD3	2.17	0.45
1:A:1952:GLN:O	1:A:1956:GLU:HG2	2.16	0.45
1:A:2297:LYS:O	1:A:2300:SER:OG	2.31	0.45
1:C:3696:ASP:O	1:C:3700:GLN:HG3	2.17	0.45
1:D:2868:SER:O	1:D:2872:GLN:NE2	2.49	0.45
1:D:4774:LYS:HE2	1:D:4774:LYS:HB3	1.73	0.45
1:D:4963:ILE:HB	1:D:4968:PHE:HE1	1.81	0.45
1:C:306:LYS:HE2	1:C:306:LYS:HB3	1.86	0.45
1:C:632:LEU:O	1:C:634:GLN:NE2	2.50	0.45
1:C:1166:GLY:HA2	1:C:1216:ILE:HD13	1.99	0.45
1:D:2897:LYS:O	1:D:2897:LYS:NZ	2.48	0.45
1:D:3921:ASP:O	1:D:3925:ARG:HG3	2.16	0.45
1:B:500:ALA:HB1	1:B:505:GLU:HB2	1.98	0.44
1:B:4844:LEU:HD22	1:B:4928:LEU:HG	1.98	0.44
1:B:4960:ILE:H	1:B:4960:ILE:HG12	1.62	0.44
1:C:266:ARG:NH2	1:C:269:TRP:O	2.50	0.44
1:C:4067:LYS:HB2	1:C:4103:PHE:CE1	2.52	0.44
1:C:4182:GLU:HG2	1:C:4192:ARG:HG3	1.98	0.44
1:A:1094:ALA:HB3	1:A:1143:TRP:HE1	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2465:ASP:O	1:A:2469:ILE:HG12	2.17	0.44
1:A:4774:LYS:HE2	1:A:4774:LYS:HB3	1.73	0.44
1:B:663:TYR:HB3	1:B:809:ALA:HB2	2.00	0.44
1:B:914:PRO:O	1:B:918:ARG:HG3	2.17	0.44
1:B:4820:VAL:HB	1:B:4823:LEU:HB2	1.98	0.44
1:C:1106:ARG:NH1	1:C:1184:ILE:O	2.51	0.44
1:C:4791:TYR:OH	1:C:4815:ASP:O	2.35	0.44
1:D:231:LEU:HD12	1:D:245:VAL:HG11	1.99	0.44
1:A:2922:LYS:HB3	1:A:2922:LYS:HE3	1.67	0.44
1:A:3719:ASP:O	1:A:3723:MET:HG2	2.17	0.44
1:A:4207:MET:HB2	1:A:4210:VAL:HG23	1.99	0.44
1:B:583:ILE:HD12	1:B:621:ILE:HD11	1.99	0.44
1:B:1385:UNK:HA	1:B:1396:UNK:HA	1.99	0.44
1:B:1856:ASP:OD1	1:B:1856:ASP:N	2.49	0.44
1:C:553:ARG:HH21	1:C:1593:PRO:HG3	1.82	0.44
1:B:551:LEU:HG	1:B:589:LEU:HD22	1.99	0.44
1:C:2254:LEU:HD11	1:C:2334:PHE:HZ	1.82	0.44
1:D:4161:ARG:O	1:D:4165:GLU:HG2	2.17	0.44
1:A:2099:SER:O	1:A:2103:VAL:HG22	2.17	0.44
1:A:2261:SER:HA	1:A:2272:PRO:HG2	1.99	0.44
1:A:2466:LEU:O	1:A:2470:ILE:HD12	2.18	0.44
1:B:4105:GLY:O	1:B:4109:GLN:NE2	2.50	0.44
1:C:1856:ASP:N	1:C:1856:ASP:OD1	2.49	0.44
1:C:2145:SER:O	1:C:2148:SER:OG	2.35	0.44
1:C:4207:MET:HB2	1:C:4210:VAL:HG23	2.00	0.44
1:D:684:VAL:HG12	1:D:781:VAL:HG22	1.98	0.44
1:D:2254:LEU:HD11	1:D:2334:PHE:HZ	1.82	0.44
1:D:3877:ASP:HB2	1:D:3880:PHE:HB3	1.99	0.44
1:A:553:ARG:HH21	1:A:1593:PRO:HG3	1.83	0.44
1:A:4976:GLU:O	1:A:4980:LEU:N	2.44	0.44
1:B:4235:VAL:O	1:B:4239:GLU:HG2	2.16	0.44
1:C:27:THR:HB	1:C:33:LEU:HB2	2.00	0.44
1:C:1671:ARG:O	1:C:1675:ALA:HB2	2.17	0.44
1:D:516:LYS:HE2	1:D:516:LYS:HB3	1.66	0.44
1:D:580:GLU:O	1:D:584:LYS:HG2	2.18	0.44
1:D:879:HIS:CE1	1:D:921:ASN:HD22	2.35	0.44
1:B:975:VAL:HB	1:B:1047:LEU:HD21	2.00	0.44
1:B:1225:PRO:HG2	1:B:1228:ILE:HB	2.00	0.44
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.42	0.44
1:B:4675:LYS:HB3	1:B:4675:LYS:HE3	1.81	0.44
1:D:786:GLY:N	1:D:1630:CYS:O	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLN:O	1:A:309:THR:OG1	2.30	0.44
1:A:2145:SER:O	1:A:2148:SER:OG	2.31	0.44
1:A:4704:LEU:HD11	1:A:4778:TRP:HB2	2.00	0.44
1:B:3696:ASP:O	1:B:3700:GLN:HG3	2.17	0.44
1:C:521:LEU:HA	1:C:524:GLU:HG3	2.00	0.44
1:D:263:GLU:HG3	1:D:281:ARG:HG3	2.00	0.44
1:D:737:LEU:HD12	1:D:737:LEU:HA	1.86	0.44
1:B:2382:GLU:O	1:B:2386:ILE:HG23	2.17	0.44
1:B:3877:ASP:HB2	1:B:3880:PHE:HB3	2.00	0.44
1:D:883:ALA:O	1:D:887:ILE:HG13	2.18	0.44
1:C:126:SER:OG	1:C:130:LYS:O	2.30	0.43
1:C:500:ALA:HB1	1:C:505:GLU:HB2	2.00	0.43
1:C:2285:GLU:HG2	1:C:2286:LEU:HG	1.98	0.43
1:D:4207:MET:HB2	1:D:4210:VAL:HG23	2.00	0.43
1:A:957:LYS:HA	1:A:960:MET:HG2	1.99	0.43
1:D:1769:THR:HG23	1:D:1956:GLU:HG2	1.99	0.43
1:D:2297:LYS:O	1:D:2300:SER:OG	2.29	0.43
1:A:178:ARG:HE	1:A:195:PHE:HE1	1.65	0.43
1:A:2159:LEU:HD12	1:A:2159:LEU:HA	1.84	0.43
1:A:2897:LYS:O	1:A:2897:LYS:NZ	2.47	0.43
1:B:317:ARG:HH22	1:B:323:LEU:H	1.65	0.43
1:B:1077:ALA:HB2	1:B:1190:PRO:HG2	1.99	0.43
1:B:4207:MET:HB2	1:B:4210:VAL:HG23	2.00	0.43
1:C:955:LEU:HD13	1:C:960:MET:HE3	2.00	0.43
1:C:5036:LEU:H	1:C:5036:LEU:HD23	1.83	0.43
1:D:3811:GLU:HA	1:D:3814:GLN:HG3	2.00	0.43
1:B:4101:LYS:HG3	1:A:4730:ASP:OD2	2.19	0.43
1:B:4821:LYS:O	1:B:4825:THR:OG1	2.33	0.43
1:C:1581:LEU:HD12	1:C:1581:LEU:HA	1.91	0.43
1:C:1842:LEU:HD23	1:C:1842:LEU:HA	1.90	0.43
1:C:1931:LEU:HB2	1:C:1936:LYS:HE3	2.00	0.43
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	2.00	0.43
1:D:2205:GLU:O	1:D:2209:GLU:HG3	2.18	0.43
1:D:3834:ALA:O	1:D:3838:THR:HG22	2.19	0.43
1:A:353:SER:HB3	1:A:355:LEU:HD23	1.99	0.43
1:A:3696:ASP:N	1:A:3696:ASP:OD1	2.50	0.43
1:A:3823:LYS:HA	1:A:3823:LYS:HD3	1.62	0.43
1:B:4156:HIS:HB3	1:B:5036:LEU:HD11	2.00	0.43
1:C:4865:LYS:HA	1:C:4865:LYS:HD2	1.79	0.43
1:D:459:LEU:HD23	1:D:459:LEU:H	1.83	0.43
1:D:870:ILE:HG13	1:D:873:LYS:HD3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:VAL:HG13	1:A:713:SER:HB2	1.99	0.43
1:A:781:VAL:HG12	1:A:783:PHE:HD2	1.84	0.43
1:A:3820:LEU:HD23	1:A:3820:LEU:HA	1.90	0.43
1:B:355:LEU:HD11	1:B:378:LEU:HB3	2.00	0.43
1:C:2176:ASN:O	1:C:2180:GLN:HG2	2.18	0.43
1:D:5012:LYS:O	1:D:5016:GLU:HG2	2.19	0.43
1:A:1717:SER:HA	1:A:1721:GLU:HB2	2.01	0.43
1:B:1742:THR:HG1	1:B:1769:THR:HG1	1.67	0.43
1:C:3768:SER:HA	1:C:3771:HIS:CE1	2.53	0.43
1:D:27:THR:HB	1:D:33:LEU:HB2	2.01	0.43
1:D:4025:VAL:HA	1:D:4028:LEU:HG	2.01	0.43
1:D:4903:ASP:OD1	1:D:4903:ASP:N	2.47	0.43
1:A:545:ASP:OD1	1:A:582:HIS:NE2	2.52	0.43
1:A:786:GLY:N	1:A:1630:CYS:O	2.51	0.43
1:A:1613:LEU:HD23	1:A:1634:LEU:HD12	2.00	0.43
1:B:1204:LEU:HD12	1:B:1226:PHE:HB3	2.00	0.43
1:B:1925:GLY:N	1:B:1928:GLN:OE1	2.49	0.43
1:C:4149:ASN:HD22	1:C:4194:TYR:HE2	1.67	0.43
1:A:265:LEU:HD12	1:A:265:LEU:H	1.84	0.43
1:A:2335:LEU:O	1:A:2339:VAL:HG22	2.19	0.43
1:A:4686:LEU:HD23	1:A:4686:LEU:HA	1.86	0.43
1:B:385:ASP:OD1	1:B:385:ASP:N	2.52	0.43
1:C:231:LEU:HD12	1:C:245:VAL:HG11	2.01	0.43
1:C:4973:HIS:NE2	1:C:4976:GLU:HG2	2.34	0.43
1:D:196:MET:SD	1:D:196:MET:N	2.92	0.43
1:D:394:GLN:NE2	1:D:396:GLU:H	2.16	0.43
1:D:1106:ARG:NH1	1:D:1184:ILE:O	2.48	0.43
1:A:4966:ASP:O	1:A:4968:PHE:N	2.52	0.43
1:B:4017:LEU:HD22	1:B:4139:ILE:HG21	2.00	0.43
1:B:4182:GLU:OE1	1:B:4983:HIS:HD2	2.02	0.43
1:D:4821:LYS:O	1:D:4825:THR:OG1	2.27	0.43
1:A:2442:LEU:HD23	1:A:2443:ILE:H	1.83	0.43
1:A:3921:ASP:OD1	1:A:3922:TYR:N	2.52	0.43
1:B:243:ARG:HA	1:B:243:ARG:HD3	1.78	0.42
1:B:707:VAL:HG13	1:B:713:SER:HB2	1.99	0.42
1:B:2205:GLU:O	1:B:2209:GLU:HG3	2.19	0.42
1:B:4978:HIS:C	1:B:4980:LEU:H	2.21	0.42
1:C:196:MET:SD	1:C:196:MET:N	2.91	0.42
1:C:688:LEU:HB3	1:C:712:TYR:HB3	1.99	0.42
1:D:4214:LYS:O	1:D:4218:ILE:HG13	2.19	0.42
1:A:320:LYS:HD2	1:A:320:LYS:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1619:ARG:O	1:A:1625:GLY:N	2.52	0.42
1:D:4542:GLY:O	1:D:4546:VAL:HG13	2.19	0.42
1:A:692:TYR:HD1	1:A:826:ILE:HD12	1.83	0.42
1:A:2189:LYS:HE2	1:A:2189:LYS:HB2	1.87	0.42
1:A:3963:ASN:O	1:A:3966:THR:OG1	2.37	0.42
1:B:608:VAL:HG22	1:B:613:ALA:HB2	2.01	0.42
1:C:957:LYS:HA	1:C:960:MET:HB2	2.01	0.42
1:C:1077:ALA:HB2	1:C:1190:PRO:HG2	2.00	0.42
1:C:2335:LEU:O	1:C:2339:VAL:HG13	2.19	0.42
1:C:4555:LEU:HD12	1:C:4555:LEU:HA	1.88	0.42
1:C:4675:LYS:HB3	1:C:4675:LYS:HE3	1.82	0.42
1:D:109:LEU:HD12	1:D:118:LEU:HD22	2.01	0.42
1:D:1077:ALA:HB2	1:D:1190:PRO:HG2	2.00	0.42
1:A:774:ASP:N	1:A:774:ASP:OD1	2.49	0.42
1:A:4844:LEU:O	1:A:4848:VAL:HG23	2.19	0.42
1:B:126:SER:OG	1:B:130:LYS:O	2.35	0.42
1:B:4870:ASP:OD1	1:B:4870:ASP:N	2.53	0.42
1:C:4985:LEU:O	1:C:4988:TYR:HB2	2.19	0.42
1:D:178:ARG:HB3	1:D:193:ALA:HB1	2.02	0.42
1:A:4813:LEU:HA	1:A:4816:ILE:HG22	2.01	0.42
1:A:4961:CYS:SG	1:A:4963:ILE:HG23	2.41	0.42
1:B:1712:TYR:OH	1:B:1814:MET:SD	2.77	0.42
1:C:758:ARG:HG2	1:C:762:CYS:HA	2.02	0.42
1:C:2581:UNK:HA	1:C:2895:GLU:HG3	2.01	0.42
1:C:4680:LYS:HD2	1:C:4686:LEU:HD11	2.01	0.42
1:C:4712:PRO:HB2	1:C:4718:LYS:HD2	2.01	0.42
1:D:1676:LEU:HD23	1:D:1676:LEU:HA	1.87	0.42
1:A:530:ILE:HD13	1:A:530:ILE:HA	1.91	0.42
1:A:1072:VAL:HG12	1:A:1195:GLY:HA2	2.01	0.42
1:A:1712:TYR:O	1:A:1716:ILE:HG23	2.19	0.42
1:C:3755:GLU:O	1:C:3759:GLU:HG2	2.20	0.42
1:C:5033:GLU:OE1	1:C:5033:GLU:N	2.44	0.42
1:D:500:ALA:HB1	1:D:505:GLU:HB2	2.01	0.42
1:A:385:ASP:OD1	1:A:385:ASP:N	2.52	0.42
1:A:866:HIS:O	1:A:869:ARG:NH1	2.52	0.42
1:A:2694:UNK:HA	1:A:2929:PHE:HE1	1.84	0.42
1:B:2189:LYS:HB2	1:B:2189:LYS:HE2	1.87	0.42
1:C:3889:GLN:HB2	1:C:3964:SER:HA	2.00	0.42
1:D:707:VAL:HG13	1:D:713:SER:HB2	2.00	0.42
1:D:4966:ASP:OD1	1:D:4967:TYR:N	2.52	0.42
1:B:550:LYS:HB3	1:B:560:ILE:HG12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4555:LEU:HD11	1:C:4656:LEU:HB3	2.01	0.42
1:D:4703:ARG:HA	1:D:4706:LEU:HD12	2.02	0.42
1:D:4750:ILE:HD13	1:D:4750:ILE:HA	1.96	0.42
1:A:294:THR:HG23	1:A:295:GLU:H	1.84	0.42
1:A:580:GLU:O	1:A:584:LYS:HG3	2.19	0.42
1:B:2145:SER:O	1:B:2148:SER:OG	2.38	0.42
1:B:3670:GLU:HG2	1:B:3728:ILE:HA	2.01	0.42
1:C:1712:TYR:OH	1:C:1814:MET:SD	2.77	0.42
1:C:4962:GLY:H	1:C:5025:GLY:HA2	1.85	0.42
1:D:4160:LEU:O	1:D:4164:LEU:HD23	2.20	0.42
1:D:4857:ASN:HD21	1:A:4807:PHE:HB2	1.85	0.42
1:B:121:LEU:HB3	1:B:123:THR:HG22	2.02	0.42
1:B:4542:GLY:O	1:B:4546:VAL:HG13	2.19	0.42
