



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:53 PM UTC

PDB ID : 9E1A / pdb\_00009e1a  
EMDB ID : EMD-47387  
Title : Structure of RyR1 in the primed state in the presence of dyphylline  
Authors : Miotto, M.C.; Marks, A.R.  
Deposited on : 2024-10-21  
Resolution : 3.35 Å (reported)  
Based on initial model : 7TZC

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

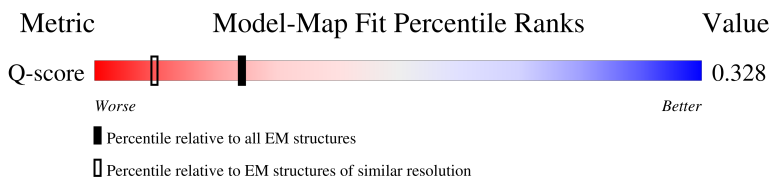
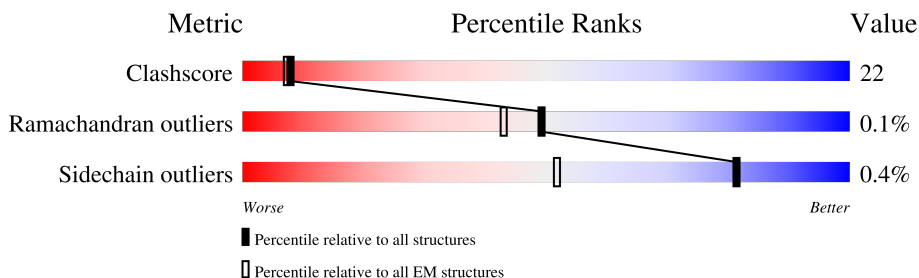
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.49

# 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 3.35 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	14390 ( 2.85 - 3.85 )

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<p>35% (Poor fit), 51% (0 outliers), 36% (1 outlier), 13% (2+ outliers)</p>
1	B	5037	<p>35% (Poor fit), 51% (0 outliers), 36% (1 outlier), 13% (2+ outliers)</p>
1	C	5037	<p>35% (Poor fit), 51% (0 outliers), 36% (1 outlier), 13% (2+ outliers)</p>
1	D	5037	<p>35% (Poor fit), 51% (0 outliers), 36% (1 outlier), 13% (2+ outliers)</p>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	E	108	 <p>66% 62% 34% ..</p>
2	F	108	 <p>65% 64% 32% ..</p>
2	G	108	 <p>64% 63% 33% ..</p>
2	H	108	 <p>64% 64% 32% ..</p>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 144128 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
			Total	C	N	O	S		
1	A	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	B	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	D	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	C	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	G	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

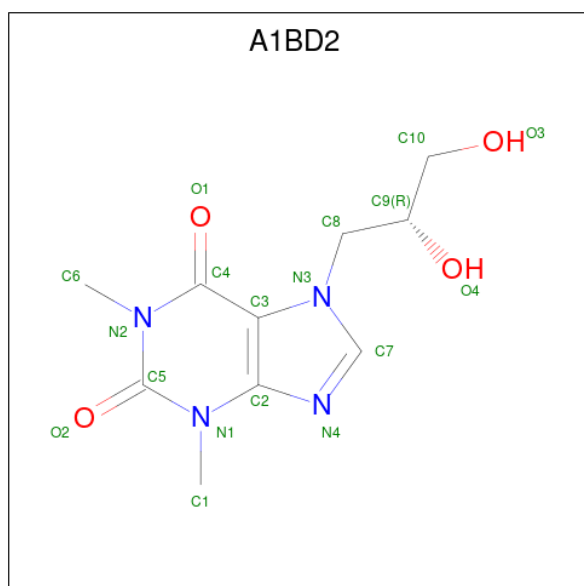
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	Total	Zn	0
			1	1	

*Continued on next page...*

Continued from previous page...

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

- Molecule 6 is dyphylline (CCD ID: A1BD2) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).

