wwPDB EM Validation Summary Report

Jul 10, 2023 – 12:08 PM EDT

PDB ID	:	8SES
EMDB ID	:	EMD-40427
Title	:	Cryo-EM Structure of RyR1 + Adenine
Authors	:	Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on	:	2023-04-10
Resolution	:	3.98 Å(reported)

This is a wwPDB EM Validation Summary 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:

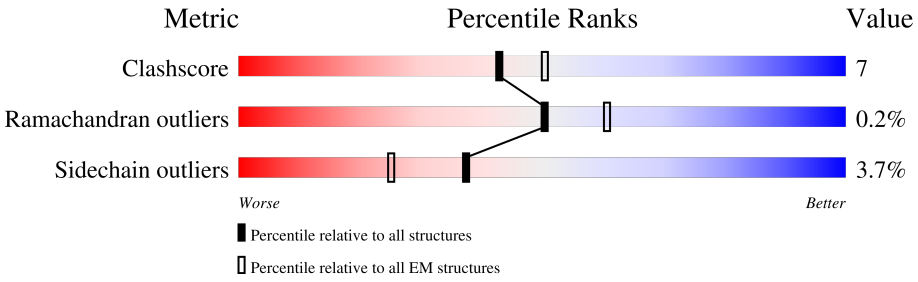
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.98 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	5037	12% 69% 18% • 13%
1	B	5037	12% 68% 18% • 13%
1	C	5037	12% 68% 18% • 13%
1	D	5037	12% 68% 18% • 13%
2	E	350	21% 9% 69%
2	F	350	21% 9% 69%
2	G	350	22% 8% 69%
2	H	350	22% 9% 69%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 142940 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4377	Total 34906	C 22208	N 6024	O 6438	S 236	9	0
1	B	4377	Total 34906	C 22208	N 6024	O 6438	S 236	9	0
1	C	4377	Total 34906	C 22208	N 6024	O 6438	S 236	9	0
1	D	4377	Total 34906	C 22208	N 6024	O 6438	S 236	9	0

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	F	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	G	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	H	107	Total 818	C 516	N 144	O 154	S 4	0	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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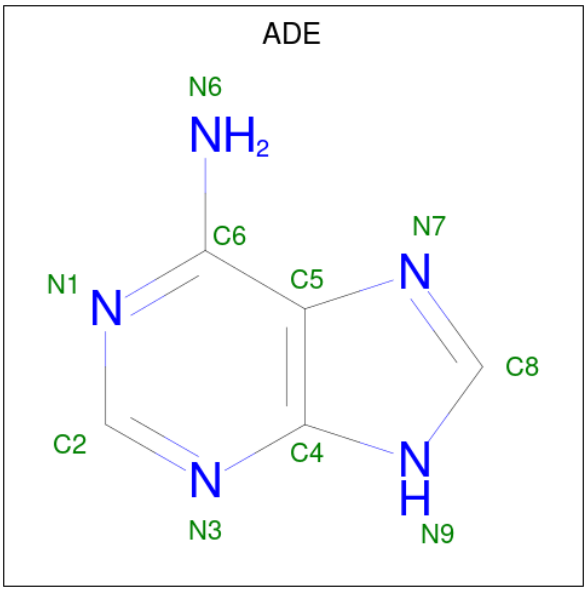
Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

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

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

- Molecule 4 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$) (labeled as "Ligand of Interest" by depositor).

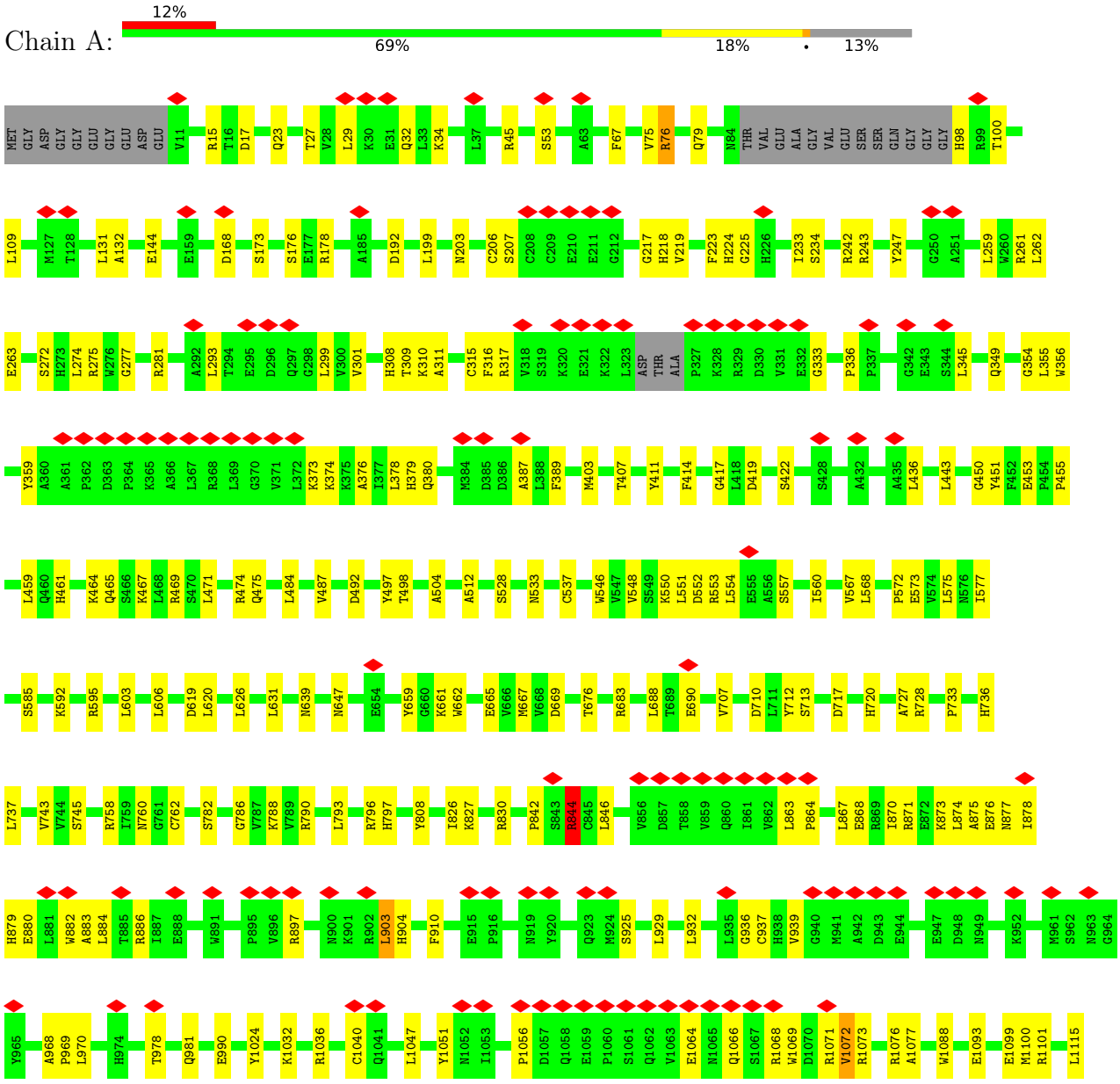


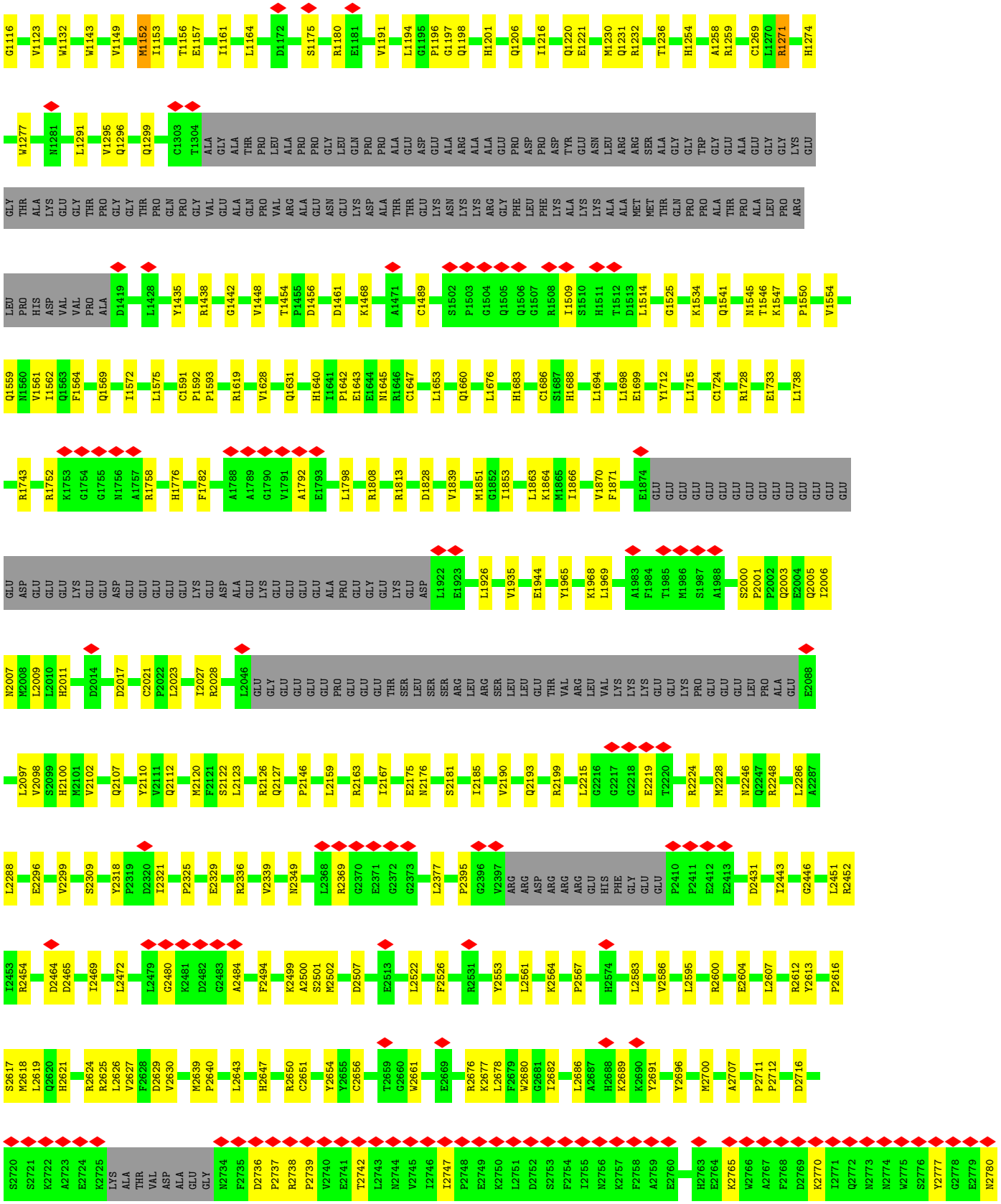
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N 10 5 5	0
4	B	1	Total C N 10 5 5	0
4	C	1	Total C N 10 5 5	0
4	D	1	Total C N 10 5 5	0

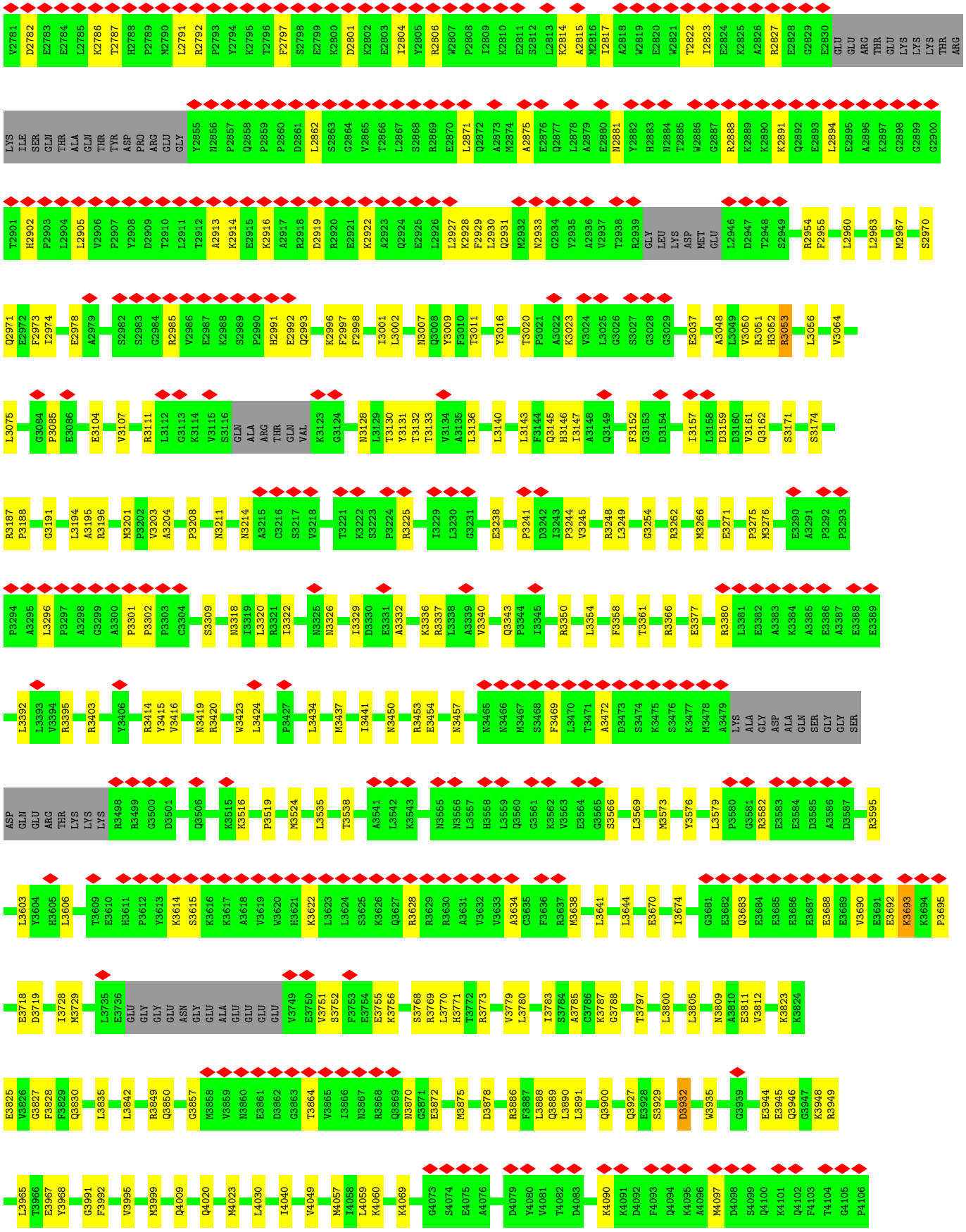
3 Residue-property plots (i)

