Full wwPDB EM Validation Report ⓘ

Nov 11, 2026 – 12:46 PM EST

PDB ID	:	9Z9U / pdb_00009z9u
EMDB ID	:	EMD-73959
Title	:	Skewed-state rabbit RyR1 with activating ligands (Ca2+/ATP) and S107
Authors	:	Chen, Y.S.; Hu, R.B.; Van Petegem, F.
Deposited on	:	2025-11-18
Resolution	:	3.02 Å(reported)
Based on initial model	:	7TZC

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:

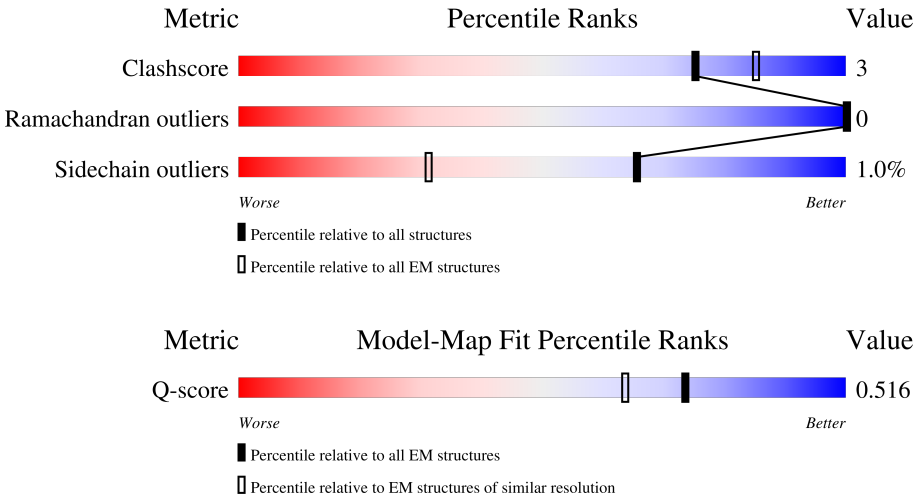
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 3.02 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.



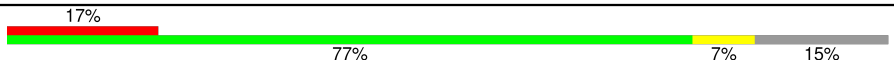
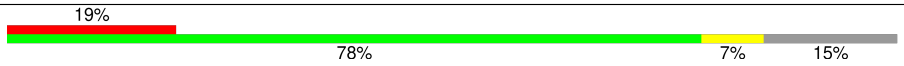
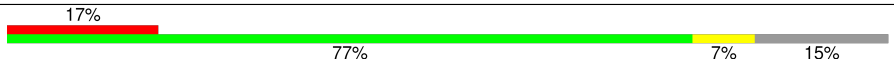
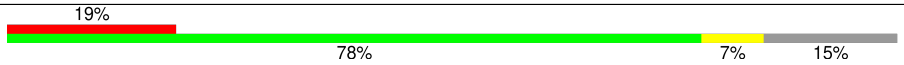
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13913 (2.52 - 3.52)

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	110	5% 85% 12%
1	C	110	88% 10%
1	E	110	5% 85% 12%
1	G	110	88% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	5037	
2	D	5037	
2	F	5037	
2	H	5037	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 136530 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	108	Total	C	N	O	S	0	0
			823	519	145	155	4		
1	C	108	Total	C	N	O	S	0	0
			823	519	145	155	4		
1	E	108	Total	C	N	O	S	0	0
			823	519	145	155	4		
1	G	108	Total	C	N	O	S	0	0
			823	519	145	155	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P68106
A	0	ASN	-	expression tag	UNP P68106
A	1	ALA	-	expression tag	UNP P68106
C	-1	SER	-	expression tag	UNP P68106
C	0	ASN	-	expression tag	UNP P68106
C	1	ALA	-	expression tag	UNP P68106
E	-1	SER	-	expression tag	UNP P68106
E	0	ASN	-	expression tag	UNP P68106
E	1	ALA	-	expression tag	UNP P68106
G	-1	SER	-	expression tag	UNP P68106
G	0	ASN	-	expression tag	UNP P68106
G	1	ALA	-	expression tag	UNP P68106

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4271	Total	C	N	O	S	1	0
			33294	21258	5756	6056	224		
2	D	4270	Total	C	N	O	S	1	0
			33259	21231	5758	6046	224		
2	F	4271	Total	C	N	O	S	1	0
			33294	21258	5756	6056	224		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	4270	Total 33259	C 21231	N 5758	O 6046	S 224	1	0

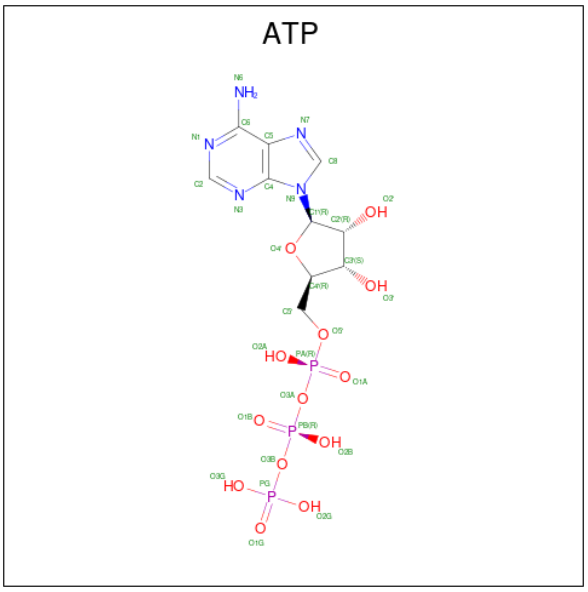
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 1	0
3	F	1	Total 1	Zn 1	0
3	H	1	Total 1	Zn 1	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	D	1	Total 1	Ca 1	0
4	F	1	Total 1	Ca 1	0
4	H	1	Total 1	Ca 1	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



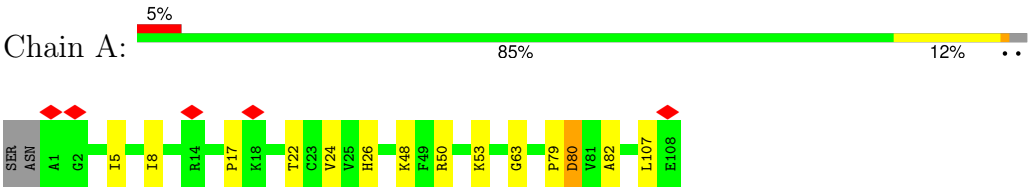
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots (i)

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

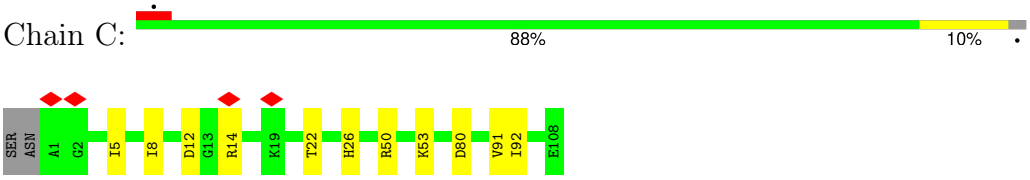
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



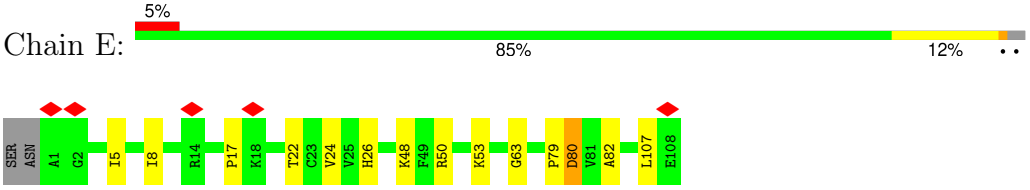
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain C:



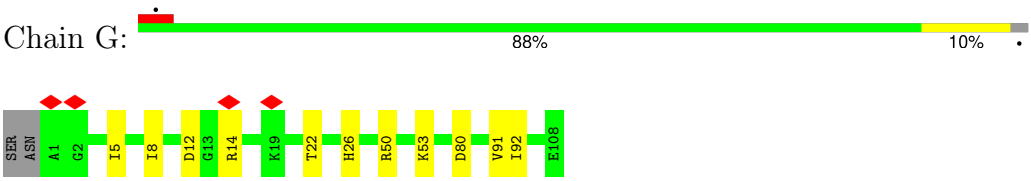
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



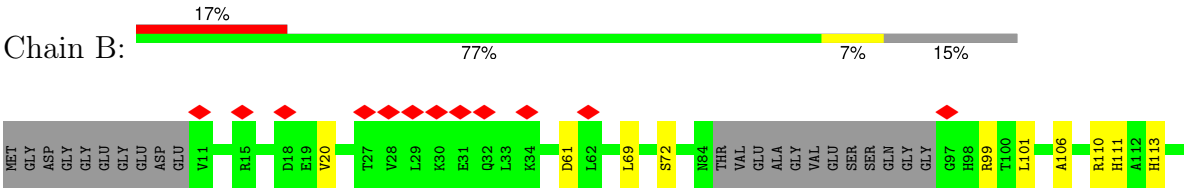
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

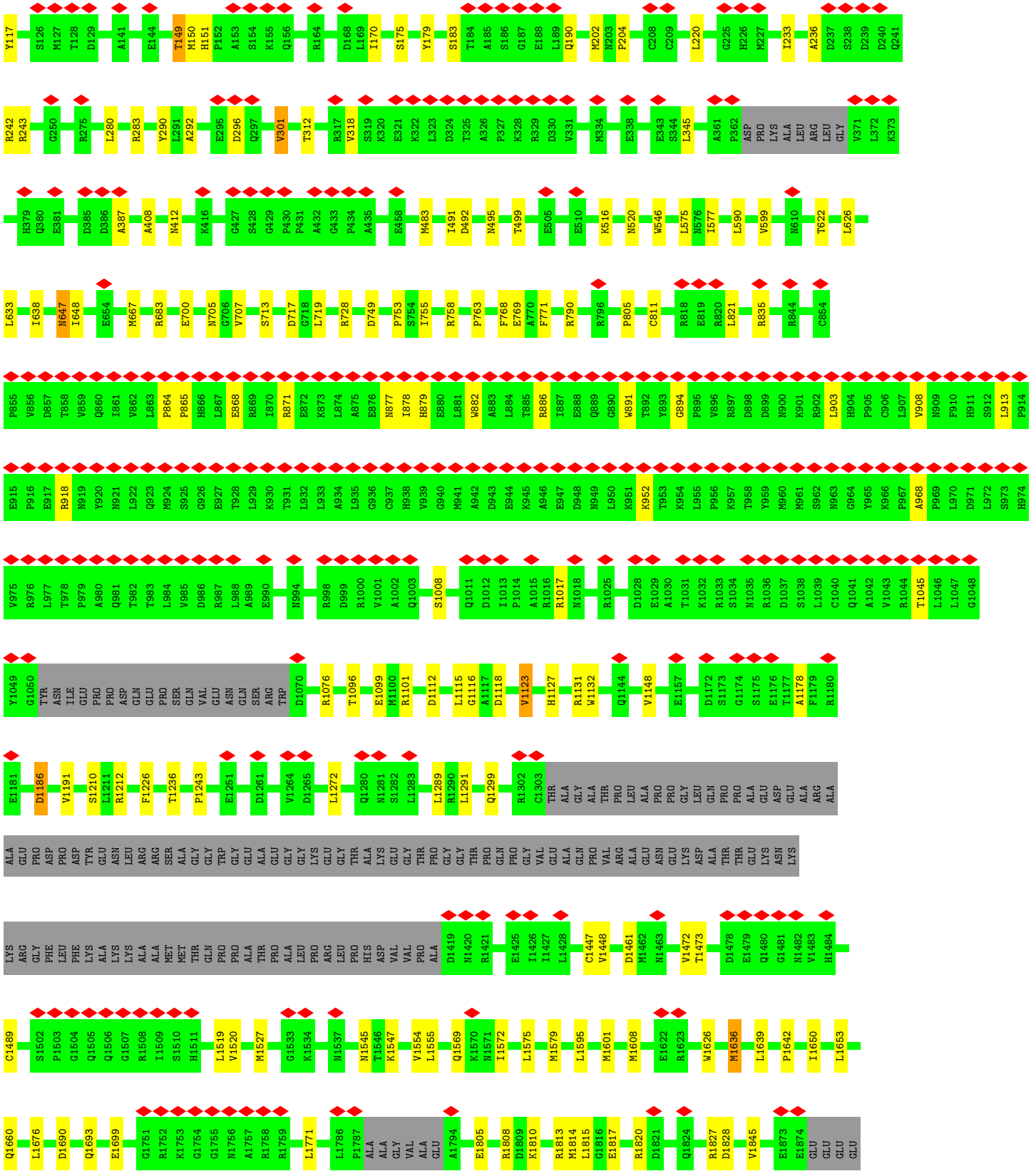
Chain G:

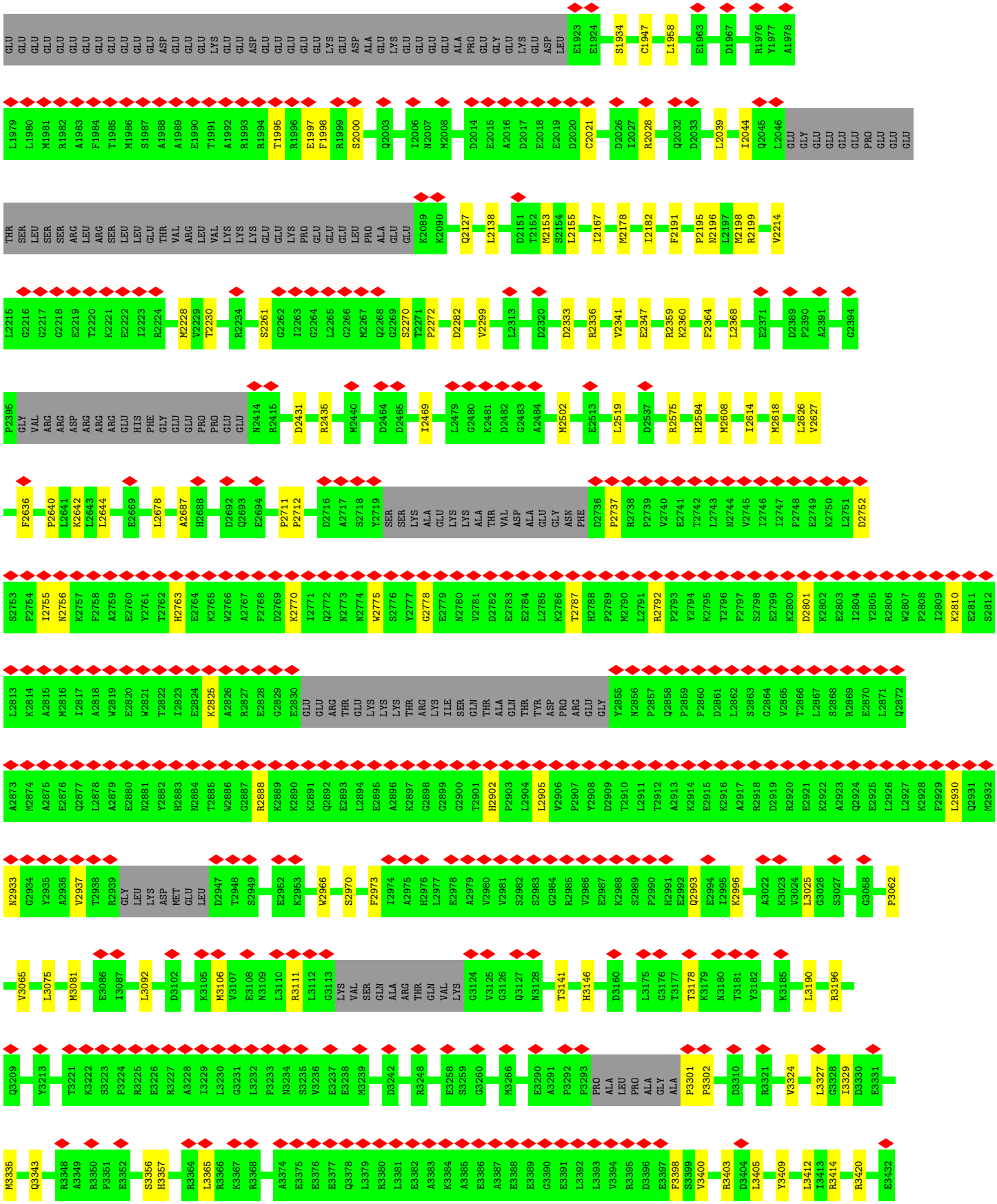


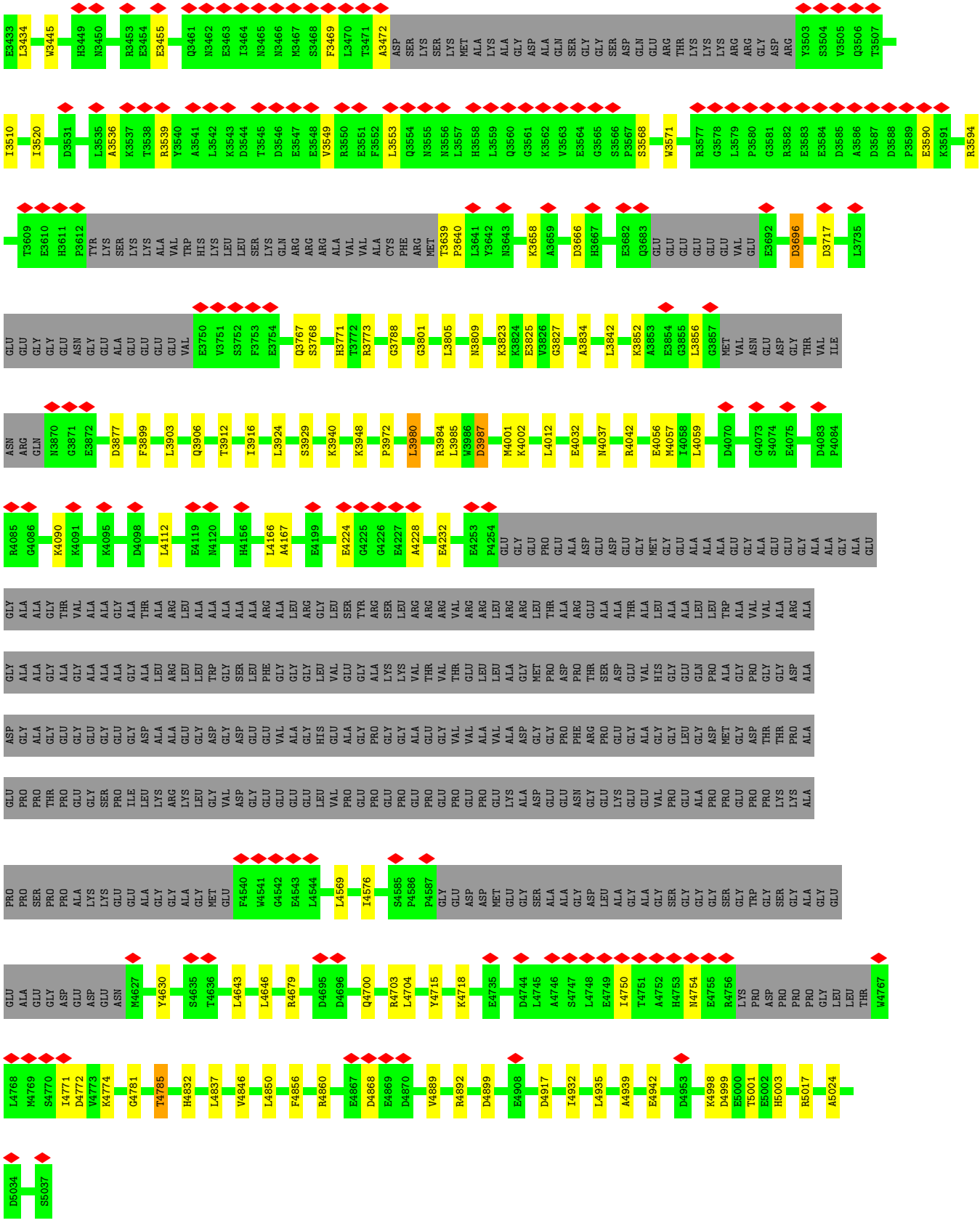
• Molecule 2: Ryanodine receptor 1

Chain B:




Y117 S126 M127 T128 D129 A141 E144 T149 M150 H151 P152 A153 S154 K155 Q156 R164 D168 L169 I170 S175 Y179 S183 T184 A185 S186 G187 E188 L189 Q190 M202 N203 P204 C208 C209 L220 G225 H226 M227 I233 A236 D237 S238 D239 D240 Q241
R242 R243 G250 R275 L280 R283 Y290 L291 A292 E295 D296 Q297 V301 T312 R317 V318 S319 K320 E321 K322 L323 D324 T325 A326 P327 K328 R329 D330 V331 W334 E338 E343 S344 L345 A361 P362 ASP PRO LYS ALA LEU ARG LEU GLY V371 L372 K373
H379 Q380 E381 D385 D386 A387 A408 N412 K416 G427 S428 G429 P430 P431 A432 G433 P434 A435 E458 M483 I491 D492 N495 T499 E505 E510 K516 N520 W546 L575 N576 I577 L590 V599 N610 T622 L626
L633 I638 N647 I648 E654 M667 R683 E700 N705 G706 V707 S713 D717 G718 L719 R728 D749 P753 S754 I755 R758 P763 F768 E769 A770 F771 R790 R796 P805 C811 R818 E819 R820 L821 R835 R844 C854
P855 V856 D857 T858 V859 Q860 I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912 L913 P914
E915 P916 E917 R918 N919 Y920 N921 L922 Q923 N924 S925 G926 E927 T928 L929 K930 T931 L932 L933 A934 L935 G936 C937 H938 V939 G940 N941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 N960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 H974
V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 V985 D986 R987 L988 A989 E990 N994 R998 D999 R1000 V1001 A1002 Q1003 S1008 Q1011 D1012 I1013 P1014 A1015 R1016 R1017 N1018 R1025 D1028 E1029 A1030 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048
Y1049 G1050 TYR ASN ILE GLU PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1076 T1096 E1099 M1100 R1101 D1112 L1115 G1116 A1117 D1118 V1123 H1127 R1131 W1132 Q1144 V1148 E1157 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179 R1180
E1181 D1186 V1191 S1210 L1211 R1212 F1226 T1236 P1243 E1251 D1261 V1264 D1265 L1272 Q1280 N1281 S1282 L1283 L1289 R1290 L1291 Q1299 R1302 C1303 THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA
ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY GLY THR ALA LYS GLU GLY GLY THR PRO GLY GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS
LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 E1425 I1426 I1427 L1428 C1447 V1448 D1461 M1462 N1463 V1472 T1473 D1478 E1479 Q1480 G1481 N1482 V1483 H1484
C1489 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 L1519 V1520 M1527 G1533 K1534 N1537 N1545 T1546 K1547 V1554 L1555 Q1569 K1570 N1571 I1572 L1575 M1579 L1595 M1601 M1608 E1622 R1623 W1626 M1636 L1639 P1642 I1650 L1653
Q1660 L1676 D1690 Q1693 E1699 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 L1771 L1786 P1787 ALA ALA GLY VAL ALA GLU A1794 E1805 R1808 D1809 K1810 R1813 M1814 L1815 G1816 E1817 R1820 D1821 Q1824 R1827 D1828 V1845 E1873 E1874 GLU GLU GLU GLU