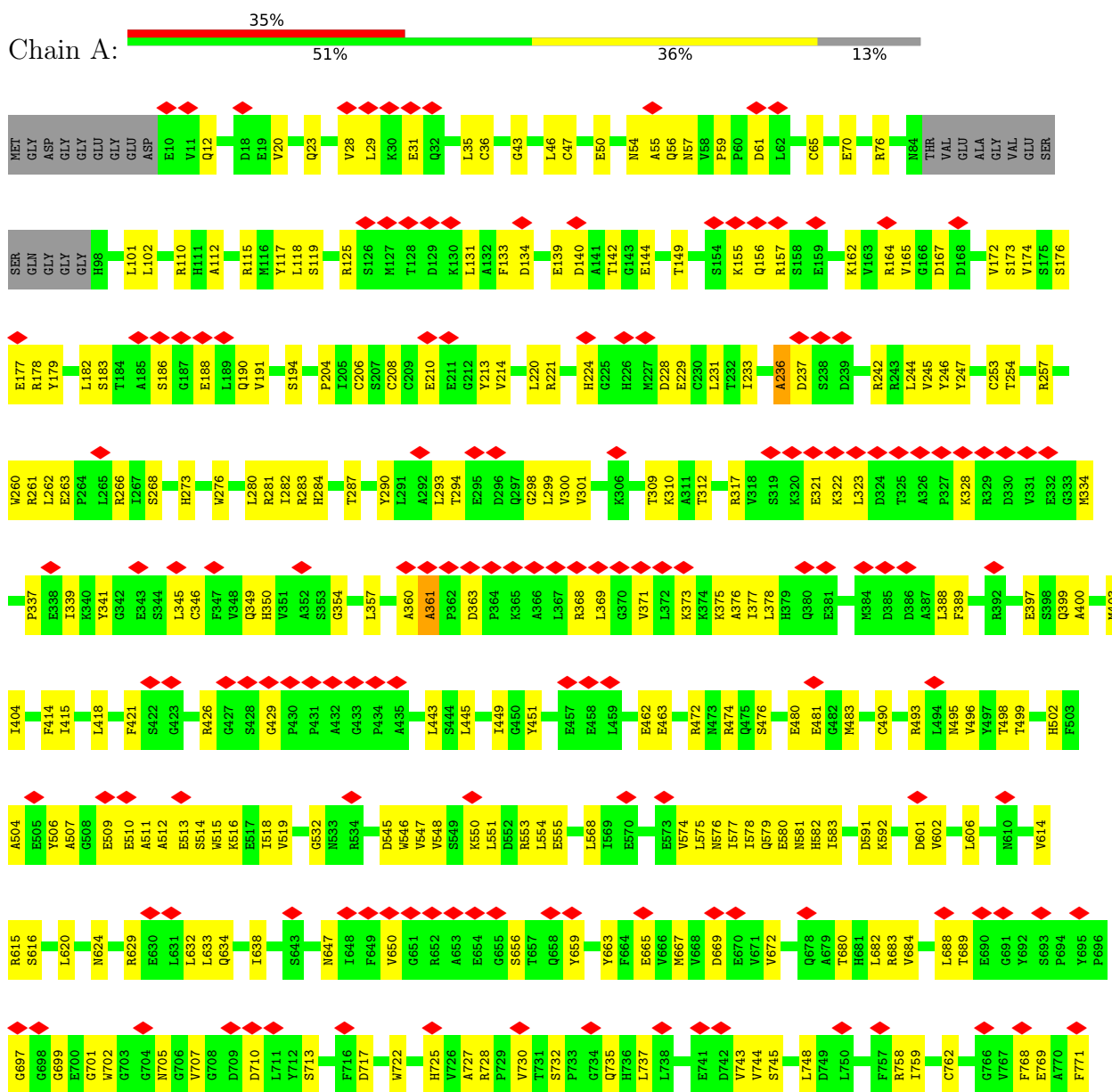


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			18	10	4	4	
6	B	1	Total	C	N	O	0
			18	10	4	4	
6	D	1	Total	C	N	O	0
			18	10	4	4	
6	C	1	Total	C	N	O	0
			18	10	4	4	