1:C:221:ARG:HH21	1:C:259:LEU:HD21	1.85	0.42
1:C:1676:LEU:HA	1:C:1725:ARG:HH22	1.85	0.42
1:C:1763:PRO:HG3	1:C:2094:LEU:HD22	2.01	0.42
1:C:4816:ILE:HD12	1:C:4816:ILE:HA	1.90	0.42
1:D:1927:LEU:HB3	1:D:2104:ARG:HH22	1.85	0.42
1:D:1969:LEU:HD21	1:D:2009:LEU:HD11	2.01	0.42
1:D:3696:ASP:O	1:D:3700:GLN:HG3	2.20	0.42
1:D:4555:LEU:HD23	1:D:4555:LEU:HA	1.89	0.42
1:A:3768:SER:HA	1:A:3771:HIS:ND1	2.35	0.42
1:B:553:ARG:HH21	1:B:1593:PRO:HG3	1.84	0.41
1:B:883:ALA:O	1:B:887:ILE:HG13	2.20	0.41
1:B:915:GLU:HA	1:B:918:ARG:HD3	2.02	0.41
1:C:626:LEU:HD11	1:C:630:GLU:H	1.85	0.41
1:D:1158:ASN:HB3	1:D:1182:ILE:HG22	2.02	0.41
1:D:2906:VAL:HG11	1:D:2914:LYS:HG3	2.01	0.41
1:D:3823:LYS:HD3	1:D:3823:LYS:HA	1.62	0.41
1:A:4072:VAL:HG13	1:A:4125:PHE:HD2	1.85	0.41
1:A:4232:GLU:OE2	1:A:4232:GLU:N	2.50	0.41
1:B:929:LEU:O	1:B:933:LEU:HG	2.21	0.41
1:B:3984:ARG:H	1:B:3984:ARG:HG2	1.69	0.41
1:B:4192:ARG:HD3	1:B:4193:ILE:N	2.34	0.41
1:B:4214:LYS:O	1:B:4218:ILE:HG13	2.19	0.41
1:D:4085:ARG:HE	1:D:4085:ARG:HB2	1.71	0.41
1:D:4783:ILE:HD13	1:D:4783:ILE:HA	1.85	0.41
1:B:1658:ASP:OD1	1:B:1659:LEU:N	2.54	0.41
1:B:2254:LEU:HD11	1:B:2334:PHE:HZ	1.85	0.41
1:B:4229:GLU:O	1:B:4233:LEU:HG	2.20	0.41
1:C:2189:LYS:HB2	1:C:2189:LYS:HE2	1.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3834:ALA:O	1:C:3838:THR:HG22	2.20	0.41
1:C:4677:LEU:HD12	1:C:4677:LEU:HA	1.88	0.41
1:D:1108:GLU:N	1:D:1108:GLU:OE1	2.53	0.41
1:D:2188:ASN:C	1:D:2188:ASN:ND2	2.71	0.41
1:D:3901:ASN:OD1	1:D:3904:ARG:NH1	2.44	0.41
1:D:4728:HIS:O	1:D:4732:PHE:N	2.53	0.41
1:A:286:THR:HG22	1:A:401:ALA:HB1	2.01	0.41
1:A:608:VAL:HG22	1:A:613:ALA:HB2	2.01	0.41
1:A:4773:VAL:O	1:A:4777:ILE:HG22	2.19	0.41
1:A:4969:ASP:HB2	1:A:4975:PHE:CZ	2.55	0.41
1:B:947:GLU:OE2	1:B:947:GLU:N	2.51	0.41
1:B:2175:GLU:O	1:B:2179:ILE:HG12	2.21	0.41
1:B:2261:SER:HA	1:B:2272:PRO:HG2	2.02	0.41
1:B:3713:LYS:NZ	1:B:3715:LYS:H	2.18	0.41
1:B:3834:ALA:O	1:B:3838:THR:HG22	2.20	0.41
1:C:3775:ALA:O	1:C:3778:MET:HG3	2.21	0.41
1:D:243:ARG:HA	1:D:243:ARG:HD3	1.79	0.41
1:D:2138:LEU:HD23	1:D:2138:LEU:HA	1.93	0.41
1:D:4039:MET:HA	1:D:4042:ARG:HD2	2.02	0.41
1:D:4725:LEU:O	1:D:4729:GLY:N	2.51	0.41
1:A:25:SER:OG	1:A:32:GLN:OE1	2.39	0.41
1:A:287:THR:HB	1:A:289:ARG:HD2	2.03	0.41
1:A:291:LEU:HD23	1:A:291:LEU:H	1.86	0.41
1:A:1155:LEU:HD13	1:A:1184:ILE:HD12	2.02	0.41
1:A:1251:GLU:OE2	1:A:1251:GLU:N	2.53	0.41
1:A:4931:ILE:O	1:A:4935:LEU:HG	2.20	0.41
1:B:957:LYS:HA	1:B:960:MET:HB2	2.02	0.41
1:B:4644:TRP:O	1:B:4648:LEU:HG	2.20	0.41
1:C:294:THR:HG23	1:C:295:GLU:H	1.86	0.41
1:C:2175:GLU:O	1:C:2179:ILE:HG12	2.20	0.41
1:C:4024:VAL:HA	1:C:4027:LEU:HD12	2.02	0.41
1:C:4973:HIS:CE1	1:C:4976:GLU:HG2	2.55	0.41
1:D:2814:LYS:HB2	1:D:2814:LYS:HE2	1.86	0.41
1:D:4229:GLU:O	1:D:4233:LEU:HG	2.21	0.41
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	2.02	0.41
1:A:3654:LEU:HD23	1:A:3654:LEU:HA	1.94	0.41
1:A:4020:GLN:HG2	1:A:4139:ILE:HD11	2.02	0.41
1:A:4834:GLY:O	1:A:4838:VAL:HG13	2.21	0.41
1:B:2906:VAL:HG11	1:B:2914:LYS:HG3	2.03	0.41
1:B:3824:LYS:HE2	1:B:3824:LYS:HB3	1.93	0.41
1:B:4991:PHE:O	1:B:4995:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2205:GLU:O	1:C:2209:GLU:HG2	2.21	0.41
1:C:2297:LYS:O	1:C:2300:SER:OG	2.29	0.41
1:C:4639:MET:O	1:C:4639:MET:HG2	2.21	0.41
1:D:758:ARG:HG2	1:D:762:CYS:HA	2.01	0.41
1:A:1095:VAL:HB	1:A:1199:VAL:HB	2.03	0.41
1:A:2433:LEU:HD23	1:A:2433:LEU:HA	1.90	0.41
1:A:4850:LEU:O	1:A:4854:VAL:HG12	2.19	0.41
1:C:291:LEU:HD23	1:C:299:LEU:HD11	2.01	0.41
1:C:2814:LYS:HE2	1:C:2814:LYS:HB2	1.86	0.41
1:C:4229:GLU:O	1:C:4233:LEU:HG	2.20	0.41
1:D:2175:GLU:O	1:D:2179:ILE:HG12	2.21	0.41
1:D:2176:ASN:O	1:D:2180:GLN:HG2	2.21	0.41
1:D:2679:UNK:HA	1:D:2741:GLU:HA	2.03	0.41
1:A:139:GLU:OE1	1:A:139:GLU:N	2.51	0.41
1:A:805:PRO:HA	1:A:806:PRO:HD3	1.98	0.41
1:A:2331:TYR:HD1	1:A:2331:TYR:HA	1.78	0.41
1:B:1673:VAL:HG12	1:B:1681:VAL:HG21	2.03	0.41
1:B:3719:ASP:O	1:B:3723:MET:HG2	2.21	0.41
1:B:4698:LYS:HB3	1:B:4698:LYS:HE2	1.92	0.41
1:C:786:GLY:N	1:C:1630:CYS:O	2.54	0.41
1:C:2196:ASN:OD1	1:C:2199:ARG:NH2	2.51	0.41
1:D:299:LEU:HD12	1:D:299:LEU:HA	1.93	0.41
1:D:2382:GLU:O	1:D:2386:ILE:HG23	2.20	0.41
1:D:4039:MET:O	1:D:4043:GLN:HG3	2.21	0.41
1:A:758:ARG:HG2	1:A:762:CYS:HA	2.03	0.41
1:A:1863:LEU:HD23	1:A:1863:LEU:HA	1.88	0.41
1:A:1969:LEU:HD21	1:A:2009:LEU:HD11	2.03	0.41
1:B:684:VAL:HG12	1:B:781:VAL:HG22	2.02	0.41
1:B:1742:THR:OG1	1:B:1769:THR:OG1	2.36	0.41
1:B:1968:LYS:NZ	1:B:2030:ASP:OD2	2.54	0.41
1:B:2128:TYR:OH	1:B:3672:ARG:NH1	2.54	0.41
1:B:2176:ASN:O	1:B:2180:GLN:HG2	2.20	0.41
1:B:2187:ASN:OD1	1:B:2187:ASN:N	2.48	0.41
1:B:2679:UNK:HA	1:B:2741:GLU:HA	2.02	0.41
1:B:3971:GLY:HA2	1:B:3972:PRO:HD2	1.91	0.41
1:C:385:ASP:OD1	1:C:385:ASP:N	2.52	0.41
1:C:4743:MET:H	1:C:4743:MET:HG2	1.66	0.41
1:C:4844:LEU:HD22	1:C:4928:LEU:HG	2.03	0.41
1:C:4968:PHE:HE2	1:C:4978:HIS:CG	2.39	0.41
1:D:67:PHE:HD1	1:D:67:PHE:HA	1.81	0.41
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1673:VAL:HG12	1:D:1681:VAL:HG21	2.03	0.41
1:D:1717:SER:HA	1:D:1721:GLU:HB2	2.01	0.41
1:D:4077:PHE:HZ	1:D:4088:ILE:HG12	1.86	0.41
1:D:4644:TRP:O	1:D:4648:LEU:HG	2.21	0.41
1:D:4743:MET:H	1:D:4743:MET:HG2	1.57	0.41
1:A:360:ALA:HB2	1:A:377:ILE:HG22	2.03	0.41
1:A:457:GLU:HG2	1:A:464:LYS:HE2	2.03	0.41
1:A:4104:THR:HG22	1:A:4106:PRO:HD2	2.03	0.41
1:A:4157:ASP:HB3	1:A:4160:LEU:HD12	2.03	0.41
1:A:4160:LEU:O	1:A:4164:LEU:HD23	2.20	0.41
1:A:4677:LEU:HD12	1:A:4677:LEU:HA	1.88	0.41
1:A:4865:LYS:HA	1:A:4865:LYS:HD3	1.78	0.41
1:B:590:LEU:HB2	1:B:599:VAL:HG11	2.02	0.41
1:B:4960:ILE:HD11	2:B:5101:ACP:N6	2.35	0.41
1:C:195:PHE:HB3	1:D:2361:PRO:HG3	2.02	0.41
1:C:353:SER:HB3	1:C:355:LEU:HD22	2.02	0.41
1:C:883:ALA:O	1:C:887:ILE:HG13	2.20	0.41
1:C:1969:LEU:HD11	1:C:2009:LEU:HD11	2.02	0.41
1:C:4013:LEU:HD12	1:C:4013:LEU:HA	1.93	0.41
1:D:3951:PHE:O	1:D:3955:MET:HG3	2.19	0.41
1:D:4666:VAL:HG13	1:D:4783:ILE:HD11	2.03	0.41
1:A:1131:ARG:HE	1:A:1137:GLU:HB2	1.86	0.41
1:A:4041:ALA:O	1:A:4045:VAL:HG22	2.21	0.41
1:A:4150:LEU:HD12	1:A:4150:LEU:HA	1.90	0.41
1:A:4966:ASP:HA	1:A:4969:ASP:HB3	2.02	0.41
1:B:1842:LEU:HD23	1:B:1842:LEU:HA	1.91	0.40
1:B:2902:HIS:HA	1:B:2903:PRO:HD3	1.98	0.40
1:B:4555:LEU:HD11	1:B:4656:LEU:HD22	2.02	0.40
1:C:379:HIS:CD2	1:C:382:GLY:H	2.39	0.40
1:C:3699:HIS:O	1:C:3703:LEU:HG	2.21	0.40
1:A:539:LEU:H	1:A:539:LEU:HD12	1.86	0.40
1:A:544:LEU:HD21	1:A:578:ILE:HG13	2.03	0.40
1:B:294:THR:HG23	1:B:295:GLU:H	1.86	0.40
1:B:1095:VAL:HB	1:B:1199:VAL:HB	2.04	0.40
1:B:4215:ARG:NH2	2:B:5101:ACP:O1B	2.55	0.40
1:B:4865:LYS:HA	1:B:4865:LYS:HD2	1.78	0.40
1:B:4983:HIS:O	2:B:5101:ACP:N6	2.54	0.40
1:C:590:LEU:HB2	1:C:599:VAL:HG11	2.04	0.40
1:C:1152:MET:HG3	1:C:1161:ILE:HB	2.02	0.40
1:C:4646:LEU:HD23	1:C:4646:LEU:HA	1.91	0.40
1:D:21:VAL:HB	1:D:205:ILE:HD11	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:ASP:OD1	1:D:385:ASP:N	2.52	0.40
1:D:3775:ALA:O	1:D:3778:MET:HG3	2.22	0.40
1:D:4071:ILE:HD13	1:D:4071:ILE:HA	1.92	0.40
1:D:4100:GLN:HB3	1:D:4102:GLN:OE1	2.21	0.40
1:D:4870:ASP:OD1	1:D:4870:ASP:N	2.53	0.40
1:A:4097:MET:HG3	1:A:4108:ILE:HG23	2.02	0.40
1:B:76:ARG:HD3	1:B:76:ARG:HA	1.95	0.40
1:B:758:ARG:HG2	1:B:762:CYS:HA	2.02	0.40
1:B:4677:LEU:HD21	1:B:4702:ASP:HB3	2.03	0.40
1:C:544:LEU:HD23	1:C:544:LEU:HA	1.96	0.40
1:D:2188:ASN:ND2	1:D:2188:ASN:O	2.41	0.40
1:D:3670:GLU:HG2	1:D:3728:ILE:HA	2.03	0.40
1:A:4984:ASN:O	1:A:4985:LEU:HB3	2.20	0.40
1:B:379:HIS:CD2	1:B:382:GLY:H	2.40	0.40
1:B:2469:ILE:HD13	1:B:2469:ILE:HA	1.86	0.40
1:C:121:LEU:HB3	1:C:123:THR:HG22	2.04	0.40
1:C:1204:LEU:HD12	1:C:1226:PHE:HB3	2.02	0.40
1:C:2182:ILE:HD13	1:C:2182:ILE:HA	2.00	0.40
1:C:3814:GLN:NE2	1:C:3818:ASP:OD2	2.55	0.40
1:C:3845:ASN:N	1:C:3845:ASN:OD1	2.55	0.40
1:C:4177:TYR:HA	1:C:4197:ILE:HB	2.04	0.40
1:D:3699:HIS:O	1:D:3703:LEU:HG	2.21	0.40
1:D:3812:VAL:O	1:D:3816:MET:HG3	2.21	0.40
1:D:4675:LYS:HB3	1:D:4675:LYS:HE3	1.83	0.40
1:A:1842:LEU:HD23	1:A:1842:LEU:HA	1.90	0.40
1:A:2656:UNK:O	1:A:2924:GLN:NE2	2.52	0.40
1:A:3917:ILE:HA	1:A:3920:VAL:HG22	2.02	0.40
1:B:150:MET:HB3	1:B:169:LEU:HD13	2.03	0.40
1:B:1231:GLN:HE22	1:B:1826:ALA:HB2	1.86	0.40
1:B:3696:ASP:OD2	1:B:3773:ARG:NH2	2.54	0.40
1:B:4850:LEU:O	1:B:4854:VAL:HG12	2.21	0.40
1:B:4966:ASP:OD1	1:B:4967:TYR:N	2.55	0.40
1:C:2332:LEU:HD11	1:C:2428:ALA:HB1	2.02	0.40
1:C:4085:ARG:HE	1:C:4085:ARG:HB2	1.72	0.40
1:C:4999:ASP:HB3	1:C:5002:GLU:HG2	2.03	0.40
1:D:121:LEU:HB3	1:D:123:THR:HG22	2.03	0.40
1:A:2030:ASP:N	1:A:2030:ASP:OD1	2.55	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	3203/5037 (64%)	3060 (96%)	140 (4%)	3 (0%)	51	81
1	B	3203/5037 (64%)	3055 (95%)	143 (4%)	5 (0%)	47	77
1	C	3203/5037 (64%)	3056 (95%)	145 (4%)	2 (0%)	51	81
1	D	3203/5037 (64%)	3059 (96%)	141 (4%)	3 (0%)	51	81
All	All	12812/20148 (64%)	12230 (96%)	569 (4%)	13 (0%)	54	81