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

- Molecule 1: Ryanodine receptor 1




G1116 V1123 W1132 W1143 V1149 M1152 I1153 T1156 E1157 I1161 L1164 D1172 S1175 R1180 E1181 V1191 L1194 G1195 P1196 G1197 Q1198 H1201 Q1206 I1216 Q1220 E1221 M1230 Q1231 R1232 T1236 H1254 A1258 R1259 C1269 L1270 R1271 H1274
W1277 N1281 L1291 V1295 Q1296 Q1299 C1303 T1304 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 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 L1428 Y1435 R1438 G1442 V1448 T1454 P1455 D1456 D1461 K1468 A1471 C1489 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 T1512 D1513 L1514 G1525 K1534 Q1541 N1545 T1546 K1547 P1550 V1554
Q1559 N1560 V1561 I1562 Q1563 F1564 Q1569 I1572 L1575 C1591 P1592 P1593 R1619 V1628 Q1631 H1640 I1641 P1642 E1643 E1644 N1645 R1646 C1647 L1653 Q1660 L1676 H1683 C1686 S1687 H1688 L1694 L1698 E1699 Y1712 L1715 C1724 R1728 E1733 L1738
R1743 R1752 K1753 G1754 G1755 N1756 A1757 R1758 H1776 F1782 A1788 A1789 G1790 V1791 A1792 E1793 L1798 R1808 R1813 D1828 V1839 M1851 G1852 I1853 L1863 K1864 M1865 I1866 V1870 F1871 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU
GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 L1926 V1935 E1944 Y1965 K1968 L1969 A1983 F1984 T1985 M1986 S1987 A1988 S2000 P2001 P2002 Q2003 E2004 Q2005 I2006
N2007 M2008 L2009 L2010 H2011 D2014 D2017 C2021 P2022 L2023 I2027 R2028 L2046 GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088
L2097 V2098 S2099 H2100 M2101 V2102 Q2107 Y2110 V2111 Q2112 M2120 F2121 S2122 L2123 R2126 Q2127 P2146 L2159 R2163 I2167 E2175 N2176 S2181 I2185 V2190 Q2193 R2199 L2215 G2216 G2217 G2218 E2219 T2220 R2224 M2228 N2246 Q2247 R2248 L2286 A2287
L2288 E2296 V2299 S2309 Y2318 P2319 D2320 I2321 P2325 E2329 R2336 V2339 N2349 L2368 R2369 G2370 E2371 G2372 G2373 L2377 P2395 G2396 V2397 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2410 P2411 E2412 E2413 D2431 I2443 G2446 L2451 R2452
I2453 R2454 D2464 D2465 I2469 L2472 L2479 G2480 K2481 D2482 G2483 A2484 F2494 K2499 A2500 S2501 M2502 D2507 E2513 L2522 F2526 R2531 Y2553 L2561 K2564 P2567 H2574 L2583 V2586 L2595 R2600 E2604 L2607 R2612 Y2613 P2616
S2617 M2618 L2619 Q2620 H2621 R2624 R2625 L2626 V2627 F2628 D2629 V2630 M2639 P2640 L2643 H2647 R2650 C2651 Y2654 Y2655 C2656 T2659 G2660 W2661 E2669 R2676 K2677 L2678 F2679 W2680 G2681 I2682 L2686 A2687 H2688 K2689 K2690 Y2691 Y2696 M2700 A2707 P2711 P2712 D2716
S2720 S2721 K2722 A2723 E2724 K2725 LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780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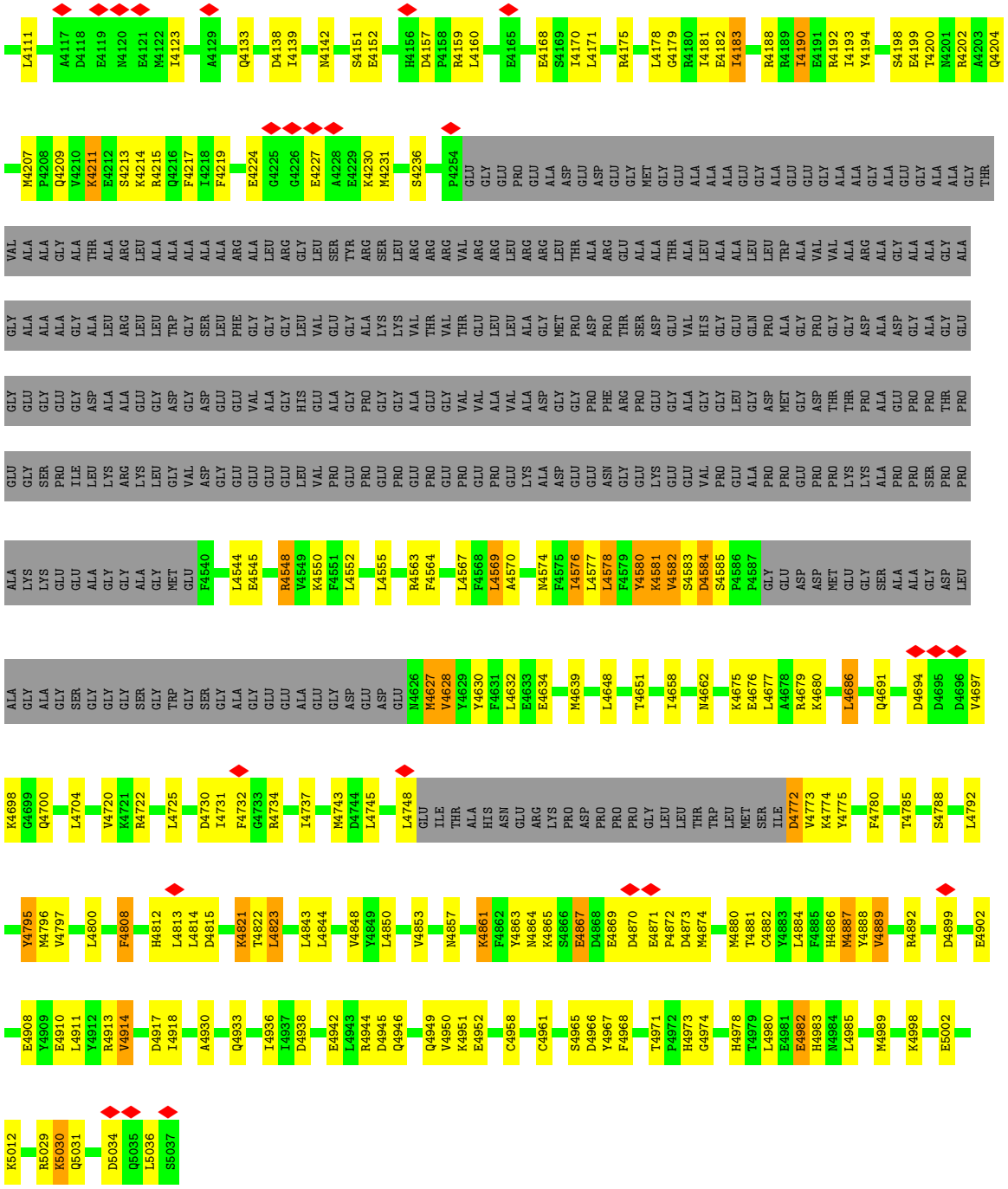
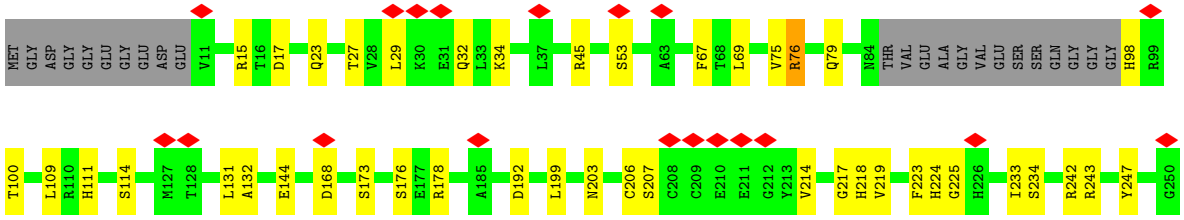
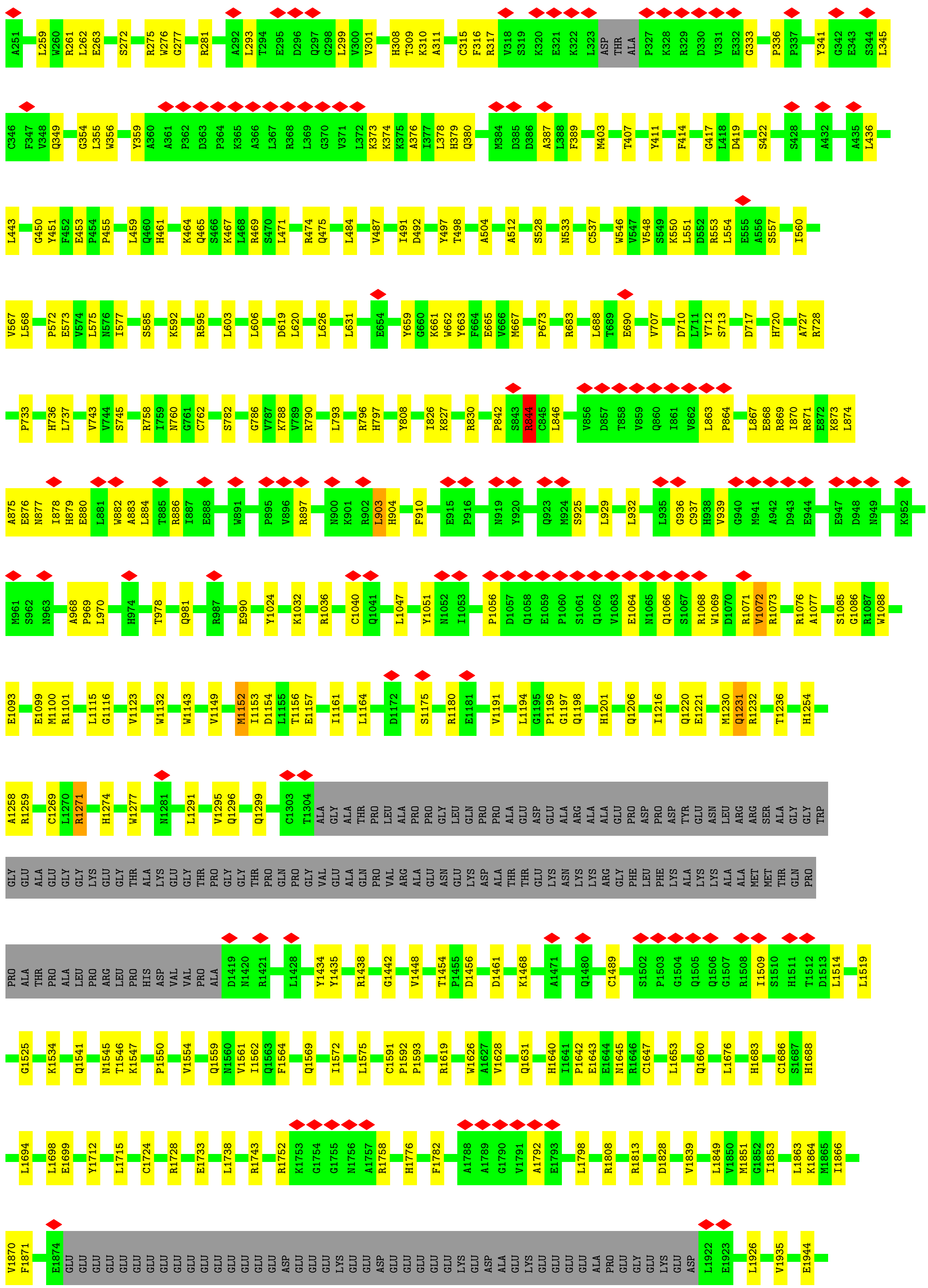
LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 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 L2946 D2947 T2948 S2949 R2954 F2955 L2960 L2963 M2967 S2970
Q2971 E2972 F2973 I2974 E2978 A2979 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 Q2993 K2996 F2997 F2998 I3001 L3002 N3007 Q3008 Y3009 F3010 T3011 Y3016 T3020 P3021 A3022 K3023 V3024 L3025 G3026 S3027 G3028 G3029 E3037 A3048 L3049 V3050 R3051 H3052 R3053 L3056 V3064
L3075 G3084 P3085 E3086 E3104 V3107 R3111 L3112 G3113 K3114 V3115 S3116 GLN ALA ARG THR GLN VAL K3123 G3124 N3128 L3129 T3130 Y3131 T3132 T3133 V3134 A3135 L3136 L3140 L3143 F3144 Q3145 H3146 I3147 A3148 Q3149 F3152 G3153 D3154 I3157 L3158 D3159 D3160 V3161 Q3162 S3171 S3174
R3187 P3188 G3191 L3194 A3195 R3196 M3201 P3202 V3203 A3204 P3208 N3211 N3214 A3215 C3216 S3217 V3218 T3221 K3222 S3223 P3224 R3225 I3229 L3230 G3231 E3238 P3241 D3242 I3243 P3244 V3245 R3248 L3249 G3254 R3262 M3266 E3271 P3275 M3276 E3290 A3291 P3292 P3293
P3294 A3295 L3296 P3297 A3298 G3299 A3300 P3301 P3302 P3303 C3304 S3309 N3318 I3319 L3320 R3321 I3322 N3325 M3326 I3329 D3330 E3331 A3332 K3336 R3337 L3338 A3339 V3340 Q3343 P3344 I3345 R3350 L3354 F3358 T3361 R3366 E3377 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389
L3392 L3393 V3394 R3395 R3403 Y3406 R3414 Y3415 V3416 N3419 R3420 W3423 L3424 P3427 L3434 M3437 I3441 N3450 R3453 E3454 N3457 N3465 N3466 M3467 S3468 F3469 L3470 T3471 A3472 D3473 S3474 K3475 S3476 K3477 M3478 A3479 LYS ALA GLY ASP ALA GLN SER GLY GLY SER
ASP GLN GLU ARG THR LYS LYS LYS R3498 R3499 G3500 D3501 Q3506 K3515 K3516 P3519 M3524 L3535 T3538 A3541 L3542 K3543 N3555 N3556 L3557 H3558 L3559 Q3560 G3561 K3562 V3563 E3564 G3565 S3566 L3569 M3573 Y3576 L3579 P3580 G3581 R3582 E3583 E3584 D3585 A3586 D3587 R3595
L3603 Y3604 H3605 L3606 T3609 E3610 H3611 P3612 Y3613 K3614 S3615 K3616 K3617 A3618 V3619 W3620 H3621 K3622 L3623 L3624 S3625 K3626 Q3627 R3628 R3629 R3630 A3631 V3632 V3633 A3634 C3635 F3636 R3637 M3638 L3641 L3644 E3670 I3674 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 K3694 P3695
E3718 D3719 I3728 M3729 L3735 E3736 GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU V3749 E3750 V3751 S3752 F3753 E3754 E3755 K3756 S3768 R3769 L3770 H3771 T3772 R3773 V3779 L3780 I3783 S3784 A3785 C3786 K3787 G3788 T3797 L3800 L3805 N3809 A3810 E3811 V3812 K3823 K3824
E3825 V3826 G3827 F3828 F3829 Q3830 L3835 L3842 R3849 Q3850 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 M3875 D3878 R3886 F3887 L3888 Q3889 L3890 L3891 Q3900 Q3927 E3928 S3929 D3932 W3935 G3939 E3944 E3945 Q3946 G3947 K3948 R3949
L3965 T3966 E3967 Y3968 G3991 F3992 V3995 M3999 Q4009 Q4020 M4023 L4030 I4040 V4049 M4057 T4058 L4059 K4060 K4069 G4073 S4074 E4075 A4076 D4079 Y4080 V4081 T4082 D4083 K4090 K4091 D4092 F4093 Q4094 K4095 A4096 M4097 D4098 S4099 Q4100 K4101 Q4102 F4103 T4104 G4105 P4106



• Molecule 1: Ryanodine receptor 1

Chain B:

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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 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 L1428 Y1434 Y1435 R1438 G1442 V1448 T1454 P1455 D1456 D1461 K1468 A1471 Q1480 C1489 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 T1512 D1513 L1514 L1519
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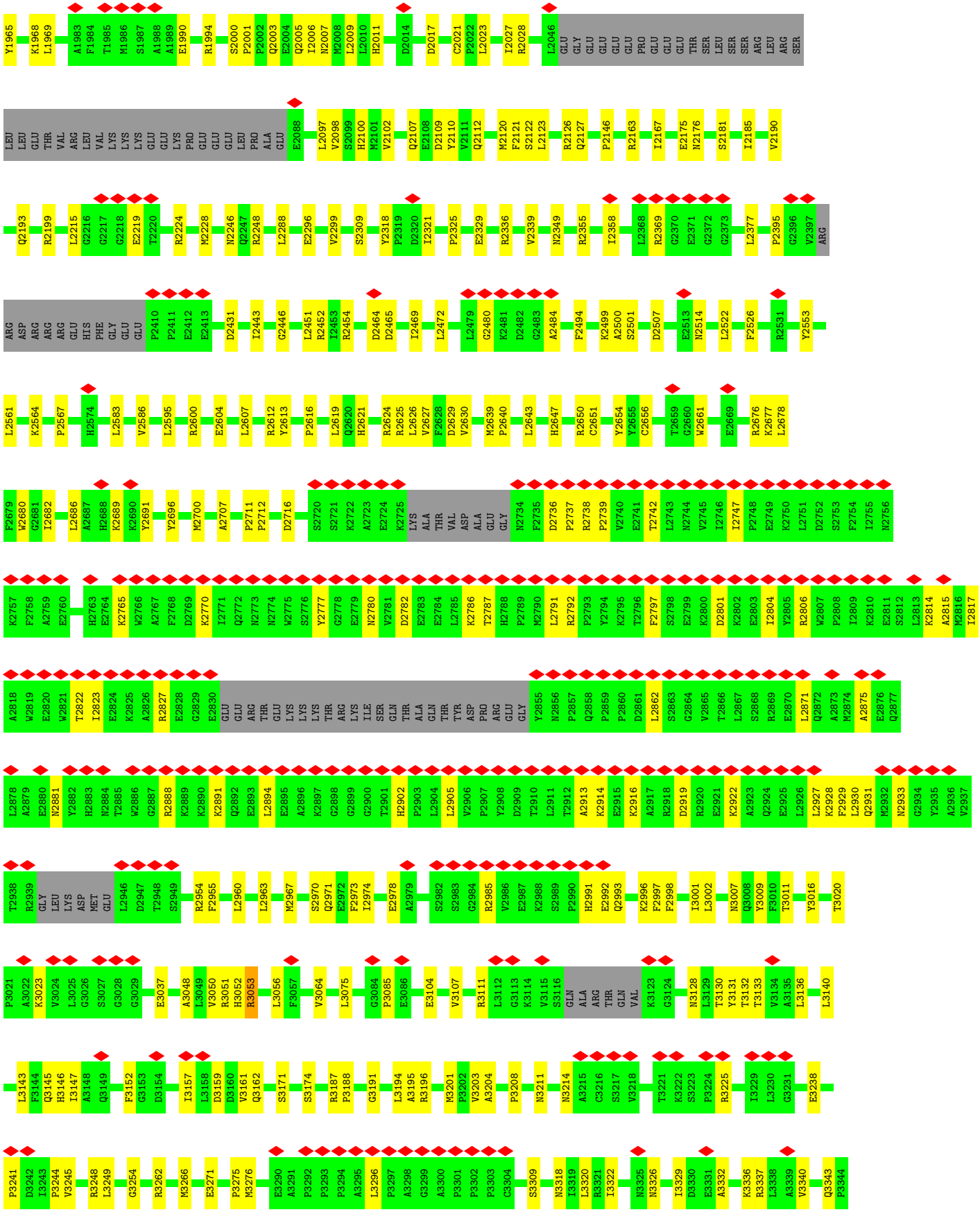
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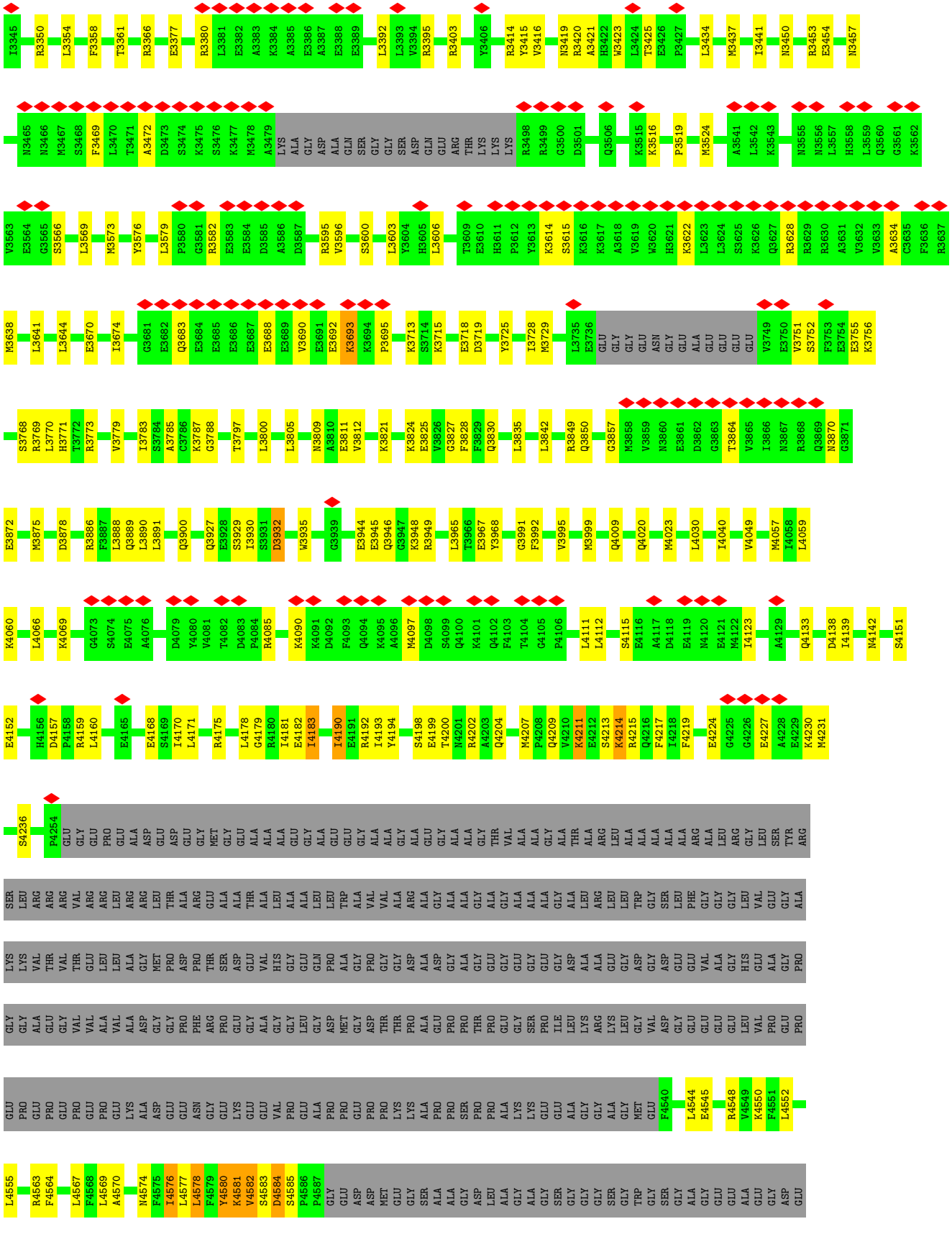
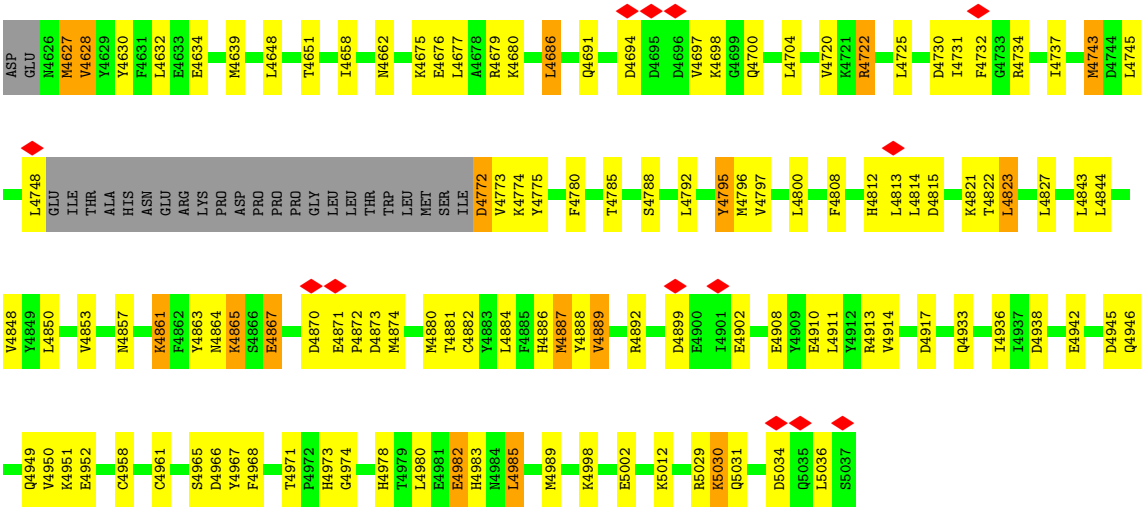
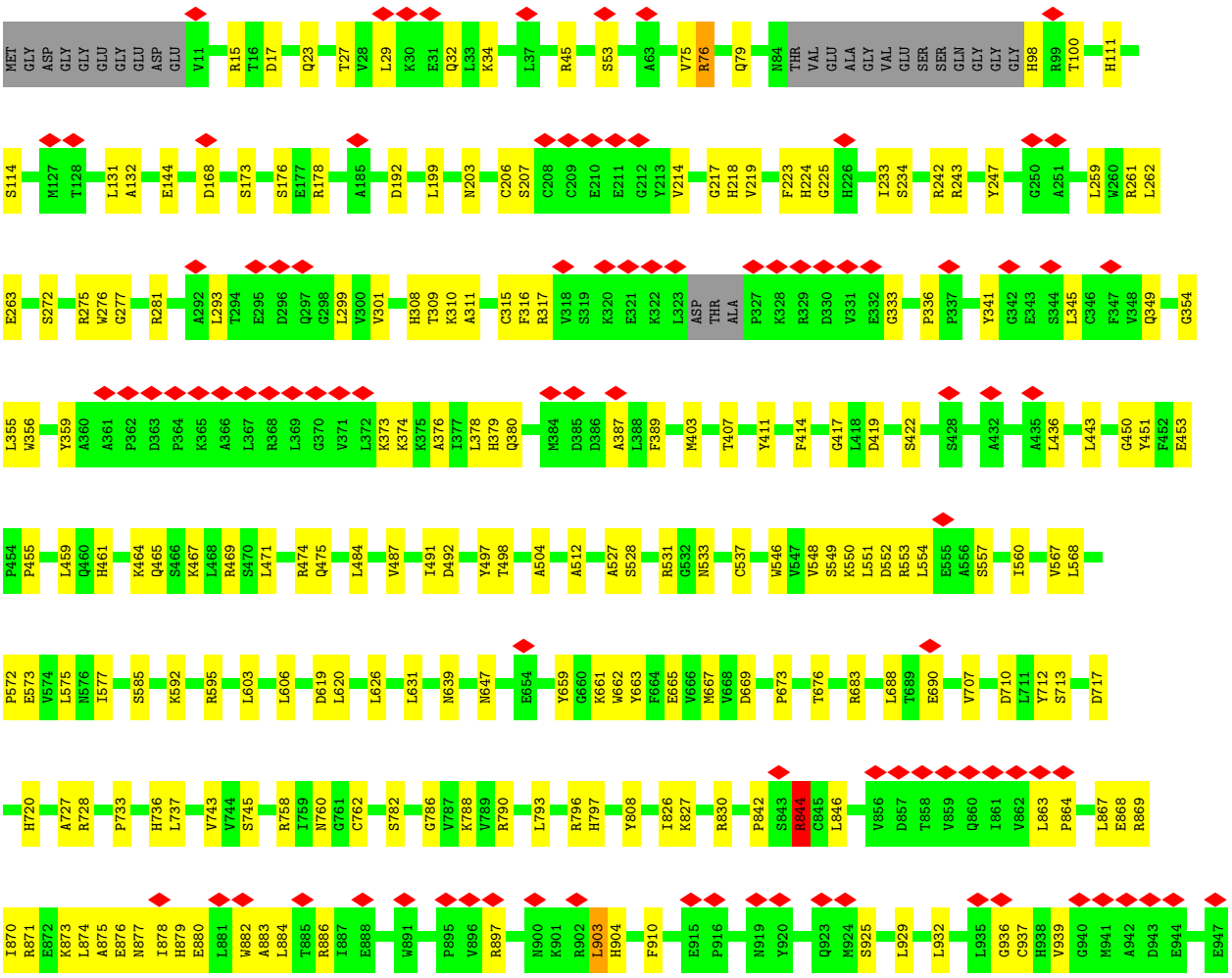
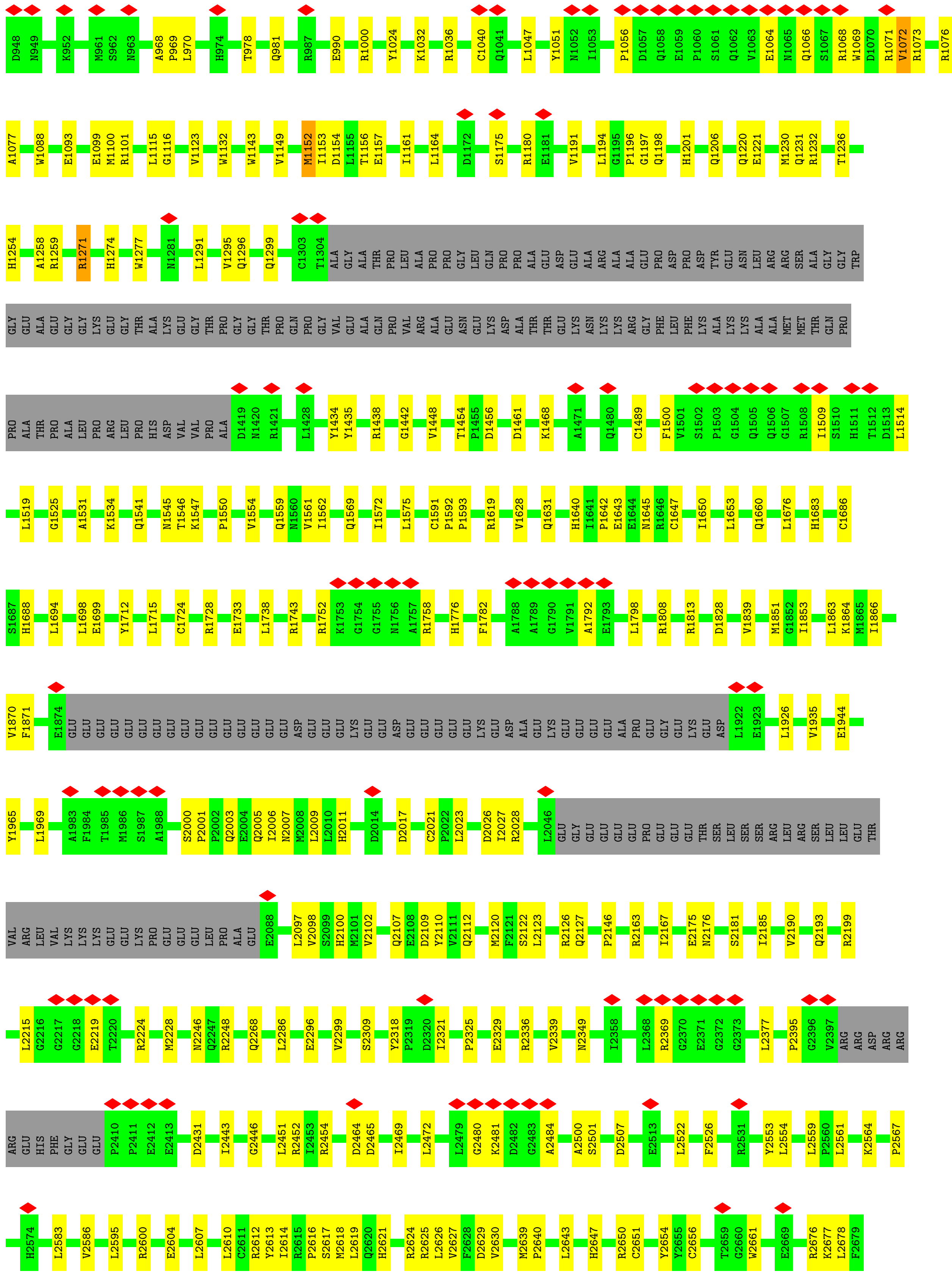




• Molecule 1: Ryanodine receptor 1

Chain C:

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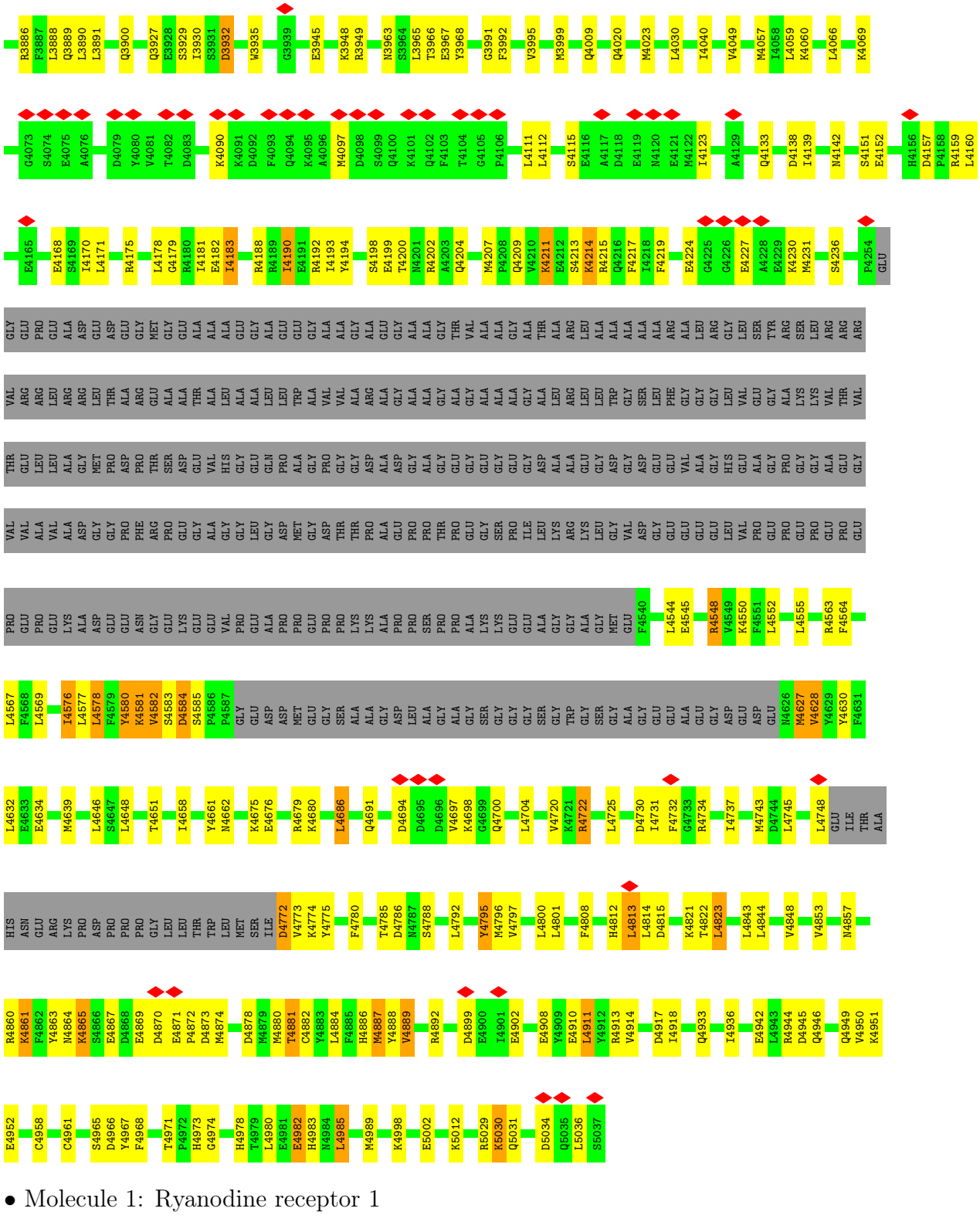
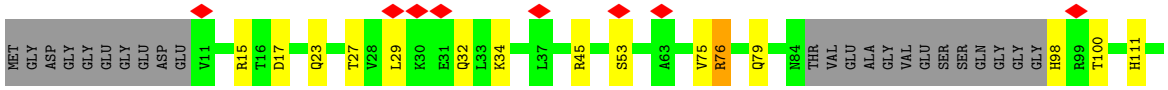
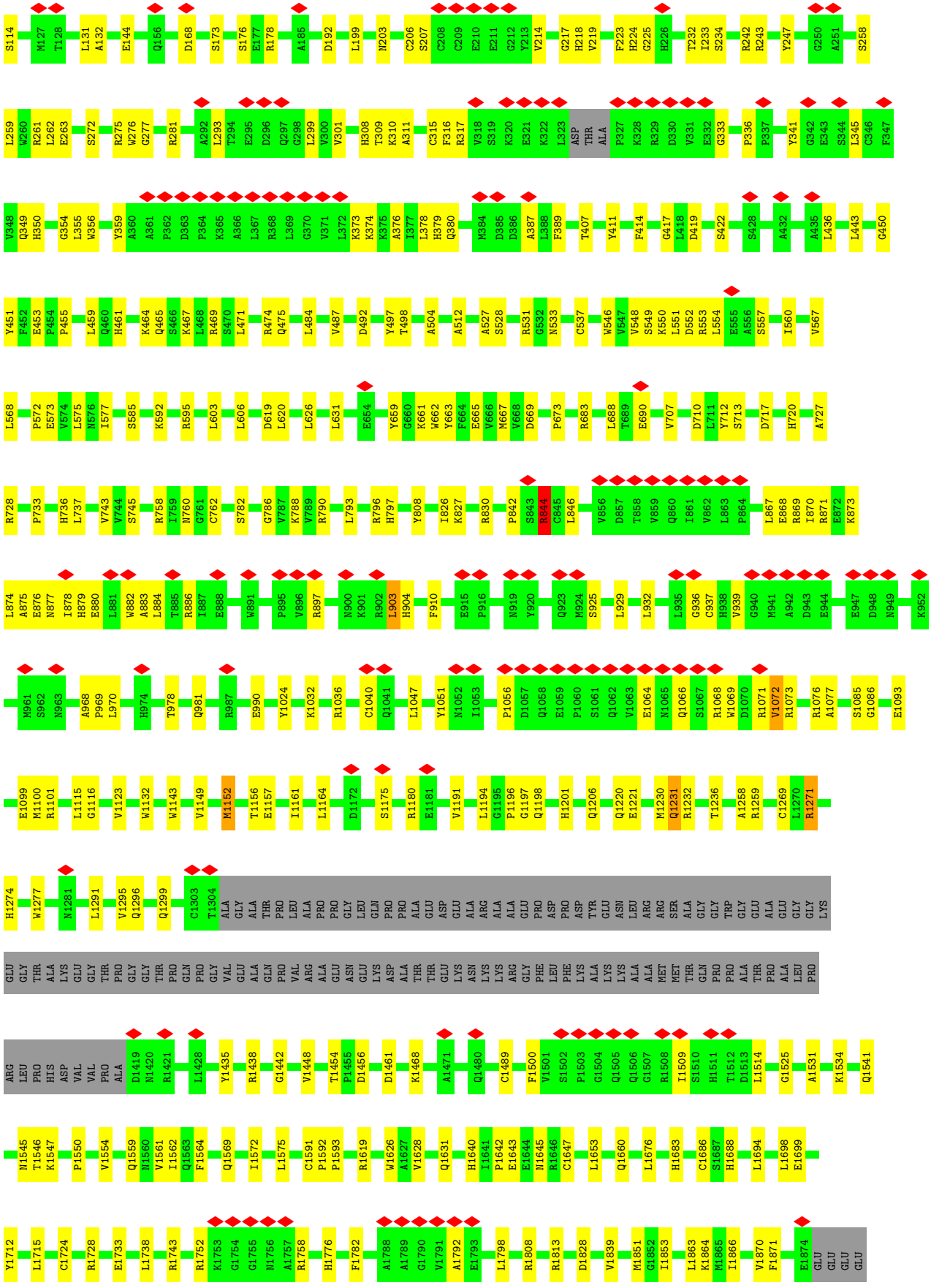


• Molecule 1: Ryanodine receptor 1

Chain D:

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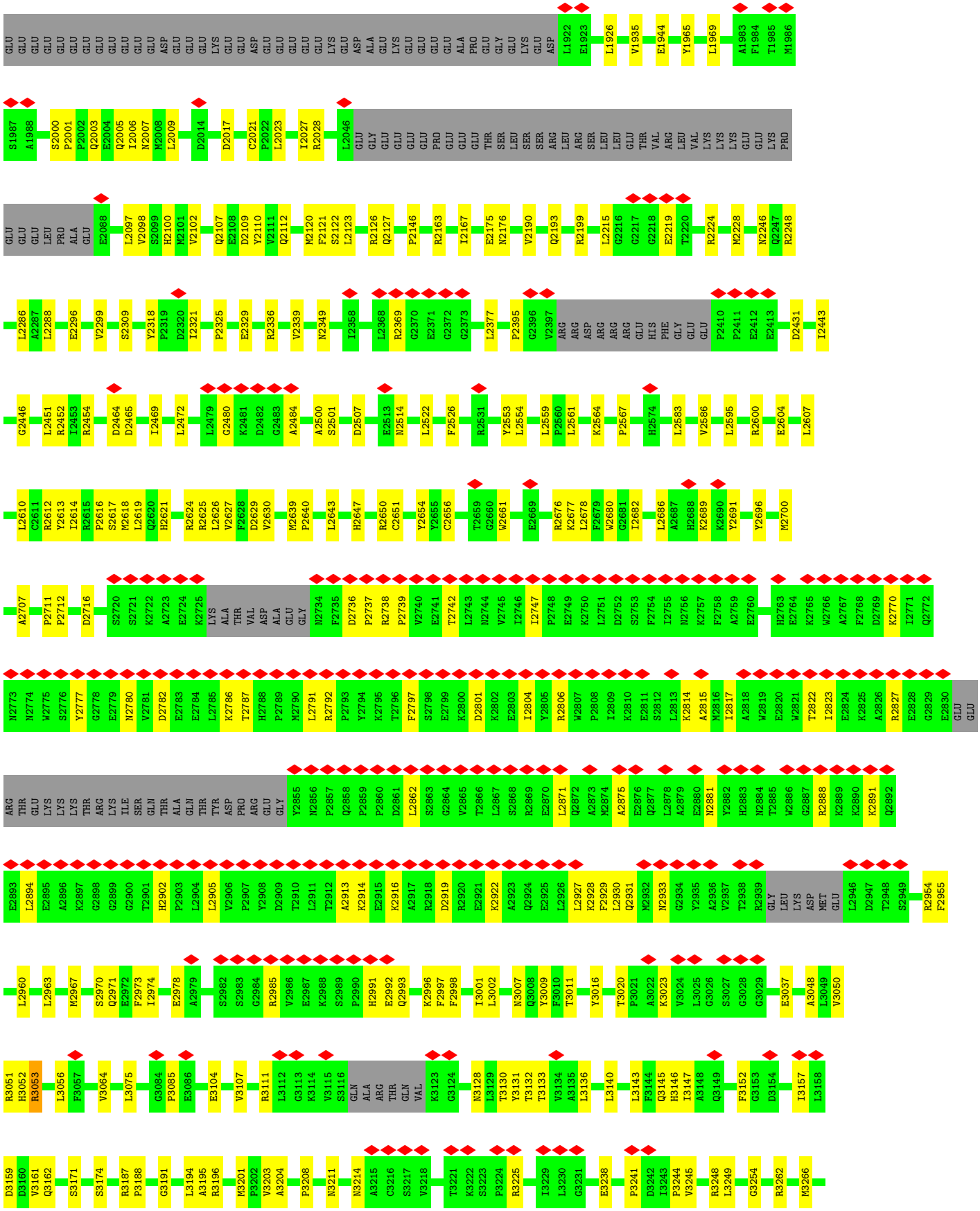
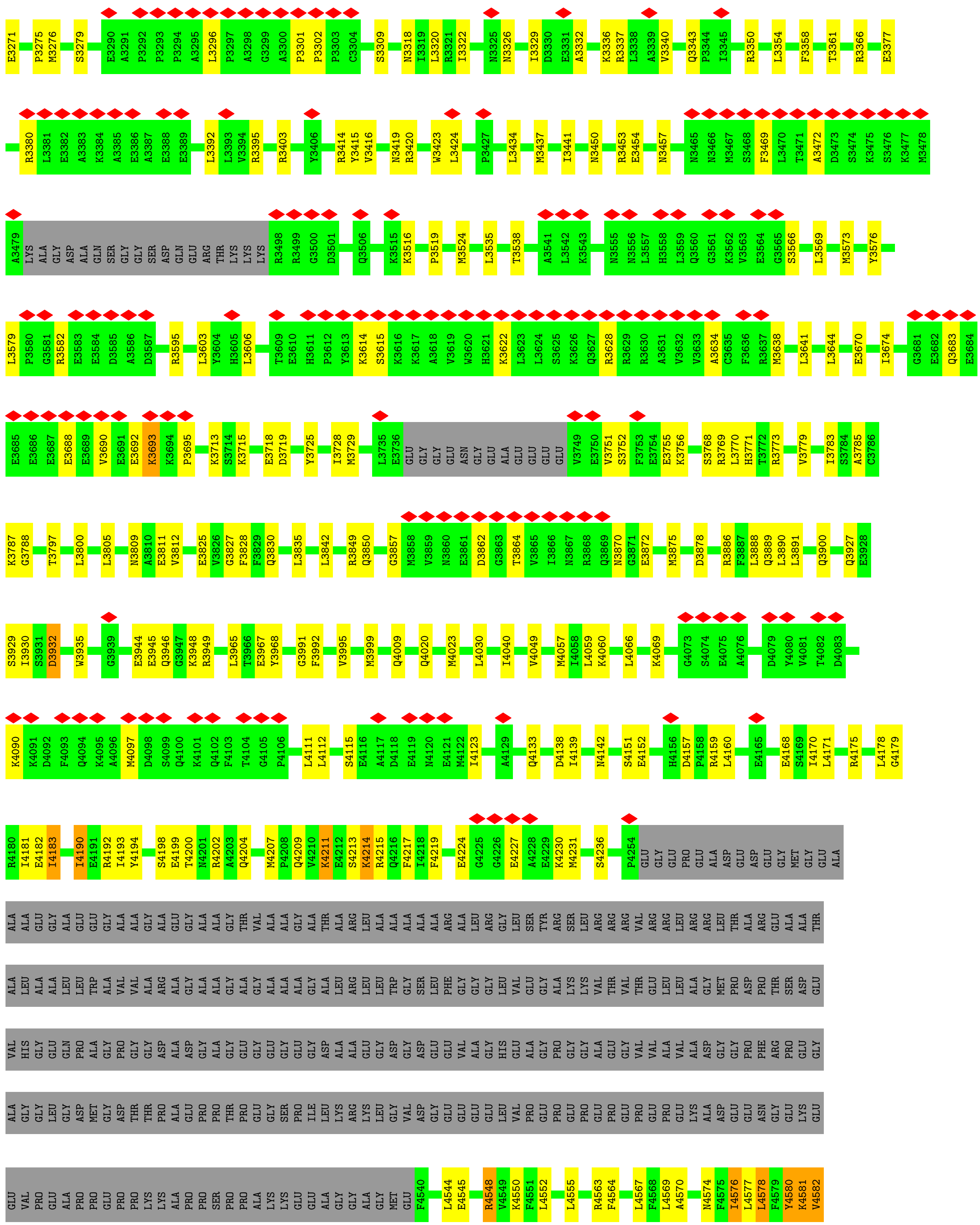
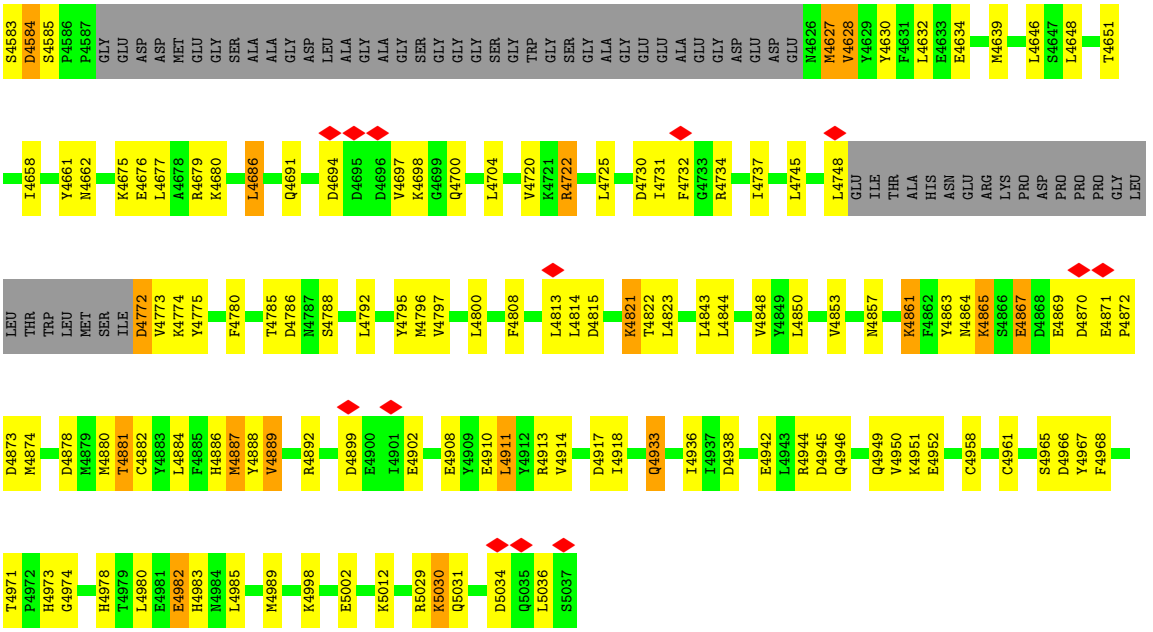
L259 W260 R261 L262 E263 S272 R275 W276 G277 R281 A292 L293 T294 E295 D296 Q297 G298 L299 V300 V301 H308 T309 K310 A311 C315 F316 R317 V318 S319 K320 E321 K322 L323 ASP THR ALA P327 K328 R329 D330 V331 E332 G333 P336 P337 Y341 G342 E343 S344 L345 C346 F347
V348 Q349 H350 G354 L355 W356 Y359 A360 A361 P362 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 K373 K374 K375 A376 I377 L378 H379 Q380 M384 D385 D386 A387 L388 F389 T407 Y411 F414 G417 L418 D419 S422 S428 A432 A435 L436 L443 G450
Y451 F452 E453 P454 P455 L459 Q460 H461 K464 Q465 S466 K467 L468 R469 S470 L471 R474 Q475 L484 V487 D492 Y497 T498 A504 A512 A527 S528 R531 G532 N533 C537 W546 V547 V548 S549 K550 L551 D552 R553 L554 E555 A556 S557 I560 V567
L568 P572 E573 V574 L575 N576 I577 S585 K592 R595 L603 L606 D619 L620 L626 L631 E654 Y659 G660 K661 W662 Y663 F664 E665 V666 M667 V668 D669 P673 R683 L688 T689 E690 V707 D710 L711 Y712 S713 D717 H720 A727
R728 P733 H736 L737 V743 Y744 S745 R758 I759 N760 C761 C762 S782 G786 Y787 K788 V789 R790 L793 R796 H797 Y808 I826 K827 R830 P842 S843 R844 C845 L846 V856 D857 T858 V859 Q860 I861 V862 L863 P864 L867 E868 R869 I870 R871 E872 K873
L874 A875 E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 W891 P895 V896 R897 N900 K901 R902 L903 H904 F910 E915 P916 N919 Y920 Q923 M924 S925 L929 L932 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 E947 D948 N949 K952
M961 S962 N963 A968 P969 L970 H974 T978 Q981 R987 E990 Y1024 K1032 R1036 C1040 Q1041 L1047 Y1051 N1052 I1053 P1056 D1057 Q1058 E1059 P1060 S1061 Q1062 V1063 E1064 N1065 Q1066 S1067 R1068 W1069 D1070 R1071 V1072 R1073 R1076 A1077 S1085 G1086 E1093
E1099 M1100 R1101 L1115 G1116 V1123 W1132 W1143 V1149 M1152 T1156 E1157 I1161 L1164 D1172 S1175 R1180 E1181 V1191 L1194 G1195 P1196 G1197 Q1198 H1201 Q1206 Q1220 E1221 M1230 Q1231 R1232 T1236 A1258 R1259 C1269 L1270 R1271
H1274 W1277 N1281 L1291 V1295 Q1296 Q1299 C1303 T1304 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 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 PRO ALA THR PRO ALA LEU PRO
ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 L1428 Y1435 R1438 G1442 V1448 T1454 P1455 D1456 D1461 K1468 A1471 Q1480 C1489 F1500 V1501 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 T1512 D1513 L1514 G1525 A1531 K1534 Q1541
N1545 T1546 K1547 P1550 V1554 Q1559 N1560 V1561 I1562 Q1563 F1564 Q1569 I1572 L1575 C1591 P1592 P1593 R1619 W1626 A1627 V1628 Q1631 H1640 I1641 P1642 E1643 E1644 N1645 R1646 C1647 L1653 Q1660 L1676 H1683 C1686 S1687 H1688 L1694 L1698 E1699
Y1712 L1715 C1724 R1728 E1733 L1738 R1743 R1752 K1753 G1754 G1755 N1756 A1757 R1758 H1776 F1782 A1788 A1789 G1790 V1791 A1792 E1793 L1798 R1808 R1813 D1828 V1839 M1851 G1852 I1853 L1863 K1864 M1865 I1866 V1870 F1871 E1874 GLU GLU GLU GLU