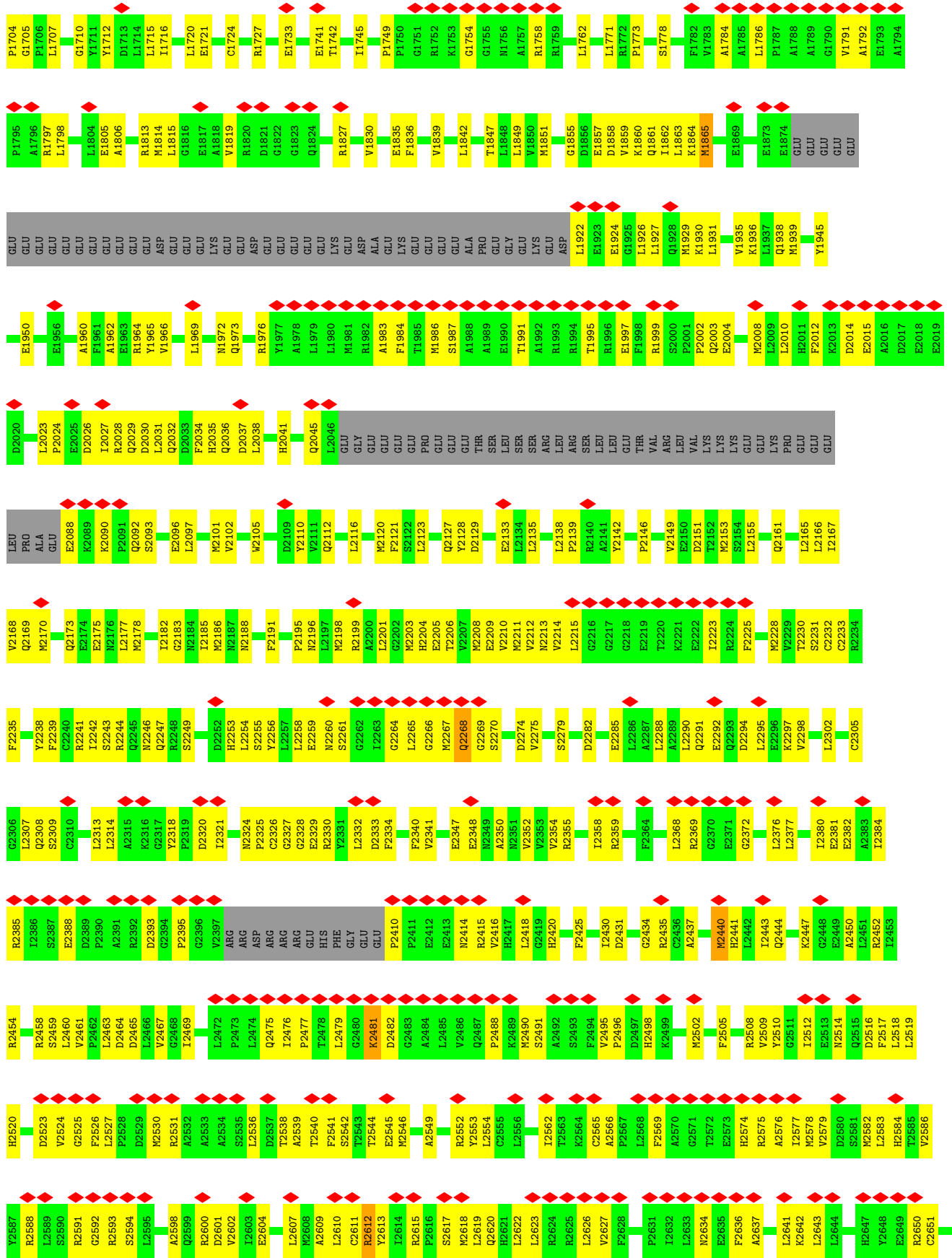
### 3 Residue-property plots

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

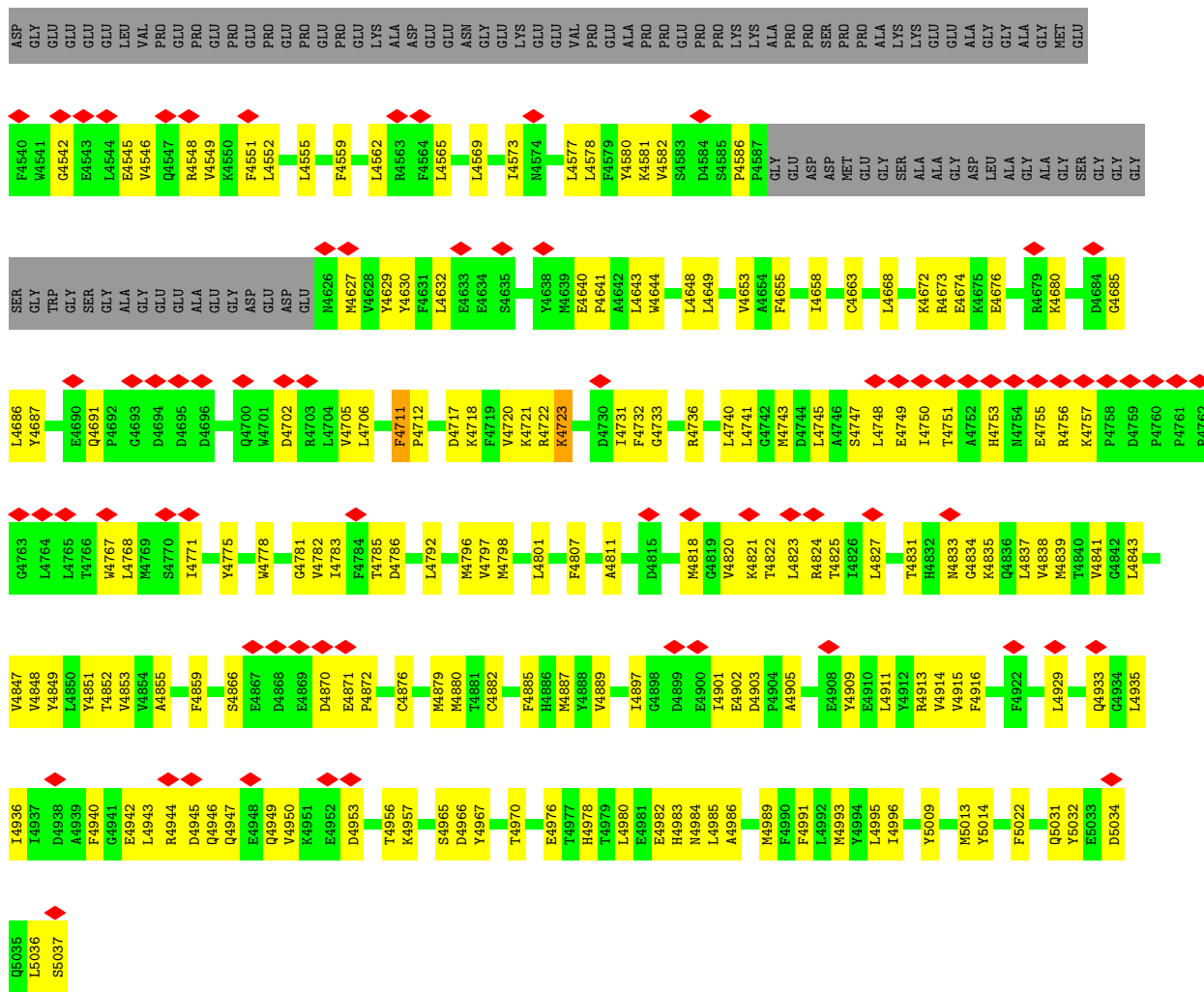


N772	N773	L774	D774	L776	F777	V781	S782	F783	G786	V787	K788	V789	R790	F791	L792	L793	R796	E799	F800	K801	F802	P806	G807	C811	H812	E813	A814	V815	L816	P817	R818	E819	R820	L821	R822	L823	K827	E828	Y829	R830	R831	R835	L839	V840	G841	S842	S843	R844	C845	L846									
S847	H848	T849	D850	F851	V852	P853	C854	F855	V856	D857	T858	V859	Q860	L861	V862	L863	P864	P865	H866	L867	E868	F869	I870	R871	E872	K873	L874	A875	E876	N877	I878	H879	E880	L881	A882	A883	L884	T885	R886	I887	E888	Q889	G890	V891	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	M924	S925	G926	E927	L928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	M941	A942	A943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	Y958	Y959	M960	M961	S962	N963	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	N991	G992	H993	N994	V995	A996	A997	R998	V1001	A1002	Q1003	M1004	W1005	S1006	Y1007	S1008	A1009	V1010	Q1011	P1014	A1015	R1016	R1017	R1020	L1021	L1022	V1023	Y1024	R1025	L1026	L1027	D1028	E1029			
A1030	T1031	K1032	R1033	S1034	N1035	N1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	P1055	P1056	D1057	Q1058	A1059	P1060	S1061	Q1062	E1063	E1064	N1065	Q1066	S1067	R1068	W1069	D1070	R1071	V1072	R1073	I1074	K1079	Q1084	R1087	W1088	E1093	E1099	M1100	R1101	L1102	G1103						
W1104	A1105	R1106	P1107	E1108	L1109	P1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	V1123	F1124	M1125	G1126	H1127	R1128	G1129	W1132	H1133	L1134	G1135	S1136	R1141	G1146	D1147	V1148	V1149	L1153	D1154	L1155	T1156	E1157	N1158	I1161	F1162	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179							