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3915	ILE
1	D	3915	ILE
1	B	3788	GLY
1	B	4198	SER
1	C	3788	GLY
1	D	4198	SER
1	A	4967	TYR
1	B	4956	THR
1	C	4198	SER
1	D	3788	GLY
1	A	3788	GLY
1	A	4198	SER
1	B	4972	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	2513/3264 (77%)	2401 (96%)	112 (4%)	27	58
1	B	2513/3264 (77%)	2396 (95%)	117 (5%)	26	57
1	C	2513/3264 (77%)	2416 (96%)	97 (4%)	32	62
1	D	2513/3264 (77%)	2405 (96%)	108 (4%)	29	59
All	All	10052/13056 (77%)	9618 (96%)	434 (4%)	33	59

All (434) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	17	ASP
1	B	150	MET
1	B	168	ASP
1	B	178	ARG
1	B	218	HIS
1	B	222	LEU
1	B	223	PHE
1	B	226	HIS
1	B	306	LYS
1	B	379	HIS
1	B	384	MET
1	B	389	PHE
1	B	451	TYR
1	B	452	PHE
1	B	478	PHE
1	B	533	ASN
1	B	539	LEU
1	B	588	SER
1	B	597	HIS
1	B	674	PHE
1	B	710	ASP
1	B	869	ARG
1	B	933	LEU
1	B	961	MET
1	B	1047	LEU
1	B	1100	MET
1	B	1180	ARG
1	B	1214	PHE
1	B	1219	LEU
1	B	1580	PHE
1	B	1608	MET
1	B	1637	MET
1	B	1713	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1846	SER
1	B	1929	MET
1	B	2122	SER
1	B	2128	TYR
1	B	2225	PHE
1	B	2267	MET
1	B	2331	TYR
1	B	2334	PHE
1	B	2340	PHE
1	B	2348	GLU
1	B	2440	MET
1	B	2442	LEU
1	B	2806	ARG
1	B	2872	GLN
1	B	2874	MET
1	B	2884	ASN
1	B	2888	ARG
1	B	2920	ARG
1	B	3652	MET
1	B	3657	TYR
1	B	3669	PHE
1	B	3675	ASP
1	B	3706	SER
1	B	3713	LYS
1	B	3718	GLU
1	B	3750	GLU
1	B	3770	LEU
1	B	3803	SER
1	B	3875	MET
1	B	3936	TYR
1	B	3937	TYR
1	B	3951	PHE
1	B	3979	SER
1	B	3984	ARG
1	B	3986	TRP
1	B	4022	ASP
1	B	4034	ASN
1	B	4039	MET
1	B	4047	MET
1	B	4083	ASP
1	B	4099	SER
1	B	4101	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4110	PHE
1	B	4114	CYS
1	B	4138	ASP
1	B	4156	HIS
1	B	4161	ARG
1	B	4252	SER
1	B	4568	PHE
1	B	4584	ASP
1	B	4630	TYR
1	B	4631	PHE
1	B	4684	ASP
1	B	4711	PHE
1	B	4730	ASP
1	B	4741	LEU
1	B	4772	ASP
1	B	4775	TYR
1	B	4784	PHE
1	B	4789	PHE
1	B	4795	TYR
1	B	4809	PHE
1	B	4818	MET
1	B	4832	HIS
1	B	4858	PHE
1	B	4861	LYS
1	B	4873	ASP
1	B	4888	TYR
1	B	4900	GLU
1	B	4957	LYS
1	B	4960	ILE
1	B	4965	SER
1	B	4969	ASP
1	B	4973	HIS
1	B	4975	PHE
1	B	4980	LEU
1	B	4981	GLU
1	B	4982	GLU
1	B	4984	ASN
1	B	4985	LEU
1	B	4987	ASN
1	B	5020	ASP
1	B	5028	PHE
1	B	5035	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	168	ASP
1	C	178	ARG
1	C	218	HIS
1	C	220	LEU
1	C	226	HIS
1	C	306	LYS
1	C	329	ARG
1	C	334	MET
1	C	379	HIS
1	C	478	PHE
1	C	481	GLU
1	C	588	SER
1	C	674	PHE
1	C	710	ASP
1	C	869	ARG
1	C	961	MET
1	C	1047	LEU
1	C	1124	PHE
1	C	1180	ARG
1	C	1214	PHE
1	C	1580	PHE
1	C	1608	MET
1	C	1846	SER
1	C	2122	SER
1	C	2128	TYR
1	C	2225	PHE
1	C	2331	TYR
1	C	2334	PHE
1	C	2340	PHE
1	C	2348	GLU
1	C	2442	LEU
1	C	2806	ARG
1	C	2810	LYS
1	C	2869	ARG
1	C	2872	GLN
1	C	2874	MET
1	C	2884	ASN
1	C	2888	ARG
1	C	2920	ARG
1	C	3652	MET
1	C	3653	PHE
1	C	3669	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3675	ASP
1	C	3696	ASP
1	C	3706	SER
1	C	3750	GLU
1	C	3809	ASN
1	C	3937	TYR
1	C	3979	SER
1	C	3986	TRP
1	C	3992	PHE
1	C	3996	PHE
1	C	3999	MET
1	C	4034	ASN
1	C	4039	MET
1	C	4047	MET
1	C	4060	LYS
1	C	4101	LYS
1	C	4103	PHE
1	C	4114	CYS
1	C	4138	ASP
1	C	4161	ARG
1	C	4192	ARG
1	C	4252	SER
1	C	4551	PHE
1	C	4564	PHE
1	C	4568	PHE
1	C	4580	TYR
1	C	4584	ASP
1	C	4630	TYR
1	C	4684	ASP
1	C	4711	PHE
1	C	4727	LYS
1	C	4741	LEU
1	C	4772	ASP
1	C	4789	PHE
1	C	4795	TYR
1	C	4809	PHE
1	C	4821	LYS
1	C	4823	LEU
1	C	4832	HIS
1	C	4849	TYR
1	C	4858	PHE
1	C	4859	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4860	ARG
1	C	4861	LYS
1	C	4873	ASP
1	C	4874	MET
1	C	4959	PHE
1	C	4965	SER
1	C	4975	PHE
1	C	4976	GLU
1	C	4977	THR
1	C	4980	LEU
1	C	5020	ASP
1	C	5028	PHE
1	C	5035	GLN
1	D	17	ASP
1	D	67	PHE
1	D	168	ASP
1	D	178	ARG
1	D	218	HIS
1	D	220	LEU
1	D	222	LEU
1	D	226	HIS
1	D	316	PHE
1	D	336	PRO
1	D	379	HIS
1	D	384	MET
1	D	389	PHE
1	D	452	PHE
1	D	478	PHE
1	D	516	LYS
1	D	553	ARG
1	D	588	SER
1	D	597	HIS
1	D	674	PHE
1	D	710	ASP
1	D	783	PHE
1	D	869	ARG
1	D	874	LEU
1	D	910	PHE
1	D	961	MET
1	D	1046	LEU
1	D	1047	LEU
1	D	1124	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1152	MET
1	D	1180	ARG
1	D	1213	PHE
1	D	1214	PHE
1	D	1219	LEU
1	D	1580	PHE
1	D	1608	MET
1	D	1827	ARG
1	D	1846	SER
1	D	2128	TYR
1	D	2188	ASN
1	D	2225	PHE
1	D	2334	PHE
1	D	2340	PHE
1	D	2348	GLU
1	D	2442	LEU
1	D	2806	ARG
1	D	2872	GLN
1	D	2874	MET
1	D	2884	ASN
1	D	2920	ARG
1	D	3653	PHE
1	D	3657	TYR
1	D	3669	PHE
1	D	3699	HIS
1	D	3706	SER
1	D	3718	GLU
1	D	3753	PHE
1	D	3936	TYR
1	D	3937	TYR
1	D	3951	PHE
1	D	3964	SER
1	D	3979	SER
1	D	3986	TRP
1	D	4039	MET
1	D	4050	GLU
1	D	4052	SER
1	D	4083	ASP
1	D	4098	ASP
1	D	4099	SER
1	D	4114	CYS
1	D	4161	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4164	LEU
1	D	4192	ARG
1	D	4252	SER
1	D	4551	PHE
1	D	4564	PHE
1	D	4579	PHE
1	D	4580	TYR
1	D	4630	TYR
1	D	4652	LEU
1	D	4684	ASP
1	D	4725	LEU
1	D	4726	ASP
1	D	4727	LYS
1	D	4731	ILE
1	D	4741	LEU
1	D	4743	MET
1	D	4772	ASP
1	D	4795	TYR
1	D	4809	PHE
1	D	4821	LYS
1	D	4832	HIS
1	D	4851	TYR
1	D	4858	PHE
1	D	4861	LYS
1	D	4873	ASP
1	D	4879	MET
1	D	4959	PHE
1	D	4965	SER
1	D	4975	PHE
1	D	4979	THR
1	D	4980	LEU
1	D	4981	GLU
1	D	4982	GLU
1	D	4984	ASN
1	D	5020	ASP
1	D	5028	PHE
1	D	5035	GLN
1	A	29	LEU
1	A	116	MET
1	A	178	ARG
1	A	213	TYR
1	A	218	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	262	LEU
1	A	265	LEU
1	A	384	MET
1	A	393	CYS
1	A	403	MET
1	A	418	LEU
1	A	452	PHE
1	A	453	GLU
1	A	459	LEU
1	A	539	LEU
1	A	588	SER
1	A	597	HIS
1	A	604	CYS
1	A	674	PHE
1	A	710	ASP
1	A	796	ARG
1	A	829	TYR
1	A	869	ARG
1	A	882	TRP
1	A	910	PHE
1	A	1112	ASP
1	A	1118	ASP
1	A	1180	ARG
1	A	1213	PHE
1	A	1214	PHE
1	A	1219	LEU
1	A	1608	MET
1	A	1702	HIS
1	A	1731	LEU
1	A	1846	SER
1	A	2128	TYR
1	A	2163	ARG
1	A	2191	PHE
1	A	2194	HIS
1	A	2331	TYR
1	A	2340	PHE
1	A	2451	LEU
1	A	2474	LEU
1	A	2806	ARG
1	A	2810	LYS
1	A	2872	GLN
1	A	2884	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2888	ARG
1	A	2920	ARG
1	A	3657	TYR
1	A	3675	ASP
1	A	3699	HIS
1	A	3706	SER
1	A	3732	SER
1	A	3771	HIS
1	A	3786	CYS
1	A	3835	LEU
1	A	3836	MET
1	A	3951	PHE
1	A	3962	PHE
1	A	3968	TYR
1	A	3980	LEU
1	A	3983	SER
1	A	3996	PHE
1	A	4022	ASP
1	A	4031	LEU
1	A	4032	GLU
1	A	4034	ASN
1	A	4039	MET
1	A	4098	ASP
1	A	4100	GLN
1	A	4101	LYS
1	A	4109	GLN
1	A	4110	PHE
1	A	4114	CYS
1	A	4132	PHE
1	A	4153	HIS
1	A	4159	ARG
1	A	4164	LEU
1	A	4192	ARG
1	A	4219	PHE
1	A	4234	PHE
1	A	4551	PHE
1	A	4559	PHE
1	A	4560	TYR
1	A	4564	PHE
1	A	4575	PHE
1	A	4580	TYR
1	A	4631	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4661	TYR
1	A	4690	GLU
1	A	4741	LEU
1	A	4743	MET
1	A	4768	LEU
1	A	4809	PHE
1	A	4821	LYS
1	A	4823	LEU
1	A	4832	HIS
1	A	4849	TYR
1	A	4858	PHE
1	A	4859	PHE
1	A	4861	LYS
1	A	4879	MET
1	A	4886	HIS
1	A	4888	TYR
1	A	4965	SER
1	A	4967	TYR
1	A	4979	THR
1	A	4980	LEU
1	A	4985	LEU
1	A	5020	ASP
1	A	5032	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	201	ASN
1	B	308	HIS
1	B	963	ASN
1	C	201	ASN
1	C	963	ASN
1	C	2744	ASN
1	C	4983	HIS
1	D	201	ASN
1	D	597	HIS
1	D	879	HIS
1	D	963	ASN
1	D	2744	ASN
1	D	4100	GLN
1	A	203	ASN
1	A	495	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2107	GLN
1	A	4978	HIS
1	A	4984	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACP	A	5101	-	27,33,33	4.68	10 (37%)	32,52,52	2.05	5 (15%)
2	ACP	D	5101	-	27,33,33	4.69	10 (37%)	32,52,52	2.05	5 (15%)
2	ACP	C	5101	-	27,33,33	4.68	10 (37%)	32,52,52	2.05	5 (15%)
2	ACP	B	5101	-	27,33,33	4.68	10 (37%)	32,52,52	2.05	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACP	A	5101	-	-	6/15/38/38	0/3/3/3
2	ACP	D	5101	-	-	6/15/38/38	0/3/3/3
2	ACP	C	5101	-	-	6/15/38/38	0/3/3/3
2	ACP	B	5101	-	-	6/15/38/38	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5101	ACP	C2'-C1'	-15.14	1.30	1.53
2	A	5101	ACP	C2'-C1'	-15.07	1.30	1.53
2	C	5101	ACP	C2'-C1'	-15.07	1.30	1.53
2	B	5101	ACP	O4'-C1'	15.03	1.62	1.41
2	B	5101	ACP	C2'-C1'	-15.02	1.31	1.53
2	D	5101	ACP	O4'-C1'	15.01	1.62	1.41
2	C	5101	ACP	O4'-C1'	15.00	1.62	1.41
2	A	5101	ACP	O4'-C1'	15.00	1.62	1.41
2	A	5101	ACP	PB-O3A	6.30	1.65	1.58
2	C	5101	ACP	PB-O3A	6.29	1.65	1.58
2	B	5101	ACP	O4'-C4'	-6.27	1.31	1.45
2	B	5101	ACP	PB-O3A	6.26	1.65	1.58
2	D	5101	ACP	PB-O3A	6.26	1.65	1.58
2	C	5101	ACP	O4'-C4'	-6.23	1.31	1.45
2	D	5101	ACP	O4'-C4'	-6.22	1.31	1.45
2	A	5101	ACP	O4'-C4'	-6.20	1.31	1.45
2	C	5101	ACP	C6-N6	3.18	1.45	1.34
2	B	5101	ACP	C6-N6	3.17	1.45	1.34
2	D	5101	ACP	C6-N6	3.16	1.45	1.34
2	A	5101	ACP	C6-N6	3.16	1.45	1.34
2	C	5101	ACP	O2'-C2'	2.96	1.49	1.43
2	B	5101	ACP	O2'-C2'	2.95	1.49	1.43
2	D	5101	ACP	O2'-C2'	2.95	1.49	1.43
2	A	5101	ACP	O2'-C2'	2.94	1.49	1.43
2	A	5101	ACP	O3'-C3'	-2.92	1.36	1.43
2	B	5101	ACP	O3'-C3'	-2.91	1.36	1.43
2	D	5101	ACP	O3'-C3'	-2.89	1.36	1.43
2	C	5101	ACP	O3'-C3'	-2.86	1.36	1.43
2	D	5101	ACP	C5-C4	-2.60	1.34	1.40
2	C	5101	ACP	C5-C4	-2.59	1.34	1.40
2	B	5101	ACP	C5-C4	-2.58	1.34	1.40
2	A	5101	ACP	C5-C4	-2.55	1.34	1.40
2	D	5101	ACP	C2-N3	2.29	1.35	1.32
2	C	5101	ACP	C2-N3	2.26	1.35	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5101	ACP	C2-N3	2.22	1.35	1.32
2	B	5101	ACP	C2-N3	2.21	1.35	1.32
2	B	5101	ACP	PB-O2B	-2.16	1.51	1.56
2	C	5101	ACP	PB-O2B	-2.11	1.51	1.56
2	D	5101	ACP	PB-O2B	-2.09	1.51	1.56
2	A	5101	ACP	PB-O2B	-2.09	1.51	1.56