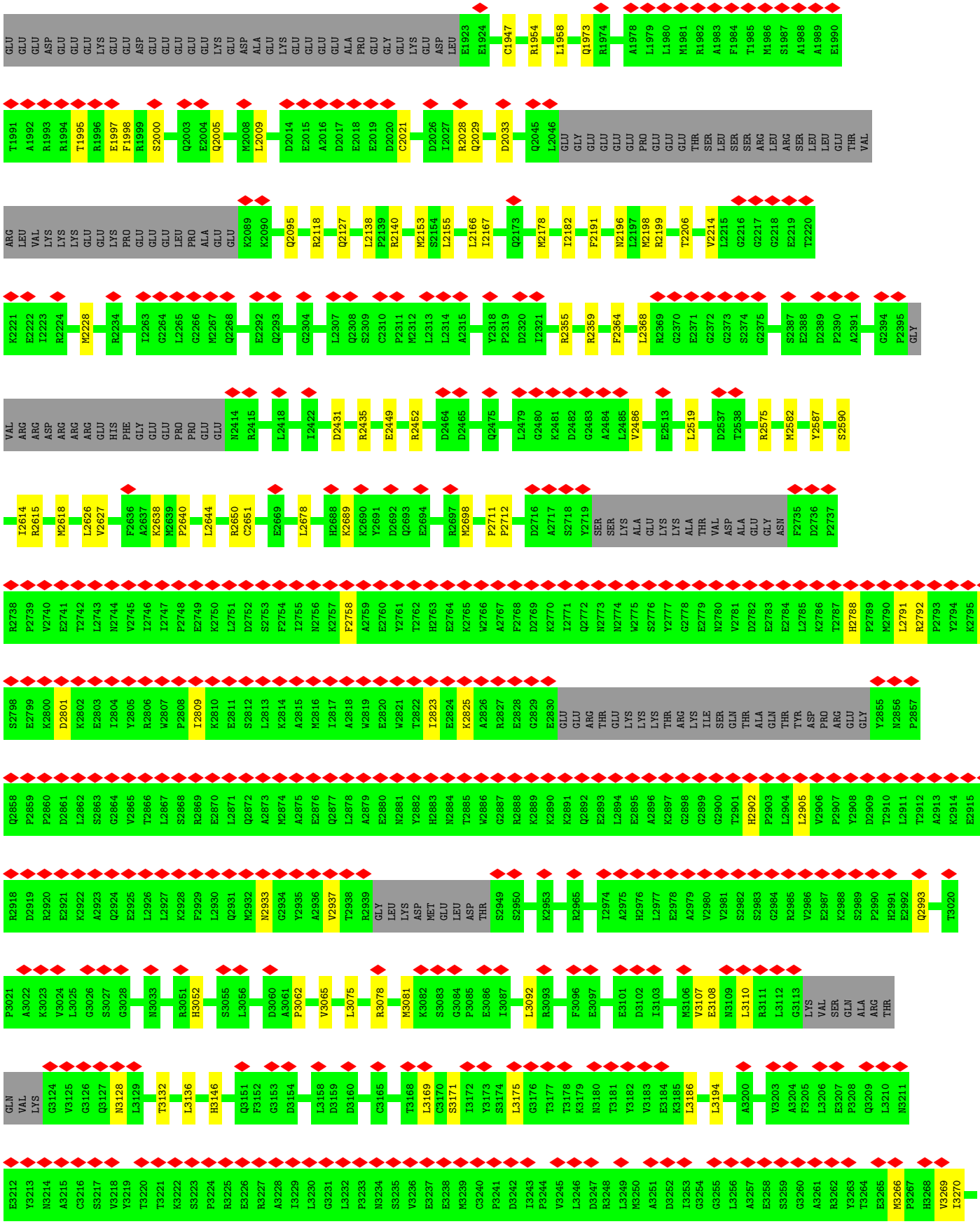

GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU LYS GLU GLU GLU LYS GLU GLU ASP ALA GLU LYS GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU
E1923 E1924 S1934 C1947 L1958 E1963 D1967 R1976 Y1977 A1978
L1979 L1980 M1981 R1982 A1983 A1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 Q2003 I2006 N2007 M2008 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021 D2026 I2027 R2028 Q2032 D2033 L2039 I2044 Q2045 L2046 GLU GLY 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 Q2127 L2138 D2151 T2152 M2153 S2154 L2155 I2167 M2178 I2182 F2191 P2195 N2196 L2197 M2198 R2199 V2214
L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 R2224 M2228 V2229 T2230 R2234 S2261 G2262 I2263 G2264 L2265 G2266 M2267 Q2268 G2269 S2270 T2271 P2272 D2282 V2299 L2313 D2320 D2333 R2336 V2341 E2347 R2359 K2360 F2364 L2368 E2371 D2389 P2390 A2391 G2394
P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU
N2414 R2415 D2431 R2435 M2440 D2464 D2465 I2469 L2479 G2480 K2481 D2482 G2483 A2484 M2502 E2513 L2519 D2537 R2575 H2584 M2608 I2614 M2618 L2626 V2627
F2636 P2640 L2641 K2642 L2643 L2644 E2669 L2678 A2687 H2688 D2692 Q2693 E2694 P2711 P2712 D2716 A2717 S2718 Y2719 SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY ASN PHE D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752
S2753 F2754 I2755 N2756 K2757 P2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812
L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872
A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932
N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU LEU D2947 T2948 S2949 E2952 K2953 W2966 S2970 F2973 I2974 A2975 H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 Q2993 E2994 I2995 K2996 A3022 K3023 V3024 L3025 G3026 S3027 G3058 P3062
V3065 L3075 M3081 E3086 I3087 L3092 D3102 K3105 M3106 V3107 E3108 N3109 L3110 R3111 L3112 G3113 LYS VAL SER GLN ALA ARG THR GLN VAL LYS G3124 V3125 G3126 Q3127 N3128 T3141 H3146 D3160 L3175 G3176 T3177 T3178 K3179 N3180 T3181 Y3182 K3185 L3190 R3196
Q3209 Y3213 T3221 K3222 S3223 P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233 N3234 S3235 V3236 E3237 E3238 M3239 D3242 R3248 E3258 S3259 G3260 M3266 E3290 A3291 P3292 P3293 PRO ALA LEU PRO ALA GLY ALA P3301 P3302 D3310 R3321 V3324 L3327 G3328 I3329 D3330 E3331
M3335 Q3343 R3348 A3349 R3350 P3351 E3352 S3356 H3357 R3364 L3365 R3366 K3367 R3368 A3374 E3375 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 L3393 V3394 R3395 D3396 E3397 F3398 S3399 V3400 R3403 D3404 L3405 Y3409 L3412 I3413 R3414 R3420 E3432

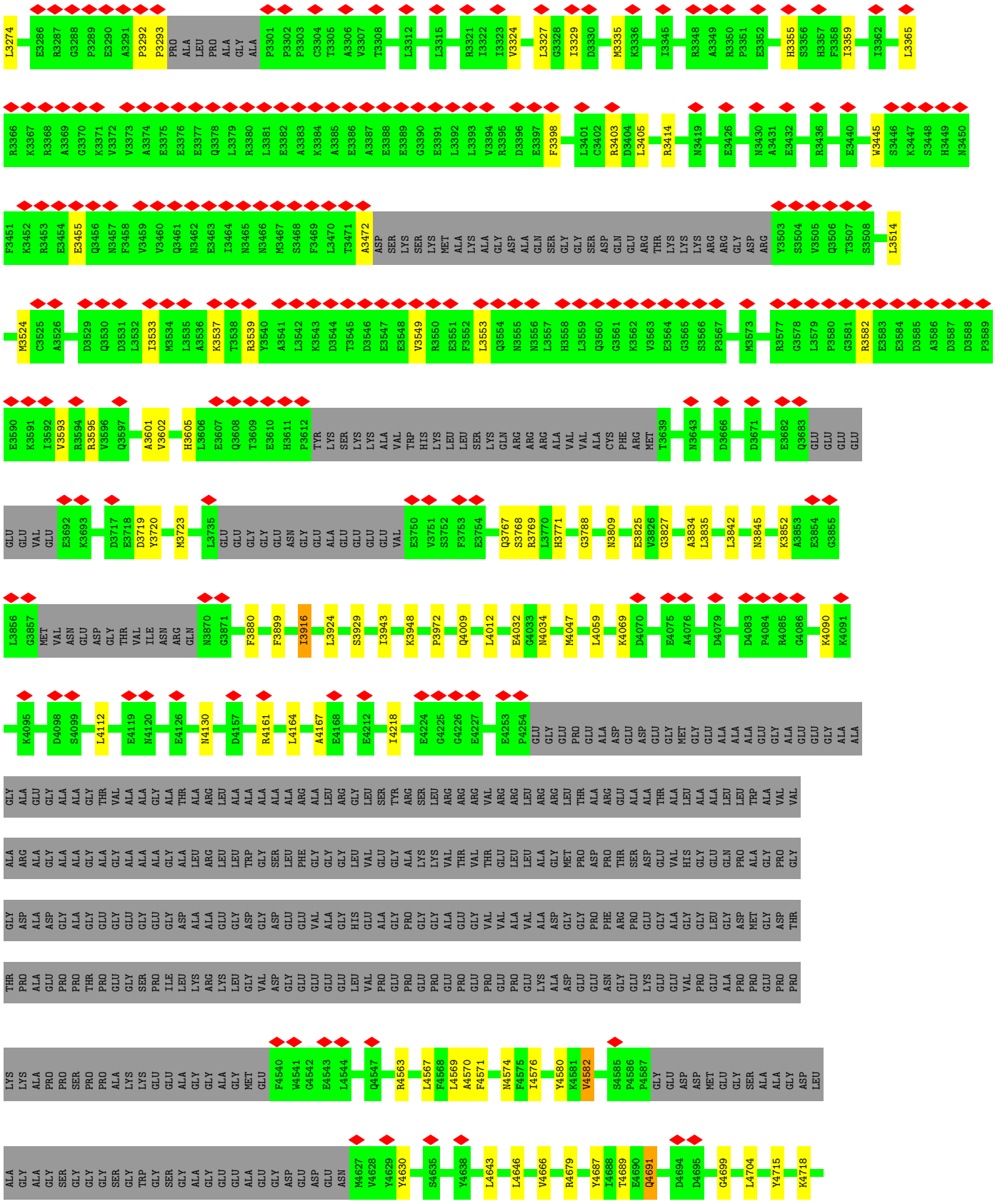


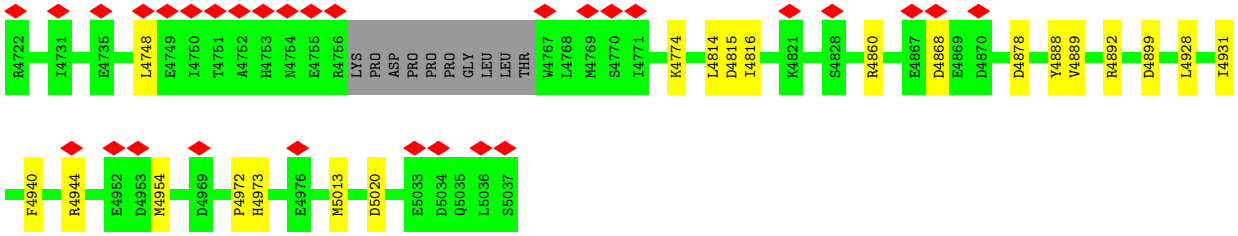
• Molecule 2: Ryanodine receptor 1

Chain D:




GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU
E1923 E1924 C1947 R1954 L1958 Q1973 R1974 A1978 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990
T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 Q2003 E2004 Q2005 M2008 L2009 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021 D2026 I2027 R2028 Q2029 D2033 Q2045 L2046 GLU GLY 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 LEU PRO ALA GLU GLU
K2089 K2090 Q2095 R2118 Q2127 L2138 P2139 R2140 M2153 S2154 L2155 L2166 I2167 Q2173 M2178 I2182 F2191 N2196 L2197 M2198 R2199 T2206 V2214 L2215 G2216 G2217 G2218 E2219 T2220
K2221 E2222 I2223 R2224 M2228 R2234 I2263 G2264 L2265 G2266 M2267 Q2268 E2292 Q2293 G2304 L2307 Q2308 S2309 C2310 P2311 M2312 L2313 L2314 A2315 Y2318 P2319 D2320 I2321 R2355 R2359 F2364 L2368 R2369 G2370 E2371 G2372 G2373 S2374 G2375 S2387 E2388 D2389 P2390 A2391 G2394 P2395 GLY
VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO PRO GLU GLU
N2414 R2415 L2418 I2422 D2431 R2435 E2449 R2452 D2464 D2465 Q2475 L2479 G2480 K2481 D2482 G2483 A2484 L2485 V2486 E2513 L2519 D2537 T2538 R2575 M2582 Y2587 S2590
I2614 R2615 M2618 L2626 V2627 F2636 A2637 K2638 M2639 P2640 L2644 R2650 C2651 E2669 L2678 H2688 K2689 K2690 Y2691 D2692 Q2693 E2694 R2697 M2698 P2711 P2712 D2716 A2717 S2718 Y2719 SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY ASN F2735 D2736 P2737
R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797
S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 A2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857
Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917
R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP THR S2949 S2950 K2953 R2965 I2974 A2975 H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 Q2993 T3020
P3021 A3022 K3023 V3024 L3025 G3026 S3027 G3028 N3033 R3051 H3052 S3055 L3056 D3060 A3061 P3062 V3065 L3075 R3078 M3081 K3082 S3083 G3084 P3085 E3086 I3087 L3092 R3093 F3096 E3097 E3101 D3102 I3103 M3106 V3107 E3108 N3109 L3110 R3111 L3112 G3113 LYS VAL SER GLN ALA ARG THR
GLN VAL LYS G3124 V3125 G3126 Q3127 N3128 L3129 T3132 L3136 H3146 Q3151 F3152 G3153 D3154 L3158 D3159 D3160 C3165 T3168 L3169 C3170 S3171 I3172 Y3173 S3174 L3175 G3176 T3177 T3178 K3179 N3180 T3181 Y3182 V3183 E3184 K3185 L3186 L3194 A3200 V3203 A3204 F3205 L3206 E3207 P3208 Q3209 L3210 N3211
E3212 Y3213 N3214 A3215 C3216 S3217 Y3218 Y3219 T3220 T3221 K3222 S3223 P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233 N3234 S3235 V3236 E3237 E3238 M3239 C3240 P3241 D3242 I3243 P3244 V3245 L3246 D3247 R3248 L3249 M3250 A3251 D3252 I3253 G3254 G3255 L3256 A3257 E3258 S3259 G3260 A3261 R3262 Y3263 T3264 E3265 M3266 P3267 H3268 V3269 I3270

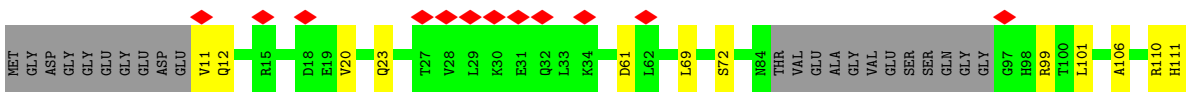

L3274 E3286 R3287 G3288 P3289 E3290 A3291 P3292 P3293 PRO ALA LEU PRO ALA GLY ALA P3301 P3302 P3303 C3304 T3305 A3306 V3307 T3308 L3312 L3315 R3321 I3322 I3323 V3324 L3327 G3328 I3329 D3330 M3335 K3336 I3345 R3348 A3349 R3350 P3351 E3362 H3355 S3356 H3357 F3358 I3359 I3362 L3365
R3366 K3367 R3368 A3369 G3370 K3371 V3372 V3373 A3374 E3375 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 L3393 V3394 R3395 D3396 E3397 F3398 L3401 C3402 R3403 D3404 L3405 R3414 N3419 E3426 N3430 A3431 E3432 R3436 E3440 W3445 S3446 K3447 S3448 H3449 N3450
F3451 K3452 R3453 E3454 E3455 Q3456 N3457 F3458 V3459 V3460 Q3461 N3462 E3463 I3464 N3465 N3466 M3467 S3468 F3469 L3470 T3471 A3472 ASP SER LYS SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG Y3503 S3504 V3505 Q3506 T3507 S3508 L3514
M3524 C3525 A3526 D3529 Q3530 D3531 L3532 I3533 M3534 L3535 A3536 K3537 T3538 R3539 Y3540 A3541 L3542 K3543 D3544 T3545 D3546 E3547 E3548 V3549 R3550 E3551 F3552 L3553 Q3554 N3555 N3556 L3557 H3558 L3559 Q3560 G3561 K3562 V3563 E3564 G3565 S3566 P3567 M3573 R3577 G3578 L3579 P3580 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 P3589
E3590 K3591 I3592 V3593 R3594 R3595 V3596 Q3597 A3601 V3602 H3605 L3606 E3607 Q3608 T3609 E3610 H3611 P3612 TYR 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 N3643 D3666 D3671 E3682 Q3683 GLU GLU GLU GLU
GLU GLU VAL GLU E3692 K3693 D3717 E3718 D3719 Y3720 M3723 L3735 GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 V3751 S3752 F3753 E3754 Q3767 S3768 R3769 L3770 H3771 G3788 N3809 E3825 V3826 G3827 A3834 L3835 L3842 N3845 K3852 A3853 E3854 G3855
L3856 G3857 MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN N3870 G3871 F3880 F3899 I3916 L3924 S3929 I3943 K3948 P3972 Q4009 L4012 E4032 G4033 N4034 M4047 L4059 K4069 D4070 E4075 A4076 D4079 D4083 P4084 R4085 G4086 K4090 K4091
K4095 D4098 S4099 L4112 E4119 N4120 E4126 N4130 D4157 R4161 L4164 A4167 E4168 E4212 I4218 E4224 G4225 G4226 E4227 E4253 P4254 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
GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA ALA GLY ALA THR ALA ALA ARG LEU ALA ALA ALA ALA ALA ALA GLY ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG ARG VAL ARG ARG ARG LEU ARG ARG ARG LEU THR ALA ARG GLU GLU ALA ALA THR ALA LEU ALA ALA ALA LEU LEU TRP ALA VAL VAL
ALA ARG ALA GLY ALA GLY ALA ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU 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 ASP GLY ALA GLY GLU GLY GLU GLY ASP GLY ALA ALA GLU GLY GLY ASP GLY GLU GLU VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY GLY LEU GLY ASP MET GLY PRO THR
THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU



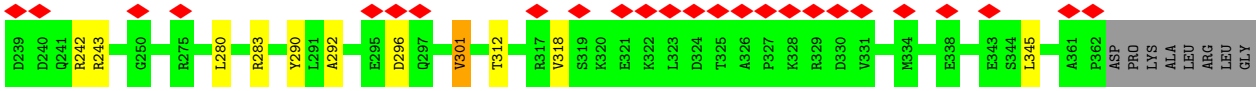
• Molecule 2: Ryanodine receptor 1

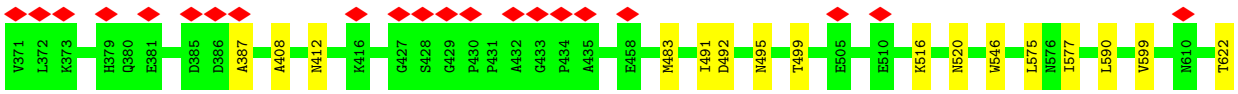
Chain F:



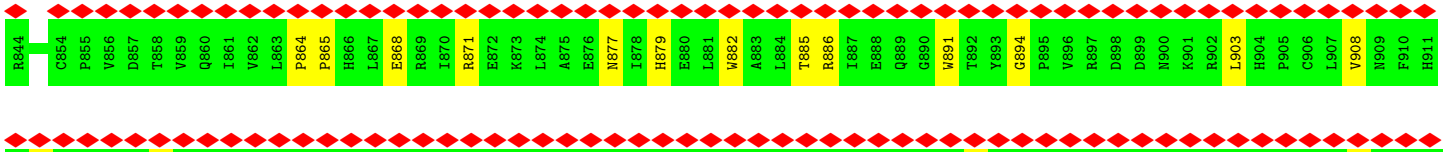


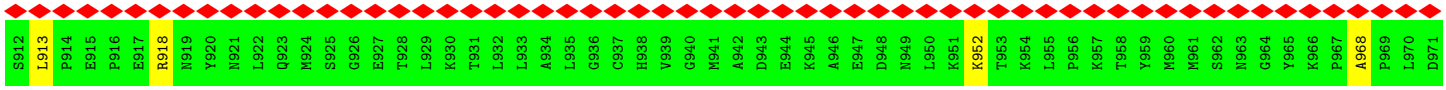




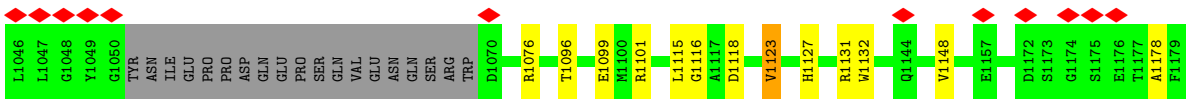


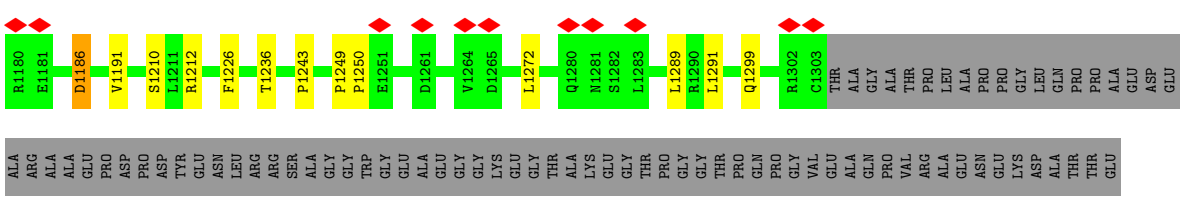


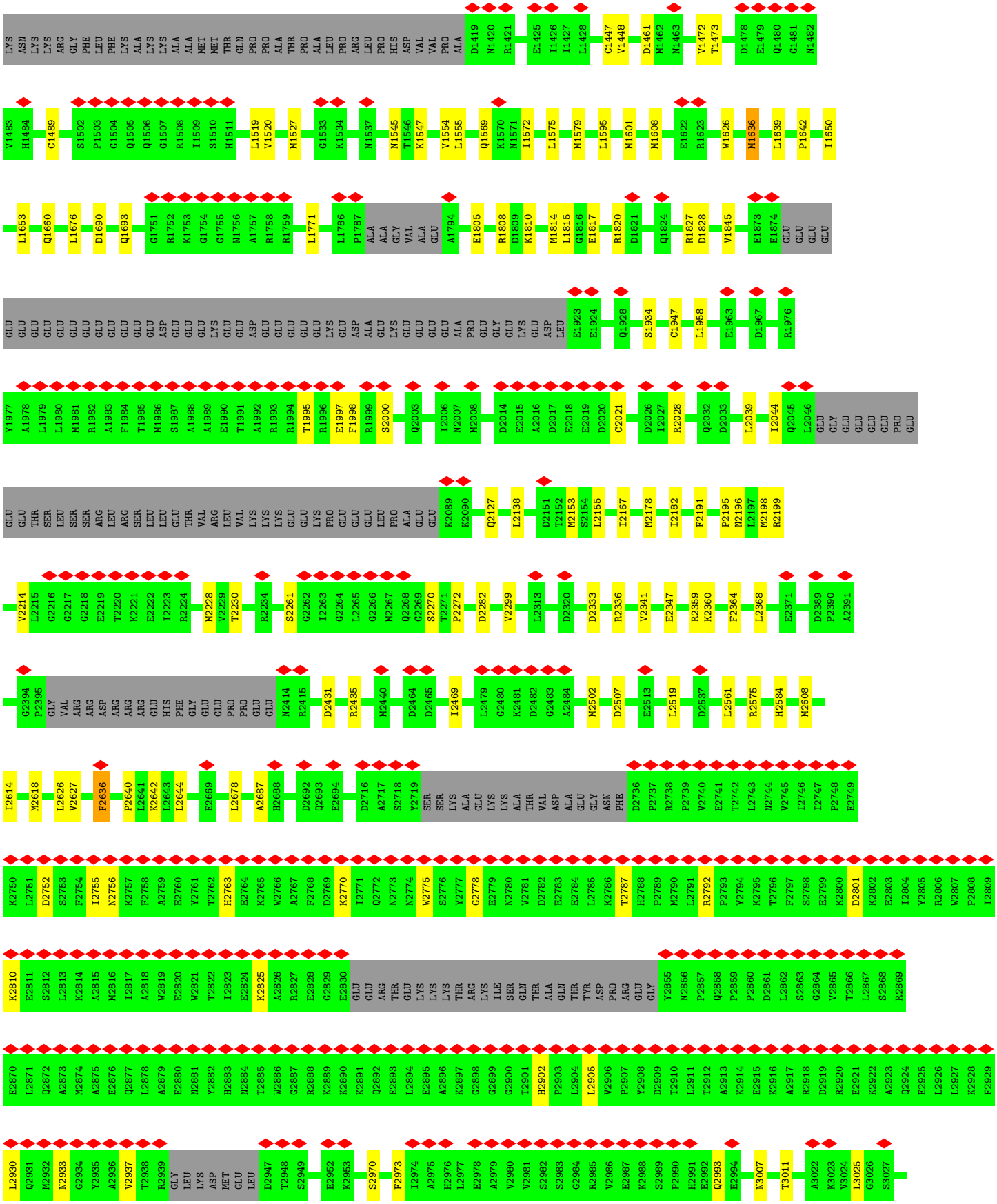


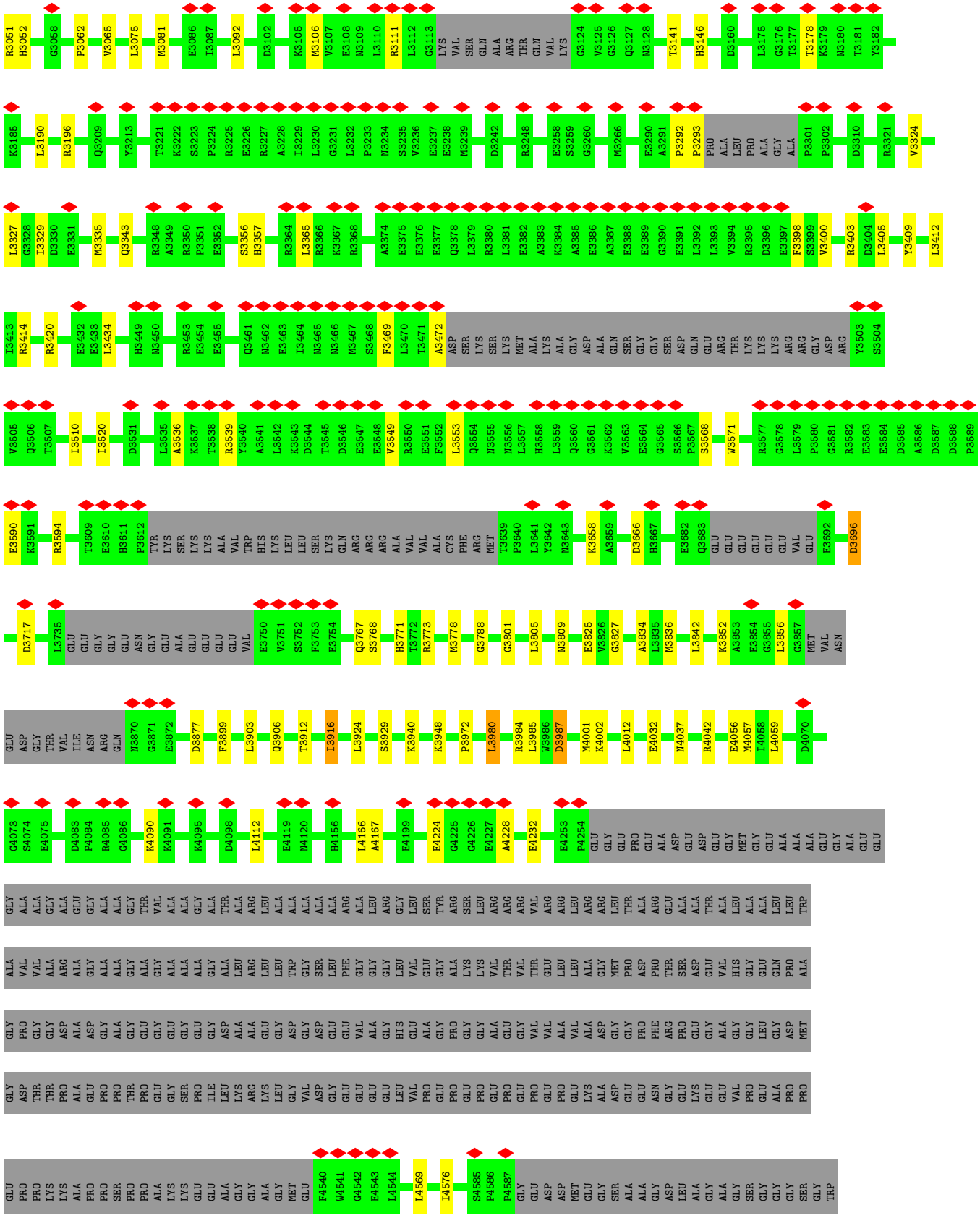


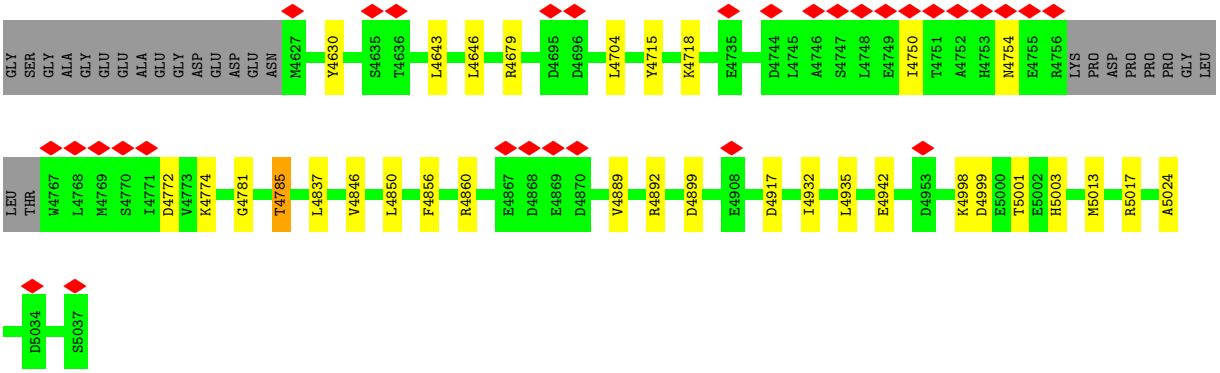








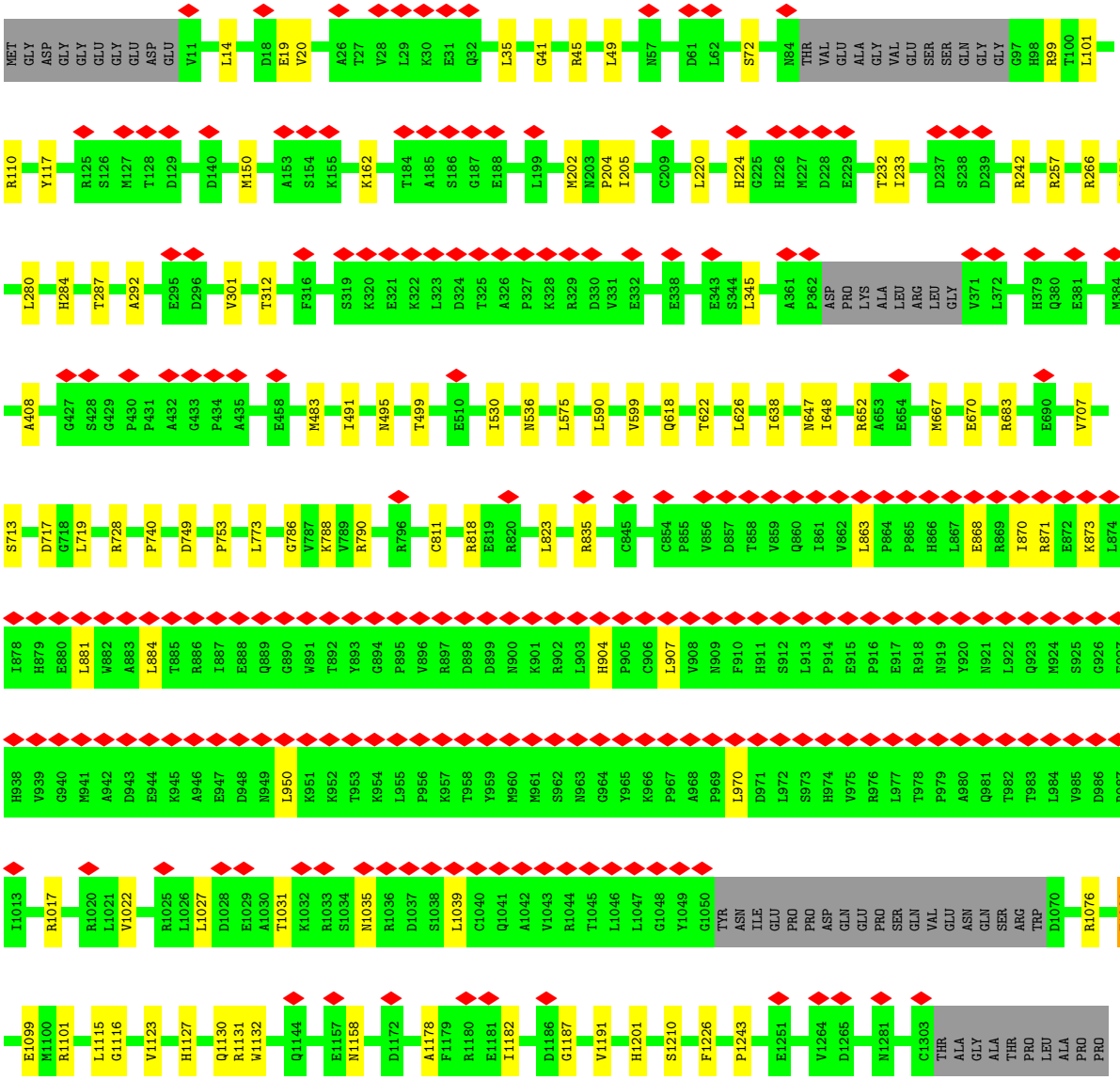


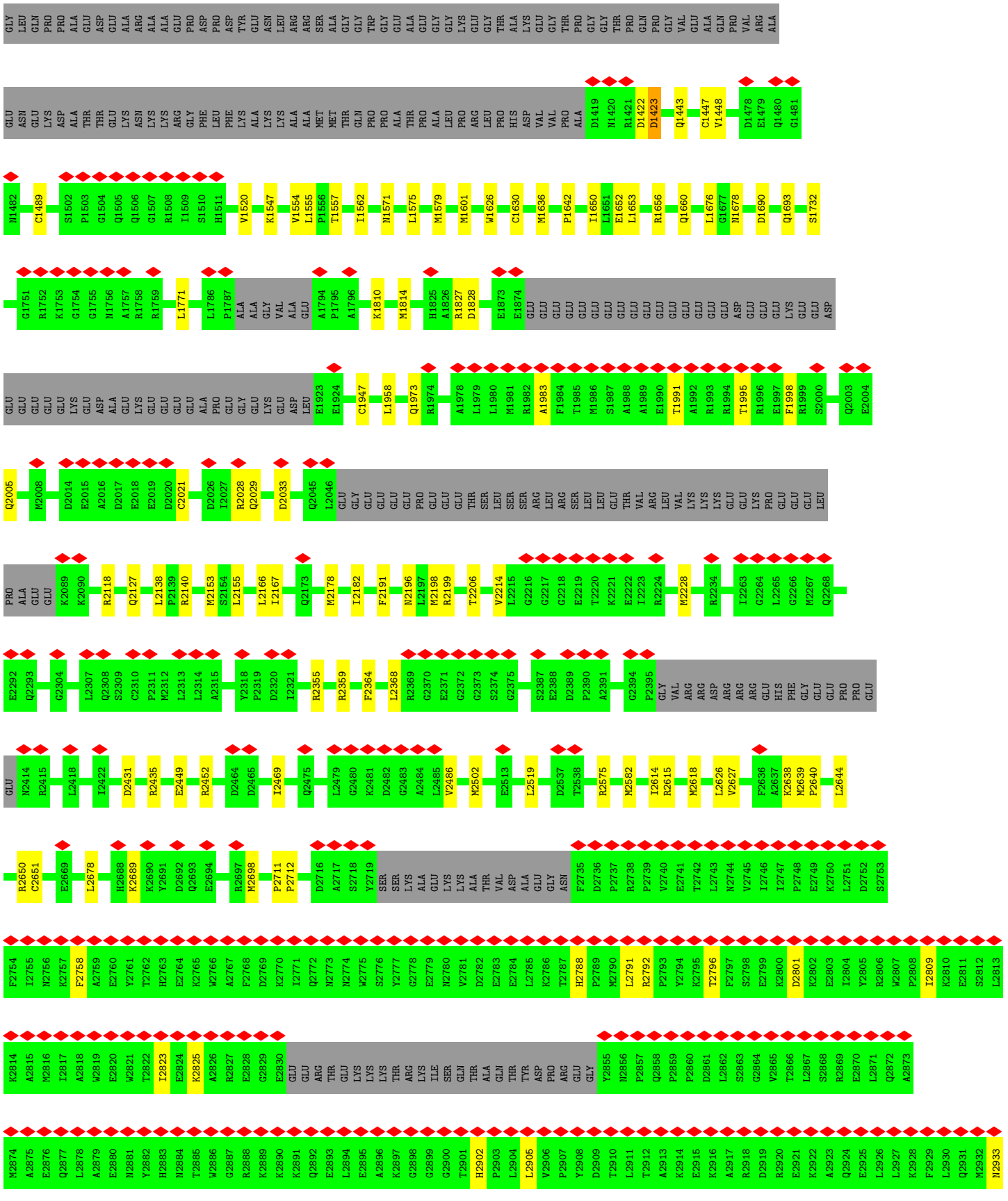


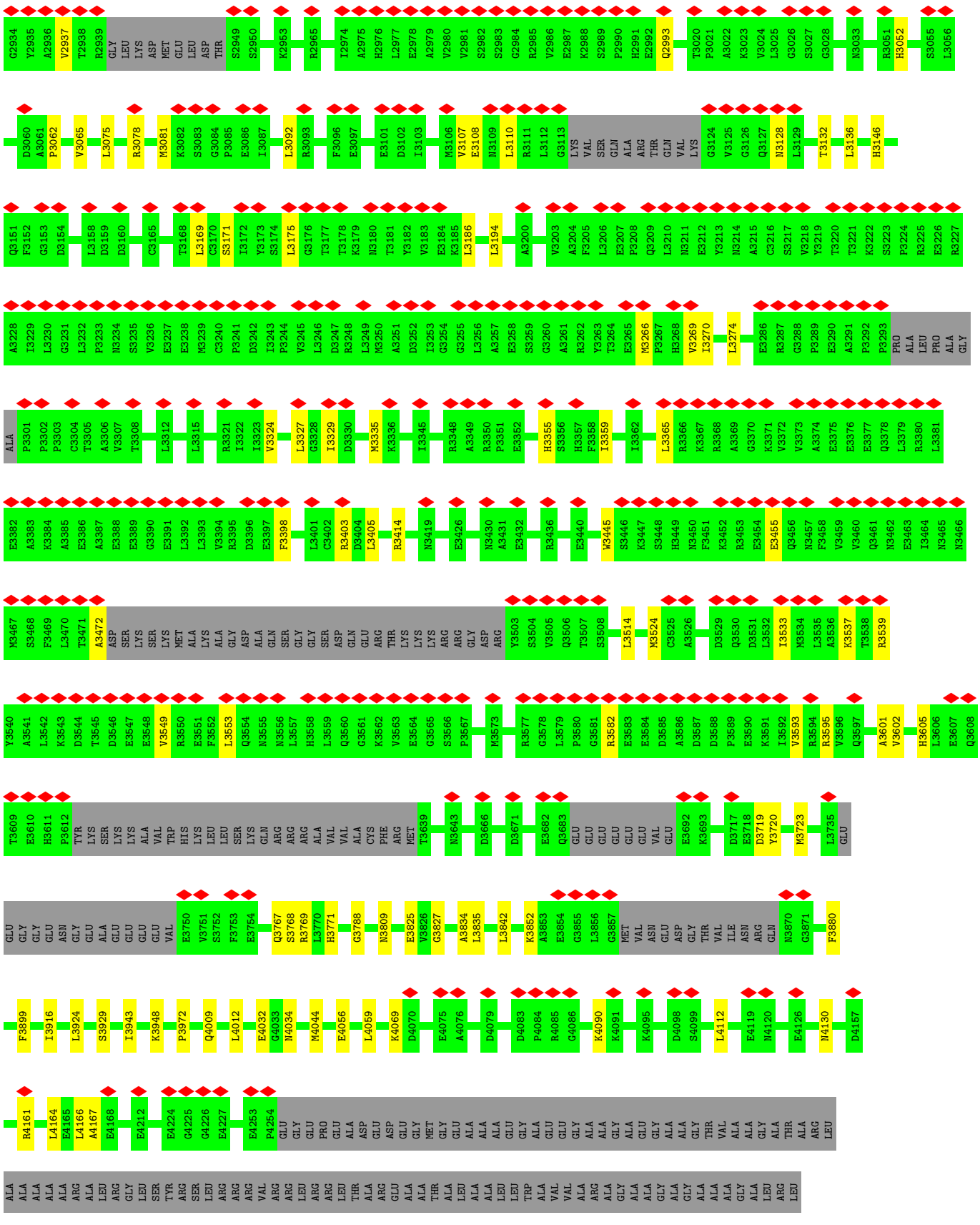
• Molecule 2: Ryanodine receptor 1

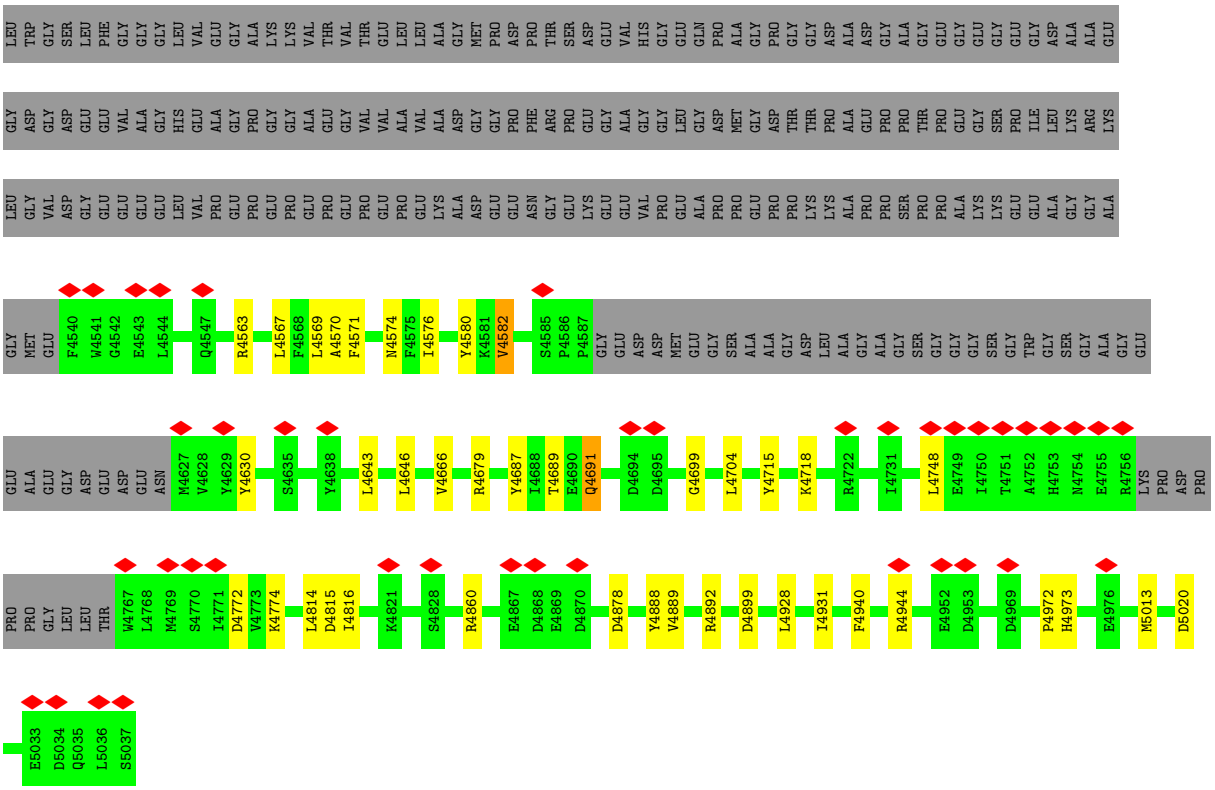
Chain H:






GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ALA ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA
GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 Q1443 C1447 V1448 D1478 E1479 Q1480 G1481
N1482 C1489 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 V1520 K1547 V1554 L1555 P1556 T1557 I1562 N1571 L1575 M1579 M1601 W1626 C1630 M1636 P1642 I1650 L1651 E1652 L1653 R1656 Q1660 L1676 G1677 N1678 D1690 Q1693 S1732
G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 L1771 L1786 P1787 ALA ALA GLY VAL ALA GLU A1794 P1795 A1796 K1810 M1814 H1825 A1826 R1827 D1828 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 LYS GLU ASP ALA GLU LYS GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU E1923 E1924 C1947 L1958 Q1973 R1974 A1978 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 Q2003 E2004
Q2005 M2008 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021 D2026 I2027 R2028 Q2029 D2033 Q2045 L2046 GLU GLY GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU LEU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU
PRO ALA GLU GLU K2089 K2090 R2118 Q2127 L2138 P2139 R2140 M2153 S2154 L2155 L2166 I2167 Q2173 M2178 I2182 F2191 N2196 L2197 M2198 R2199 T2206 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 R2224 M2228 R2234 I2263 G2264 L2265 G2266 M2267 Q2268
E2292 Q2293 G2304 L2307 Q2308 S2309 C2310 P2311 M2312 L2313 L2314 A2315 Y2318 P2319 D2320 I2321 R2355 R2359 F2364 L2368 R2369 G2370 E2371 G2372 G2373 S2374 G2375 S2387 E2388 D2389 P2390 A2391 G2394 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU
GLU N2414 R2415 L2418 I2422 D2431 R2435 E2449 R2452 D2464 D2465 I2469 Q2475 L2479 G2480 K2481 D2482 G2483 A2484 L2485 V2486 M2502 E2513 L2519 D2537 T2538 R2575 M2582 I2614 R2615 M2618 L2626 V2627 F2636 A2637 K2638 M2639 P2640 L2644
R2650 C2651 E2669 L2678 H2688 K2689 K2690 Y2691 D2692 Q2693 E2694 R2697 M2698 P2711 P2712 D2716 A2717 S2718 Y2719 SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY ASN F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753
F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813
K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873
M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933




LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU 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 ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU
GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA ALA VAL ALA ASP GLY GLY PRO GLU 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 GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU 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 PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA
GLY MET GLU F4540 W4541 G4542 E4543 L4544 Q4547 R4563 L4567 F4568 L4569 A4570 F4571 N4574 F4575 I4576 Y4580 K4581 V4582 S4585 P4586 P4587 GLY GLU ASP ASP MET GLU GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU
GLU ALA GLU GLY ASP GLU ASP GLU ASN M4627 V4628 Y4629 Y4630 S4635 Y4638 L4643 L4646 V4666 R4679 Y4687 I4688 T4689 E4690 Q4691 D4694 D4695 G4699 L4704 Y4715 K4718 R4722 I4731 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 LYS PRO ASP PRO
PRO PRO GLY LEU LEU THR W4767 L4768 M4769 S4770 I4771 D4772 V4773 K4774 L4814 D4815 I4816 K4821 S4828 R4860 E4867 D4868 E4869 D4870 D4878 Y4888 V4889 R4892 D4899 L4928 I4931 F4940 R4944 E4952 D4953 D4969 P4972 H4973 E4976 M5013 D5020
E5033 D5034 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	91956	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.469	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.068	Depositor
Map size (Å)	477.696, 477.696, 477.696	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.933, 0.933, 0.933	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	0.12	0/839	0.30	0/1130
1	C	0.13	0/839	0.34	0/1130
1	E	0.12	0/839	0.30	0/1130
1	G	0.13	0/839	0.34	0/1130
2	B	0.14	0/34057	0.32	0/46206
2	D	0.13	0/34021	0.31	0/46159
2	F	0.14	0/34057	0.32	0/46206
2	H	0.13	0/34021	0.31	0/46159
All	All	0.14	0/139512	0.31	0/189250

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	823	0	829	8	0
1	C	823	0	829	5	0
1	E	823	0	829	9	0
1	G	823	0	829	5	0
2	B	33294	0	32507	223	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	33259	0	32447	207	0
2	F	33294	0	32507	223	0
2	H	33259	0	32447	200	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
5	B	31	0	12	0	0
5	D	31	0	12	0	0
5	F	31	0	12	0	0
5	H	31	0	12	0	0
All	All	136530	0	133272	824	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 3.