R1180	E1181	L1182	E1183	H1184	G1185	D1186	L1187	F1188	L1189	P1190	V1191	P1196	V1199	L1204	G1205	D1207	S1208	S1209	S1210	L1211	R1212	I1216	C1217	G1218	L1219	Q1220	E1221	G1222	F1223	E1224	A1227	I1228	M1229	M1230	Q1231	R1232	P1233	V1234	T1235	T1236	K1240	S1241	Q1244	F1245	E1251	H1252	Y1255	E1256											
R1259	M1260	D1261	G1262	T1263	V1264	D1265	T1266	C1269	L1270	R1271	L1272	R1276	T1276	W1277	S1278	Q1280	N1281	S1282	L1283	V1284	E1285	M1286	L1287	F1288	L1289	R1290	L1293	Q1296	F1297	H1298	Q1299	H1300	F1301	R1302	C1303	L1304	ALA	GLY	ALA	THR	PRO	ALA	PRO	PRO	PRO	GLY	LEU	GLN	PRO	GLU									
ALA	ARG	ALA	ALA	GLU	PRO	ASP	ASP	TYR	GLU	ASN	LEU	ARG	ARG	SER	GLY	GLY	TRP	GLY	ALA	ALA	GLU	THR	ALA	LYS	GLU	GLY	VAL	THR	PRO	GLY	GLY	THR	VAL	GLY	GLU	ALA	ALA	ARG	ALA	GLU	ASN	LYS	ASP	ALA	PRO	GLY	THR	THR	GLU										
LYS	ASN	LYS	LYS	ARG	GLY	PHE	LEU	PHE	ALA	LYS	LYS	ALA	ALA	MET	MET	THR	GLN	PRO	PRO	ALA	THR	PRO	ALA	ALA	LEU	ARG	VAL	PRO	ALA	D1419	N1420	R1421	D1422	D1423	P1424	E1425	I1426	I1427	L1428	N1429	T1430	T1431	T1432	Y1433	Y1434	Y1435	S1436	V1439	F1440	A1441	P1445								
S1446	C1447	V1448	W1449	V1453	T1454	P1455	D1456	D1461	M1462	F1464	D1465	L1466	S1467	K1468	V1469	R1470	V1474	T1475	M1476	G1477	D1478	E1479	Q1480	G1481	M1482	V1483	H1484	S1485	S1486	L1487	K1488	C1489	S1490	N1491	C1492	T1493	M1494	V1495	W1496	G1497	G1498	D1499	F1500	V1501	S1502	P1503	Q1504	Q1505	Q1506	G1507	I1508	S1510	H1511	T1512					
D1513	L1514	V1515	I1516	A1523	M1527	A1531	N1532	G1533	K1534	M1537	T1538	F1539	F1540	Q1541	V1542	K1547	L1548	F1549	P1550	A1551	V1554	L1555	V1561	I1562	Q1563	F1564	N1565	L1566	G1567	K1568	Q1569	K1570	N1571	M1572	M1573	P1574	L1575	S1576	A1577	A1578	M1579	F1580	E1583	L1584	K1585	N1586	Q1590	A1591	P1592	P1593									
R1594	L1595	Q1598	M1599	L1600	M1601	P1602	V1603	M1608	P1609	N1610	E1616	T1617	R1618	R1619	A1620	W1626	A1627	V1628	D1632	M1636	M1637	L1639	H1640	I1641	P1642	E1643	E1644	N1645	R1646	C1647	M1648	D1649	D1658	R1663	R1671	L1676	N1679	R1680	L1694	L1698	E1699	D1700	A1701	H1702	L1703														