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	5101	ACP	C5-C6-N6	7.01	131.00	120.35
2	D	5101	ACP	C5-C6-N6	6.99	130.98	120.35
2	B	5101	ACP	C5-C6-N6	6.96	130.93	120.35
2	A	5101	ACP	C5-C6-N6	6.95	130.91	120.35
2	D	5101	ACP	N3-C2-N1	-5.62	119.89	128.68
2	A	5101	ACP	N3-C2-N1	-5.61	119.90	128.68
2	C	5101	ACP	N3-C2-N1	-5.61	119.91	128.68
2	B	5101	ACP	N3-C2-N1	-5.59	119.94	128.68
2	D	5101	ACP	N6-C6-N1	-4.61	109.00	118.57
2	C	5101	ACP	N6-C6-N1	-4.61	109.01	118.57
2	B	5101	ACP	N6-C6-N1	-4.60	109.03	118.57
2	A	5101	ACP	N6-C6-N1	-4.56	109.11	118.57
2	D	5101	ACP	PB-O3A-PA	-2.83	123.58	132.56
2	A	5101	ACP	PB-O3A-PA	-2.82	123.63	132.56
2	B	5101	ACP	PB-O3A-PA	-2.81	123.66	132.56
2	C	5101	ACP	PB-O3A-PA	-2.80	123.68	132.56
2	A	5101	ACP	C3'-C2'-C1'	2.79	105.19	100.98
2	B	5101	ACP	C3'-C2'-C1'	2.74	105.10	100.98
2	D	5101	ACP	C3'-C2'-C1'	2.73	105.09	100.98
2	C	5101	ACP	C3'-C2'-C1'	2.73	105.08	100.98