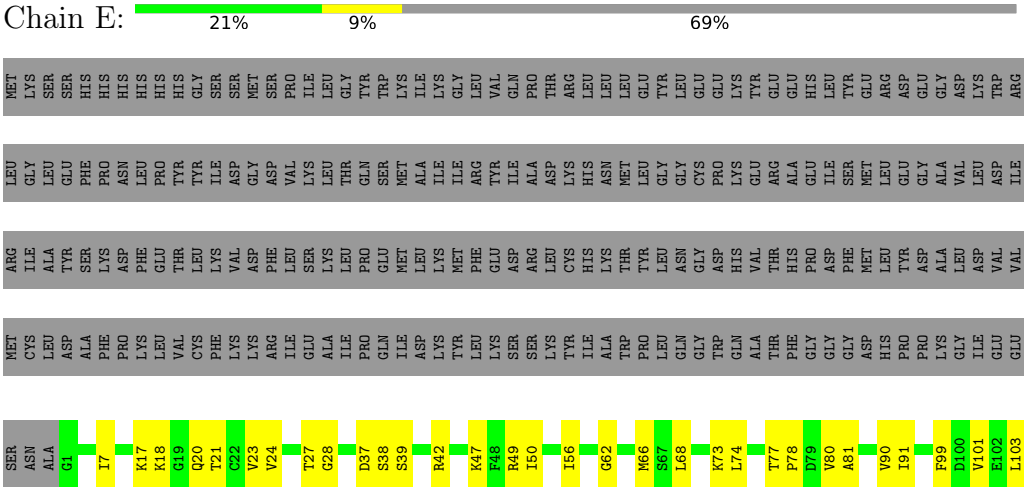






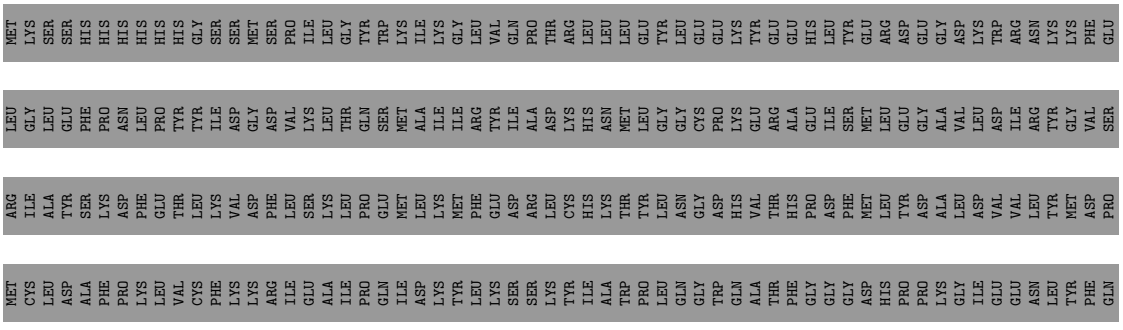
• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

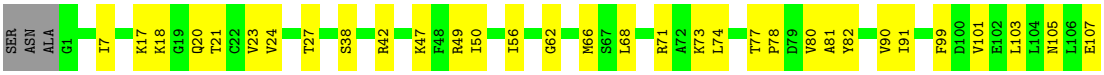
Chain E:



• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

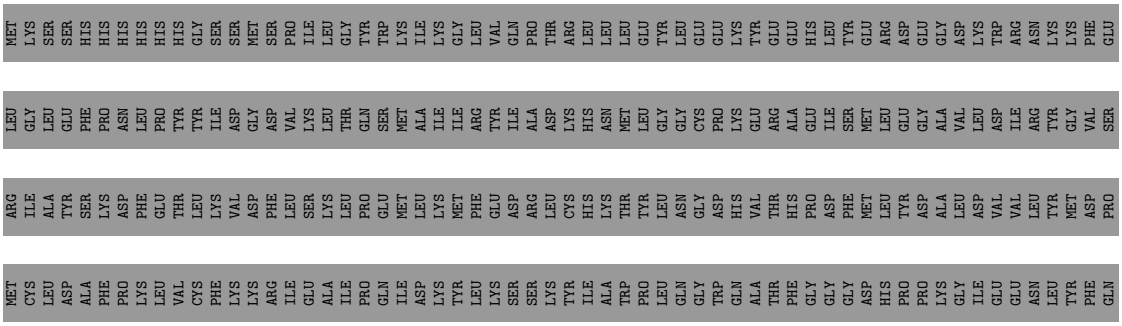
Chain F:

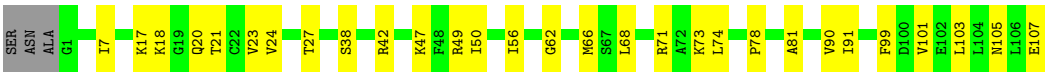




• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

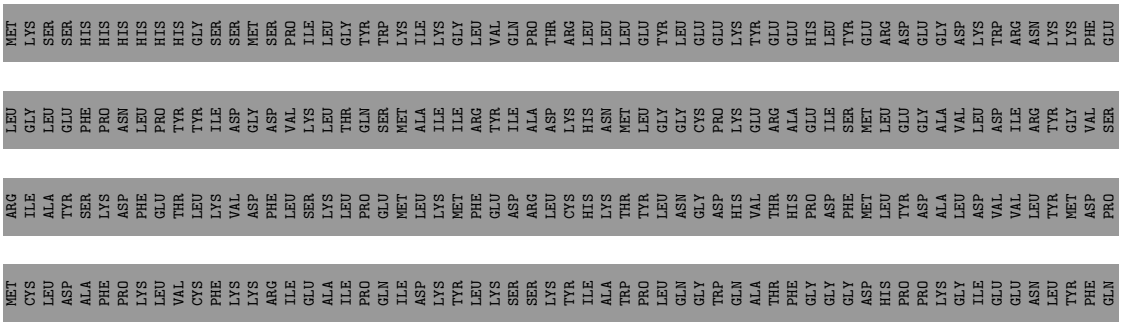
Chain G:





• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21706	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.200	Depositor
Minimum map value	-0.744	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.305	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.35	0/35720	0.68	15/48374 (0.0%)
1	B	0.35	0/35720	0.68	16/48374 (0.0%)
1	C	0.35	0/35720	0.68	16/48374 (0.0%)
1	D	0.35	0/35720	0.68	15/48374 (0.0%)
2	E	0.33	0/834	0.67	0/1123
2	F	0.33	0/834	0.67	0/1123
2	G	0.33	0/834	0.67	0/1123
2	H	0.33	0/834	0.67	0/1123
All	All	0.35	0/146216	0.68	62/197988 (0.0%)

There are no bond length outliers.

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	76	ARG	CG-CD-NE	7.00	126.51	111.80
1	C	844	ARG	CA-CB-CG	6.99	128.78	113.40
1	D	844	ARG	CA-CB-CG	6.99	128.78	113.40
1	A	844	ARG	CA-CB-CG	6.99	128.77	113.40
1	B	76	ARG	CG-CD-NE	6.98	126.46	111.80

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	34906	0	34529	480	0
1	B	34906	0	34529	492	0
1	C	34906	0	34529	496	0
1	D	34906	0	34529	491	0
2	E	818	0	824	20	0
2	F	818	0	824	20	0
2	G	818	0	824	18	0
2	H	818	0	824	19	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	10	0	4	1	0
4	B	10	0	4	1	0
4	C	10	0	4	1	0
4	D	10	0	4	1	0
All	All	142940	0	141428	2006	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 7.

The worst 5 of 2006 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:844:ARG:HH12	1:C:1197:GLY:HA3	1.45	0.80
1:B:844:ARG:HH12	1:B:1197:GLY:HA3	1.45	0.80
1:A:844:ARG:HH12	1:A:1197:GLY:HA3	1.45	0.79
1:D:844:ARG:HH12	1:D:1197:GLY:HA3	1.45	0.79
1:B:34:LYS:H	1:B:53:SER:HB3	1.49	0.78

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	4353/5037 (86%)	4129 (95%)	217 (5%)	7 (0%)	47	79
1	B	4353/5037 (86%)	4128 (95%)	218 (5%)	7 (0%)	47	79
1	C	4353/5037 (86%)	4131 (95%)	215 (5%)	7 (0%)	47	79
1	D	4353/5037 (86%)	4129 (95%)	217 (5%)	7 (0%)	47	79
2	E	105/350 (30%)	95 (90%)	10 (10%)	0	100	100
2	F	105/350 (30%)	96 (91%)	9 (9%)	0	100	100
2	G	105/350 (30%)	95 (90%)	10 (10%)	0	100	100
2	H	105/350 (30%)	95 (90%)	10 (10%)	0	100	100
All	All	17832/21548 (83%)	16898 (95%)	906 (5%)	28 (0%)	50	79

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1069	TRP
1	A	3615	SER
1	A	4910	GLU
1	B	1069	TRP
1	B	3615	SER

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	3805/4276 (89%)	3656 (96%)	149 (4%)	32	58
1	B	3805/4276 (89%)	3655 (96%)	150 (4%)	32	58
1	C	3805/4276 (89%)	3655 (96%)	150 (4%)	32	58
1	D	3805/4276 (89%)	3656 (96%)	149 (4%)	32	58
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	15572/18320 (85%)	14974 (96%)	598 (4%)	37 58

5 of 598 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2224	ARG
1	D	4917	ASP
1	D	3225	ARG
1	D	2100[B]	HIS
1	D	4632	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3214	ASN
1	D	877	ASN
1	C	3457	ASN
1	D	98	HIS
1	D	1545	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
4	ADE	B	5102	-	9,11,11	0.95	0	7,15,15	1.08	0
4	ADE	A	5102	-	9,11,11	0.95	0	7,15,15	1.08	0
4	ADE	D	5102	-	9,11,11	0.95	0	7,15,15	1.08	0
4	ADE	C	5102	-	9,11,11	0.95	0	7,15,15	1.08	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
4	ADE	B	5102	-	-	-	0/2/2/2
4	ADE	A	5102	-	-	-	0/2/2/2
4	ADE	D	5102	-	-	-	0/2/2/2
4	ADE	C	5102	-	-	-	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

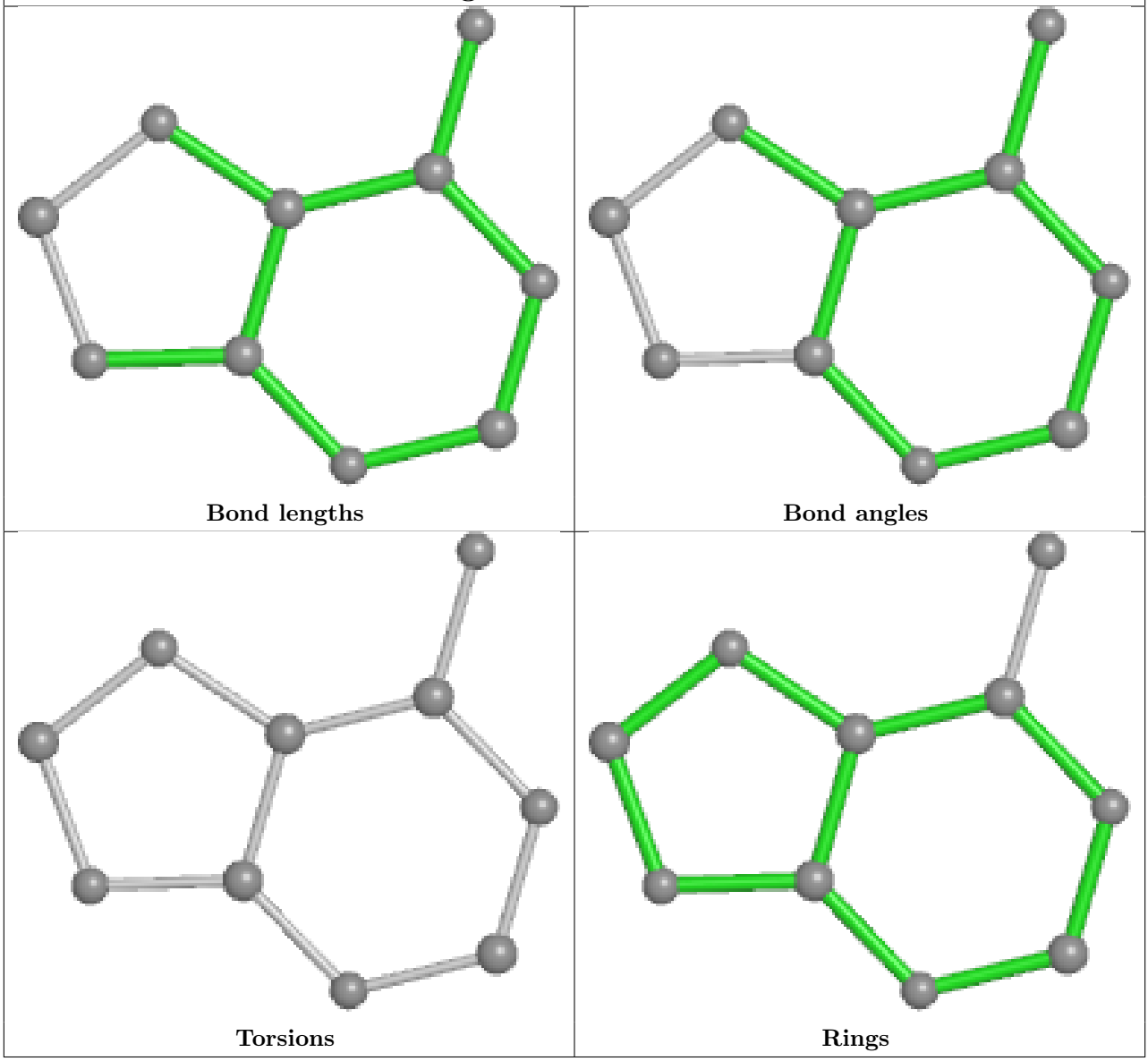
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5102	ADE	1	0
4	A	5102	ADE	1	0
4	D	5102	ADE	1	0
4	C	5102	ADE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