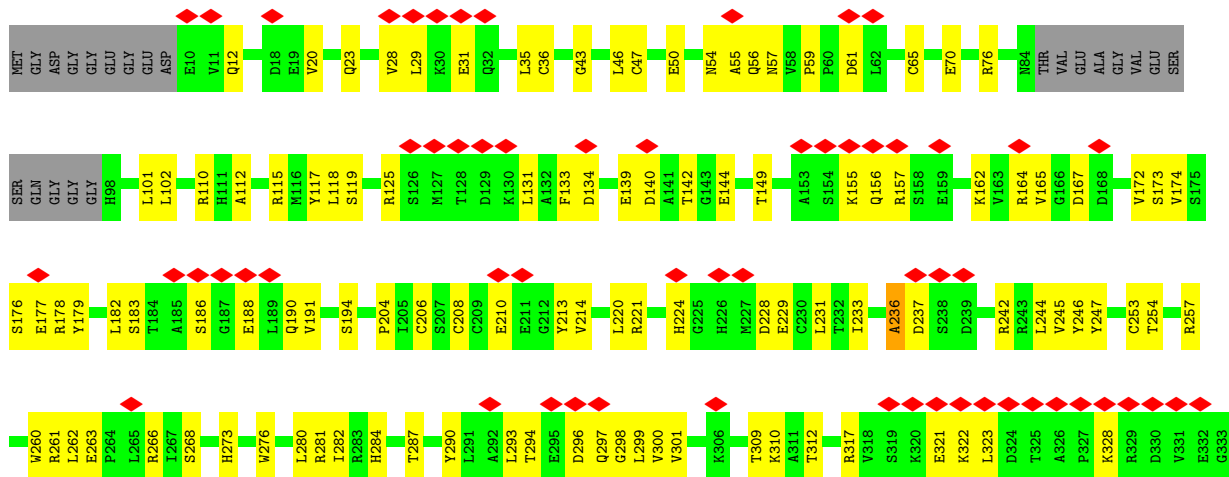


Y2655	D2716	S2776	L2896	K2986	Y3016	D3076	L3136	L3197	A3257	G3317	E3377
C2656	A2717	Y2777	K2897	F2957	F3017	A3077	L3137	A3198	E3258	M3318	Q3378
L2657	S2718	G2778	G2898	L2958	L3018	R3078	P3138	A3199	S3259	I3319	L3379
P2658	Y2719	E2779	G2899	L2959	S3019	T3079	V3139	A3200	G3260	L3320	R3380
G2660	L2720	M2780	G2900	L2960	T3020	V3080	T3140	M3201	A3261	R3321	L3381
	S2721	D2781	T2901	Q2961	P3021	M3081	T3141	P3202	R3262	I3322	E3382
	K2722	D2782	H2902	Q2962	A3022	K3082	T3142	V3203	Y3263	L3323	A3383
	A2723	E2783	H2902	L2963	K3023	S3083	L3143	A3204	T3264	V3324	K3384
	E2724	P2784	P2903	L2964	V3024	G3084	F3144	F3205	E3265	M3325	A3385
	K2725	L2785	L2905	K2965	L3025	P3085	Q3145	L3206	M3266	M3326	A3386
	LYS	K2786	V2906	W2966	G3026	E3086	H3146	E3207	P3267	L3327	A3387
	ALA	T2787	P2907	D2967	S3027	I3087	A3148	P3208	H3268	G3328	E3388
	THR	H2788	Y2908	D2968	G3028	V3088	Q3149	Q3209	V3269	I3329	E3389
	VAL	P2789	Y2908	I2969	G3029	K3089	H3150	L3210	I3270	D3330	G3390
	ASP	P2790	G2909	S2970	H3030	A3090	Q3151	M3211	E3271	E3331	E3391
	ALA	M2790	T2910	Q2971	A3031	G3091	F3152	E3212	T3272	A3332	L3392
	GLU	L2791	L2911	E2972	S3032	L3092	G3153	F3213	T3273	T3333	L3393
	GLY	R2792	T2912	F2973	N3033	R3093	D3154	M3214	L3274	W3334	V3394
	N2734	R2793	A2913	I2974	K3034	S3094	D3155	A3215	P3275	M3335	R3395
	F2735	P2794	K2914	A2975	E2975	F3095	V3156	C3216	M3276	K3336	D3396
	D2736	K2795	E2915	H2976	H2976	F3096	I3157	S3217	L3277	R3337	I3397
	P2737	T2796	K2916	L2977	E3037	E3097	I3158	V3218	C3278	L3338	F3398
	R2738	P2797	A2917	E2978	G3038	S3098	D3159	Y3219	S3279	A3339	S3399
	P2739	S2798	R2918	L2862	M3038	A3099	D3160	T3220	Y3280	V3340	V3400
	P2740	E2799	R2919	L2862	I3039	S3100	D3161	T3221	L3281	F3341	L3401
	E2741	R2800	D2920	Q2864	T3040	E3101	V3161	Q3222	P3282	C3402	C3402
	T2742	K2801	E2921	S2866	L3042	D3102	Q3162	K3223	R3283	R3403	R3403
	L2743	K2802	K2922	T2866	S3041	I3103	V3163	S3223	W3284	P3404	D3404
	N2744	K2802	A2923	L2867	F3043	E3104	S3164	P3224	W3285	P3405	L3405
	V2745	E2803	Q2924	Q2984	C3044	K3105	C3165	R3225	E3286	I3406	L3406
	I2746	I2804	Q2925	R2869	K3045	M3106	V3166	R3226	R3287	R3407	A3407