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5101	ACP	C5'-O5'-PA-O2A
2	B	5101	ACP	C5'-O5'-PA-O3A
2	B	5101	ACP	C4'-C5'-O5'-PA
2	C	5101	ACP	C5'-O5'-PA-O2A
2	C	5101	ACP	C5'-O5'-PA-O3A
2	C	5101	ACP	C4'-C5'-O5'-PA
2	D	5101	ACP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	5101	ACP	C5'-O5'-PA-O3A
2	D	5101	ACP	C4'-C5'-O5'-PA
2	D	5101	ACP	C3'-C4'-C5'-O5'
2	A	5101	ACP	C5'-O5'-PA-O2A
2	A	5101	ACP	C5'-O5'-PA-O3A
2	A	5101	ACP	C4'-C5'-O5'-PA
2	A	5101	ACP	C3'-C4'-C5'-O5'
2	B	5101	ACP	C3'-C4'-C5'-O5'
2	C	5101	ACP	C3'-C4'-C5'-O5'
2	D	5101	ACP	O4'-C4'-C5'-O5'
2	A	5101	ACP	O4'-C4'-C5'-O5'
2	B	5101	ACP	O4'-C4'-C5'-O5'
2	C	5101	ACP	O4'-C4'-C5'-O5'
2	B	5101	ACP	PB-C3B-PG-O1G
2	C	5101	ACP	PB-C3B-PG-O1G
2	D	5101	ACP	PB-C3B-PG-O1G
2	A	5101	ACP	PB-C3B-PG-O1G

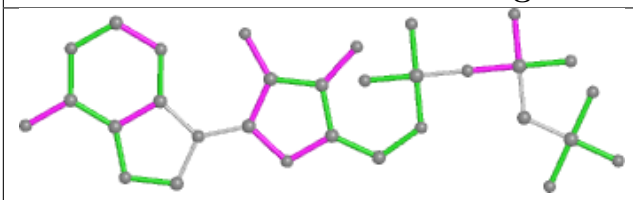
There are no ring outliers.

1 monomer is involved in 4 short contacts:

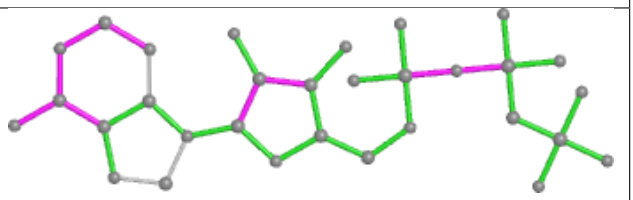
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5101	ACP	4	0

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

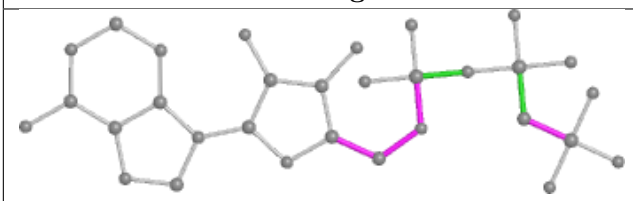
Ligand ACP A 5101



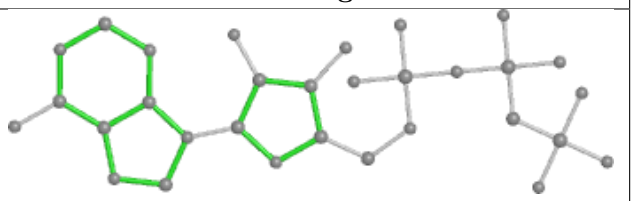
Bond lengths



Bond angles

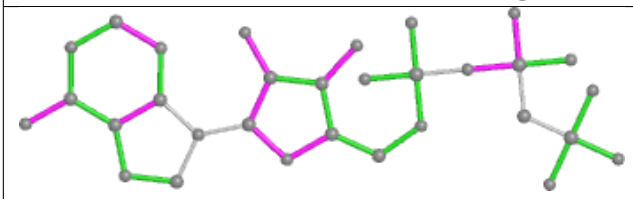


Torsions

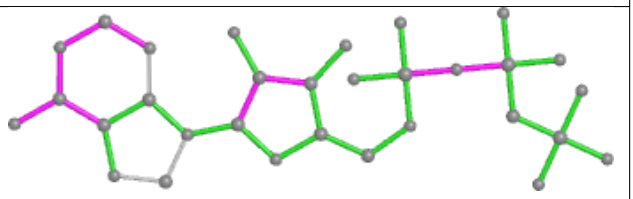


Rings

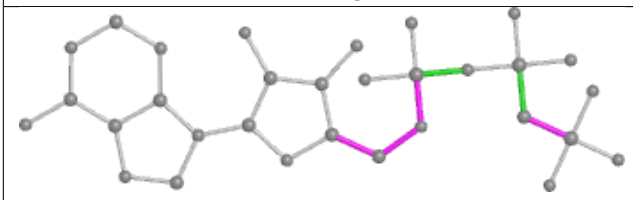
Ligand ACP D 5101



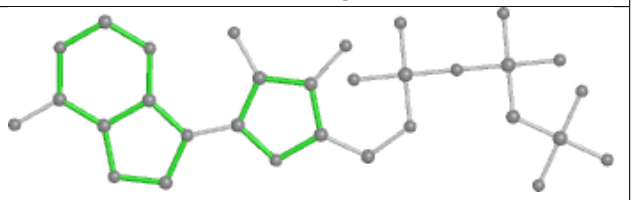
Bond lengths



Bond angles

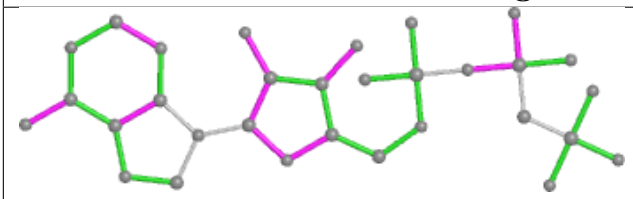


Torsions

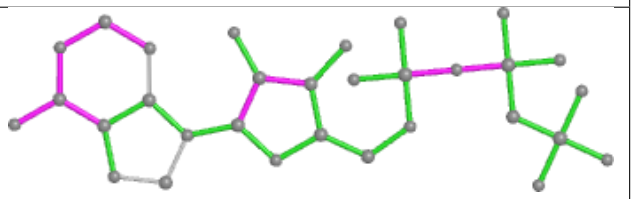


Rings

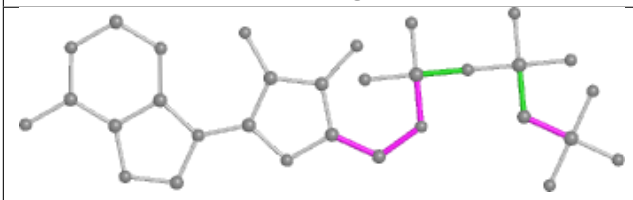
Ligand ACP C 5101



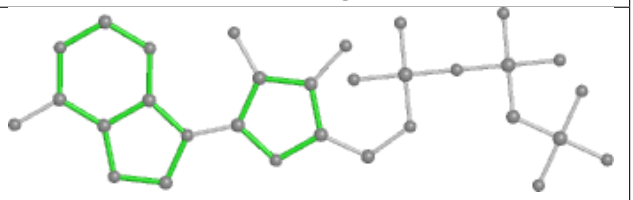
Bond lengths



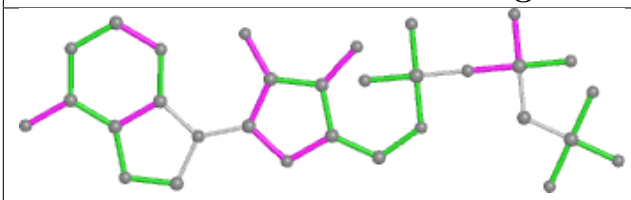
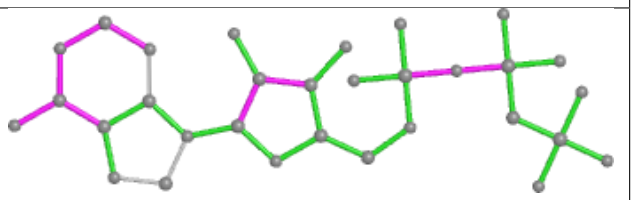
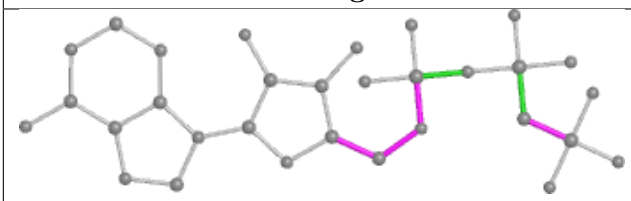
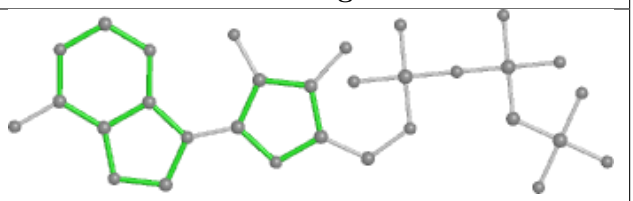
Bond angles