All (824) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2359:ARG:NH1	2:F:179:TYR:CE2	2.35	0.95
2:B:179:TYR:CE2	2:H:2359:ARG:NH1	2.35	0.95
2:D:4944:ARG:HH21	2:F:4942:GLU:HG3	1.40	0.86
2:B:4942:GLU:HG3	2:H:4944:ARG:HH21	1.40	0.84
2:H:868:GLU:O	2:H:871:ARG:HB3	1.83	0.78
2:D:868:GLU:O	2:D:871:ARG:HB3	1.83	0.77
2:D:2359:ARG:NH1	2:F:179:TYR:HE2	1.87	0.72
2:B:868:GLU:O	2:B:871:ARG:HB3	1.91	0.70
2:B:4856:PHE:CZ	2:H:4582:VAL:HG13	2.27	0.70
2:F:868:GLU:O	2:F:871:ARG:HB3	1.91	0.70
2:B:4942:GLU:CG	2:H:4944:ARG:HH21	2.05	0.69
2:D:4582:VAL:HG13	2:F:4856:PHE:CZ	2.27	0.69
2:B:749:ASP:O	2:B:753:PRO:HA	1.93	0.69
2:B:4942:GLU:HG3	2:H:4944:ARG:NH2	2.07	0.69
2:D:4944:ARG:HH21	2:F:4942:GLU:CG	2.05	0.69
2:D:4944:ARG:NH2	2:F:4942:GLU:HG3	2.07	0.69
2:B:179:TYR:HE2	2:H:2359:ARG:NH1	1.87	0.69
2:F:749:ASP:O	2:F:753:PRO:HA	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1116:GLY:HA3	2:F:1132:TRP:HB3	1.77	0.67
2:B:1116:GLY:HA3	2:B:1132:TRP:HB3	1.77	0.66
2:B:647:ASN:HD21	2:B:821:LEU:HA	1.61	0.66
2:B:179:TYR:HE2	2:H:2359:ARG:HH11	1.43	0.66
2:D:2359:ARG:HH11	2:F:179:TYR:HE2	1.43	0.66
2:B:4899:ASP:OD1	2:H:4892:ARG:NH2	2.29	0.65
2:H:3110:LEU:HD12	2:H:3175:LEU:HD21	1.80	0.64
2:B:2261:SER:HB2	2:B:2272:PRO:HB2	1.80	0.64
2:F:647:ASN:HD21	2:F:821:LEU:HA	1.61	0.64
2:D:4582:VAL:CG1	2:F:4856:PHE:CZ	2.80	0.64
2:D:4892:ARG:NH2	2:F:4899:ASP:OD1	2.29	0.64
2:B:4856:PHE:CZ	2:H:4582:VAL:CG1	2.80	0.64
2:F:2627:VAL:HG22	2:F:2678:LEU:HB2	1.79	0.63
2:F:2261:SER:HB2	2:F:2272:PRO:HB2	1.80	0.63
2:B:2627:VAL:HG22	2:B:2678:LEU:HB2	1.79	0.63
2:H:2214:VAL:HG21	2:H:2228:MET:HG2	1.78	0.63
2:D:3335:MET:SD	2:D:3403:ARG:NH1	2.72	0.63
2:H:3335:MET:SD	2:H:3403:ARG:NH1	2.72	0.63
2:D:2214:VAL:HG21	2:D:2228:MET:HG2	1.78	0.63
2:D:3110:LEU:HD12	2:D:3175:LEU:HD21	1.80	0.63
2:H:4704:LEU:O	2:H:4774:LYS:NZ	2.32	0.63
2:H:3075:LEU:O	2:H:3146:HIS:NE2	2.32	0.61
2:B:2902:HIS:HB3	2:B:2905:LEU:HG	1.83	0.61
2:D:4704:LEU:O	2:D:4774:LYS:NZ	2.32	0.61
2:D:863:LEU:HD23	2:D:871:ARG:HH21	1.66	0.61
2:H:863:LEU:HD23	2:H:871:ARG:HH21	1.66	0.60
2:B:758:ARG:HH12	2:B:805:PRO:HG3	1.66	0.60
2:F:2902:HIS:HB3	2:F:2905:LEU:HG	1.83	0.60
2:D:3075:LEU:O	2:D:3146:HIS:NE2	2.32	0.59
2:B:1447:CYS:HB3	2:B:1555:LEU:HB3	1.85	0.59
2:F:758:ARG:HH12	2:F:805:PRO:HG3	1.66	0.59
1:A:79:PRO:HA	1:A:82:ALA:HB3	1.85	0.59
2:B:4704:LEU:O	2:B:4774:LYS:NZ	2.36	0.59
2:F:101:LEU:HB3	2:F:150:MET:HE1	1.85	0.59
2:H:3329:ILE:O	2:H:3403:ARG:NH2	2.35	0.59
2:D:3052:HIS:HE1	2:D:3128:ASN:HD22	1.50	0.59
2:F:4704:LEU:O	2:F:4774:LYS:NZ	2.36	0.59
2:B:491:ILE:O	2:B:495:ASN:HB2	2.03	0.59
2:D:3329:ILE:O	2:D:3403:ARG:NH2	2.35	0.59
2:F:491:ILE:O	2:F:495:ASN:HB2	2.03	0.59
2:H:1116:GLY:HA3	2:H:1132:TRP:HB3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1569:GLN:HB2	2:B:1572:ILE:HD12	1.85	0.58
2:B:4001:MET:HG3	2:B:4057:MET:HE2	1.84	0.58
2:F:4001:MET:HG3	2:F:4057:MET:HE2	1.84	0.58
2:H:3052:HIS:HE1	2:H:3128:ASN:HD22	1.50	0.58
2:B:2614:ILE:HG23	2:B:2618:MET:HE3	1.85	0.58
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.85	0.58
1:E:79:PRO:HA	1:E:82:ALA:HB3	1.85	0.58
2:B:4860:ARG:NH1	2:H:4630:TYR:OH	2.37	0.58
2:F:1569:GLN:HB2	2:F:1572:ILE:HD12	1.85	0.58
2:F:1447:CYS:HB3	2:F:1555:LEU:HB3	1.85	0.57
2:D:648:ILE:HD13	2:D:811:CYS:HB3	1.85	0.57
2:F:700:GLU:H	2:F:705:ASN:HD21	1.52	0.57
2:F:1123:VAL:HG23	2:F:1132:TRP:HB2	1.86	0.57
2:H:101:LEU:HB3	2:H:150:MET:HE1	1.86	0.57
2:D:4630:TYR:OH	2:F:4860:ARG:NH1	2.37	0.57
2:H:648:ILE:HD13	2:H:811:CYS:HB3	1.85	0.57
2:F:2614:ILE:HG23	2:F:2618:MET:HE3	1.85	0.57
2:H:749:ASP:O	2:H:753:PRO:HA	2.05	0.57
2:D:101:LEU:HB3	2:D:150:MET:HE1	1.86	0.57
2:D:1116:GLY:HA3	2:D:1132:TRP:HB3	1.85	0.57
2:H:2519:LEU:HD13	2:H:2575:ARG:HG3	1.87	0.57
2:B:700:GLU:H	2:B:705:ASN:HD21	1.52	0.56
2:D:749:ASP:O	2:D:753:PRO:HA	2.05	0.56
2:D:2650:ARG:NH1	2:D:2651:CYS:SG	2.78	0.56
2:F:3825:GLU:HG2	2:F:3827:GLY:H	1.70	0.56
2:F:4232:GLU:OE2	2:F:5017:ARG:NH2	2.38	0.56
2:D:3948:LYS:HG2	2:D:4012:LEU:HD22	1.87	0.56
2:F:3329:ILE:O	2:F:3403:ARG:NH2	2.38	0.56
2:H:1101:ARG:NH1	2:H:1115:LEU:O	2.38	0.56
2:H:3948:LYS:HG2	2:H:4012:LEU:HD22	1.87	0.56
2:B:1123:VAL:HG23	2:B:1132:TRP:HB2	1.86	0.56
2:D:1031:THR:O	2:D:1035:ASN:ND2	2.36	0.56
2:F:3335:MET:SD	2:F:3403:ARG:NH1	2.79	0.56
2:B:2195:PRO:HA	2:B:2198:MET:HG2	1.88	0.56
2:B:3825:GLU:HG2	2:B:3827:GLY:H	1.70	0.56
2:B:4892:ARG:NH2	2:D:4899:ASP:OD1	2.39	0.56
2:D:35:LEU:HD13	2:D:49:LEU:HD13	1.88	0.56
2:D:2519:LEU:HD13	2:D:2575:ARG:HG3	1.87	0.56
2:F:4892:ARG:NH2	2:H:4899:ASP:OD1	2.39	0.56
2:D:728:ARG:NH2	2:D:1489:CYS:SG	2.79	0.56
2:B:771:PHE:HB3	2:B:1472:VAL:HG23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2650:ARG:NH1	2:H:2651:CYS:SG	2.78	0.56
2:F:1771:LEU:HD22	2:F:2153:MET:HE2	1.88	0.56
2:F:2195:PRO:HA	2:F:2198:MET:HG2	1.88	0.56
2:B:3335:MET:SD	2:B:3403:ARG:NH1	2.79	0.56
2:D:638:ILE:HD11	2:D:1636:MET:HE2	1.88	0.56
2:D:3445:TRP:NE1	2:D:3455:GLU:OE1	2.39	0.56
2:F:3400:VAL:HG13	2:F:3403:ARG:HH21	1.71	0.56
2:B:3329:ILE:O	2:B:3403:ARG:NH2	2.38	0.56
2:B:3400:VAL:HG13	2:B:3403:ARG:HH21	1.71	0.55
2:D:110:ARG:NH2	2:D:117:TYR:OH	2.39	0.55
2:F:2214:VAL:HG21	2:F:2228:MET:HG2	1.87	0.55
2:F:2825:LYS:NZ	2:F:2933:ASN:O	2.39	0.55
2:F:4781:GLY:O	2:F:4785:THR:OG1	2.23	0.55
2:H:345:LEU:HB3	2:H:387:ALA:HB1	1.88	0.55
2:H:728:ARG:NH2	2:H:1489:CYS:SG	2.79	0.55
2:H:3825:GLU:HG2	2:H:3827:GLY:H	1.70	0.55
2:B:894:GLY:HA3	2:B:903:LEU:HB3	1.87	0.55
2:D:4679:ARG:NH2	2:D:4715:TYR:OH	2.39	0.55
2:D:3825:GLU:HG2	2:D:3827:GLY:H	1.70	0.55
2:B:1520:VAL:HG12	2:B:1527:MET:HG2	1.89	0.55
2:B:2214:VAL:HG21	2:B:2228:MET:HG2	1.87	0.55
2:B:3081:MET:HE2	2:B:3092:LEU:HD23	1.89	0.55
2:H:35:LEU:HD13	2:H:49:LEU:HD13	1.88	0.55
2:H:638:ILE:HD11	2:H:1636:MET:HE2	1.88	0.55
2:D:345:LEU:HB3	2:D:387:ALA:HB1	1.88	0.55
2:B:835:ARG:NH2	2:B:1210:SER:O	2.40	0.55
1:C:22:THR:HG22	1:C:50:ARG:HG2	1.89	0.55
2:F:1520:VAL:HG12	2:F:1527:MET:HG2	1.89	0.55
2:H:3445:TRP:NE1	2:H:3455:GLU:OE1	2.39	0.55
2:F:771:PHE:HB3	2:F:1472:VAL:HG23	1.88	0.55
2:H:110:ARG:NH2	2:H:117:TYR:OH	2.39	0.55
2:D:2021:CYS:O	2:D:2028:ARG:NH2	2.40	0.55
2:F:894:GLY:HA3	2:F:903:LEU:HB3	1.87	0.55
2:F:3414:ARG:HH12	2:F:3472:ALA:HA	1.72	0.55
2:H:2364:PHE:HB3	2:H:2368:LEU:HB2	1.88	0.55
2:B:4232:GLU:OE2	2:B:5017:ARG:NH2	2.38	0.54
2:D:2364:PHE:HB3	2:D:2368:LEU:HB2	1.88	0.54
2:D:2627:VAL:HG22	2:D:2678:LEU:HB2	1.88	0.54
2:B:3414:ARG:HH12	2:B:3472:ALA:HA	1.72	0.54
2:B:4942:GLU:CG	2:H:4944:ARG:NH2	2.69	0.54
2:H:2021:CYS:O	2:H:2028:ARG:NH2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.90	0.54
2:F:3081:MET:HE2	2:F:3092:LEU:HD23	1.89	0.54
1:G:22:THR:HG22	1:G:50:ARG:HG2	1.89	0.54
2:B:1771:LEU:HD22	2:B:2153:MET:HE2	1.88	0.54
2:F:2230:THR:HG23	2:F:2270:SER:H	1.71	0.54
2:B:2230:THR:HG23	2:B:2270:SER:H	1.71	0.54
2:B:3343:GLN:HE22	2:B:3469:PHE:HA	1.73	0.54
2:D:3110:LEU:HD11	2:D:3186:LEU:HD12	1.89	0.54
2:H:3110:LEU:HD11	2:H:3186:LEU:HD12	1.89	0.54
2:D:1243:PRO:HA	2:D:1601:MET:O	2.08	0.54
2:F:835:ARG:NH2	2:F:1210:SER:O	2.40	0.54
2:H:818:ARG:NH1	2:H:1027:LEU:O	2.41	0.54
2:H:2627:VAL:HG22	2:H:2678:LEU:HB2	1.88	0.54
2:B:516:LYS:O	2:B:520:ASN:ND2	2.40	0.54
2:B:3111:ARG:NH1	2:B:3178:THR:OG1	2.41	0.54
2:D:1101:ARG:NH1	2:D:1115:LEU:O	2.38	0.54
2:B:3536:ALA:HB2	2:B:3553:LEU:HD21	1.90	0.54
2:D:818:ARG:NH1	2:D:1027:LEU:O	2.41	0.54
2:F:3111:ARG:NH1	2:F:3178:THR:OG1	2.41	0.54
2:F:4837:LEU:HD22	2:F:4932:ILE:HG23	1.89	0.54
2:B:2687:ALA:O	2:B:2993:GLN:NE2	2.41	0.53
2:D:2614:ILE:HG23	2:D:2618:MET:HE3	1.90	0.53
2:F:3343:GLN:HE22	2:F:3469:PHE:HA	1.73	0.53
2:B:3590:GLU:OE2	2:B:3594:ARG:NH2	2.41	0.53
2:B:3984:ARG:HH12	2:D:162:LYS:HG3	1.73	0.53
2:B:3666:ASP:OD1	2:B:3666:ASP:N	2.41	0.53
2:B:4837:LEU:HD22	2:B:4932:ILE:HG23	1.89	0.53
2:H:41:GLY:O	2:H:45:ARG:NH1	2.42	0.53
2:H:1243:PRO:HA	2:H:1601:MET:O	2.08	0.53
1:G:50:ARG:HE	1:G:53:LYS:HG3	1.73	0.53
2:H:2118:ARG:NH2	2:H:3719:ASP:OD1	2.38	0.53
2:B:3906:GLN:H	2:B:3912:THR:HG23	1.74	0.53
2:D:2355:ARG:NH2	2:D:2449:GLU:OE2	2.42	0.53
2:F:886:ARG:HB3	2:F:891:TRP:HB2	1.90	0.53
2:F:3536:ALA:HB2	2:F:3553:LEU:HD21	1.90	0.53
2:F:3590:GLU:OE2	2:F:3594:ARG:NH2	2.41	0.53
2:H:1031:THR:O	2:H:1035:ASN:ND2	2.36	0.53
2:H:2355:ARG:NH2	2:H:2449:GLU:OE2	2.42	0.53
2:B:2825:LYS:NZ	2:B:2933:ASN:O	2.39	0.53
2:B:3940:LYS:O	2:B:4002:LYS:NZ	2.42	0.53
2:D:881:LEU:O	2:D:884:LEU:HB3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3414:ARG:HH12	2:D:3472:ALA:HA	1.74	0.53
2:F:4772:ASP:OD1	2:F:4772:ASP:N	2.41	0.53
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.90	0.53
2:B:2644:LEU:HD13	2:B:2678:LEU:HD21	1.91	0.53
1:C:50:ARG:HE	1:C:53:LYS:HG3	1.73	0.53
2:D:652:ARG:HD3	2:D:773:LEU:HD13	1.91	0.53
2:F:2687:ALA:O	2:F:2993:GLN:NE2	2.41	0.53
2:F:3412:LEU:HD11	2:F:3434:LEU:HD21	1.91	0.53
2:F:3906:GLN:H	2:F:3912:THR:HG23	1.74	0.53
2:H:2198:MET:SD	2:H:2198:MET:N	2.82	0.53
2:H:3414:ARG:HH12	2:H:3472:ALA:HA	1.74	0.53
2:B:1995:THR:HA	2:B:1998:PHE:HD2	1.74	0.52
2:B:3539:ARG:HB3	2:B:3549:VAL:HG22	1.91	0.52
2:D:3081:MET:HE2	2:D:3092:LEU:HD23	1.91	0.52
2:F:3984:ARG:HH12	2:H:162:LYS:HG3	1.73	0.52
2:H:622:THR:HG23	2:H:626:LEU:HD12	1.91	0.52
2:F:2626:LEU:HD22	2:F:2640:PRO:HB3	1.90	0.52
2:H:881:LEU:O	2:H:884:LEU:HB3	2.08	0.52
2:H:2614:ILE:HG23	2:H:2618:MET:HE3	1.90	0.52
2:D:622:THR:HG23	2:D:626:LEU:HD12	1.91	0.52
2:F:1815:LEU:HD22	2:F:1845:VAL:HG21	1.90	0.52
2:H:950:LEU:HD13	2:H:970:LEU:HD13	1.91	0.52
2:B:758:ARG:HG2	2:B:763:PRO:HA	1.92	0.52
2:F:3539:ARG:HB3	2:F:3549:VAL:HG22	1.91	0.52
2:B:638:ILE:HD11	2:B:1636:MET:HE2	1.91	0.52
2:B:4090:LYS:HG3	2:B:4112:LEU:HD22	1.92	0.52
2:D:41:GLY:O	2:D:45:ARG:NH1	2.42	0.52
2:D:2198:MET:SD	2:D:2198:MET:N	2.82	0.52
2:F:758:ARG:HG2	2:F:763:PRO:HA	1.92	0.52
2:F:1299:GLN:NE2	2:F:1545:ASN:OD1	2.41	0.52
2:B:4781:GLY:O	2:B:4785:THR:OG1	2.23	0.52
2:F:638:ILE:HD11	2:F:1636:MET:HE2	1.91	0.52
2:B:1101:ARG:NH1	2:B:1115:LEU:O	2.43	0.52
2:F:1995:THR:HA	2:F:1998:PHE:HD2	1.74	0.52
2:H:652:ARG:HD3	2:H:773:LEU:HD13	1.91	0.52
2:H:3132:THR:HA	2:H:3136:LEU:HB3	1.92	0.52
2:D:1131:ARG:NH1	2:D:1178:ALA:O	2.43	0.52
2:H:1771:LEU:HD22	2:H:2153:MET:HE2	1.92	0.52
2:B:2021:CYS:O	2:B:2028:ARG:NH2	2.42	0.52
2:B:3412:LEU:HD11	2:B:3434:LEU:HD21	1.91	0.52
2:D:950:LEU:HD13	2:D:970:LEU:HD13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1448:VAL:HG22	2:F:1554:VAL:HG23	1.92	0.52
2:F:2021:CYS:O	2:F:2028:ARG:NH2	2.42	0.52
2:F:4090:LYS:HG3	2:F:4112:LEU:HD22	1.92	0.52
2:F:492:ASP:OD1	2:F:546:TRP:NE1	2.35	0.51
2:H:2191:PHE:HD1	2:H:2198:MET:HE2	1.75	0.51
2:D:3132:THR:HA	2:D:3136:LEU:HB3	1.92	0.51
2:F:2333:ASP:OD1	2:F:2336:ARG:NH1	2.43	0.51
2:H:4772:ASP:OD1	2:H:4772:ASP:N	2.43	0.51
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.92	0.51
2:B:4056:GLU:HG2	2:B:4166:LEU:HD13	1.92	0.51
2:B:4935:LEU:HD23	2:H:4940:PHE:CZ	2.45	0.51
2:D:2191:PHE:HD1	2:D:2198:MET:HE2	1.75	0.51
2:D:2825:LYS:NZ	2:D:2933:ASN:O	2.39	0.51
2:D:4940:PHE:CZ	2:F:4935:LEU:HD23	2.45	0.51
2:D:4944:ARG:NH2	2:F:4942:GLU:CG	2.69	0.51
2:F:2191:PHE:HD1	2:F:2198:MET:HE2	1.75	0.51
2:F:2644:LEU:HD13	2:F:2678:LEU:HD21	1.91	0.51
2:H:4928:LEU:HD23	2:H:4931:ILE:HD12	1.93	0.51
2:F:683:ARG:HG2	2:F:717:ASP:HB3	1.92	0.51
2:H:3081:MET:HE2	2:H:3092:LEU:HD23	1.91	0.51
2:B:2155:LEU:HD21	2:B:2198:MET:HE1	1.92	0.51
2:B:2333:ASP:OD1	2:B:2336:ARG:NH1	2.43	0.51
2:B:4772:ASP:OD1	2:B:4772:ASP:N	2.41	0.51
2:F:2778:GLY:HA3	2:F:2787:THR:HB	1.92	0.51
2:F:3696:ASP:OD2	2:F:3773:ARG:NE	2.33	0.51
2:H:408:ALA:HB2	2:H:483:MET:HE1	1.93	0.51
2:H:4090:LYS:HG3	2:H:4112:LEU:HD22	1.93	0.51
2:B:2626:LEU:HD22	2:B:2640:PRO:HB3	1.90	0.51
1:A:22:THR:HG22	1:A:50:ARG:HG2	1.92	0.51
2:F:2155:LEU:HD21	2:F:2198:MET:HE1	1.92	0.51
2:B:1810:LYS:HG2	2:B:1814:MET:HE2	1.93	0.51
2:D:408:ALA:HB2	2:D:483:MET:HE1	1.93	0.51
2:D:4928:LEU:HD23	2:D:4931:ILE:HD12	1.93	0.51
2:F:590:LEU:HB2	2:F:599:VAL:HG11	1.92	0.51
2:H:2689:LYS:O	2:H:2993:GLN:NE2	2.44	0.51
2:D:1226:PHE:O	2:D:1827:ARG:NH2	2.44	0.51
2:D:1676:LEU:HD22	2:D:2167:ILE:HD12	1.93	0.51
2:D:1771:LEU:HD22	2:D:2153:MET:HE2	1.92	0.51
2:D:1973:GLN:NE2	2:D:2005:GLN:OE1	2.40	0.51
2:D:2638:LYS:HG3	2:D:2698:MET:HG3	1.93	0.51
2:D:4569:LEU:HD22	2:D:4646:LEU:HD22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3801:GLY:O	2:F:3805:LEU:HB2	2.11	0.51
2:H:1973:GLN:NE2	2:H:2005:GLN:OE1	2.40	0.51
2:H:2792:ARG:NH2	2:H:2801:ASP:OD2	2.44	0.51
2:D:2792:ARG:NH2	2:D:2801:ASP:OD2	2.44	0.51
2:F:4715:TYR:O	2:F:4718:LYS:NZ	2.44	0.51
2:H:4679:ARG:NH2	2:H:4715:TYR:OH	2.39	0.51
2:B:1243:PRO:HA	2:B:1601:MET:O	2.11	0.50
2:D:1422:ASP:OD1	2:D:1422:ASP:N	2.43	0.50
2:D:1447:CYS:HB3	2:D:1555:LEU:HB3	1.94	0.50
2:D:4090:LYS:HG3	2:D:4112:LEU:HD22	1.93	0.50
2:H:1226:PHE:O	2:H:1827:ARG:NH2	2.44	0.50
2:B:590:LEU:HB2	2:B:599:VAL:HG11	1.92	0.50
2:B:1653:LEU:O	2:B:1660:GLN:NE2	2.45	0.50
2:D:2902:HIS:HB3	2:D:2905:LEU:HG	1.93	0.50
2:F:1131:ARG:NH1	2:F:1178:ALA:O	2.45	0.50
2:F:1243:PRO:HA	2:F:1601:MET:O	2.11	0.50
2:F:2431:ASP:OD1	2:F:2435:ARG:NE	2.40	0.50
2:H:1676:LEU:HD22	2:H:2167:ILE:HD12	1.93	0.50
2:B:2178:MET:HE3	2:B:2182:ILE:HD11	1.92	0.50
2:F:2178:MET:HE3	2:F:2182:ILE:HD11	1.92	0.50
2:H:4059:LEU:HD13	2:H:4167:ALA:HB2	1.94	0.50
2:H:4569:LEU:HD22	2:H:4646:LEU:HD22	1.93	0.50
2:B:1299:GLN:NE2	2:B:1545:ASN:OD1	2.41	0.50
2:D:1732:SER:O	2:D:2140:ARG:NH1	2.43	0.50
2:F:1101:ARG:NH1	2:F:1115:LEU:O	2.43	0.50
2:H:1131:ARG:NH1	2:H:1178:ALA:O	2.43	0.50
2:B:1448:VAL:HG22	2:B:1554:VAL:HG23	1.92	0.50
2:B:4850:LEU:HD11	2:H:4814:LEU:HD21	1.93	0.50
2:B:2191:PHE:HD1	2:B:2198:MET:HE2	1.75	0.50
2:D:2118:ARG:NH2	2:D:3719:ASP:OD1	2.38	0.50
2:D:2689:LYS:O	2:D:2993:GLN:NE2	2.44	0.50
2:F:110:ARG:NH2	2:F:117:TYR:OH	2.45	0.50
2:H:2638:LYS:HG3	2:H:2698:MET:HG3	1.93	0.50
2:B:2431:ASP:OD1	2:B:2435:ARG:NE	2.40	0.50
2:B:3696:ASP:OD2	2:B:3773:ARG:NE	2.33	0.50
2:D:530:ILE:HG22	2:D:536:ASN:HB3	1.94	0.50
1:E:22:THR:HG22	1:E:50:ARG:HG2	1.92	0.50
2:F:1461:ASP:OD1	2:F:1461:ASP:N	2.42	0.50
2:F:1653:LEU:O	2:F:1660:GLN:NE2	2.45	0.50
2:B:647:ASN:HD22	2:B:647:ASN:H	1.59	0.50
2:F:647:ASN:H	2:F:647:ASN:HD22	1.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:913:LEU:O	2:F:918:ARG:NH2	2.45	0.50
2:F:3940:LYS:O	2:F:4002:LYS:NZ	2.42	0.50
2:B:877:ASN:ND2	2:B:1045:THR:OG1	2.45	0.49
2:B:3801:GLY:O	2:B:3805:LEU:HB2	2.11	0.49
2:D:870:ILE:HD12	2:D:873:LYS:HB2	1.94	0.49
2:D:4715:TYR:O	2:D:4718:LYS:NZ	2.45	0.49
2:D:4814:LEU:HD21	2:F:4850:LEU:HD11	1.93	0.49
2:D:4868:ASP:OD1	2:D:4868:ASP:N	2.44	0.49
2:F:3062:PRO:HA	2:F:3065:VAL:HG22	1.93	0.49
2:H:2902:HIS:HB3	2:H:2905:LEU:HG	1.93	0.49
2:B:1131:ARG:NH1	2:B:1178:ALA:O	2.45	0.49
2:B:1690:ASP:OD2	2:B:1693:GLN:NE2	2.45	0.49
2:D:790:ARG:HA	2:D:1626:TRP:O	2.12	0.49
2:F:4056:GLU:HG2	2:F:4166:LEU:HD13	1.92	0.49
2:H:3270:ILE:HA	2:H:3274:LEU:HD12	1.94	0.49
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.93	0.49
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.95	0.49
2:B:4846:VAL:HG21	2:H:4816:ILE:CD1	2.43	0.49
2:D:1448:VAL:HG22	2:D:1554:VAL:HG23	1.94	0.49
2:H:670:GLU:HA	2:H:740:PRO:HG3	1.94	0.49
2:H:683:ARG:HG2	2:H:717:ASP:HB3	1.94	0.49
2:H:790:ARG:HA	2:H:1626:TRP:O	2.12	0.49
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.92	0.49
2:B:4715:TYR:O	2:B:4718:LYS:NZ	2.44	0.49
2:B:913:LEU:O	2:B:918:ARG:NH2	2.45	0.49
2:B:4846:VAL:HG21	2:H:4816:ILE:HD11	1.94	0.49
2:D:683:ARG:HG2	2:D:717:ASP:HB3	1.94	0.49
2:F:877:ASN:ND2	2:F:1045:THR:OG1	2.45	0.49
2:F:1810:LYS:HG2	2:F:1814:MET:HE2	1.93	0.49
2:F:4576:ILE:HG21	2:F:4643:LEU:HB2	1.94	0.49
2:H:1447:CYS:HB3	2:H:1555:LEU:HB3	1.94	0.49
2:H:1448:VAL:HG22	2:H:1554:VAL:HG23	1.94	0.49
2:D:4878:ASP:OD1	2:D:4878:ASP:N	2.46	0.49
2:F:516:LYS:O	2:F:520:ASN:ND2	2.40	0.49
2:H:1422:ASP:N	2:H:1422:ASP:OD1	2.43	0.49
2:B:492:ASP:OD1	2:B:546:TRP:NE1	2.35	0.49
2:D:835:ARG:NH2	2:D:1210:SER:O	2.45	0.49
2:D:3601:ALA:O	2:D:3605:HIS:ND1	2.41	0.49
2:F:20:VAL:HG12	2:F:204:PRO:HA	1.93	0.49
2:F:952:LYS:HB3	2:F:968:ALA:HB1	1.95	0.49
2:H:530:ILE:HG22	2:H:536:ASN:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:835:ARG:NH2	2:H:1210:SER:O	2.45	0.49
2:B:3062:PRO:HA	2:B:3065:VAL:HG22	1.93	0.49
2:B:4576:ILE:HG21	2:B:4643:LEU:HB2	1.94	0.49
2:H:1732:SER:O	2:H:2140:ARG:NH1	2.43	0.49
2:B:110:ARG:NH2	2:B:117:TYR:OH	2.45	0.49
2:B:1461:ASP:OD1	2:B:1461:ASP:N	2.42	0.49
2:D:670:GLU:HA	2:D:740:PRO:HG3	1.94	0.49
2:D:2452:ARG:HG3	2:F:175:SER:O	2.13	0.49
2:H:2788:HIS:HB3	2:H:2791:LEU:HG	1.95	0.49
2:D:3270:ILE:HA	2:D:3274:LEU:HD12	1.94	0.49
2:D:4059:LEU:HD13	2:D:4167:ALA:HB2	1.94	0.49
2:D:4973:HIS:HE1	2:F:4228:ALA:HB1	1.78	0.49
2:H:904:HIS:HB3	2:H:907:LEU:HG	1.95	0.49
2:H:3539:ARG:HB3	2:H:3549:VAL:HG22	1.95	0.49
2:B:175:SER:O	2:H:2452:ARG:HG3	2.13	0.48
2:B:4228:ALA:HB1	2:H:4973:HIS:HE1	1.78	0.48
2:D:4816:ILE:HD11	2:F:4846:VAL:HG21	1.94	0.48
2:F:1690:ASP:OD2	2:F:1693:GLN:NE2	2.45	0.48
2:H:3972:PRO:HB3	2:H:4032:GLU:HG3	1.95	0.48
2:D:1653:LEU:O	2:D:1660:GLN:NE2	2.43	0.48
2:D:3767:GLN:OE1	2:D:3809:ASN:ND2	2.47	0.48
2:F:1997:GLU:O	2:F:2000:SER:OG	2.29	0.48
2:H:3601:ALA:O	2:H:3605:HIS:ND1	2.41	0.48
2:H:4715:TYR:O	2:H:4718:LYS:NZ	2.45	0.48
2:B:667:MET:SD	2:B:790:ARG:NH2	2.84	0.48
2:D:4816:ILE:CD1	2:F:4846:VAL:HG21	2.43	0.48
2:F:2763:HIS:NE2	2:F:2792:ARG:O	2.42	0.48
2:H:292:ALA:HB2	2:H:312:THR:HG22	1.94	0.48
2:H:1653:LEU:O	2:H:1660:GLN:NE2	2.43	0.48
2:D:2587:TYR:O	2:D:2590:SER:OG	2.28	0.48
2:D:2792:ARG:NH1	2:D:2796:THR:O	2.46	0.48
2:F:283:ARG:NH1	2:F:290:TYR:OH	2.47	0.48
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.96	0.48
2:H:2792:ARG:NH1	2:H:2796:THR:O	2.46	0.48
2:D:2788:HIS:HB3	2:D:2791:LEU:HG	1.95	0.48
2:H:233:ILE:HD12	2:H:242:ARG:HB3	1.96	0.48
2:H:491:ILE:O	2:H:495:ASN:HB2	2.14	0.48
2:D:904:HIS:HB3	2:D:907:LEU:HG	1.95	0.48
2:D:1652:GLU:OE1	2:D:1656:ARG:NH1	2.41	0.48
2:H:2644:LEU:HD13	2:H:2678:LEU:HD21	1.95	0.48
2:H:4878:ASP:OD1	2:H:4878:ASP:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:ALA:HB2	2:B:483:MET:HE1	1.96	0.48
2:B:728:ARG:NH2	2:B:1489:CYS:SG	2.87	0.48
2:B:1519:LEU:HD11	2:B:1572:ILE:HD13	1.96	0.48
2:F:879:HIS:NE2	2:F:908:VAL:O	2.40	0.48
2:H:870:ILE:HD12	2:H:873:LYS:HB2	1.94	0.48
2:B:4630:TYR:OH	2:D:4860:ARG:NH1	2.42	0.47
2:D:3539:ARG:HB3	2:D:3549:VAL:HG22	1.95	0.47
2:F:4059:LEU:HD13	2:F:4167:ALA:HB2	1.96	0.47
2:D:292:ALA:HB2	2:D:312:THR:HG22	1.94	0.47
2:F:69:LEU:HD21	2:F:202:MET:HE1	1.96	0.47
2:F:1519:LEU:HD11	2:F:1572:ILE:HD13	1.96	0.47
2:B:1805:GLU:OE1	2:B:1808:ARG:NH2	2.41	0.47
2:D:1112:ASP:OD1	2:D:1112:ASP:N	2.47	0.47
2:B:69:LEU:HD21	2:B:202:MET:HE1	1.96	0.47
2:B:1226:PHE:O	2:B:1827:ARG:NH2	2.48	0.47
2:D:224:HIS:NE2	2:D:385:ASP:O	2.48	0.47
2:D:3972:PRO:HB3	2:D:4032:GLU:HG3	1.95	0.47
2:F:1226:PHE:O	2:F:1827:ARG:NH2	2.48	0.47
2:F:1650:ILE:O	2:F:1653:LEU:HB2	2.14	0.47
2:F:3365:LEU:HD13	2:F:3405:LEU:HD23	1.95	0.47
2:H:224:HIS:NE2	2:H:385:ASP:O	2.48	0.47
2:H:266:ARG:NH2	2:H:272:SER:OG	2.47	0.47
2:H:786:GLY:N	2:H:1630:CYS:O	2.41	0.47
2:B:2347:GLU:OE2	2:B:3852:LYS:NZ	2.39	0.47
2:D:2359:ARG:HA	2:D:2359:ARG:HD3	1.71	0.47
2:D:2644:LEU:HD13	2:D:2678:LEU:HD21	1.95	0.47
2:F:1805:GLU:OE1	2:F:1808:ARG:NH2	2.41	0.47
2:F:4630:TYR:OH	2:H:4860:ARG:NH1	2.42	0.47
2:D:233:ILE:HD12	2:D:242:ARG:HB3	1.96	0.47
2:D:266:ARG:NH2	2:D:272:SER:OG	2.47	0.47
2:F:728:ARG:NH2	2:F:1489:CYS:SG	2.87	0.47
2:H:3767:GLN:OE1	2:H:3809:ASN:ND2	2.47	0.47
2:D:491:ILE:O	2:D:495:ASN:HB2	2.14	0.47
2:D:1443:GLN:NE2	2:D:1555:LEU:O	2.48	0.47
2:D:1810:LYS:HG2	2:D:1814:MET:HE2	1.96	0.47