	L2747	R2805	E2925	E2870	L3046	V3107	R3167	R3227	G3288	L3408	L3408
	L2748	R2806	L2926	L2871	L3047	I3108	T3168	A3228	P3289	Y3409	Y3409
	P2748	R2807	L2927	Q2872	A3047	E3109	L3169	I3229	E3290	P3410	P3410
	E2749	P2808	K2928	M2874	S3048	N3109	L3170	L3230	A3291	L3411	L3411
	K2750	L2809	F2929	A2874	P3049	L3049	R3110	G3231	P3292	A3352	A3352
	L2751	K2810	L2930	A2874	V3050	L3110	R3111	G3232	P3293	L3353	L3412
	D2752	E2811	M2931	E2876	R3051	L3112	L3112	P3233	P3294	L3354	R3414
	S2753	E2812	M2932	Q2877	H3052	G3113	G3113	L3175	A3295	H3355	Y3415
	E2693	L2813	N2933	L2878	R3053	K3114	L3176	S3235	L3296	S3356	Y3416
	E2694	L2813	G2934	A2879	V3054	V3115	G3177	V3236	P3297	H3357	D3417
	L2695	K2814	Y2935	A2879	S3055	S3116	T3178	E3237	A3298	F3358	N3418
	Y2696	A2815	A2936	E2880	F3056	G3116	K3179	E3238	G3299	I3359	N3419
	R2697	W2816	L2937	M2881	F3057	ALA	N3180	M3239	G3300	P3360	R3420
	R2698	L2817	T2938	Y2882	G3058	ARG	T3181	C3240	A3300	I3361	A3421
	K2699	A2818	L2939	H2883	T3059	THR	Y3182	G3241	P3301	T3362	H3422
	L2700	W2819	M2939	H2883	D3060	GLN	T3183	P3241	P3302	L3363	H3423
	R2701	E2820	L3003	Y2882	P3062	K3123	V3183	D3242	P3303	G3363	H3423
	C2702	W2821	L3003	W2886	A3063	G3124	E3184	I3243	C3304	R3364	L3424
	L2703	E2822	L3003	G2887	A3063	V3125	K3185	P3244	C3304	L3365	T3425
	C2704	T2823	L3005	R2888	V3064	G3126	L3186	V3245	T3305	R3366	E3426
	L2706	I2824	L3005	K2888	V3065	Q3127	R3187	L3246	A3306	K3367	P3427
	A2707	E2824	L3006	L2946	V3066	M3128	P3188	D3247	V3307	R3368	N3428
	G2708	A2767	K2889	D2947	N3066	L3128	A3189	R3248	T3308	A3369	A3429
	G2708	A2767	K2890	T2948	M3067	L3129	L3190	L3249	G3309	G3370	N3430
	L2710	F2768	K2891	S2949	C3067	F3130	G3191	L3249	D3310	K3371	A3431
	P2711	D2769	Q2892	S2950	Y3009	Y3131	E3192	M3250	H3311	V3372	E3432
	P2712	Q2770	E2893	S2950	T3011	T3132	C3193	D3252	L3312	L3373	E3433
	D2713	Q2772	E2894	I2951	I3070	T3133	C3193	I3253	L3313	V3373	L3434
	Y2714	N2773	L2894	E2952	L3071	T3133	L3194	I3253	L3314	A3374	F3435
	W2715	N2774	GLU	R2954	A3072	V3134	A3195	I3254	L3315	E3375	R3436
		THR	ARG	R2954	R3073	A3135	A3195	G3255	L3316	E3376	
		THR	GLU	R2955	S3074		R3196	G3256			
		GLU	R2955	L3015	L3075		L3256	L3256			