Torsions



Rings

Ligand ACP B 5101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	7
1	B	7
1	C	7
1	A	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	3288:UNK	C	3289:UNK	N	13.33
1	B	3288:UNK	C	3289:UNK	N	13.32
1	C	3288:UNK	C	3289:UNK	N	13.32
1	A	3288:UNK	C	3289:UNK	N	13.25
1	A	3510:UNK	C	3511:UNK	N	13.22
1	D	3510:UNK	C	3511:UNK	N	13.12
1	B	3510:UNK	C	3511:UNK	N	13.11
1	C	3510:UNK	C	3511:UNK	N	13.11
1	D	3122:UNK	C	3123:UNK	N	12.59
1	A	3122:UNK	C	3123:UNK	N	12.59
1	B	3122:UNK	C	3123:UNK	N	12.51
1	C	3122:UNK	C	3123:UNK	N	12.50
1	A	3221:UNK	C	3222:UNK	N	11.37

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3221:UNK	C	3222:UNK	N	11.35
1	C	3221:UNK	C	3222:UNK	N	11.35
1	D	3221:UNK	C	3222:UNK	N	11.34
1	B	3191:UNK	C	3192:UNK	N	11.13
1	C	3191:UNK	C	3192:UNK	N	11.13
1	D	3191:UNK	C	3192:UNK	N	11.13
1	A	3191:UNK	C	3192:UNK	N	11.10
1	B	3302:UNK	C	3303:UNK	N	10.58
1	D	3302:UNK	C	3303:UNK	N	10.58
1	C	3302:UNK	C	3303:UNK	N	10.57
1	A	3302:UNK	C	3303:UNK	N	10.43
1	B	1297:UNK	C	1298:UNK	N	7.04
1	C	1297:UNK	C	1298:UNK	N	7.04
1	D	1297:UNK	C	1298:UNK	N	7.04
1	A	1297:UNK	C	1298:UNK	N	6.91

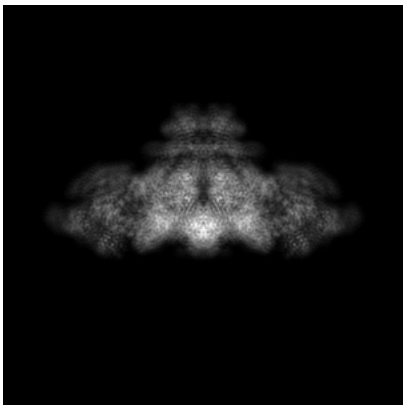
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25830. These allow visual inspection of the internal detail of the map and identification of artifacts.

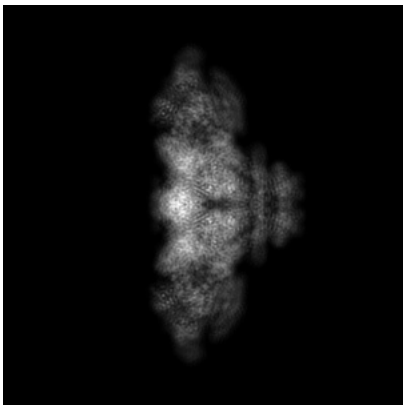
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

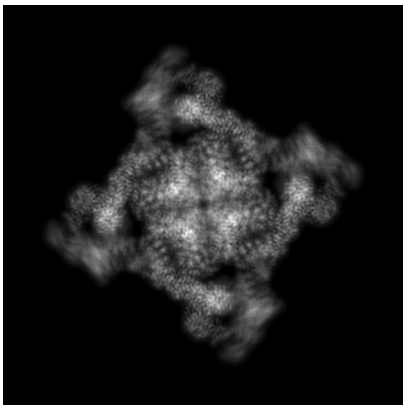
6.1.1 Primary map



X

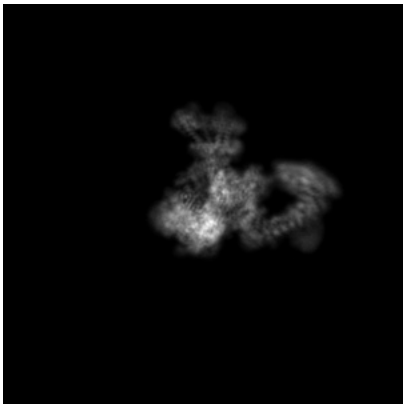


Y

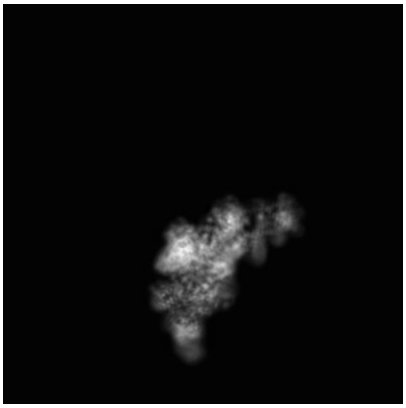


Z

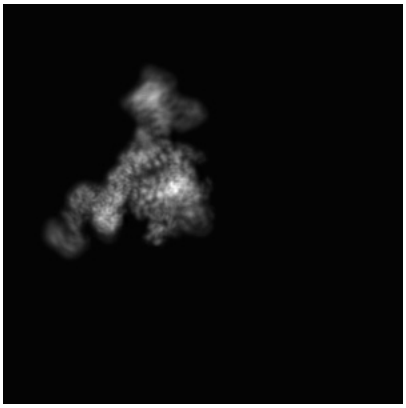
6.1.2 Raw map



X



Y



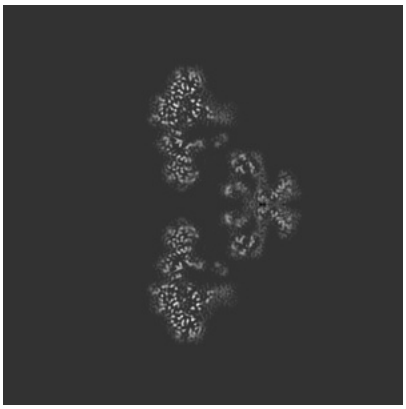
Z

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

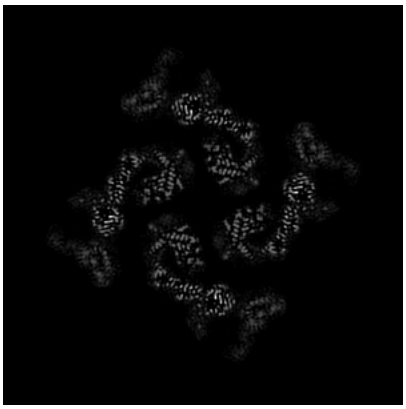
6.2 Central slices (i)

6.2.1 Primary map

X Index: 216

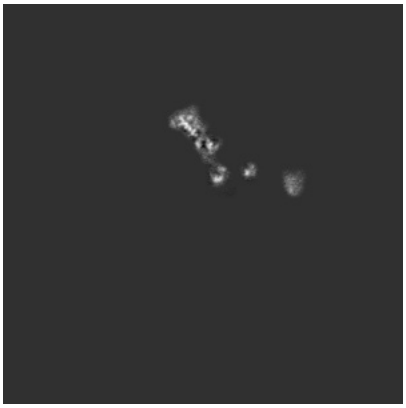


Y Index: 216

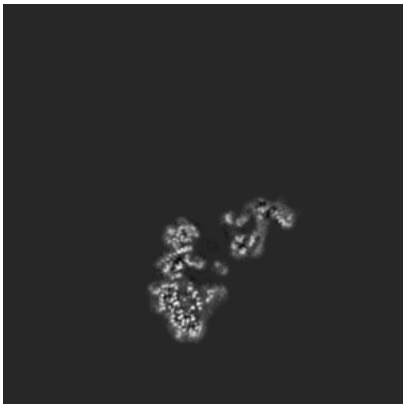


Z Index: 216

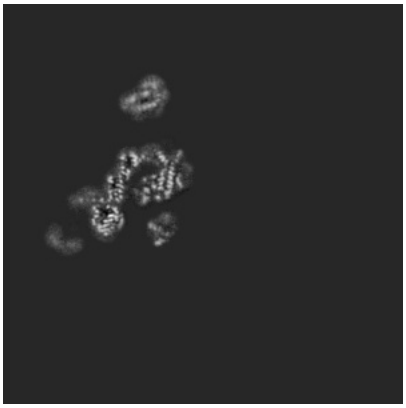
6.2.2 Raw map



X Index: 216



Y Index: 216



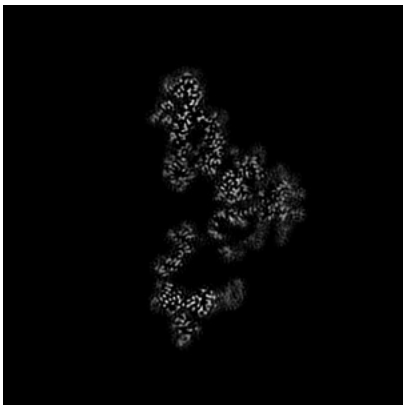
Z Index: 216

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

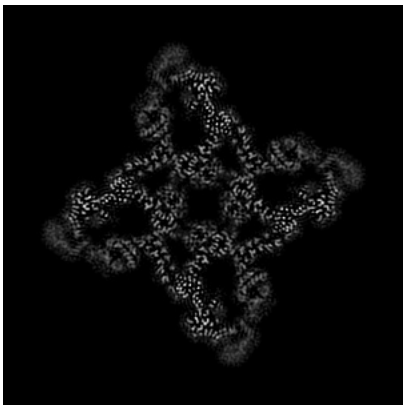
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 226