2:D:2178:MET:HE3	2:D:2182:ILE:HD11	1.96	0.47
2:D:2178:MET:HB3	2:D:2228:MET:HE1	1.97	0.47
2:F:61:ASP:OD1	2:F:61:ASP:N	2.39	0.47
2:H:1443:GLN:NE2	2:H:1555:LEU:O	2.48	0.47
2:H:1947:CYS:SG	2:H:2127:GLN:NE2	2.88	0.47
2:B:283:ARG:NH1	2:B:290:TYR:OH	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:ALA:O	2:B:412:ASN:ND2	2.45	0.47
2:B:1650:ILE:O	2:B:1653:LEU:HB2	2.14	0.47
2:B:4998:LYS:HB3	2:B:5003:HIS:HE1	1.80	0.47
2:D:1099:GLU:HA	2:D:1127:HIS:HB2	1.97	0.47
2:D:3720:TYR:HA	2:D:3723:MET:HE2	1.97	0.47
2:F:3767:GLN:OE1	2:F:3809:ASN:ND2	2.47	0.47
2:F:3788:GLY:HA3	2:F:3834:ALA:HB3	1.96	0.47
2:F:4999:ASP:OD2	2:F:5001:THR:OG1	2.32	0.47
2:H:2196:ASN:OD1	2:H:2199:ARG:NH2	2.48	0.47
2:B:345:LEU:HB3	2:B:387:ALA:HB1	1.97	0.47
2:B:3365:LEU:HD13	2:B:3405:LEU:HD23	1.95	0.47
2:D:1947:CYS:SG	2:D:2127:GLN:NE2	2.88	0.47
2:F:151:HIS:HB2	2:F:170:ILE:HG13	1.97	0.47
2:F:622:THR:HG23	2:F:626:LEU:HD12	1.96	0.47
2:F:1099:GLU:HA	2:F:1127:HIS:HB2	1.97	0.47
2:B:3141:THR:HG23	2:B:3196:ARG:HG3	1.97	0.47
1:C:91:VAL:HG12	1:C:92:ILE:HG13	1.97	0.47
2:H:2178:MET:HE3	2:H:2182:ILE:HD11	1.96	0.47
2:B:2196:ASN:OD1	2:B:2199:ARG:NH2	2.48	0.46
2:B:3356:SER:OG	2:B:3357:HIS:ND1	2.38	0.46
2:B:3767:GLN:OE1	2:B:3809:ASN:ND2	2.47	0.46
2:D:2196:ASN:OD1	2:D:2199:ARG:NH2	2.48	0.46
2:H:1958:LEU:HD23	2:H:2138:LEU:HD21	1.97	0.46
2:H:2431:ASP:OD1	2:H:2435:ARG:NE	2.48	0.46
2:H:3788:GLY:HA3	2:H:3834:ALA:HB3	1.98	0.46
2:B:622:THR:HG23	2:B:626:LEU:HD12	1.96	0.46
2:D:707:VAL:HG13	2:D:713:SER:HB2	1.97	0.46
2:F:3141:THR:HG23	2:F:3196:ARG:HG3	1.97	0.46
2:H:1093:GLU:HB3	2:H:1201:HIS:HB3	1.97	0.46
2:H:1652:GLU:OE1	2:H:1656:ARG:NH1	2.41	0.46
2:H:1810:LYS:HG2	2:H:1814:MET:HE2	1.96	0.46
1:A:5:ILE:HD11	1:A:63:GLY:HA2	1.95	0.46
2:B:707:VAL:HG13	2:B:713:SER:HB2	1.98	0.46
2:B:3980:LEU:HD13	2:B:3985:LEU:HD22	1.98	0.46
2:B:4999:ASP:OD2	2:B:5001:THR:OG1	2.32	0.46
2:F:2196:ASN:OD1	2:F:2199:ARG:NH2	2.48	0.46
2:F:3980:LEU:HD13	2:F:3985:LEU:HD22	1.98	0.46
2:H:590:LEU:HB2	2:H:599:VAL:HG11	1.98	0.46
2:H:3842:LEU:HB2	2:H:3929:SER:HB2	1.98	0.46
2:D:1997:GLU:O	2:D:2000:SER:OG	2.30	0.46
1:E:5:ILE:HD11	1:E:63:GLY:HA2	1.95	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:408:ALA:HB2	2:F:483:MET:HE1	1.96	0.46
2:B:2138:LEU:HB3	2:B:3658:LYS:HE2	1.98	0.46
2:D:1958:LEU:HD23	2:D:2138:LEU:HD21	1.97	0.46
2:D:4940:PHE:CZ	2:F:4935:LEU:CD2	2.99	0.46
2:H:2178:MET:HB3	2:H:2228:MET:HE1	1.97	0.46
2:H:2359:ARG:HD3	2:H:2359:ARG:HA	1.71	0.46
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.72	0.46
2:D:2615:ARG:HG2	2:D:2618:MET:HE2	1.98	0.46
2:D:5013:MET:HE1	2:D:5020:ASP:HB2	1.98	0.46
2:F:4998:LYS:HB3	2:F:5003:HIS:HE1	1.80	0.46
2:H:5013:MET:HE1	2:H:5020:ASP:HB2	1.98	0.46
2:B:3788:GLY:HA3	2:B:3834:ALA:HB3	1.96	0.46
2:D:2431:ASP:OD1	2:D:2435:ARG:NE	2.48	0.46
2:D:4563:ARG:NH2	2:D:4815:ASP:OD1	2.48	0.46
2:D:4888:TYR:HE1	2:F:4917:ASP:HB2	1.81	0.46
2:F:2138:LEU:HB3	2:F:3658:LYS:HE2	1.98	0.46
2:H:72:SER:O	2:H:99:ARG:NH1	2.49	0.46
2:B:61:ASP:OD1	2:B:61:ASP:N	2.39	0.46
2:B:879:HIS:NE2	2:B:908:VAL:O	2.40	0.46
2:B:2752:ASP:O	2:B:2756:ASN:ND2	2.40	0.46
2:F:667:MET:SD	2:F:790:ARG:NH2	2.84	0.46
2:F:769:GLU:HG3	2:F:1473:THR:HB	1.98	0.46
2:H:707:VAL:HG13	2:H:713:SER:HB2	1.97	0.46
2:B:769:GLU:HG3	2:B:1473:THR:HB	1.98	0.46
2:F:183:SER:HB2	2:F:190:GLN:HB2	1.98	0.46
2:B:183:SER:HB2	2:B:190:GLN:HB2	1.98	0.46
2:B:1676:LEU:HD22	2:B:2167:ILE:HD12	1.98	0.46
2:B:3717:ASP:OD1	2:B:3717:ASP:N	2.48	0.46
2:B:4750:ILE:O	2:B:4754:ASN:N	2.49	0.46
2:F:2930:LEU:HD13	2:F:2937:VAL:HG21	1.98	0.46
2:H:1123:VAL:HG23	2:H:1132:TRP:HB2	1.98	0.46
2:H:2029:GLN:NE2	2:H:2033:ASP:OD1	2.49	0.46
2:H:3720:TYR:HA	2:H:3723:MET:HE2	1.97	0.46
2:D:590:LEU:HB2	2:D:599:VAL:HG11	1.98	0.45
2:F:4750:ILE:O	2:F:4754:ASN:N	2.49	0.45
2:H:1690:ASP:OD2	2:H:1693:GLN:NE2	2.48	0.45
2:H:4563:ARG:NH2	2:H:4815:ASP:OD1	2.48	0.45
2:B:1099:GLU:HA	2:B:1127:HIS:HB2	1.97	0.45
2:D:72:SER:O	2:D:99:ARG:NH1	2.49	0.45
2:D:1690:ASP:OD2	2:D:1693:GLN:NE2	2.48	0.45
2:F:345:LEU:HB3	2:F:387:ALA:HB1	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1423:ASP:OD1	2:H:1423:ASP:N	2.49	0.45
2:B:1272:LEU:HD22	2:B:1289:LEU:HD11	1.98	0.45
2:B:3768:SER:HA	2:B:3771:HIS:CD2	2.52	0.45
2:B:4935:LEU:CD2	2:H:4940:PHE:CZ	2.99	0.45
2:D:2166:LEU:HD11	2:D:2206:THR:HG23	1.99	0.45
2:D:3788:GLY:HA3	2:D:3834:ALA:HB3	1.98	0.45
1:G:91:VAL:HG12	1:G:92:ILE:HG13	1.97	0.45
2:H:2166:LEU:HD11	2:H:2206:THR:HG23	1.99	0.45
2:H:2626:LEU:HD22	2:H:2640:PRO:HB3	1.98	0.45
2:H:3768:SER:HA	2:H:3771:HIS:CD2	2.52	0.45
2:B:3075:LEU:O	2:B:3146:HIS:NE2	2.39	0.45
2:B:4917:ASP:HB2	2:H:4888:TYR:HE1	1.81	0.45
2:D:1443:GLN:HE21	2:D:1557:THR:H	1.64	0.45
2:D:3842:LEU:HB2	2:D:3929:SER:HB2	1.98	0.45
2:F:106:ALA:HA	2:F:149:THR:HA	1.99	0.45
2:F:408:ALA:O	2:F:412:ASN:ND2	2.45	0.45
2:F:707:VAL:HG13	2:F:713:SER:HB2	1.98	0.45
2:F:1186:ASP:OD1	2:F:1186:ASP:N	2.49	0.45
2:F:1272:LEU:HD22	2:F:1289:LEU:HD11	1.98	0.45
2:B:2299:VAL:HG12	2:B:2360:LYS:HD2	1.98	0.45
2:D:257:ARG:O	2:D:284:HIS:NE2	2.40	0.45
2:D:2029:GLN:NE2	2:D:2033:ASP:OD1	2.49	0.45
2:D:4570:ALA:O	2:D:4574:ASN:ND2	2.45	0.45
2:F:1236:THR:OG1	2:F:1608:MET:SD	2.72	0.45
2:F:2299:VAL:HG12	2:F:2360:LYS:HD2	1.98	0.45
2:H:1099:GLU:HA	2:H:1127:HIS:HB2	1.97	0.45
2:B:106:ALA:HA	2:B:149:THR:HA	1.99	0.45
2:D:1093:GLU:HB3	2:D:1201:HIS:HB3	1.97	0.45
2:D:1123:VAL:HG23	2:D:1132:TRP:HB2	1.98	0.45
2:F:1676:LEU:HD22	2:F:2167:ILE:HD12	1.98	0.45
2:F:3768:SER:HA	2:F:3771:HIS:CD2	2.52	0.45
2:H:20:VAL:HG21	2:H:202:MET:HE3	1.98	0.45
2:B:2519:LEU:HD13	2:B:2575:ARG:HG3	1.98	0.45
2:D:667:MET:SD	2:D:790:ARG:NH2	2.89	0.45
2:D:2626:LEU:HD22	2:D:2640:PRO:HB3	1.98	0.45
2:H:2758:PHE:HB3	2:H:2809:ILE:HD13	1.99	0.45
2:B:151:HIS:HB2	2:B:170:ILE:HG13	1.97	0.45
2:B:1186:ASP:OD1	2:B:1186:ASP:N	2.49	0.45
2:B:2930:LEU:HD13	2:B:2937:VAL:HG21	1.98	0.45
2:D:823:LEU:HD11	2:D:1626:TRP:HB3	1.99	0.45
2:D:1423:ASP:OD1	2:D:1423:ASP:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3916:ILE:H	2:D:3916:ILE:HG12	1.60	0.45
1:E:8:ILE:HA	2:F:719:LEU:HD11	1.99	0.45
2:H:2615:ARG:HG2	2:H:2618:MET:HE2	1.98	0.45
2:D:552:ASP:OD1	2:D:552:ASP:N	2.48	0.45
2:D:4576:ILE:HG21	2:D:4643:LEU:HB2	1.99	0.45
2:H:1443:GLN:HE21	2:H:1557:THR:H	1.64	0.45
1:A:50:ARG:HE	1:A:53:LYS:HG3	1.81	0.44
2:D:1575:LEU:HD13	2:D:1579:MET:HE3	1.99	0.44
2:D:2758:PHE:HB3	2:D:2809:ILE:HD13	1.99	0.44
1:E:50:ARG:HE	1:E:53:LYS:HG3	1.81	0.44
2:F:1115:LEU:HD13	2:F:1123:VAL:HG11	1.99	0.44
2:D:3107:VAL:HG21	2:D:3171:SER:HB3	1.99	0.44
2:F:3877:ASP:OD1	2:F:3877:ASP:N	2.51	0.44
2:H:257:ARG:O	2:H:284:HIS:NE2	2.40	0.44
2:H:4161:ARG:HA	2:H:4164:LEU:HD12	1.99	0.44
1:A:24:VAL:HG22	1:A:48:LYS:HG2	1.99	0.44
2:D:3768:SER:HA	2:D:3771:HIS:CD2	2.52	0.44
2:D:4972:PRO:HB3	2:F:5024:ALA:HB3	1.99	0.44
2:F:3972:PRO:HB3	2:F:4032:GLU:HG3	1.99	0.44
2:H:1983:ALA:O	2:H:1991:THR:OG1	2.29	0.44
2:H:2582:MET:HE2	2:H:2582:MET:HB3	1.91	0.44
2:B:3324:VAL:HA	2:B:3327:LEU:HG	2.00	0.44
2:H:3107:VAL:HG21	2:H:3171:SER:HB3	1.99	0.44
2:H:3266:MET:HE3	2:H:3269:VAL:HB	1.99	0.44
1:C:12:ASP:HB3	1:C:14:ARG:HG2	1.98	0.44
2:F:2608:MET:HE1	2:F:2642:LYS:HD3	2.00	0.44
2:B:1817:GLU:HG2	2:B:1820:ARG:HH22	1.82	0.44
2:B:2763:HIS:NE2	2:B:2792:ARG:O	2.42	0.44
2:D:20:VAL:HG21	2:D:202:MET:HE3	1.98	0.44
2:D:1008:SER:HB3	2:D:1017:ARG:HB3	2.00	0.44
2:F:3717:ASP:N	2:F:3717:ASP:OD1	2.48	0.44
1:G:12:ASP:HB3	1:G:14:ARG:HG2	1.98	0.44
2:H:4567:LEU:HD11	2:H:4816:ILE:HG22	1.99	0.44
2:B:647:ASN:HD22	2:B:647:ASN:N	2.16	0.44
2:B:3972:PRO:HB3	2:B:4032:GLU:HG3	1.99	0.44
2:D:1995:THR:HA	2:D:1998:PHE:HD2	1.83	0.44
2:D:4161:ARG:HA	2:D:4164:LEU:HD12	1.99	0.44
2:F:1575:LEU:HD13	2:F:1579:MET:HE3	2.00	0.44
2:B:755:ILE:HB	2:B:768:PHE:HB2	2.00	0.44
2:F:755:ILE:HB	2:F:768:PHE:HB2	2.00	0.44
2:F:3778:MET:HE2	2:F:3778:MET:HB3	1.88	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4679:ARG:NH2	2:F:4715:TYR:OH	2.41	0.44
2:H:14:LEU:HD13	2:H:202:MET:HE2	2.00	0.44
1:A:8:ILE:HA	2:B:719:LEU:HD11	1.99	0.44
2:D:3266:MET:HE3	2:D:3269:VAL:HB	1.99	0.44
1:E:24:VAL:HG22	1:E:48:LYS:HG2	1.99	0.44
2:H:823:LEU:HD11	2:H:1626:TRP:HB3	1.99	0.44
2:H:4069:LYS:NZ	2:H:4130:ASN:OD1	2.39	0.44
2:D:3355:HIS:HA	2:D:3359:ILE:HD12	2.01	0.43
2:F:1817:GLU:HG2	2:F:1820:ARG:HH22	1.82	0.43
2:F:2519:LEU:HD13	2:F:2575:ARG:HG3	1.98	0.43
2:H:1008:SER:HB3	2:H:1017:ARG:HB3	2.00	0.43
2:H:4687:TYR:O	2:H:4691:GLN:NE2	2.51	0.43
2:B:4037:ASN:HB3	2:B:4042:ARG:HH21	1.83	0.43
2:D:3062:PRO:HA	2:D:3065:VAL:HG22	2.00	0.43
2:F:236:ALA:HA	2:F:242:ARG:HD2	2.00	0.43
2:F:3842:LEU:HB2	2:F:3929:SER:HB2	2.00	0.43
2:H:3355:HIS:HA	2:H:3359:ILE:HD12	2.01	0.43
2:H:4576:ILE:HG21	2:H:4643:LEU:HB2	1.99	0.43
2:B:3445:TRP:NE1	2:B:3455:GLU:OE1	2.50	0.43
2:B:5024:ALA:HB3	2:H:4972:PRO:HB3	1.99	0.43
2:D:4567:LEU:HD11	2:D:4816:ILE:HG22	1.99	0.43
2:H:647:ASN:OD1	2:H:647:ASN:N	2.50	0.43
2:B:233:ILE:HD12	2:B:242:ARG:HB3	2.00	0.43
2:B:236:ALA:HA	2:B:242:ARG:HD2	2.00	0.43
2:D:3835:LEU:HD22	2:D:3880:PHE:HZ	1.83	0.43
2:F:2770:LYS:HB3	2:F:2775:TRP:HB2	2.00	0.43
2:F:3324:VAL:HA	2:F:3327:LEU:HG	2.00	0.43
2:H:1575:LEU:HD13	2:H:1579:MET:HE3	1.99	0.43
2:H:2228:MET:HE2	2:H:2228:MET:HB2	1.81	0.43
2:B:3842:LEU:HB2	2:B:3929:SER:HB2	2.00	0.43
2:D:1828:ASP:OD1	2:D:1828:ASP:N	2.52	0.43
2:F:233:ILE:HD12	2:F:242:ARG:HB3	2.00	0.43
2:F:3356:SER:OG	2:F:3357:HIS:ND1	2.38	0.43
2:B:292:ALA:HB2	2:B:312:THR:HG22	2.00	0.43
2:B:1958:LEU:HD23	2:B:2138:LEU:HD21	2.00	0.43
2:B:2228:MET:HE2	2:B:2228:MET:HB2	1.77	0.43
2:H:1650:ILE:O	2:H:1653:LEU:HB2	2.19	0.43
2:B:1115:LEU:HD13	2:B:1123:VAL:HG11	1.99	0.43
2:B:3852:LYS:HE3	2:B:3852:LYS:HB2	1.87	0.43
2:B:4228:ALA:CB	2:H:4973:HIS:HE1	2.32	0.43
2:F:3106:MET:HE1	2:F:3190:LEU:HD21	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2608:MET:HE1	2:B:2642:LYS:HD3	2.00	0.43
2:B:4771:ILE:HD12	2:B:4771:ILE:HA	1.96	0.43
2:D:618:GLN:OE1	2:D:1678:ASN:ND2	2.43	0.43
2:D:786:GLY:N	2:D:1630:CYS:O	2.41	0.43
2:F:292:ALA:HB2	2:F:312:THR:HG22	2.00	0.43
2:F:864:PRO:HA	2:F:865:PRO:HD3	1.91	0.43
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.47	0.43
2:B:1575:LEU:HD13	2:B:1579:MET:HE3	2.00	0.43
2:B:3420:ARG:HG3	2:B:3520:ILE:HD11	2.01	0.43
2:B:3948:LYS:HG2	2:B:4012:LEU:HD22	2.01	0.43
2:B:4569:LEU:HD22	2:B:4646:LEU:HD22	2.01	0.43
2:B:4856:PHE:CE1	2:H:4582:VAL:HG13	2.53	0.43
2:D:1650:ILE:O	2:D:1653:LEU:HB2	2.19	0.43
2:F:647:ASN:HD22	2:F:647:ASN:N	2.16	0.43
2:F:790:ARG:HA	2:F:1626:TRP:O	2.19	0.43
2:F:1958:LEU:HD23	2:F:2138:LEU:HD21	2.00	0.43
2:H:3524:MET:HA	2:H:3582:ARG:HH22	1.84	0.43
2:B:3877:ASP:OD1	2:B:3877:ASP:N	2.51	0.43
2:B:4942:GLU:CD	2:H:4944:ARG:HH21	2.27	0.43
2:D:14:LEU:HD13	2:D:202:MET:HE2	2.00	0.43
2:D:20:VAL:HG12	2:D:204:PRO:HA	2.01	0.43
2:F:2347:GLU:OE2	2:F:3852:LYS:NZ	2.39	0.43
2:H:20:VAL:HG12	2:H:204:PRO:HA	2.01	0.43
2:H:3062:PRO:HA	2:H:3065:VAL:HG22	2.00	0.43
2:F:2359:ARG:HD3	2:F:2359:ARG:HA	1.78	0.42
2:H:667:MET:SD	2:H:790:ARG:NH2	2.89	0.42
2:H:1828:ASP:N	2:H:1828:ASP:OD1	2.52	0.42
2:H:1995:THR:HA	2:H:1998:PHE:HD2	1.83	0.42
2:H:2823:ILE:HG23	2:H:2937:VAL:HG22	2.01	0.42
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	2.00	0.42
2:B:3823:LYS:HD3	2:B:3823:LYS:HA	1.81	0.42
2:D:3292:PRO:HA	2:D:3293:PRO:HD3	1.92	0.42
2:F:1115:LEU:HB3	2:F:1123:VAL:HG21	2.01	0.42
2:B:4700:GLN:OE1	2:B:4703:ARG:NH1	2.52	0.42
2:D:601:ASP:OD1	2:D:1665:HIS:ND1	2.48	0.42
2:D:3324:VAL:HA	2:D:3327:LEU:HG	2.01	0.42
2:D:4973:HIS:HE1	2:F:4228:ALA:CB	2.32	0.42
2:F:5013:MET:HE2	2:F:5013:MET:HB3	1.94	0.42
2:B:2039:LEU:HD22	2:B:2044:ILE:HD12	2.02	0.42
2:D:2823:ILE:HG23	2:D:2937:VAL:HG22	2.01	0.42
2:F:2282:ASP:HA	2:F:2341:VAL:HG13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3916:ILE:H	2:F:3916:ILE:HG12	1.61	0.42
2:F:4037:ASN:HB3	2:F:4042:ARG:HH21	1.83	0.42
2:F:4569:LEU:HD22	2:F:4646:LEU:HD22	2.01	0.42
2:H:2825:LYS:NZ	2:H:2933:ASN:O	2.39	0.42
2:H:3324:VAL:HA	2:H:3327:LEU:HG	2.01	0.42
2:B:1947:CYS:SG	2:B:2127:GLN:NE2	2.93	0.42
2:B:2282:ASP:HA	2:B:2341:VAL:HG13	2.02	0.42
2:B:2364:PHE:HB3	2:B:2368:LEU:HB2	2.01	0.42
2:D:3524:MET:HE3	2:D:3595:ARG:HB2	2.01	0.42
2:D:4582:VAL:HG13	2:F:4856:PHE:CE1	2.53	0.42
2:D:4687:TYR:OH	2:D:4699:GLY:O	2.36	0.42
2:F:203:ASN:HA	2:F:204:PRO:HD3	1.95	0.42
2:F:1828:ASP:OD1	2:F:1828:ASP:N	2.52	0.42
2:F:3007:ASN:O	2:F:3011:THR:OG1	2.26	0.42
2:H:3514:LEU:HD11	2:H:3602:VAL:HG13	2.01	0.42
1:A:17:PRO:HG3	1:A:107:LEU:HD21	2.01	0.42
2:B:790:ARG:HA	2:B:1626:TRP:O	2.19	0.42
2:D:3524:MET:HA	2:D:3582:ARG:HH22	1.84	0.42
2:D:4687:TYR:O	2:D:4691:GLN:NE2	2.51	0.42
2:F:243:ARG:HA	2:F:301:VAL:HG23	2.01	0.42
2:F:3075:LEU:O	2:F:3146:HIS:NE2	2.39	0.42
2:B:3106:MET:HE1	2:B:3190:LEU:HD21	2.01	0.42
2:D:1076:ARG:HB3	2:D:1191:VAL:HG23	2.02	0.42
2:D:3514:LEU:HD11	2:D:3602:VAL:HG13	2.01	0.42
2:F:23:GLN:HE21	2:F:23:GLN:HB3	1.72	0.42
2:B:1997:GLU:O	2:B:2000:SER:OG	2.29	0.42
2:B:3301:PRO:HA	2:B:3302:PRO:HD3	1.96	0.42
2:D:1547:LYS:NZ	2:D:1642:PRO:O	2.53	0.42
2:D:3107:VAL:HG22	2:D:3175:LEU:HD22	2.02	0.42
2:D:3533:ILE:HG22	2:D:3537:LYS:HE3	2.02	0.42
2:F:774:ASP:OD1	2:F:774:ASP:N	2.53	0.42
2:H:3835:LEU:HD22	2:H:3880:PHE:HZ	1.83	0.42
1:A:80:ASP:OD1	1:A:80:ASP:N	2.53	0.42
2:B:878:ILE:O	2:B:882:TRP:N	2.47	0.42
2:B:1148:VAL:HG21	2:B:1212:ARG:HD2	2.02	0.42
1:E:107:LEU:HD23	1:E:107:LEU:HA	1.92	0.42
2:B:2359:ARG:HA	2:B:2359:ARG:HD3	1.78	0.42
1:C:8:ILE:HA	2:D:719:LEU:HD11	2.02	0.42
2:F:2469:ILE:HG21	2:F:2502:MET:HE3	2.02	0.42
2:F:2752:ASP:O	2:F:2756:ASN:ND2	2.40	0.42
2:F:2970:SER:HA	2:F:2973:PHE:CE2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3420:ARG:HG3	2:F:3520:ILE:HD11	2.01	0.42
2:D:3852:LYS:HE2	2:D:3852:LYS:HB3	1.89	0.41
2:F:1076:ARG:HB3	2:F:1191:VAL:HG23	2.02	0.41
2:F:3948:LYS:HG2	2:F:4012:LEU:HD22	2.01	0.41
2:H:3533:ILE:HG22	2:H:3537:LYS:HE3	2.02	0.41
2:B:2711:PRO:HA	2:B:2712:PRO:HD3	1.93	0.41
2:D:4047:MET:HE3	2:D:4047:MET:HB3	2.00	0.41
2:F:1947:CYS:SG	2:F:2127:GLN:NE2	2.93	0.41
2:H:1547:LYS:NZ	2:H:1642:PRO:O	2.53	0.41
2:H:3524:MET:HE3	2:H:3595:ARG:HB2	2.01	0.41
2:B:243:ARG:HA	2:B:301:VAL:HG23	2.01	0.41
2:B:2970:SER:HA	2:B:2973:PHE:CE2	2.55	0.41
2:B:4868:ASP:OD1	2:B:4868:ASP:N	2.47	0.41
2:F:728:ARG:HA	2:F:729:PRO:HD3	1.94	0.41
2:H:2469:ILE:HG21	2:H:2502:MET:HE3	2.02	0.41
2:H:3107:VAL:HG22	2:H:3175:LEU:HD22	2.02	0.41
2:H:3365:LEU:HD13	2:H:3405:LEU:HD23	2.02	0.41
2:B:1115:LEU:HB3	2:B:1123:VAL:HG21	2.01	0.41
2:B:1547:LYS:NZ	2:B:1642:PRO:O	2.54	0.41
2:B:2792:ARG:NH2	2:B:2801:ASP:OD2	2.53	0.41
2:D:3553:LEU:HB2	2:D:3593:VAL:HG23	2.03	0.41
1:E:17:PRO:HG3	1:E:107:LEU:HD21	2.01	0.41
2:F:1291:LEU:HD13	2:F:1595:LEU:HD11	2.02	0.41
1:G:8:ILE:HA	2:H:719:LEU:HD11	2.02	0.41
2:H:19:GLU:O	2:H:205:ILE:N	2.54	0.41
2:B:72:SER:O	2:B:99:ARG:NH1	2.54	0.41
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.42	0.41
2:B:4679:ARG:NH2	2:B:4715:TYR:OH	2.41	0.41
2:D:2228:MET:HB2	2:D:2228:MET:HE2	1.81	0.41
2:D:2582:MET:HE2	2:D:2582:MET:HB3	1.91	0.41
2:F:1039:LEU:HD13	2:F:1039:LEU:HA	1.92	0.41
2:F:2039:LEU:HD22	2:F:2044:ILE:HD12	2.02	0.41
2:F:2507:ASP:HB2	2:F:2561:LEU:HD12	2.03	0.41
2:F:2636:PHE:HD1	2:F:2636:PHE:HA	1.76	0.41
2:F:2755:ILE:HD13	2:F:2810:LYS:HG2	2.03	0.41
2:H:4570:ALA:O	2:H:4574:ASN:ND2	2.45	0.41
2:B:1076:ARG:HB3	2:B:1191:VAL:HG23	2.02	0.41
2:B:1291:LEU:HD13	2:B:1595:LEU:HD11	2.02	0.41
2:B:2469:ILE:HG21	2:B:2502:MET:HE3	2.02	0.41
2:D:4944:ARG:HH21	2:F:4942:GLU:CD	2.27	0.41
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:633:LEU:HD13	2:F:1639:LEU:HD11	2.03	0.41
2:F:2792:ARG:NH2	2:F:2801:ASP:OD2	2.53	0.41
2:D:71:GLN:HE21	2:D:147:TRP:HH2	1.69	0.41
2:D:1954:ARG:HH22	2:D:2095:GLN:HE21	1.69	0.41
2:F:1148:VAL:HG21	2:F:1212:ARG:HD2	2.02	0.41
2:F:2228:MET:HE2	2:F:2228:MET:HB2	1.77	0.41
2:F:3292:PRO:HA	2:F:3293:PRO:HD3	1.91	0.41
2:F:3987:ASP:OD1	2:F:3987:ASP:N	2.52	0.41
2:H:1575:LEU:HD23	2:H:1575:LEU:HA	1.89	0.41
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.91	0.41
2:B:1828:ASP:N	2:B:1828:ASP:OD1	2.52	0.41
2:B:3987:ASP:OD1	2:B:3987:ASP:N	2.52	0.41
2:D:788:LYS:HB2	2:D:788:LYS:HE3	1.84	0.41
2:D:1082:THR:HG23	2:D:1187:GLY:HA3	2.03	0.41
2:D:2711:PRO:HA	2:D:2712:PRO:HD3	1.94	0.41
2:D:3365:LEU:HD13	2:D:3405:LEU:HD23	2.02	0.41
2:D:5013:MET:HE2	2:D:5013:MET:HB3	1.99	0.41
2:F:2364:PHE:HB3	2:F:2368:LEU:HB2	2.01	0.41
2:F:3836:MET:HE3	2:F:3836:MET:HB2	1.93	0.41
2:H:618:GLN:OE1	2:H:1678:ASN:ND2	2.43	0.41
2:H:1076:ARG:HB3	2:H:1191:VAL:HG23	2.02	0.41
2:H:2639:MET:HE3	2:H:2639:MET:HB3	1.95	0.41
2:H:2711:PRO:HA	2:H:2712:PRO:HD3	1.94	0.41
2:H:2823:ILE:HG12	2:H:2937:VAL:HG13	2.03	0.41
2:B:1118:ASP:OD1	2:B:1118:ASP:N	2.54	0.41
2:F:3568:SER:HA	2:F:3571:TRP:CD1	2.56	0.41
2:H:1082:THR:HG23	2:H:1187:GLY:HA3	2.03	0.41
2:H:1422:ASP:HB3	2:H:1571:ASN:H	1.86	0.41
2:H:4056:GLU:HG2	2:H:4166:LEU:HD13	2.03	0.41
2:H:4687:TYR:OH	2:H:4699:GLY:O	2.36	0.41
2:B:111:HIS:CE1	2:B:113:HIS:HB3	2.56	0.40
2:B:648:ILE:HD13	2:B:811:CYS:HB3	2.03	0.40
2:F:111:HIS:CE1	2:F:113:HIS:HB3	2.56	0.40
2:F:1547:LYS:NZ	2:F:1642:PRO:O	2.54	0.40
2:H:788:LYS:HE3	2:H:788:LYS:HB2	1.84	0.40
2:H:3169:LEU:HD23	2:H:3194:LEU:HD11	2.03	0.40
2:B:1699:GLU:OE2	2:B:1813:ARG:NH2	2.54	0.40
2:B:2996:LYS:HD3	2:B:2996:LYS:HA	1.93	0.40
2:B:4832:HIS:HB3	2:B:4939:ALA:HB1	2.03	0.40
2:D:1773:PRO:HA	2:D:1774:PRO:HD3	1.89	0.40
2:D:2009:LEU:HD23	2:D:2009:LEU:HA	1.97	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:72:SER:O	2:F:99:ARG:NH1	2.54	0.40
2:F:882:TRP:O	2:F:885:THR:OG1	2.32	0.40
2:H:3553:LEU:HB2	2:H:3593:VAL:HG23	2.03	0.40
2:H:3943:ILE:H	2:H:4009:GLN:NE2	2.19	0.40
2:H:4044:MET:HE3	2:H:4044:MET:HB2	1.98	0.40
2:B:2966:TRP:O	2:B:2970:SER:OG	2.36	0.40
2:B:3639:THR:HA	2:B:3640:PRO:HD3	1.94	0.40
1:E:80:ASP:OD1	1:E:80:ASP:N	2.53	0.40
2:B:633:LEU:HD13	2:B:1639:LEU:HD11	2.03	0.40
2:B:1008:SER:HB3	2:B:1017:ARG:HB3	2.03	0.40
2:D:19:GLU:O	2:D:205:ILE:N	2.54	0.40
2:D:1422:ASP:HB3	2:D:1571:ASN:H	1.86	0.40
2:D:3943:ILE:H	2:D:4009:GLN:NE2	2.19	0.40
2:D:4069:LYS:NZ	2:D:4130:ASN:OD1	2.39	0.40
2:F:11:VAL:HB	2:F:12:GLN:H	1.72	0.40
2:F:1118:ASP:OD1	2:F:1118:ASP:N	2.54	0.40
2:F:1249:PRO:HA	2:F:1250:PRO:HD3	1.98	0.40
2:F:3051:ARG:HG2	2:F:3052:HIS:CD2	2.57	0.40
2:H:3852:LYS:HE2	2:H:3852:LYS:HB3	1.89	0.40
2:B:3568:SER:HA	2:B:3571:TRP:CD1	2.56	0.40
2:D:1502:SER:O	2:D:1506:GLN:N	2.52	0.40
2:D:3169:LEU:HD23	2:D:3194:LEU:HD11	2.03	0.40
2:D:3845:ASN:OD1	2:D:3845:ASN:N	2.55	0.40
2:D:4218:ILE:HD13	2:D:4954:MET:HE2	2.04	0.40
2:F:1008:SER:HB3	2:F:1017:ARG:HB3	2.03	0.40
2:F:3666:ASP:OD1	2:F:3666:ASP:N	2.41	0.40
2:H:1158:ASN:ND2	2:H:1182:ILE:O	2.45	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	106/110 (96%)	104 (98%)	2 (2%)	0	100	100
1	C	106/110 (96%)	105 (99%)	1 (1%)	0	100	100
1	E	106/110 (96%)	104 (98%)	2 (2%)	0	100	100
1	G	106/110 (96%)	105 (99%)	1 (1%)	0	100	100
2	B	4228/5037 (84%)	4164 (98%)	64 (2%)	0	100	100
2	D	4227/5037 (84%)	4168 (99%)	59 (1%)	0	100	100
2	F	4228/5037 (84%)	4164 (98%)	64 (2%)	0	100	100
2	H	4227/5037 (84%)	4168 (99%)	59 (1%)	0	100	100
All	All	17334/20588 (84%)	17082 (98%)	252 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/90 (98%)	86 (98%)	2 (2%)	44	72
1	C	88/90 (98%)	85 (97%)	3 (3%)	32	64
1	E	88/90 (98%)	86 (98%)	2 (2%)	44	72
1	G	88/90 (98%)	85 (97%)	3 (3%)	32	64
2	B	3514/4276 (82%)	3482 (99%)	32 (1%)	70	84
2	D	3505/4276 (82%)	3473 (99%)	32 (1%)	70	84
2	F	3514/4276 (82%)	3482 (99%)	32 (1%)	70	84
2	H	3505/4276 (82%)	3473 (99%)	32 (1%)	70	84
All	All	14390/17464 (82%)	14252 (99%)	138 (1%)	65	83