• Molecule 1: Ryanodine receptor 1



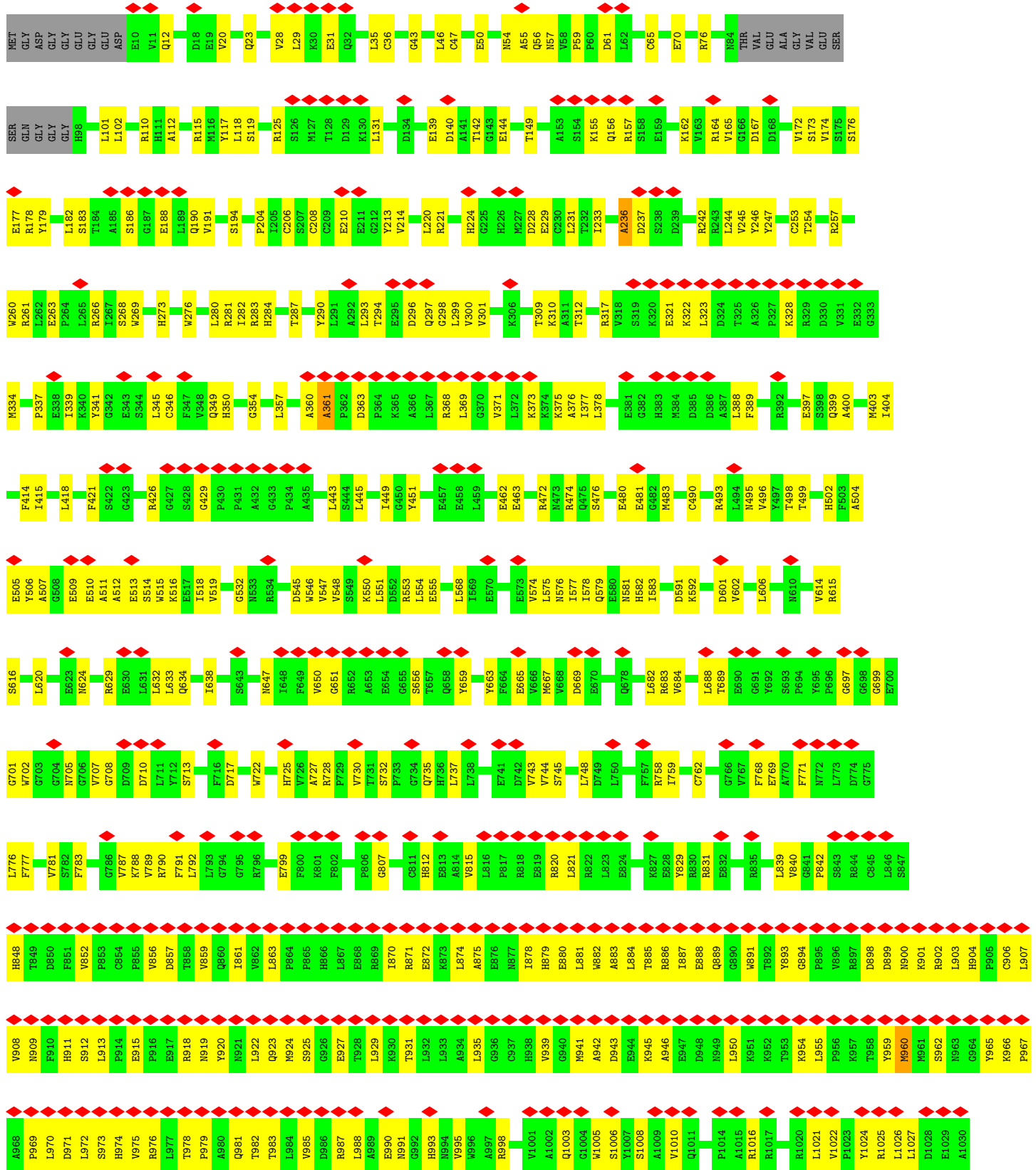
ASP	Y1255	S1175	R1101	D1028	Y965	P905	C845	L773	G898	R815	A504	I404	M334
GLU	E1256	E1176	V1102	E1029	K966	C906	L846	D774	G699	S616	E505	F414	G335
ARG		T1177	G1103	A1030	P967	L907	S847	G775	E700	L620	Y506	I415	P336
ALA	R1259	A1178	A1105	T1031	A968	Y908	H848	L776	G701	G508	E509	L418	E338
GLU	D1261	F1179	R1106	K1032	P969	R909	T849	F777	W702	G509	E510	K340	P337
PRO	G1262	R1180	P1107	R1033	D971	F910	D850	F781	G704	N624	E511	Y341	K341
ASP	E1181	E1181	E1108	S1034	S913	H911	F851	S782	G705	R629	A512	S422	G342
PRO	I1182	I1182	L1109	N1035	L972	S912	S852	F783	V707	E630	E513	G423	E343
TYR	I1184	I1184	R1110	H1036	S973	L914	P853	G786	G708	L632	E514	R426	S344
GLU	G1185	G1185	D1037	D1037	H974	P913	C854	W787	D709	L633	S514	G427	L345
ASN	D1186	D1186	S1038	L1039	V975	E915	S855	K788	D710	L634	S515	G428	C346
LEU	C1269	G1187	L1039	C1040	R976	P916	S856	W789	L711	Q634	K516	G429	F347
ARG	L1270	F1188	L1041	Q1044	L977	E917	D857	R790	W712	I638	E517	G430	V348
ARG	R1271	P1190	A1042	R1044	T978	R918	T858	F791	S713	I638	E518	P430	Q349
ALA	R1275	P1191	Q1044	R1044	T978	R918	T858	L792	F716	S943	E519	P431	H350
GLY	T1276	P1196	V1043	V1043	P979	N919	S859	L793	D717	N647	E533	A432	G354
GLY	G1278	P1199	R1044	R1044	A880	Y920	T861	G794	W722	I648	R534	G433	L357
GLY	Q1280	V1199	L1046	L1046	Q981	A921	L862	G795	F649	F649	D545	P434	
ALA	N1281	L1204	L1046	L1046	T982	L922	L863	R796	W725	V650	W546	A435	A360
GLY	S1282	L1204	L1047	L1047	T983	Q923	L864	E799	H725	V650	W547	L443	A361
GLY	L1283	Q1206	G1048	G1048	V985	M924	P864	F800	V726	V651	V548	L444	P362
LYS	L1284	Q1206	Y1049	Y1049	S925	S925	A727	A801	A727	R652	S549	L445	D363
GLU	E1285	D1207	G1050	G1050	R987	G926	H866	F802	R728	A653	K550	L449	P364
GLY	S1208	V1209	Y1051	Y1051	R988	T928	E868	P806	V730	R654	D552	G450	K365