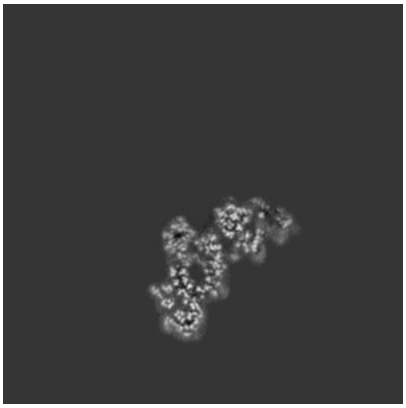
Y Index: 206



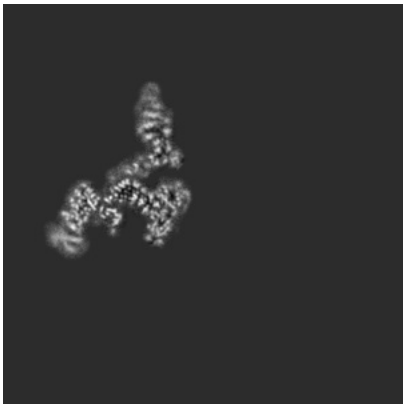
Z Index: 198

6.3.2 Raw map

X Index: 167



Y Index: 226

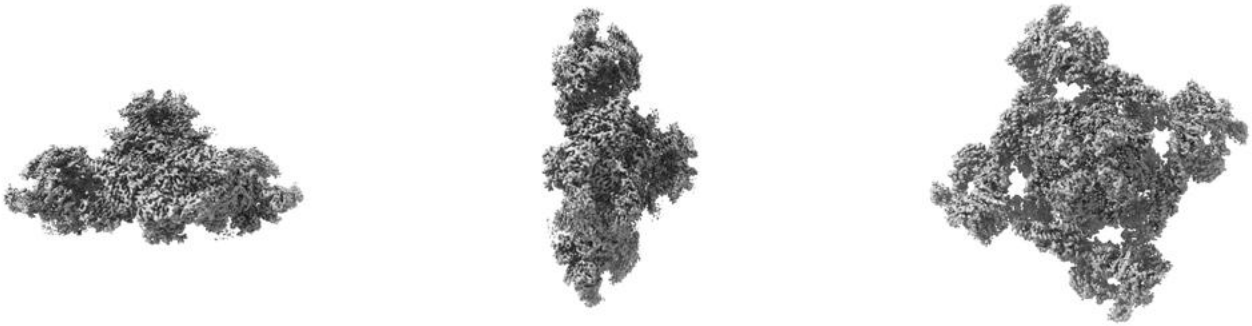


Z Index: 192

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

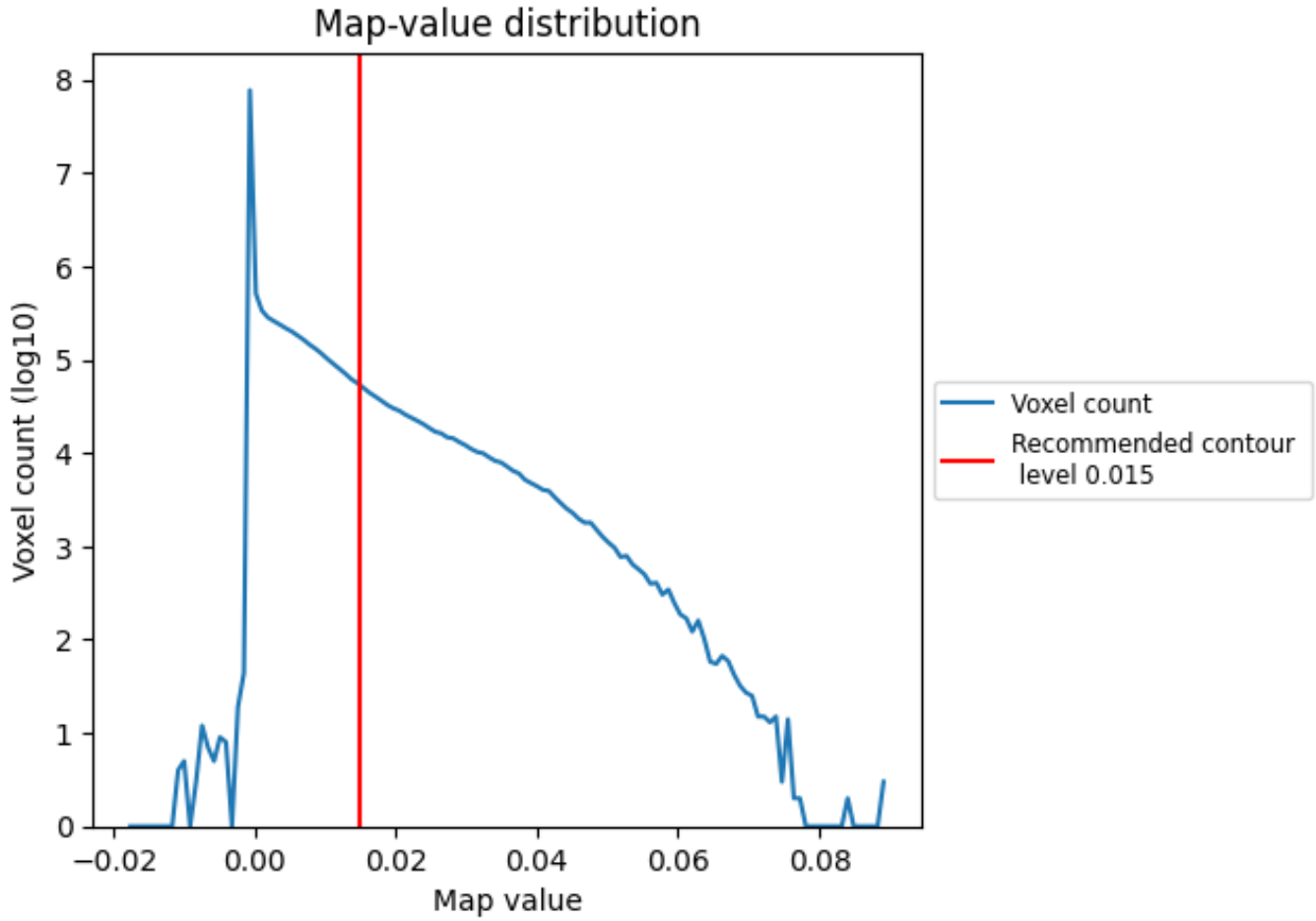
6.5 Mask visualisation (i)

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

7 Map analysis

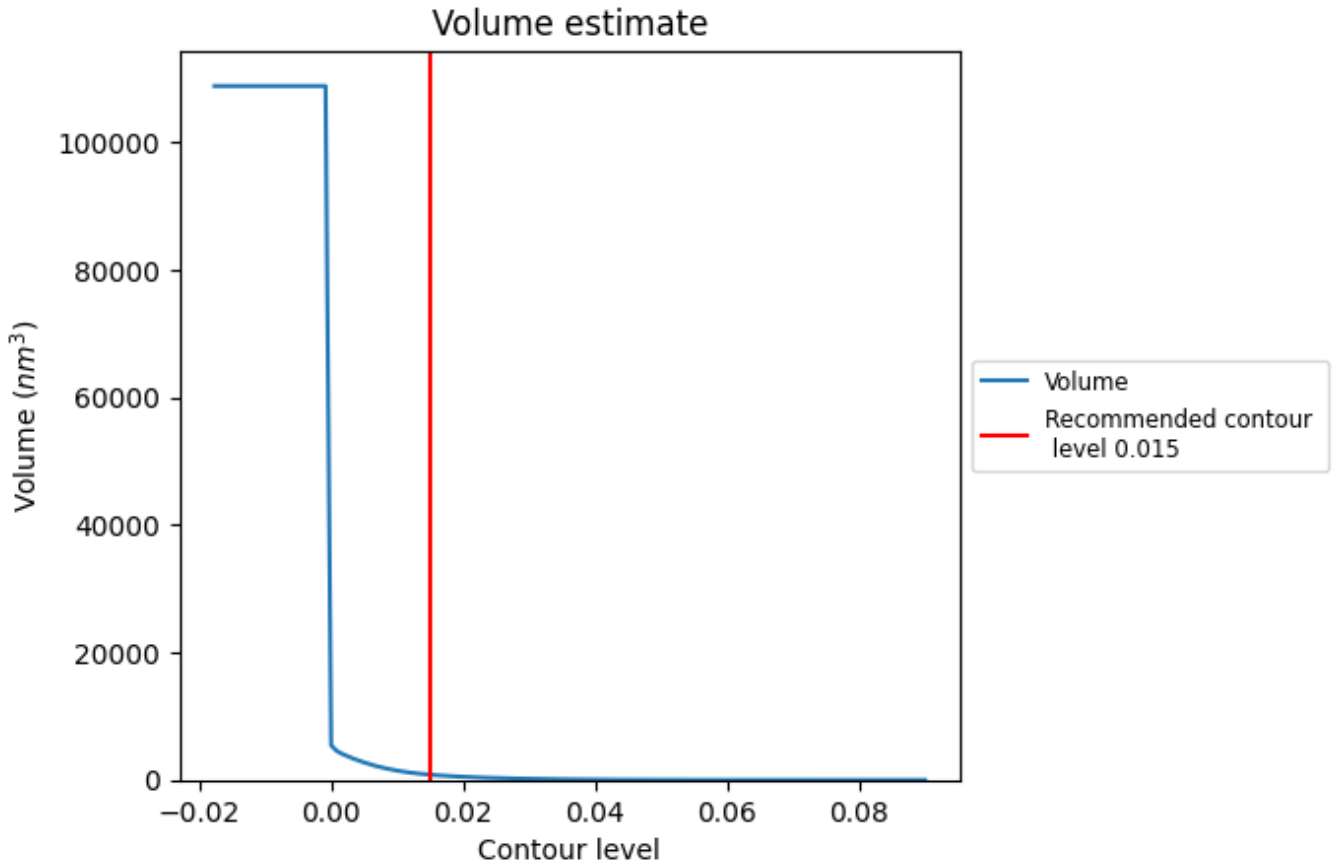
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

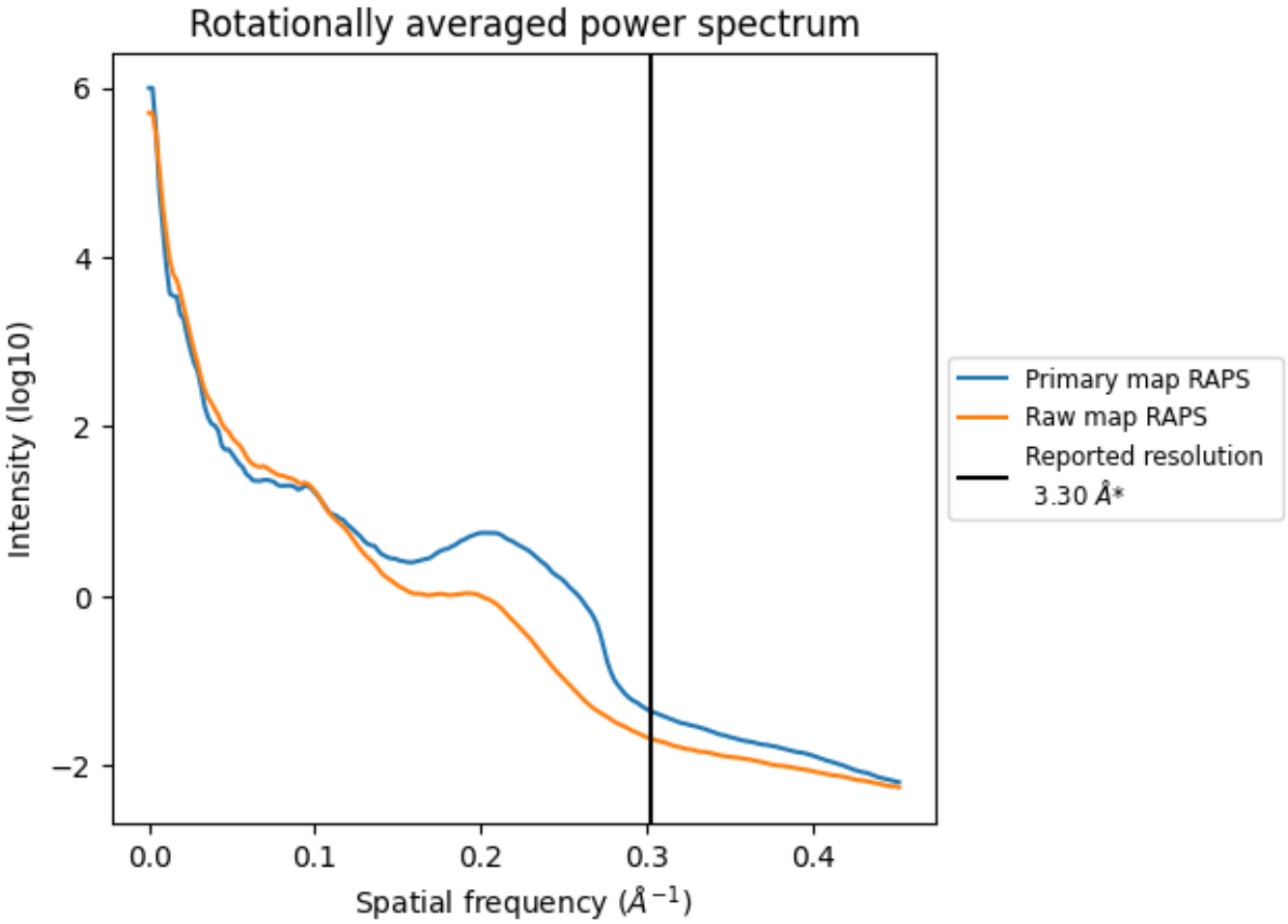
7.2 Volume estimate



The volume at the recommended contour level is 826 nm^3; this corresponds to an approximate mass of 746 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)