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	80	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	149	THR
2	B	220	LEU
2	B	280	LEU
2	B	296	ASP
2	B	301	VAL
2	B	318	VAL
2	B	499	THR
2	B	575	LEU
2	B	577	ILE
2	B	647	ASN
2	B	1096	THR
2	B	1123	VAL
2	B	1186	ASP
2	B	1636	MET
2	B	1934	SER
2	B	2584	HIS
2	B	2636	PHE
2	B	3025	LEU
2	B	3398	PHE
2	B	3409	TYR
2	B	3510	ILE
2	B	3696	ASP
2	B	3856	LEU
2	B	3899	PHE
2	B	3903	LEU
2	B	3916	ILE
2	B	3924	LEU
2	B	3980	LEU
2	B	3987	ASP
2	B	4224	GLU
2	B	4785	THR
2	B	4889	VAL
1	C	5	ILE
1	C	26	HIS
1	C	80	ASP
2	D	220	LEU
2	D	232	THR
2	D	280	LEU
2	D	287	THR
2	D	301	VAL
2	D	499	THR
2	D	575	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	1022	VAL
2	D	1039	LEU
2	D	1082	THR
2	D	1130	GLN
2	D	1423	ASP
2	D	1520	VAL
2	D	1562	ILE
2	D	2155	LEU
2	D	2486	VAL
2	D	3078	ARG
2	D	3108	GLU
2	D	3398	PHE
2	D	3769	ARG
2	D	3899	PHE
2	D	3916	ILE
2	D	3924	LEU
2	D	4034	ASN
2	D	4571	PHE
2	D	4580	TYR
2	D	4582	VAL
2	D	4666	VAL
2	D	4689	THR
2	D	4691	GLN
2	D	4748	LEU
2	D	4889	VAL
1	E	26	HIS
1	E	80	ASP
2	F	149	THR
2	F	220	LEU
2	F	280	LEU
2	F	296	ASP
2	F	301	VAL
2	F	318	VAL
2	F	499	THR
2	F	575	LEU
2	F	577	ILE
2	F	647	ASN
2	F	1096	THR
2	F	1123	VAL
2	F	1186	ASP
2	F	1636	MET
2	F	1934	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	2584	HIS
2	F	2636	PHE
2	F	3025	LEU
2	F	3398	PHE
2	F	3409	TYR
2	F	3510	ILE
2	F	3696	ASP
2	F	3856	LEU
2	F	3899	PHE
2	F	3903	LEU
2	F	3916	ILE
2	F	3924	LEU
2	F	3980	LEU
2	F	3987	ASP
2	F	4224	GLU
2	F	4785	THR
2	F	4889	VAL
1	G	5	ILE
1	G	26	HIS
1	G	80	ASP
2	H	220	LEU
2	H	232	THR
2	H	280	LEU
2	H	287	THR
2	H	301	VAL
2	H	499	THR
2	H	575	LEU
2	H	1022	VAL
2	H	1039	LEU
2	H	1082	THR
2	H	1130	GLN
2	H	1423	ASP
2	H	1520	VAL
2	H	1562	ILE
2	H	2155	LEU
2	H	2486	VAL
2	H	3078	ARG
2	H	3108	GLU
2	H	3398	PHE
2	H	3769	ARG
2	H	3899	PHE
2	H	3916	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	3924	LEU
2	H	4034	ASN
2	H	4571	PHE
2	H	4580	TYR
2	H	4582	VAL
2	H	4666	VAL
2	H	4689	THR
2	H	4691	GLN
2	H	4748	LEU
2	H	4889	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (231) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
2	B	23	GLN
2	B	71	GLN
2	B	79	GLN
2	B	113	HIS
2	B	138	GLN
2	B	241	GLN
2	B	461	HIS
2	B	465	GLN
2	B	582	HIS
2	B	647	ASN
2	B	705	ASN
2	B	765	GLN
2	B	877	ASN
2	B	993	HIS
2	B	1133	HIS
2	B	1206	GLN
2	B	1229	ASN
2	B	1300	HIS
2	B	1460	HIS
2	B	1511	HIS
2	B	1558	HIS
2	B	1614	GLN
2	B	1660	GLN
2	B	1938	GLN
2	B	2003	GLN
2	B	2007	ASN
2	B	2095	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	2176	ASN
2	B	2184	ASN
2	B	2260	ASN
2	B	2284	ASN
2	B	2515	GLN
2	B	2574	HIS
2	B	2673	HIS
2	B	2772	GLN
2	B	2877	GLN
2	B	2962	GLN
2	B	3012	ASN
2	B	3030	HIS
2	B	3052	HIS
2	B	3128	ASN
2	B	3162	GLN
2	B	3343	GLN
2	B	3378	GLN
2	B	3418	ASN
2	B	3456	GLN
2	B	3523	ASN
2	B	3530	GLN
2	B	3572	GLN
2	B	3914	ASN
2	B	4034	ASN
2	B	4120	ASN
2	B	4162	ASN
2	B	4209	GLN
2	B	4246	GLN
2	B	4547	GLN
2	B	4558	ASN
2	B	4707	ASN
2	B	4997	ASN
2	B	5003	HIS
1	C	32	GLN
1	C	66	GLN
2	D	23	GLN
2	D	44	ASN
2	D	71	GLN
2	D	79	GLN
2	D	201	ASN
2	D	203	ASN
2	D	241	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	383	HIS
2	D	461	HIS
2	D	579	GLN
2	D	705	ASN
2	D	765	GLN
2	D	797	HIS
2	D	866	HIS
2	D	949	ASN
2	D	1041	GLN
2	D	1125	ASN
2	D	1220	GLN
2	D	1229	ASN
2	D	1443	GLN
2	D	1532	ASN
2	D	1702	HIS
2	D	1719	HIS
2	D	1938	GLN
2	D	2003	GLN
2	D	2169	GLN
2	D	2173	GLN
2	D	2176	ASN
2	D	2184	ASN
2	D	2194	HIS
2	D	2520	HIS
2	D	2772	GLN
2	D	2877	GLN
2	D	3008	GLN
2	D	3012	ASN
2	D	3052	HIS
2	D	3128	ASN
2	D	3378	GLN
2	D	3456	GLN
2	D	3556	ASN
2	D	3704	HIS
2	D	4223	ASN
2	D	4547	GLN
2	D	4558	ASN
2	D	4707	ASN
2	D	4832	HIS
2	D	4836	GLN
2	D	4946	GLN
2	D	4973	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	4997	ASN
2	D	5003	HIS
1	E	32	GLN
2	F	23	GLN
2	F	57	ASN
2	F	71	GLN
2	F	79	GLN
2	F	113	HIS
2	F	138	GLN
2	F	241	GLN
2	F	461	HIS
2	F	465	GLN
2	F	582	HIS
2	F	647	ASN
2	F	705	ASN
2	F	877	ASN
2	F	993	HIS
2	F	1133	HIS
2	F	1206	GLN
2	F	1229	ASN
2	F	1300	HIS
2	F	1460	HIS
2	F	1558	HIS
2	F	1614	GLN
2	F	1660	GLN
2	F	1938	GLN
2	F	2003	GLN
2	F	2007	ASN
2	F	2095	GLN
2	F	2161	GLN
2	F	2176	ASN
2	F	2184	ASN
2	F	2260	ASN
2	F	2284	ASN
2	F	2515	GLN
2	F	2673	HIS
2	F	2772	GLN
2	F	2877	GLN
2	F	2962	GLN
2	F	3012	ASN
2	F	3030	HIS
2	F	3052	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	3128	ASN
2	F	3162	GLN
2	F	3343	GLN
2	F	3378	GLN
2	F	3418	ASN
2	F	3456	GLN
2	F	3523	ASN
2	F	3530	GLN
2	F	3572	GLN
2	F	3914	ASN
2	F	4034	ASN
2	F	4120	ASN
2	F	4162	ASN
2	F	4209	GLN
2	F	4246	GLN
2	F	4547	GLN
2	F	4558	ASN
2	F	4707	ASN
2	F	4997	ASN
2	F	5003	HIS
1	G	32	GLN
2	H	23	GLN
2	H	44	ASN
2	H	71	GLN
2	H	79	GLN
2	H	201	ASN
2	H	203	ASN
2	H	241	GLN
2	H	273	HIS
2	H	383	HIS
2	H	461	HIS
2	H	579	GLN
2	H	705	ASN
2	H	765	GLN
2	H	797	HIS
2	H	866	HIS
2	H	949	ASN
2	H	1041	GLN
2	H	1203	ASN
2	H	1220	GLN
2	H	1229	ASN
2	H	1443	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	1532	ASN
2	H	1702	HIS
2	H	1719	HIS
2	H	1938	GLN
2	H	2003	GLN
2	H	2169	GLN
2	H	2173	GLN
2	H	2176	ASN
2	H	2184	ASN
2	H	2194	HIS
2	H	2260	ASN
2	H	2520	HIS
2	H	2663	ASN
2	H	2772	GLN
2	H	2877	GLN
2	H	3013	HIS
2	H	3052	HIS
2	H	3127	GLN
2	H	3128	ASN
2	H	3211	ASN
2	H	3268	HIS
2	H	3378	GLN
2	H	3456	GLN
2	H	3556	ASN
2	H	3704	HIS
2	H	3901	ASN
2	H	4043	GLN
2	H	4223	ASN
2	H	4547	GLN
2	H	4558	ASN
2	H	4707	ASN
2	H	4836	GLN
2	H	4946	GLN
2	H	4973	HIS
2	H	4997	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
5	ATP	F	5303	-	32,33,33	0.26	0	48,52,52	0.30	0
5	ATP	B	5303	-	32,33,33	0.26	0	48,52,52	0.30	0
5	ATP	H	5303	-	32,33,33	0.26	0	48,52,52	0.30	0
5	ATP	D	5303	-	32,33,33	0.26	0	48,52,52	0.30	0