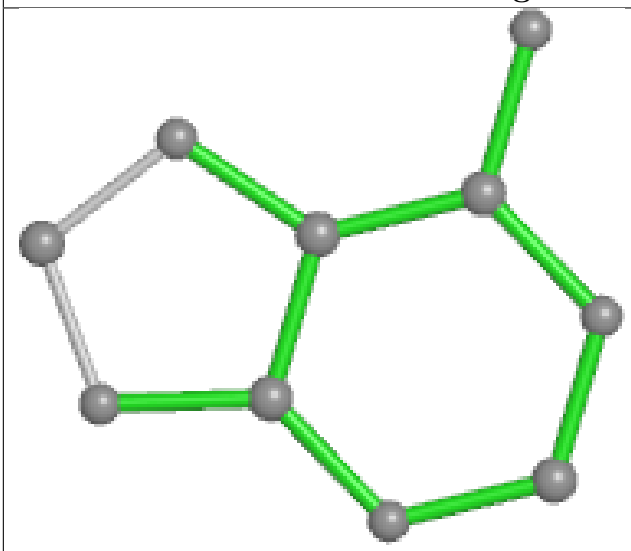
Ligand ADE B 5102



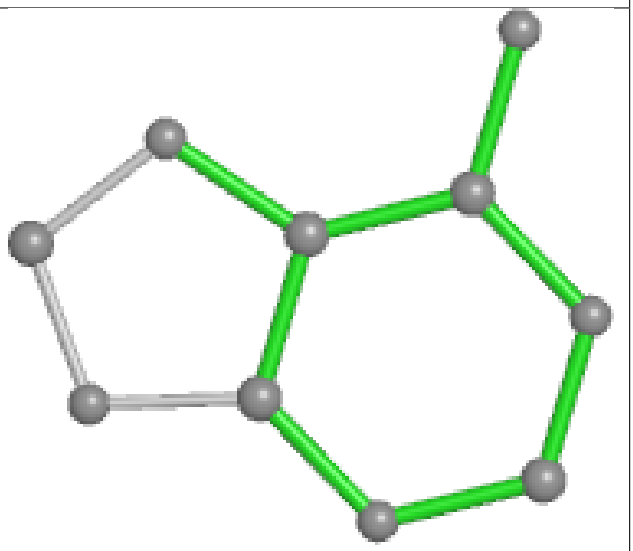
Bond lengths | **Bond angles**

Torsions | **Rings**

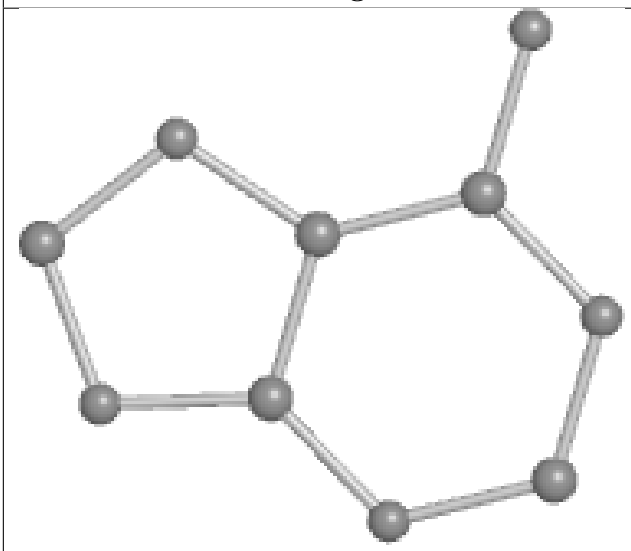
Ligand ADE A 5102



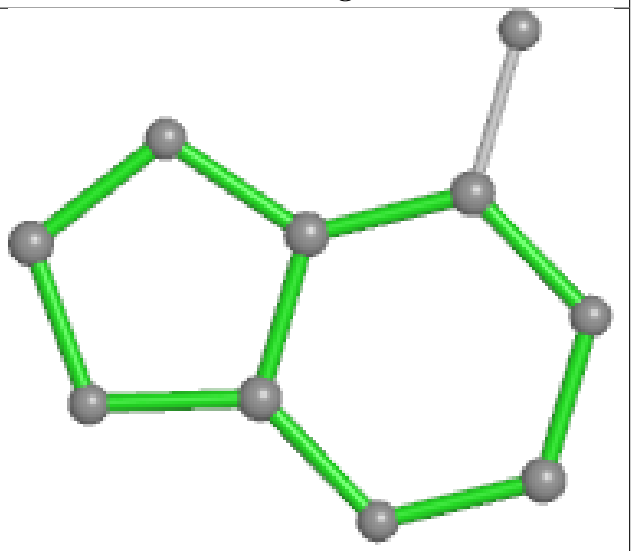
Bond lengths



Bond angles

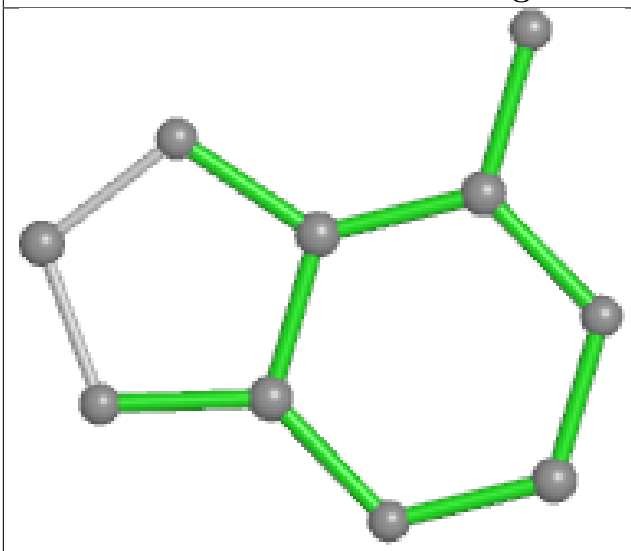


Torsions

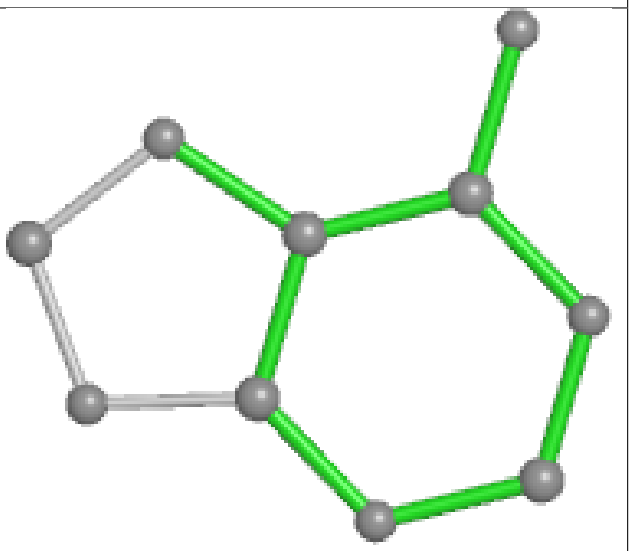


Rings

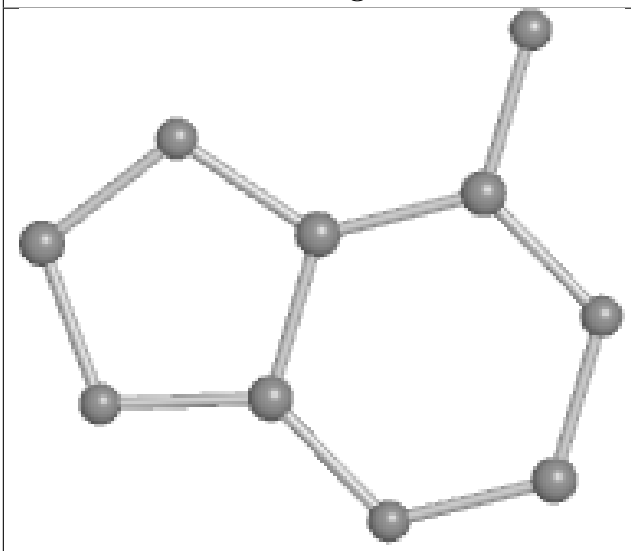
Ligand ADE D 5102



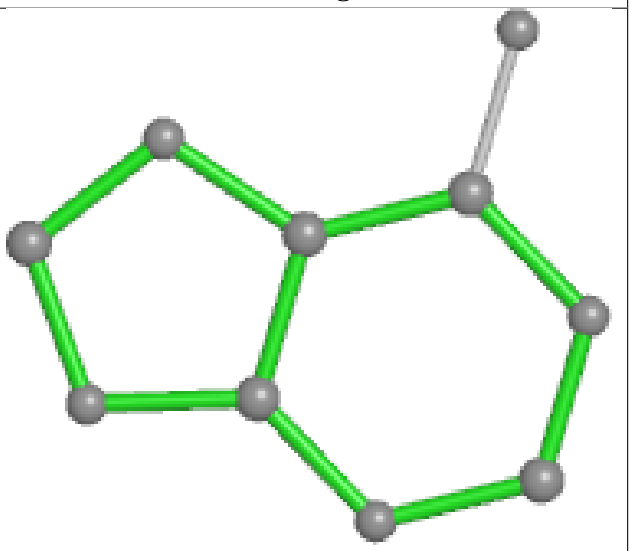
Bond lengths



Bond angles

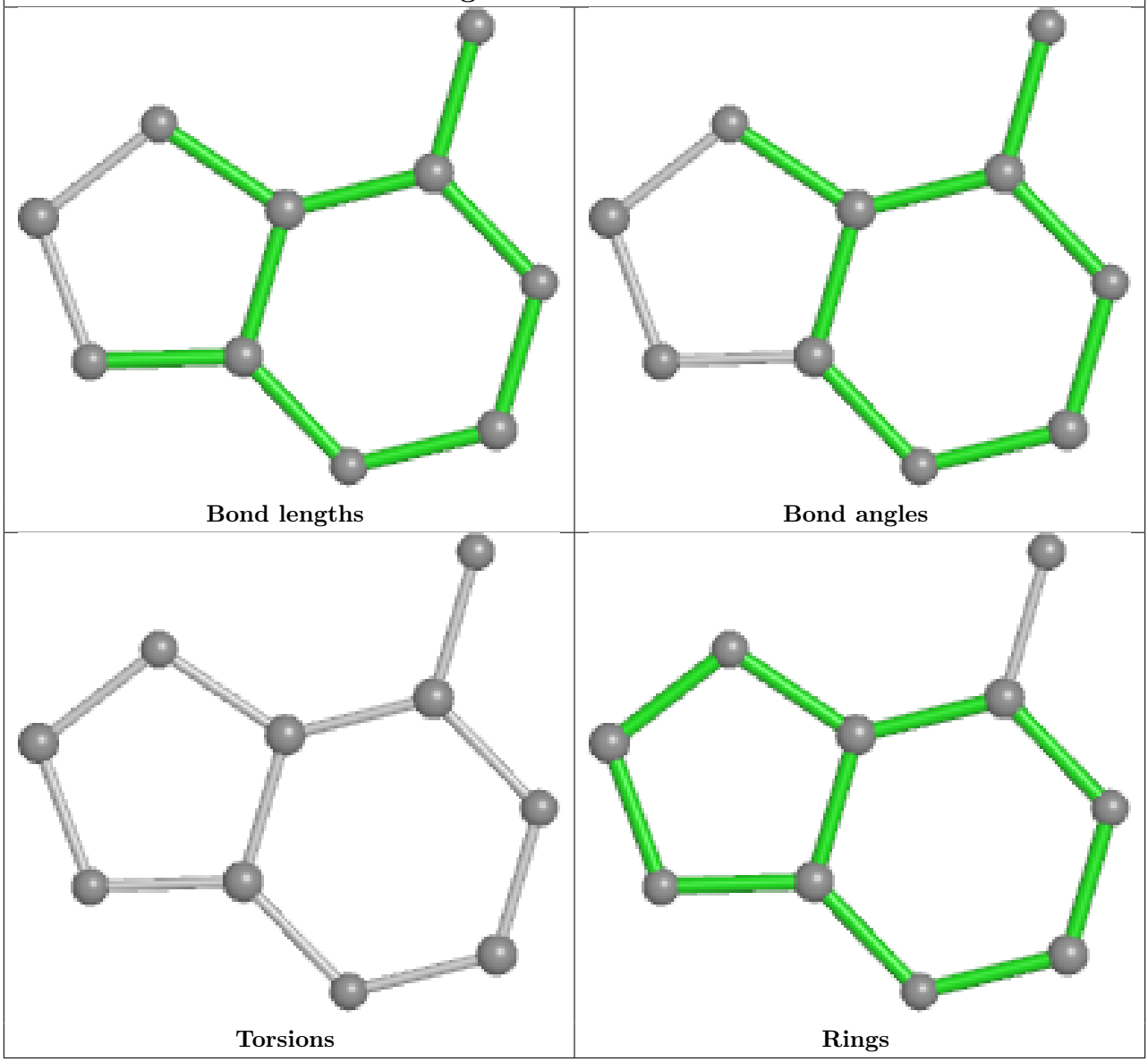


Torsions



Rings

Ligand ADE C 5102



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.

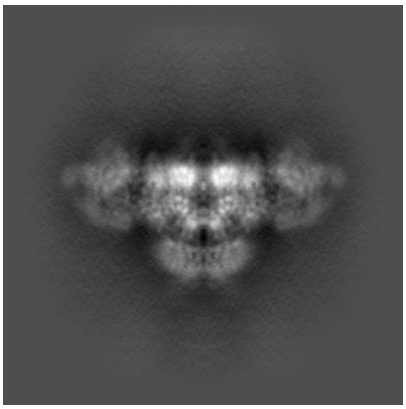
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40427. These allow visual inspection of the internal detail of the map and identification of artifacts.

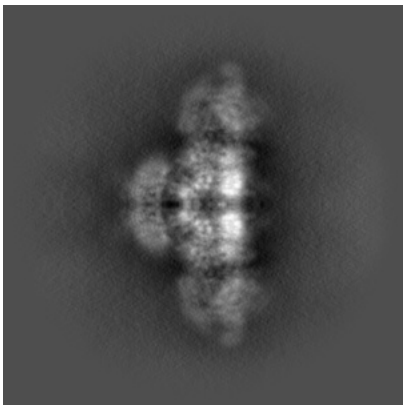
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

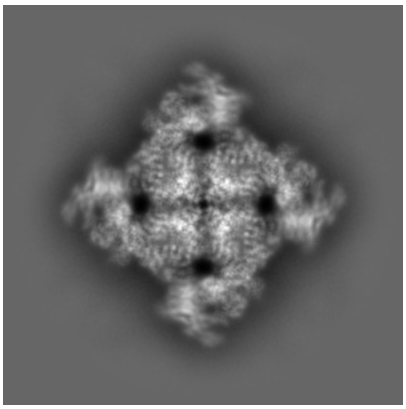
6.1.1 Primary map



X

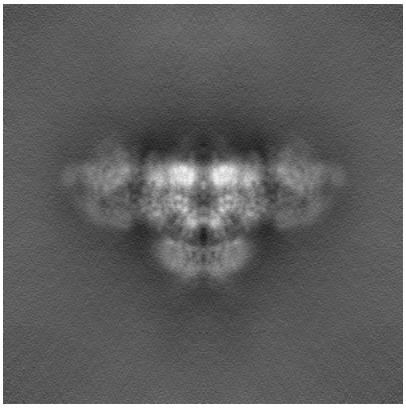


Y

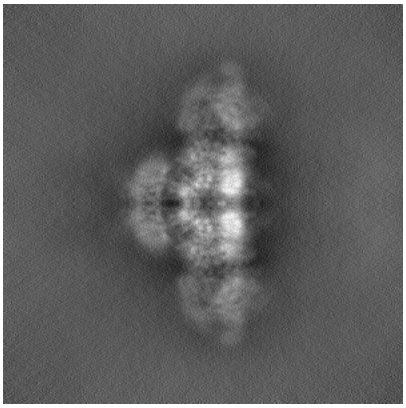


Z

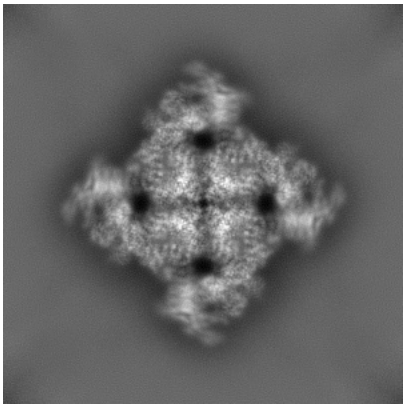
6.1.2 Raw map



X



Y

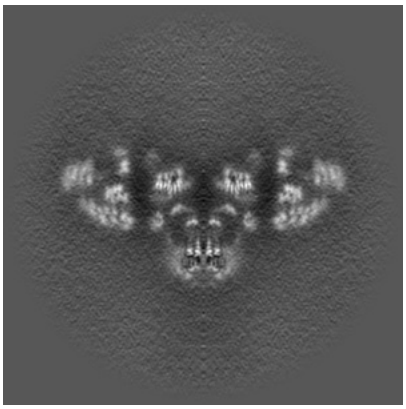


Z

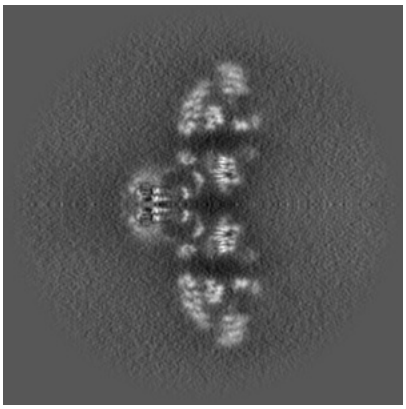
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

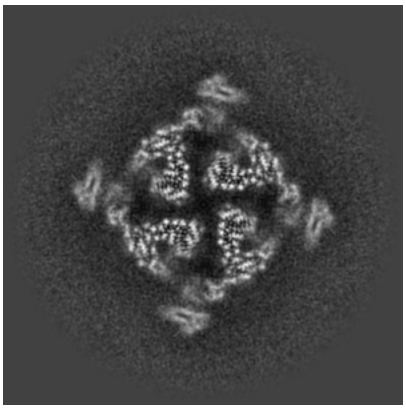
6.2.1 Primary map



X Index: 200

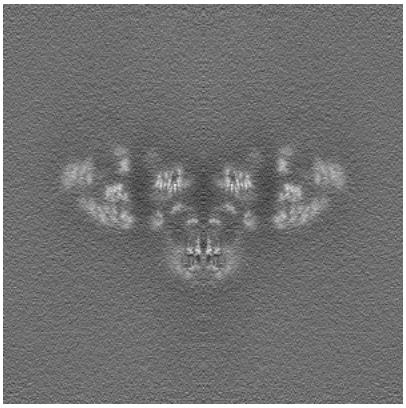


Y Index: 200

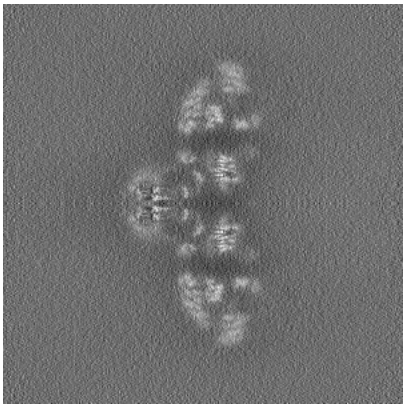


Z Index: 200

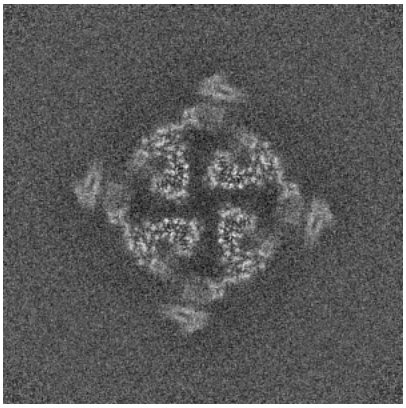
6.2.2 Raw map



X Index: 200



Y Index: 200

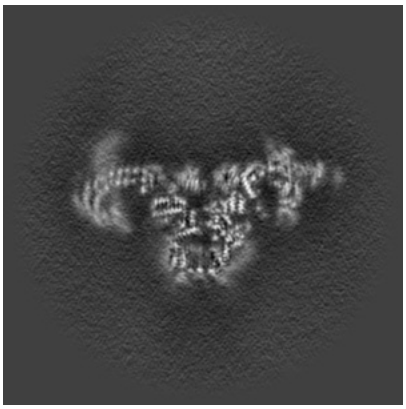


Z Index: 200

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

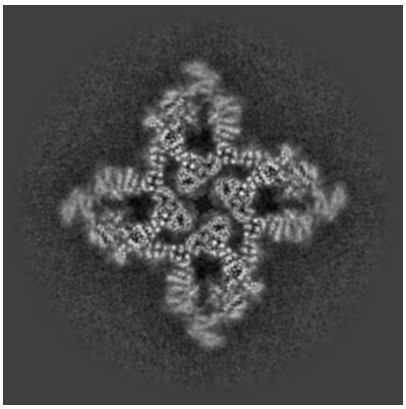
6.3 Largest variance slices (i)