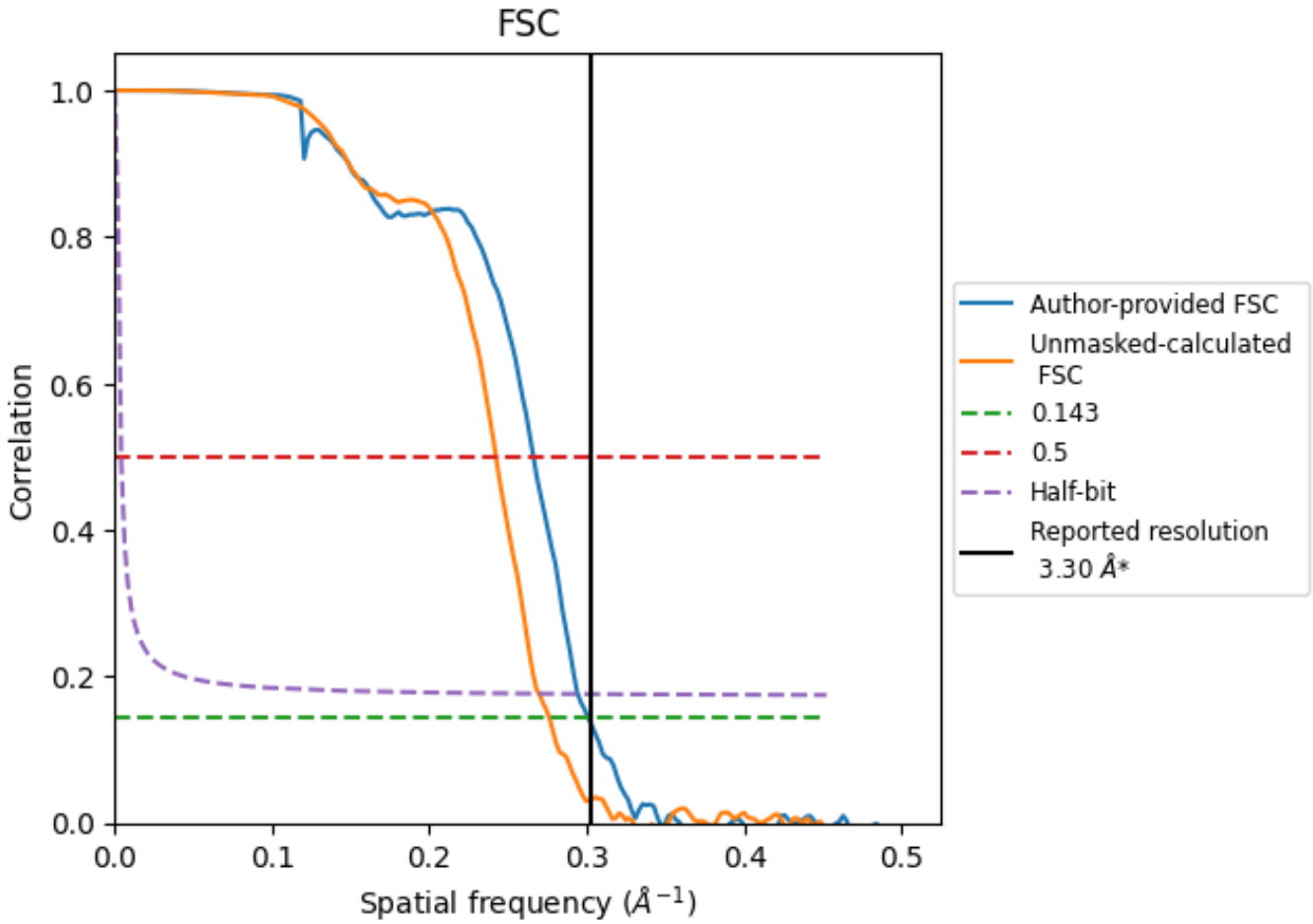


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

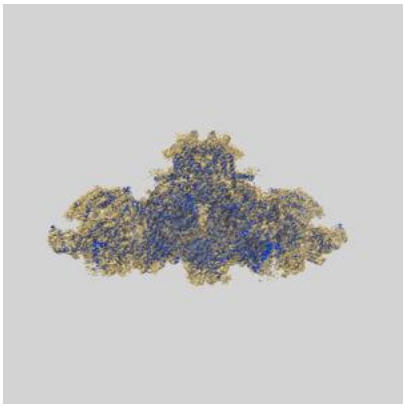
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.76	3.40
Unmasked-calculated*	3.62	4.13	3.71

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

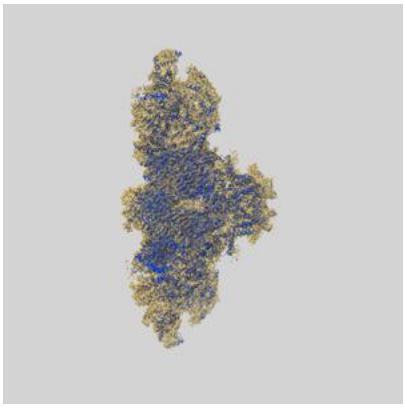
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25830 and PDB model 7TDI. Per-residue inclusion information can be found in section 3 on page 5.

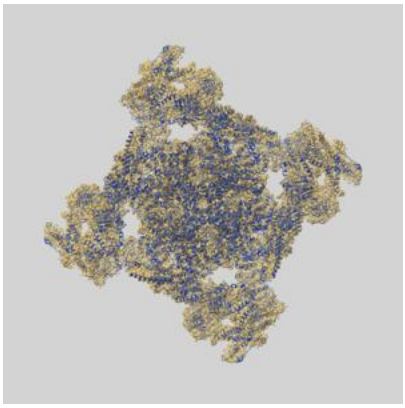
9.1 Map-model overlay



X



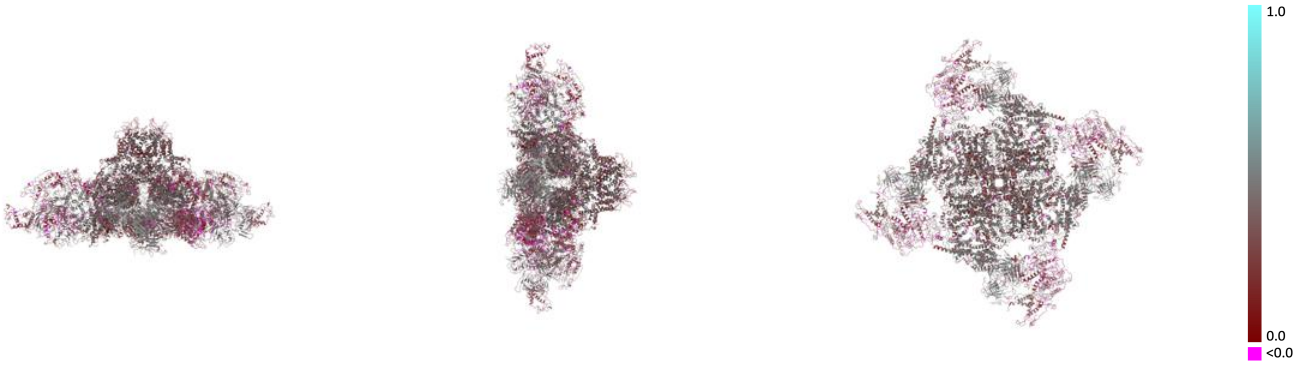
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

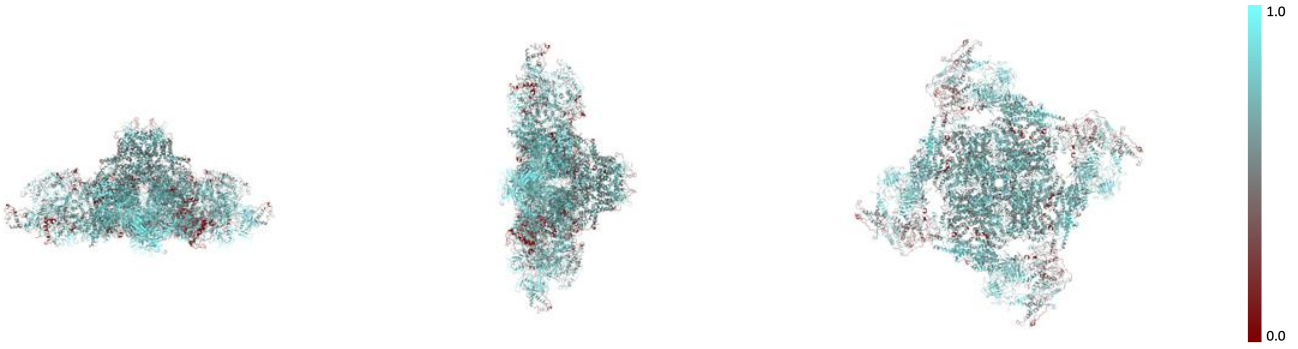
9.2 Q-score mapped to coordinate model (i)



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.

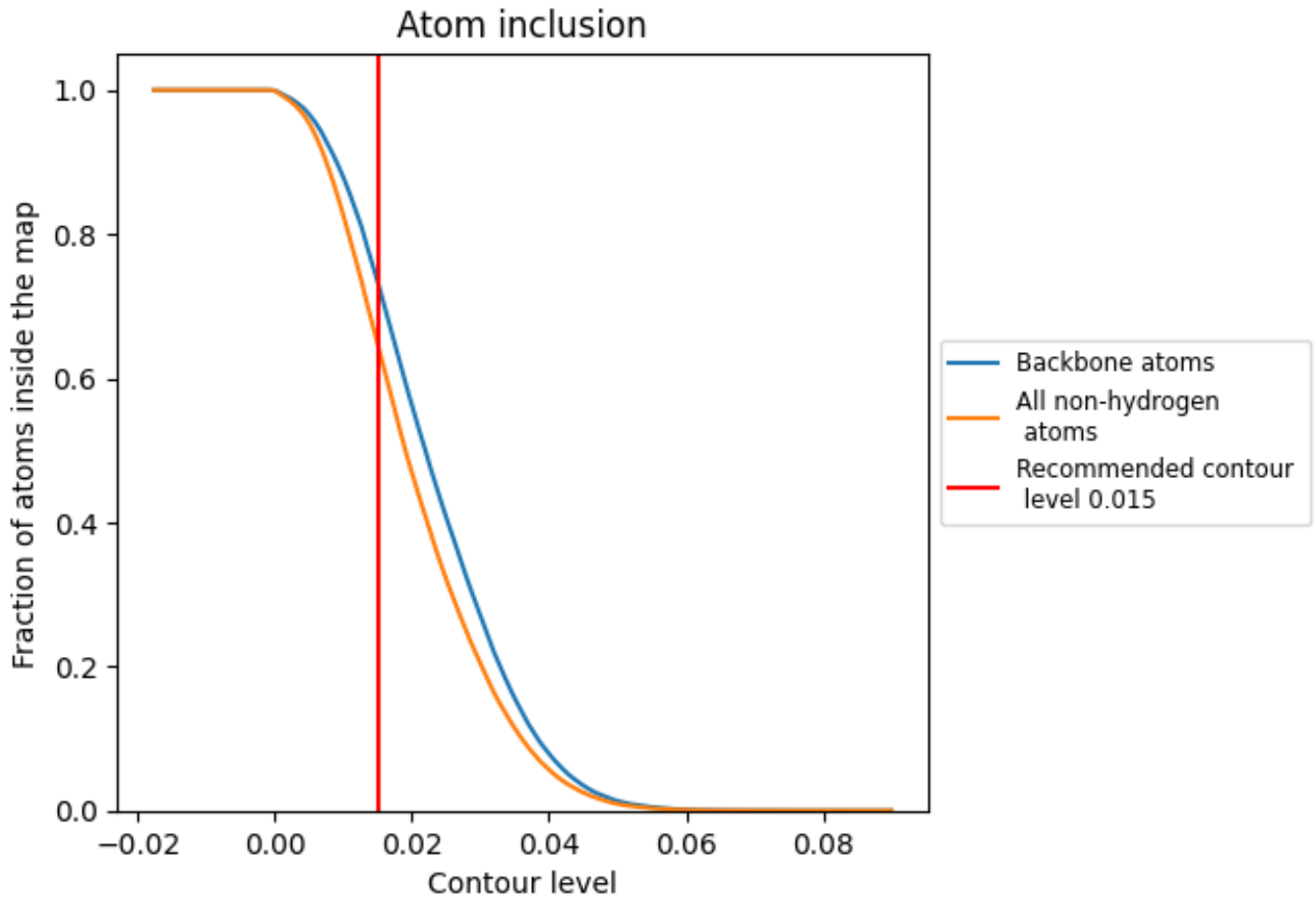
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 65% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6479	0.3320
A	0.6394	0.3250
B	0.6492	0.3350
C	0.6512	0.3350
D	0.6517	0.3350