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
5	ATP	F	5303	-	-	4/22/38/38	0/3/3/3
5	ATP	B	5303	-	-	4/22/38/38	0/3/3/3
5	ATP	H	5303	-	-	7/22/38/38	0/3/3/3
5	ATP	D	5303	-	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

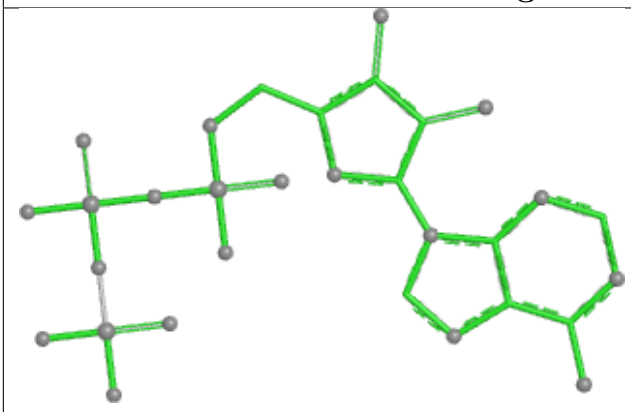
Mol	Chain	Res	Type	Atoms
5	B	5303	ATP	C5'-O5'-PA-O2A
5	B	5303	ATP	C5'-O5'-PA-O3A
5	B	5303	ATP	C4'-C5'-O5'-PA
5	D	5303	ATP	C5'-O5'-PA-O2A
5	D	5303	ATP	C5'-O5'-PA-O3A
5	D	5303	ATP	C4'-C5'-O5'-PA
5	F	5303	ATP	C5'-O5'-PA-O2A
5	F	5303	ATP	C5'-O5'-PA-O3A
5	F	5303	ATP	C4'-C5'-O5'-PA
5	H	5303	ATP	C5'-O5'-PA-O2A
5	H	5303	ATP	C5'-O5'-PA-O3A
5	H	5303	ATP	C4'-C5'-O5'-PA
5	D	5303	ATP	O4'-C4'-C5'-O5'
5	H	5303	ATP	O4'-C4'-C5'-O5'
5	D	5303	ATP	C3'-C4'-C5'-O5'
5	H	5303	ATP	C3'-C4'-C5'-O5'
5	D	5303	ATP	PB-O3A-PA-O5'
5	H	5303	ATP	PB-O3A-PA-O5'
5	B	5303	ATP	O4'-C1'-N9-C8
5	D	5303	ATP	O4'-C1'-N9-C8
5	F	5303	ATP	O4'-C1'-N9-C8
5	H	5303	ATP	O4'-C1'-N9-C8

There are no ring outliers.

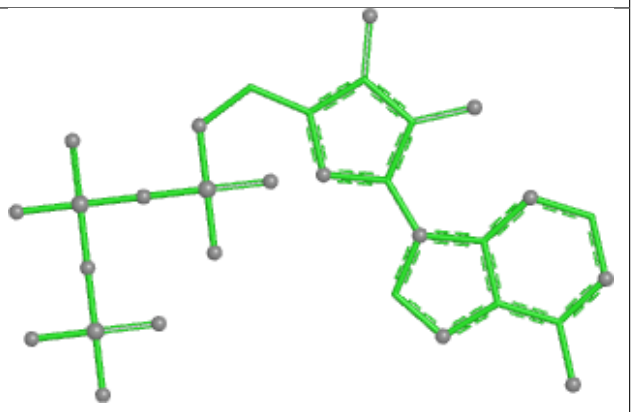
No monomer is involved in short contacts.

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

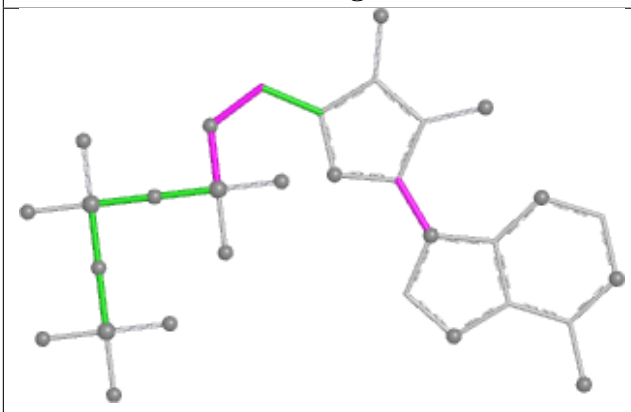
Ligand ATP F 5303



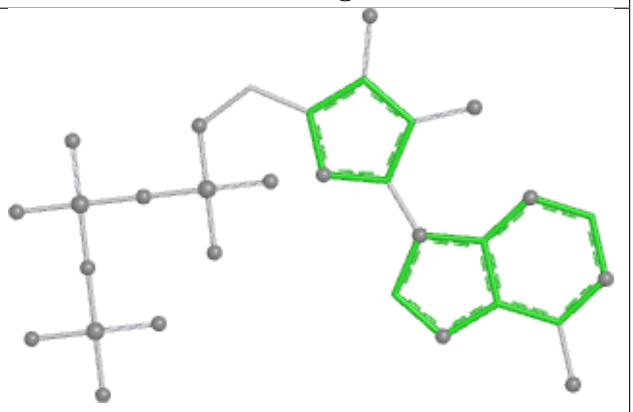
Bond lengths



Bond angles

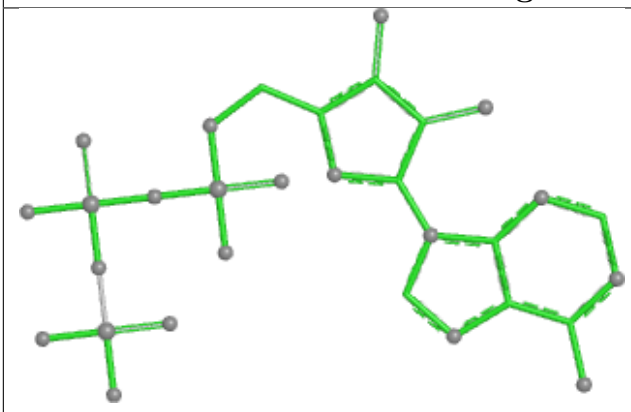


Torsions

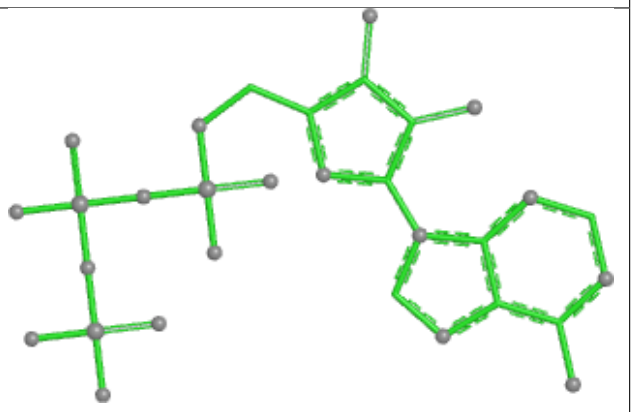


Rings

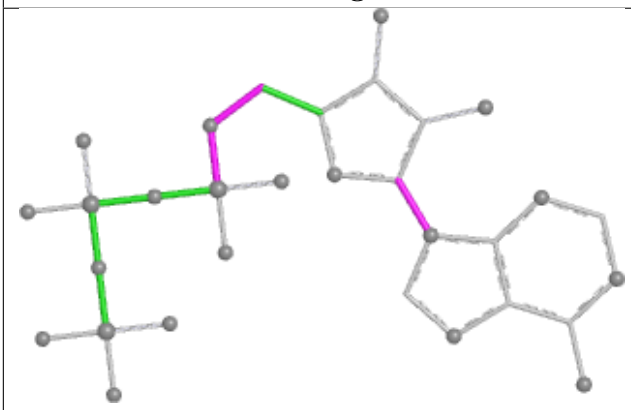
Ligand ATP B 5303



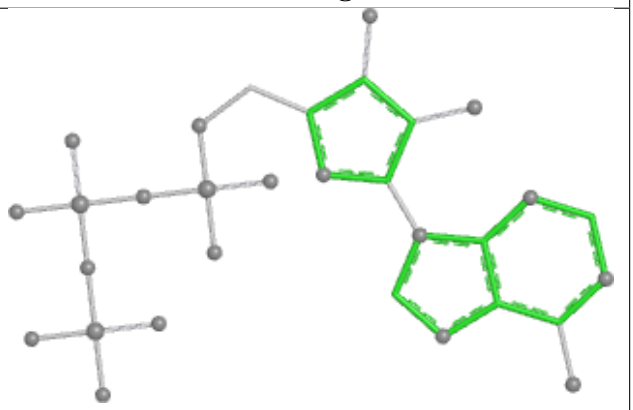
Bond lengths



Bond angles

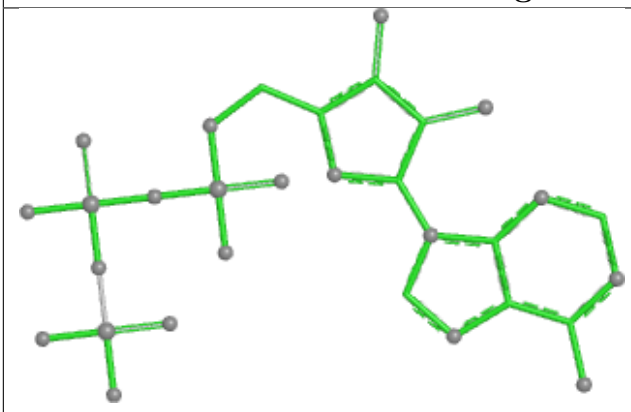


Torsions

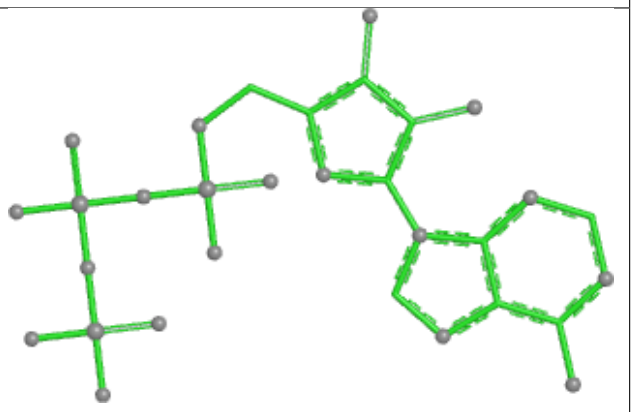


Rings

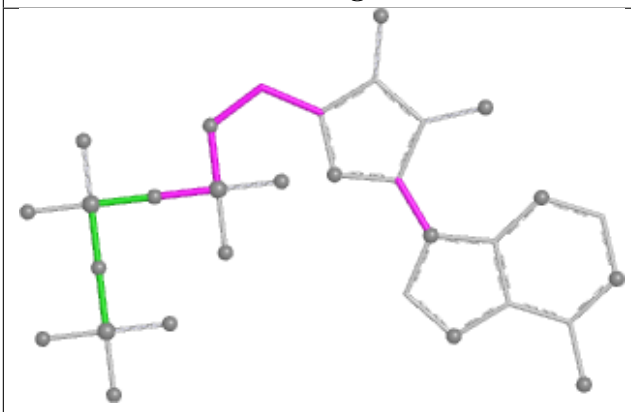
Ligand ATP H 5303



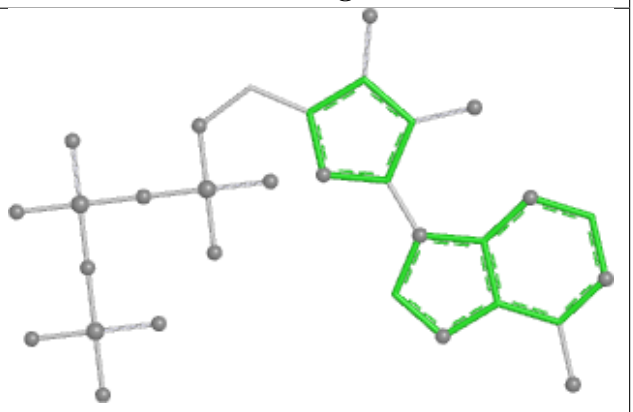
Bond lengths



Bond angles

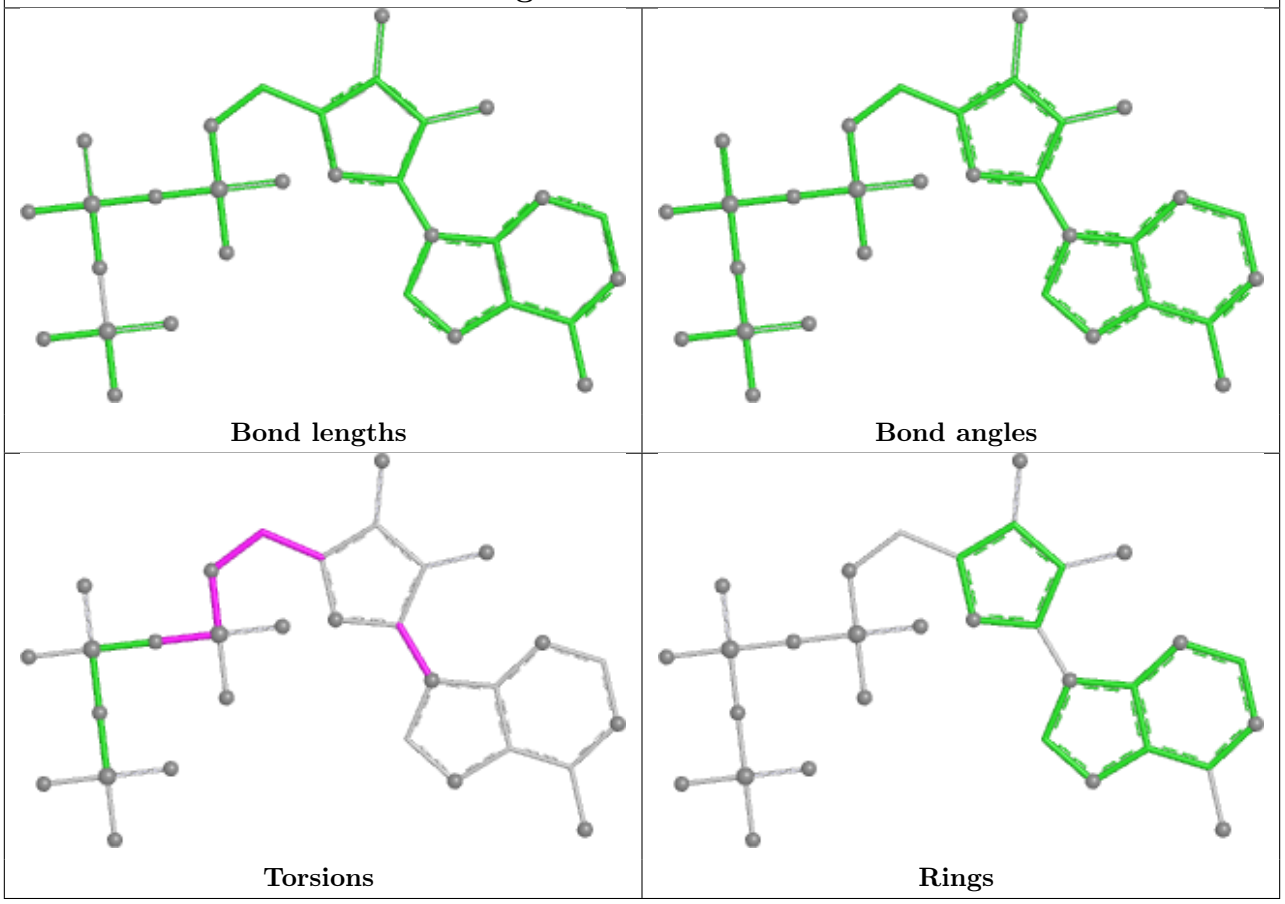


Torsions



Rings

Ligand ATP D 5303



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

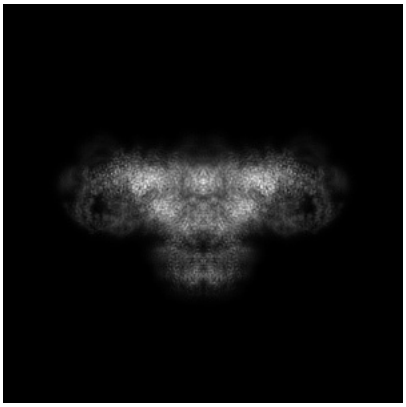
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73959. These allow visual inspection of the internal detail of the map and identification of artifacts.

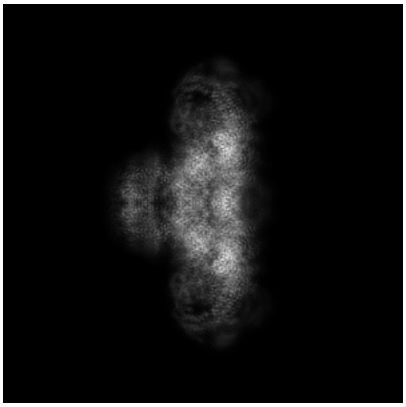
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

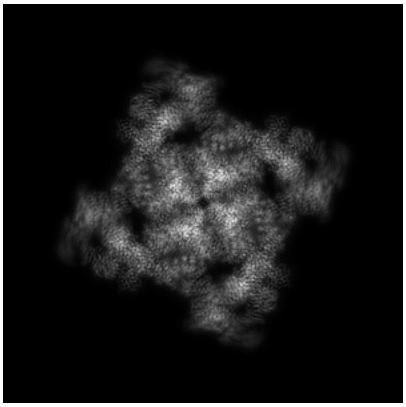
6.1.1 Primary map



X



Y

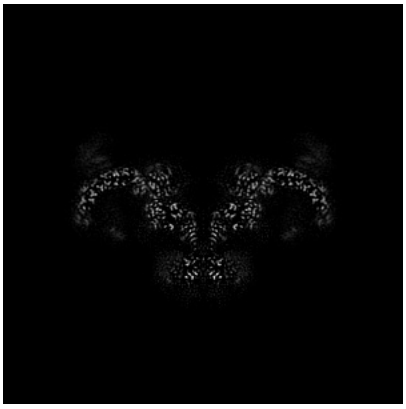


Z

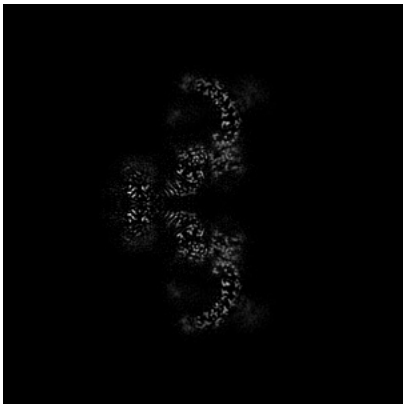
The images above show the map projected in three orthogonal directions.