6.3.1 Primary map



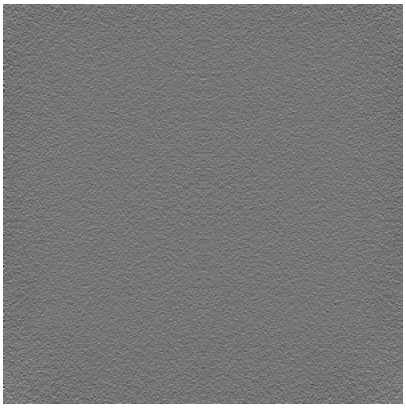
X Index: 182

Y Index: 182

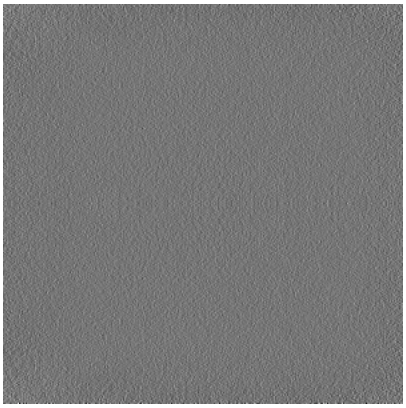


Z Index: 225

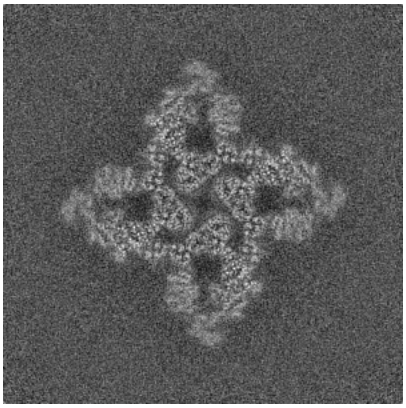
6.3.2 Raw map



X Index: 0



Y Index: 0

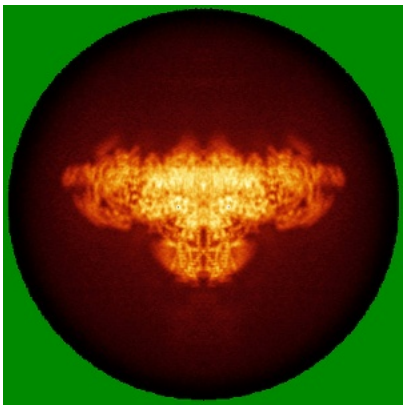


Z Index: 224

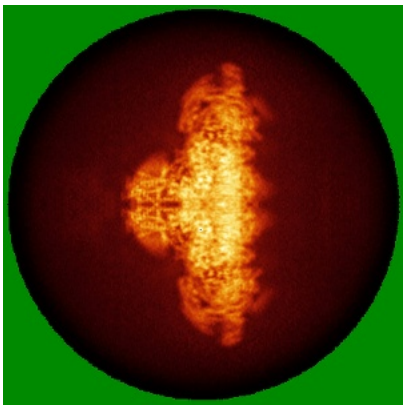
The images above show the largest variance slices of the map in three orthogonal directions.

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

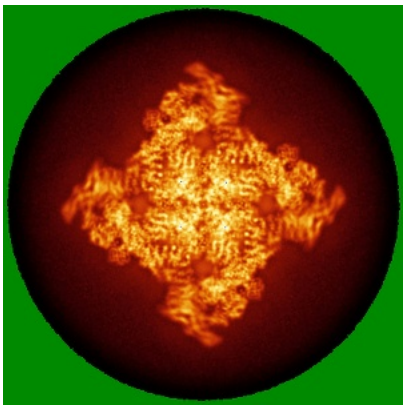
6.4.1 Primary map



X

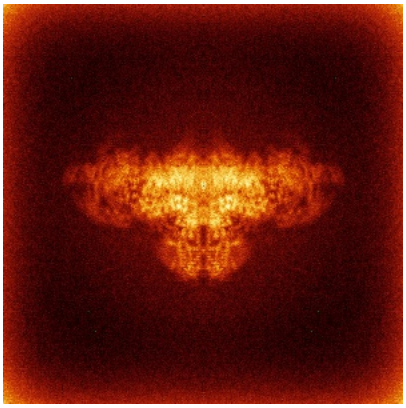


Y

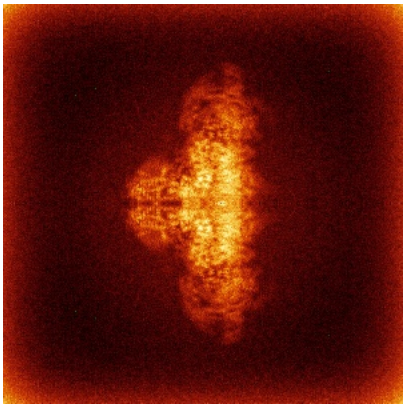


Z

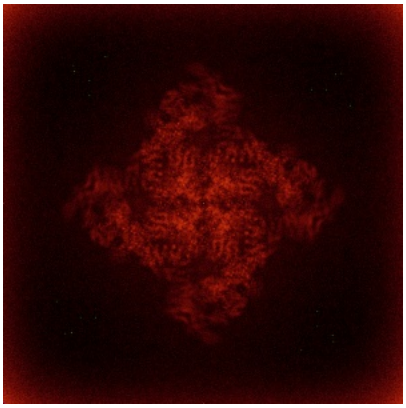
6.4.2 Raw map



X



Y

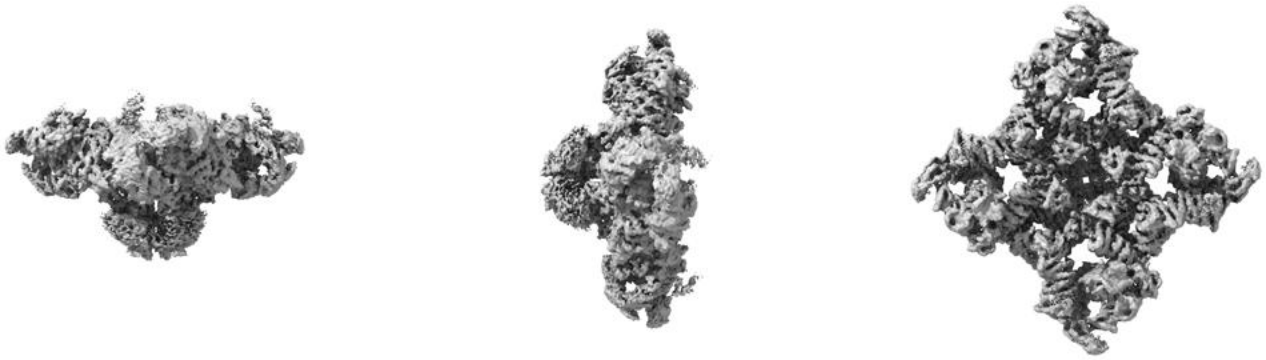


Z

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

6.5 Orthogonal surface views (i)

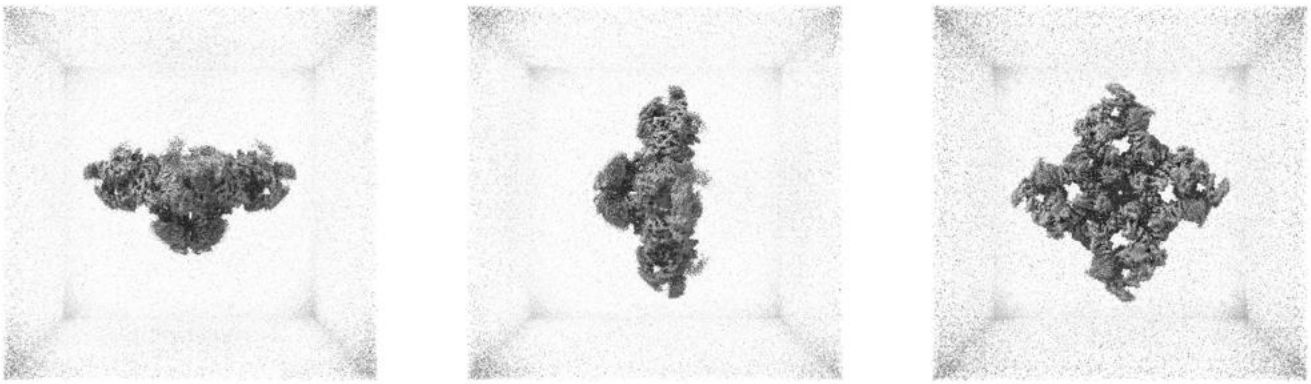
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.305. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

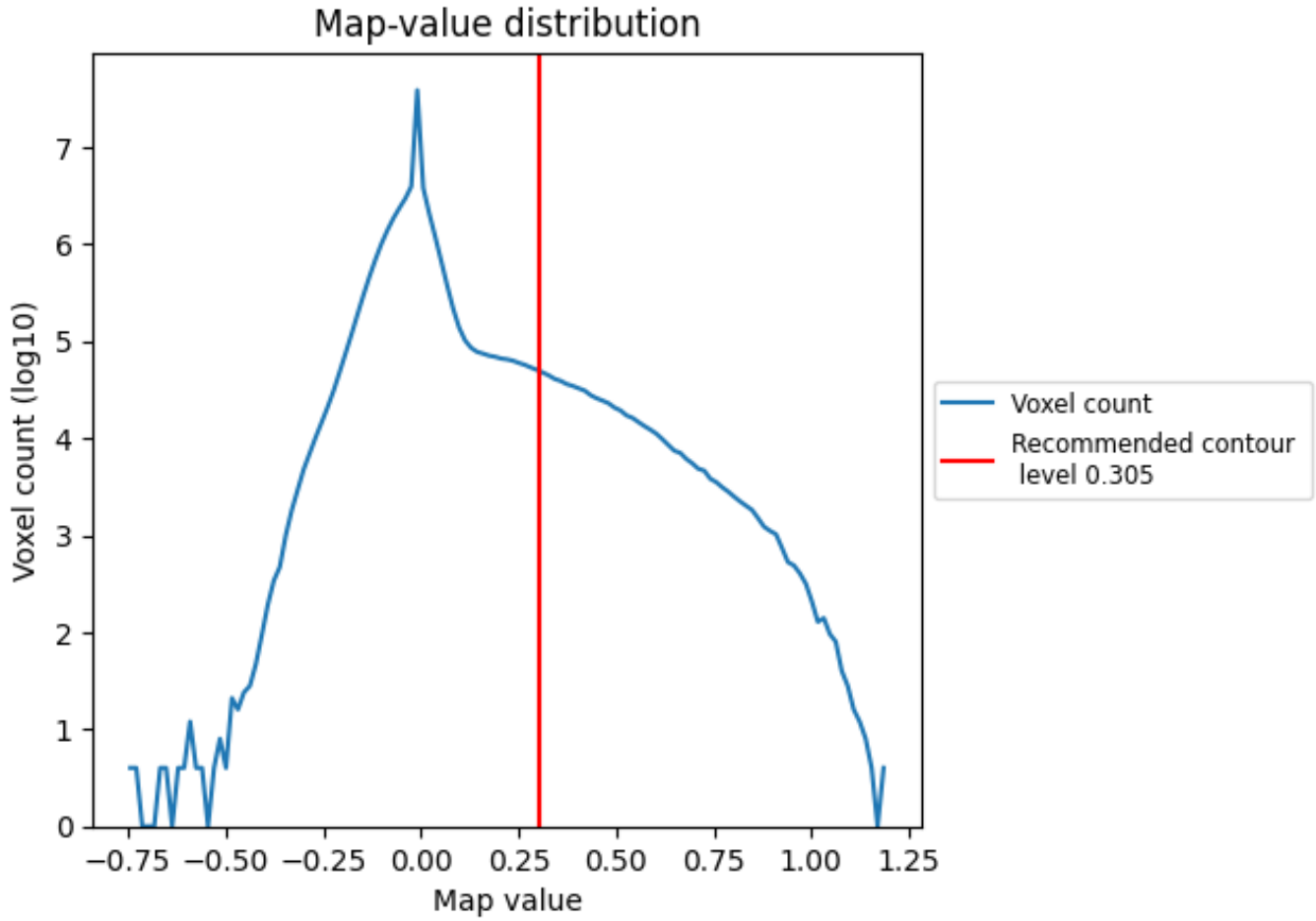
6.6 Mask visualisation (i)

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

7 Map analysis

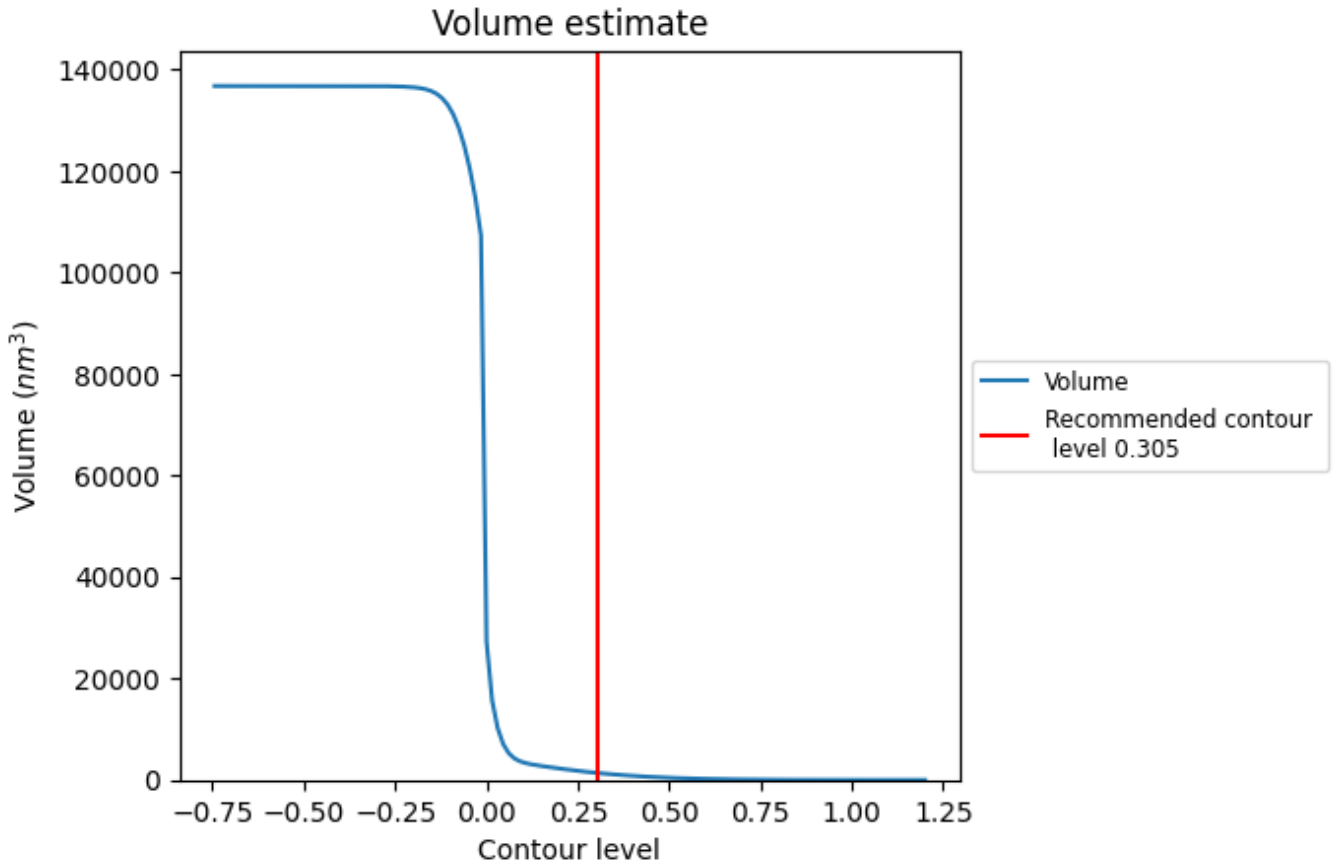
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