6.2 Central slices

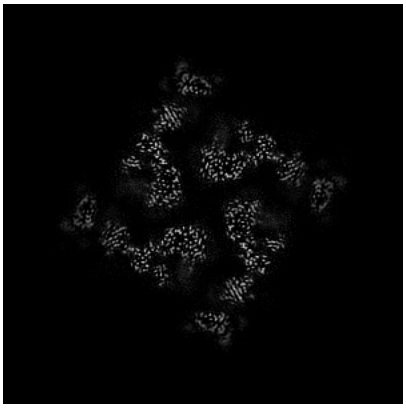
6.2.1 Primary map



X Index: 256



Y Index: 256

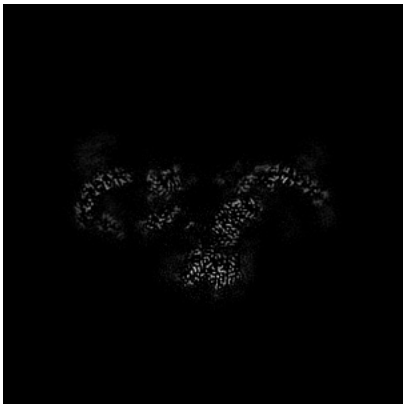


Z Index: 256

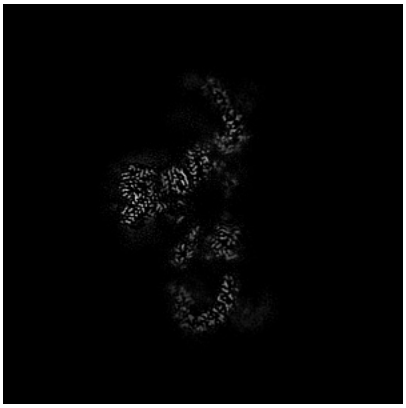
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

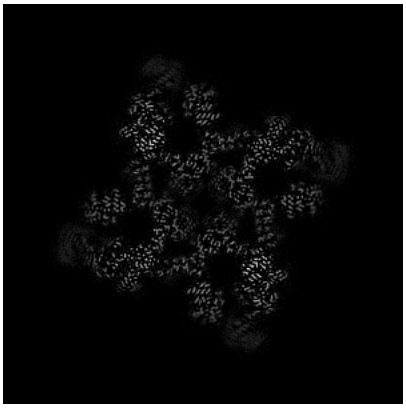
6.3.1 Primary map



X Index: 264



Y Index: 246

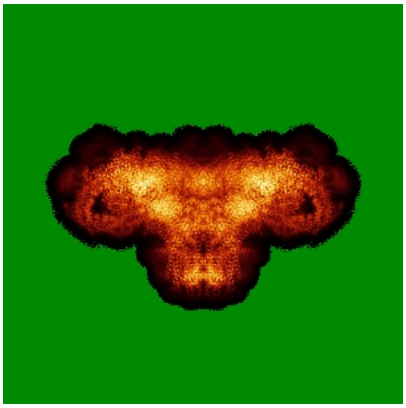


Z Index: 282

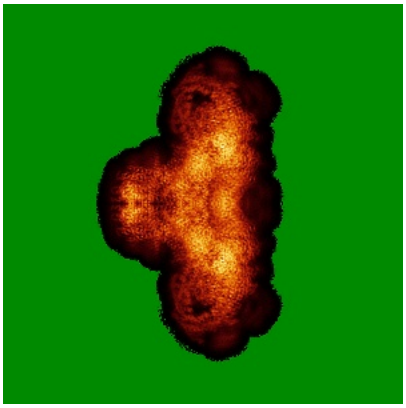
The images above show the largest variance slices of the map in three orthogonal directions.

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

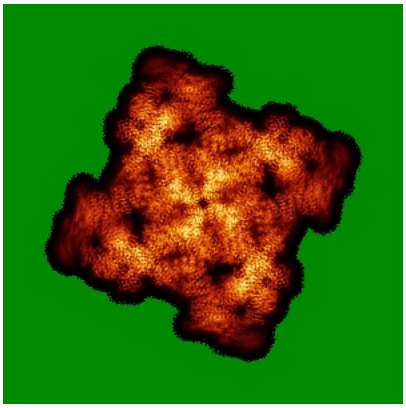
6.4.1 Primary map



X



Y

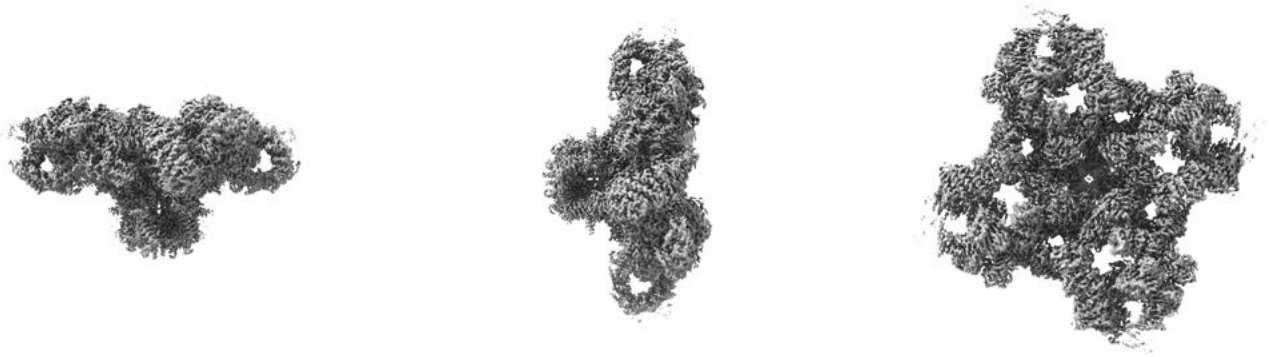


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.068. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

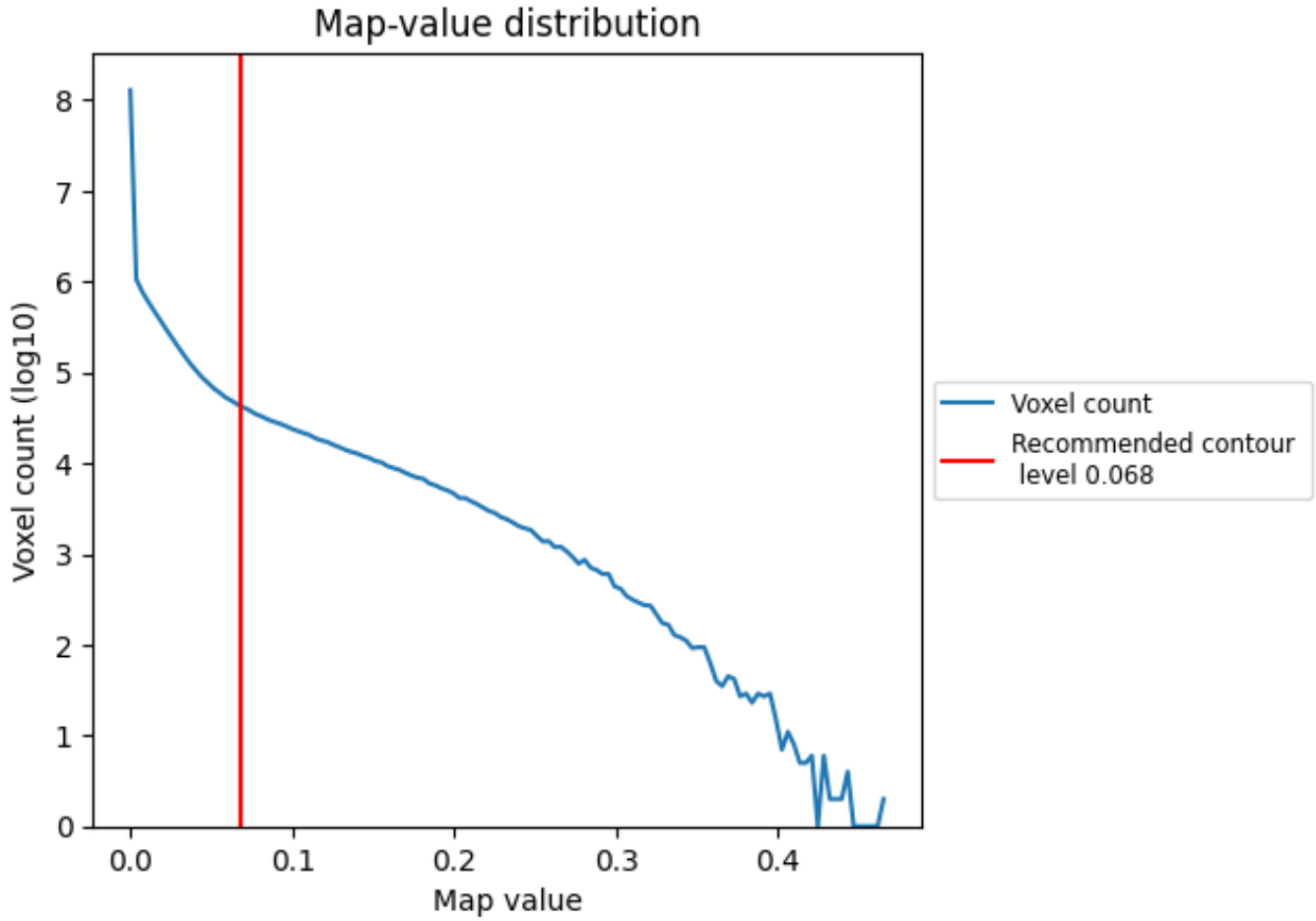
6.6 Mask visualisation (i)

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

7 Map analysis

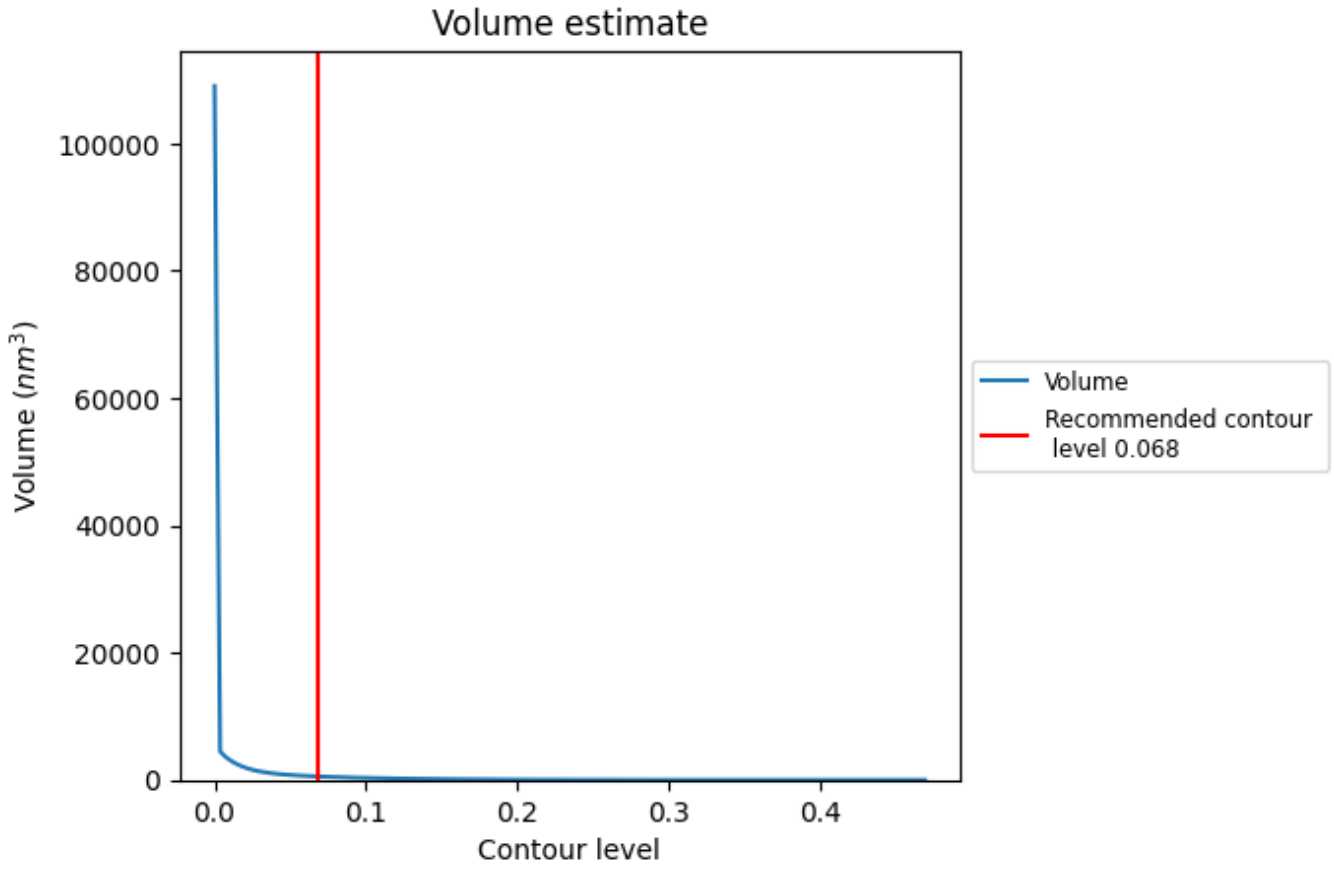
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

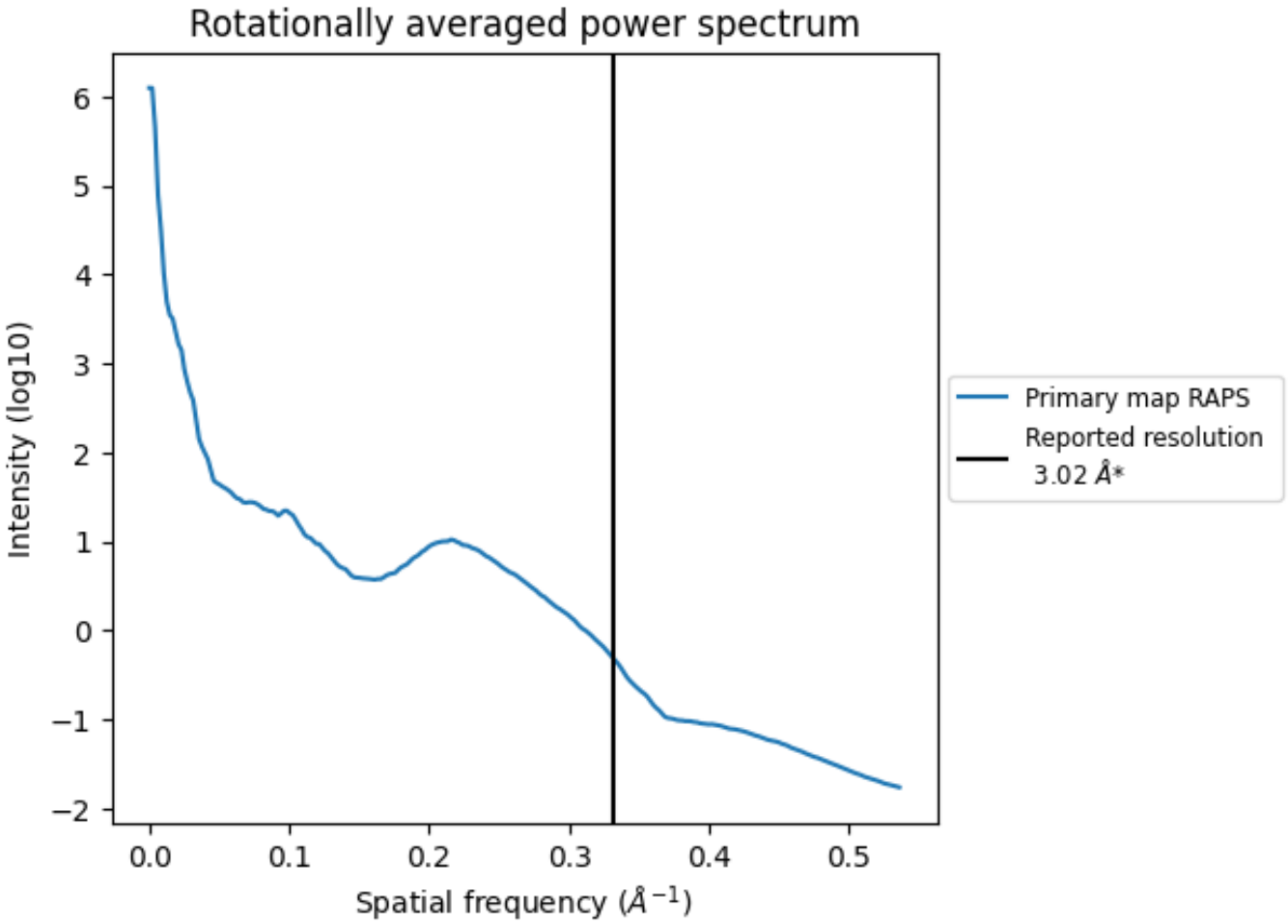
7.2 Volume estimate



The volume at the recommended contour level is 551 nm^3; this corresponds to an approximate mass of 498 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 0.331 Å^{-1}

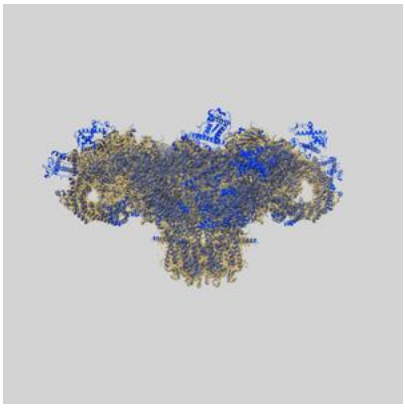
8 Fourier-Shell correlation (i)

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

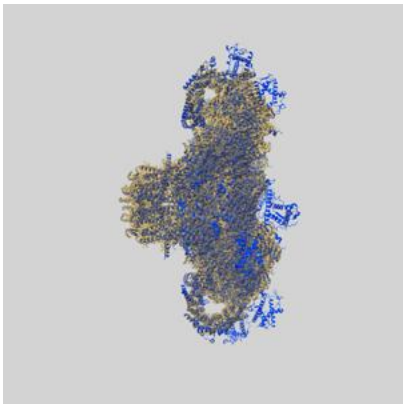
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73959 and PDB model 9Z9U. Per-residue inclusion information can be found in section 3 on page 7.

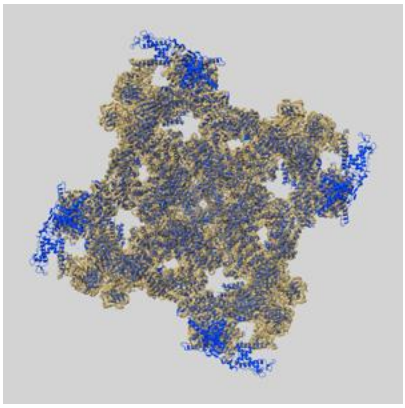
9.1 Map-model overlay



X



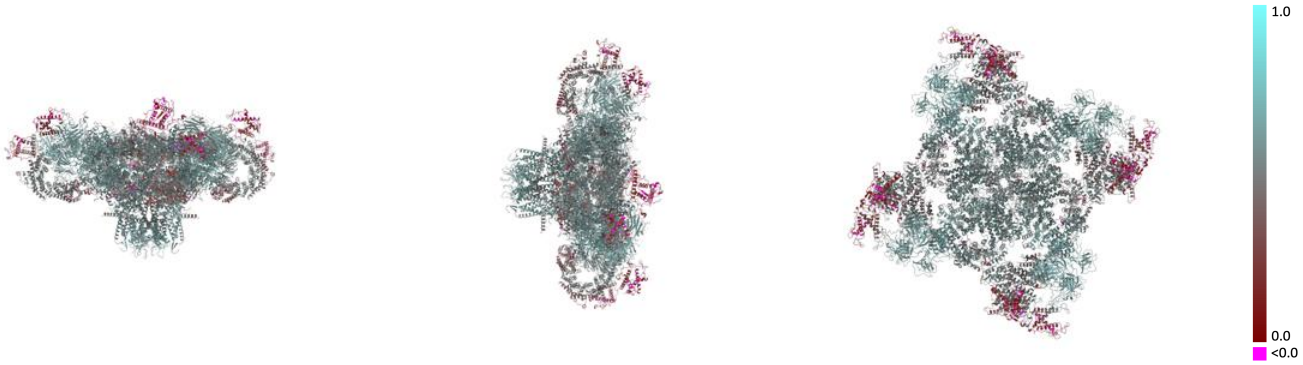
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.068 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.

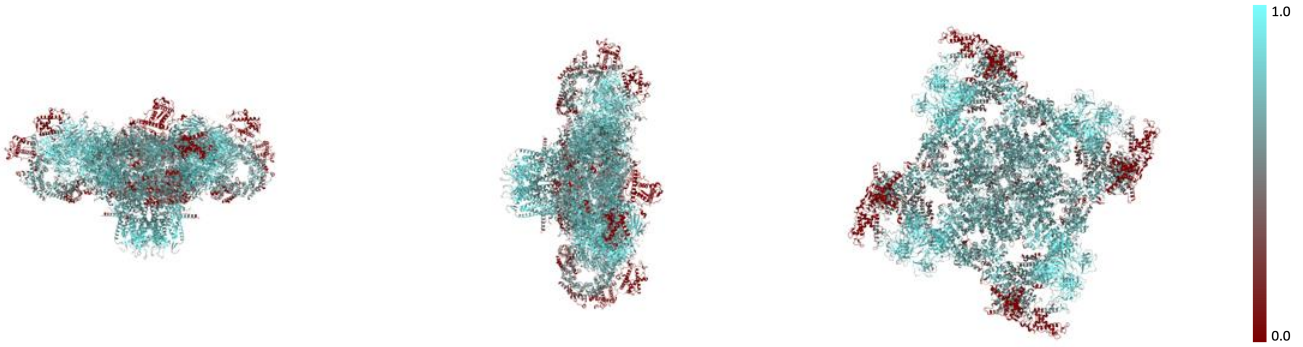
9.2 Q-score mapped to coordinate model (i)



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.

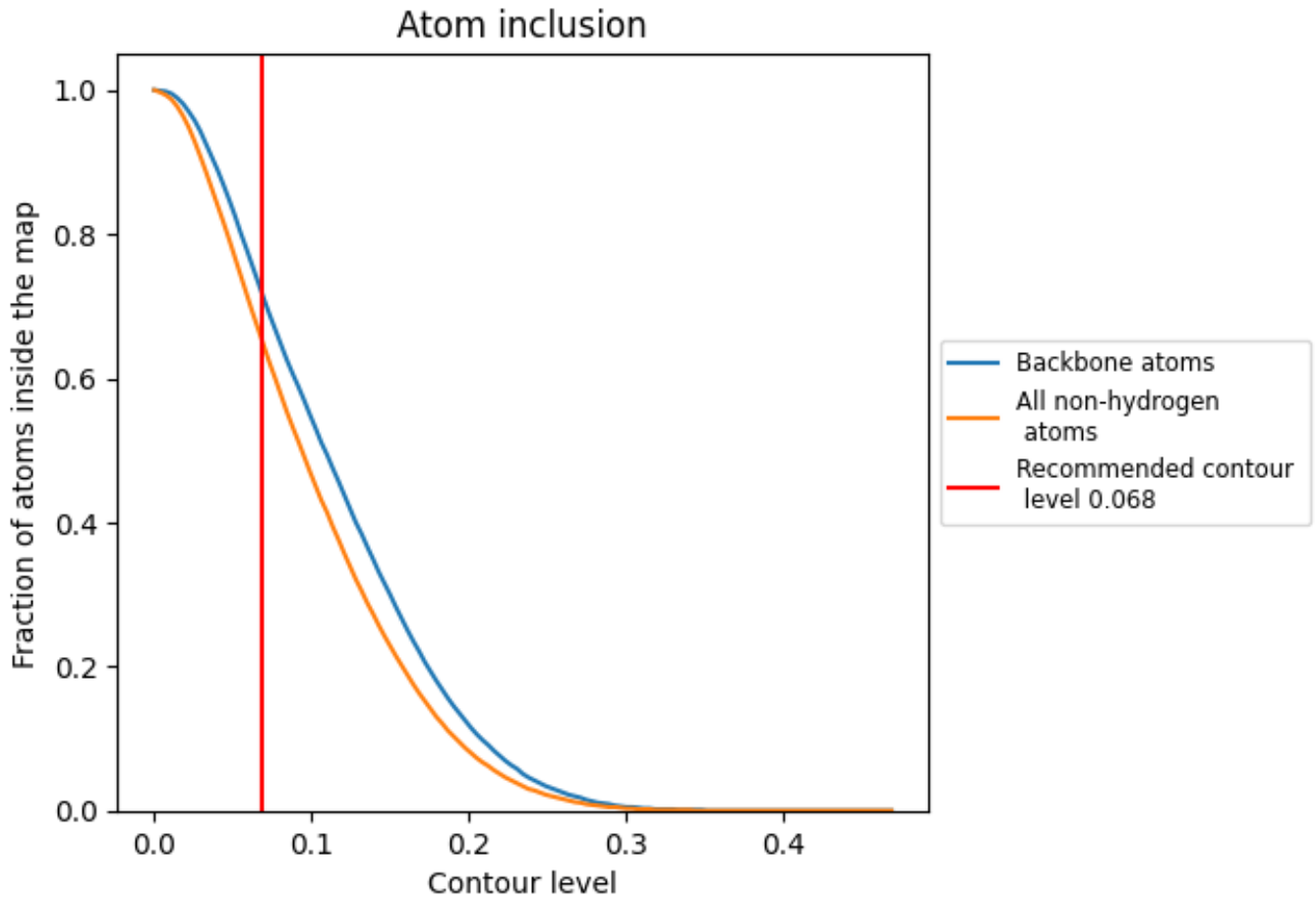
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.068).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.068) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.5160
A	0.7710	0.5790
B	0.6600	0.5190
C	0.7950	0.5910
D	0.6460	0.5100
E	0.7680	0.5800
F	0.6600	0.5190
G	0.7940	0.5910
H	0.6460	0.5100