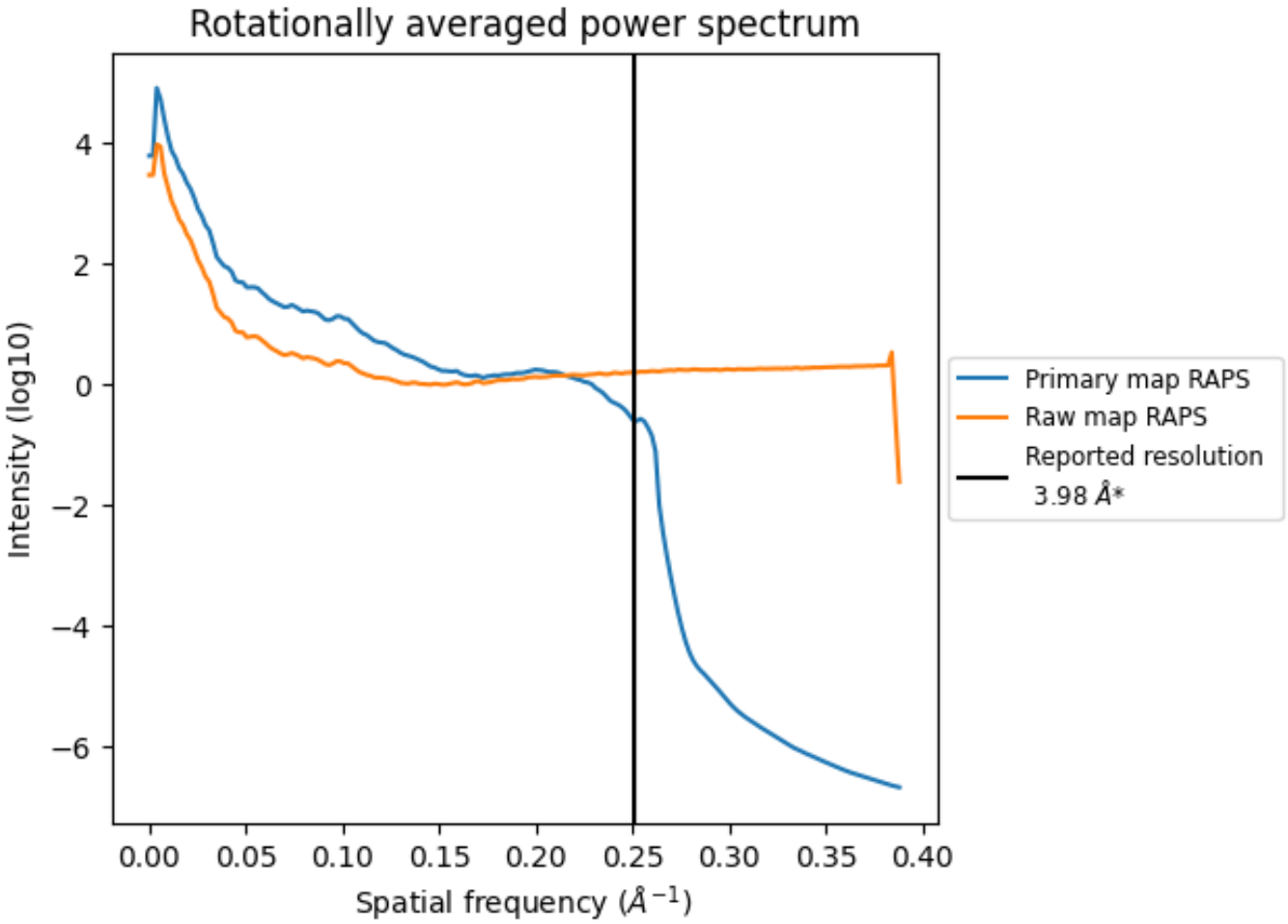
7.2 Volume estimate (i)



The volume at the recommended contour level is 1365 nm^3; this corresponds to an approximate mass of 1233 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)

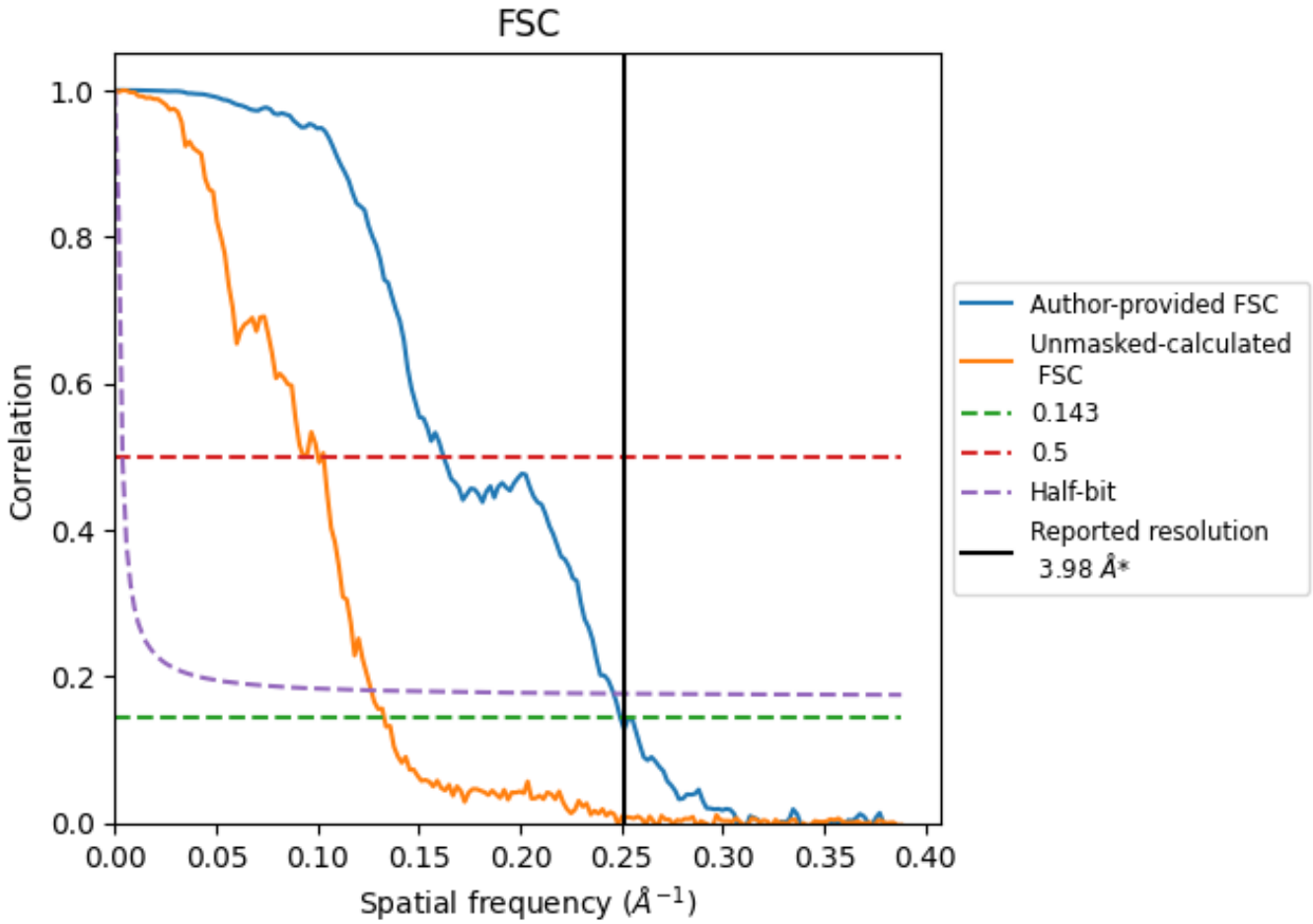


*Reported resolution corresponds to spatial frequency of 0.251 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.251 Å^{-1}

8.2 Resolution estimates (i)

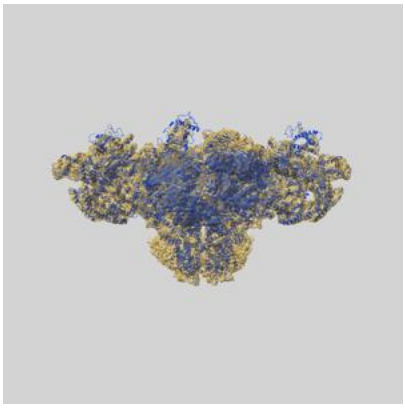
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.98	-	-
Author-provided FSC curve	4.01	6.17	4.06
Unmasked-calculated*	7.52	10.75	7.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.52 differs from the reported value 3.98 by more than 10 %

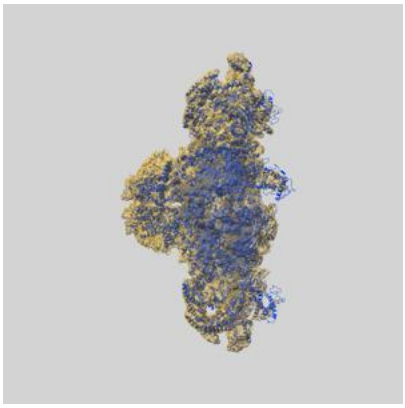
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40427 and PDB model 8SES. Per-residue inclusion information can be found in section 3 on page 8.

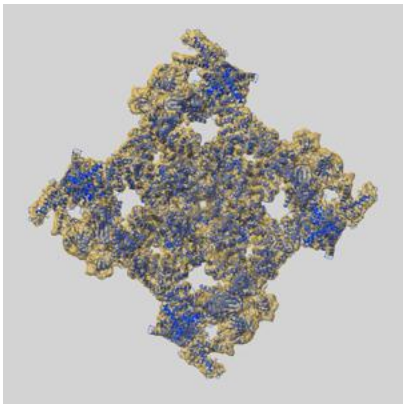
9.1 Map-model overlay



X



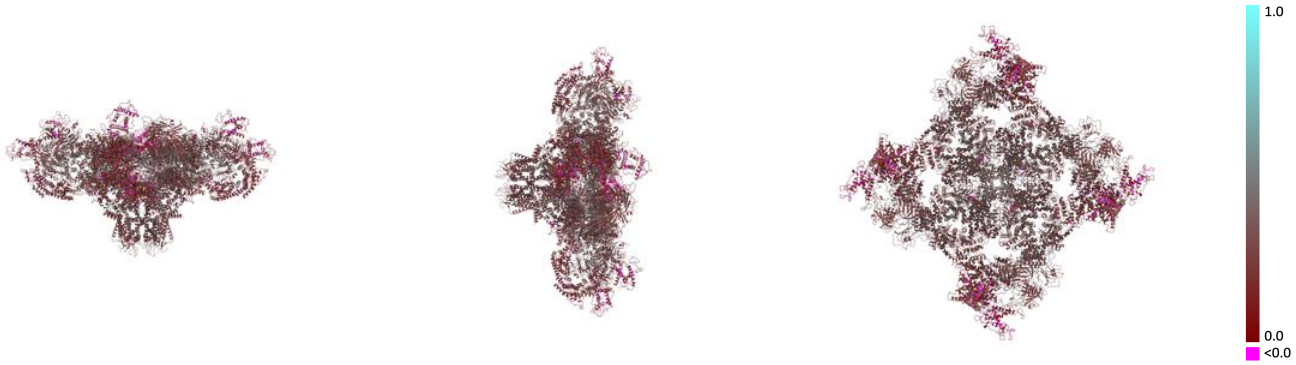
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.305 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

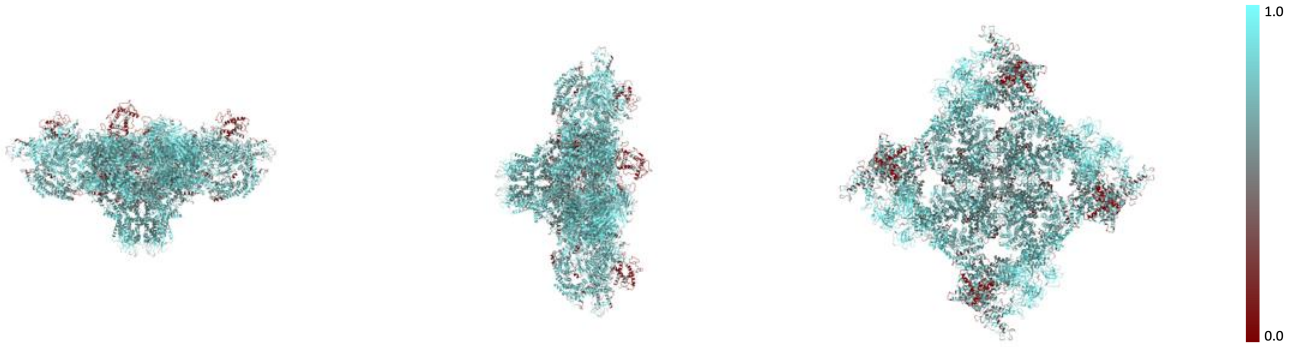
9.2 Q-score mapped to coordinate model



X Y Z

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

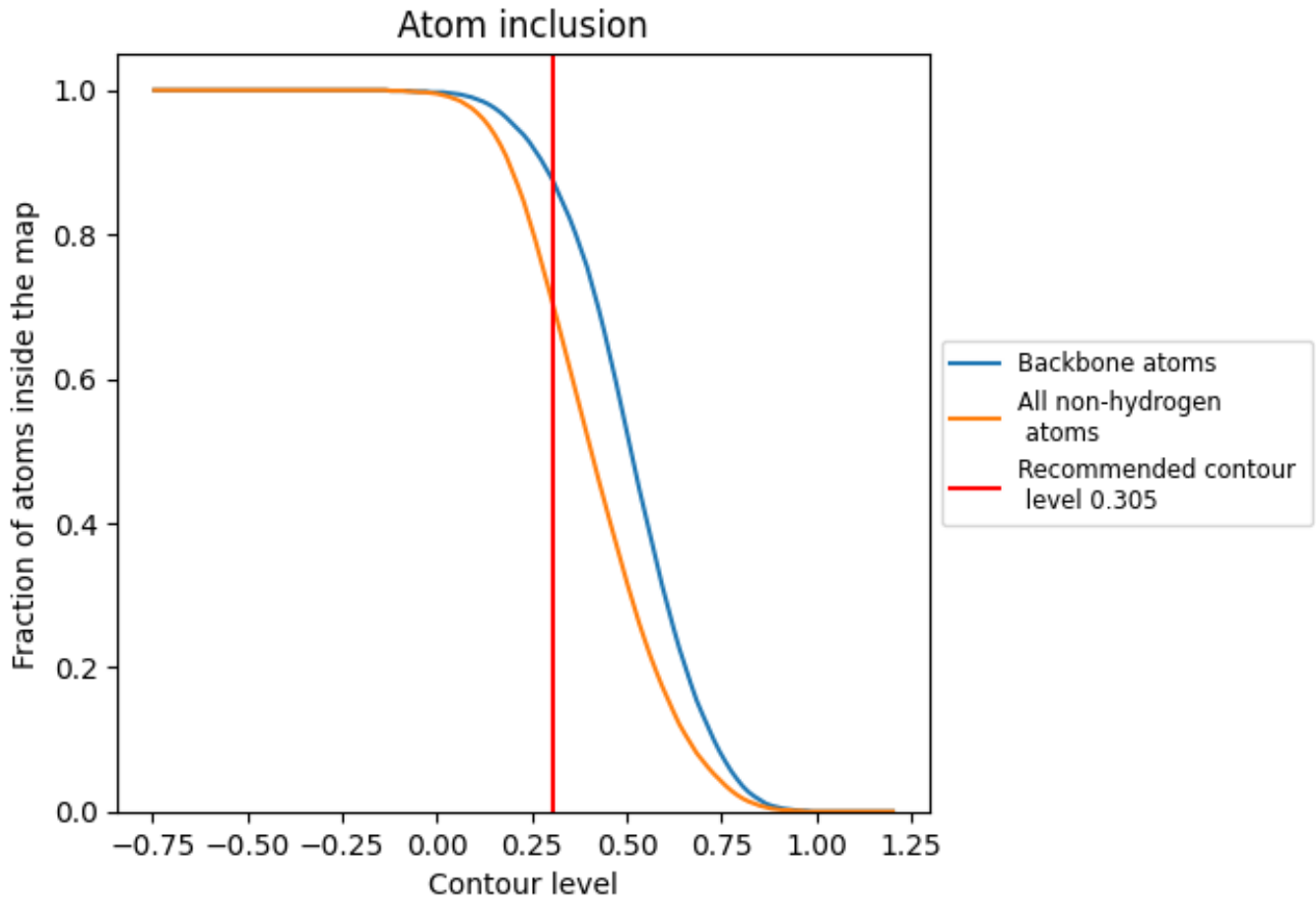
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.305).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.305) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7040	0.2840
A	0.7000	0.2820
B	0.7010	0.2820
C	0.7010	0.2820
D	0.7010	0.2830
E	0.8610	0.3440
F	0.8610	0.3430
G	0.8610	0.3420
H	0.8610	0.3450