THR	M1286	S1209	M1052	M1052	A889	R929	R869	G807	T731	S656	R553	Y451	A366
ALA	L1287	S1210	E1054	E1054	E990	K930	L870	C811	P733	Q858	L568	E457	R368
LYS	F1288	L1211	P1055	P1055	N991	R931	R871	H612	Q735	Y659	I569	E458	L369
GLU	R1289	L1212	P1056	P1056	H993	L932	E872	ES13	H736	I569	I569	L459	L370
THR	R1290	L1216	P1056	P1056	V994	L933	L874	A814	L737	Y663	E573	E462	L372
PRO	L1293	Q1220	D1057	D1057	V995	A934	A875	W815	L738	F664	V574	E463	K373
GLY	Q1296	E1221	Q1058	Q1058	A997	L935	A875	L816	E741	E665	L575	R472	K374
PRO	F1297	G1222	E1059	E1059	G936	G936	E876	P817	D742	D669	N576	M473	K375
GLN	H1298	F1223	P1060	P1060	C937	C937	N877	R818	V743	E670	I577	R474	A376
PRO	Q1299	E1224	S1061	S1061	H938	H938	L878	ES19	W744	V671	I578	Q475	I377
GLY	H1300	A1227	Q1062	Q1062	V939	V939	H879	R820	S745	V672	Q579	S476	L378
VAL	F1301	I1228	V1063	V1063	G940	G940	E880	L821	L748	E480	E580	E480	E381
ALA	R1302	N1229	E1064	E1064	M941	M941	L881	R822	D749	Q678	N581	E481	G382
GLN	C1303	M1230	V1065	V1065	A942	A942	W882	L823	L750	A879	H862	M483	H383
PRO	T1304	Q1231	Q1066	Q1066	D943	D943	A883	E824	F757	T880	I583	C490	M384
VAL	ALA	R1232	S1067	S1067	E944	E944	L884	K827	R758	L682	D591	C490	D385
ALA	GLY	P1233	S1068	S1068	A945	A945	R886	E828	I759	R683	K592	C490	D386
ALA	ALA	V1234	A1009	A1009	A946	A946	R886	Y829	W684	L684	D601	R493	D387
ASN	THR	T1236	V1010	V1010	E947	E947	T887	Y830	C762	V684	D601	R493	D388
PRO	LEU	K1240	Q1011	Q1011	P1014	P1014	E888	R831	G766	L688	V602	R493	D388
ALA	ALA	S1241	P1014	P1014	A1015	A1015	Q889	E832	V767	T689	V602	L494	L388
ALA	PRO	Q1244	A1015	A1015	R1016	R1016	G890	G835	F768	E690	L606	M495	F389
ALA	GLY	F1245	R1017	R1017	L1017	L1017	A891	R835	F768	G692	L606	M496	F389
LEU	GLY	H1251	K1079	K1079	R1020	R1020	T892	L839	A770	N610	L606	T497	R392
GLN	GLN	E1252	Q1084	Q1084	L1021	L1021	S893	V840	E769	T498	L606	T499	E397
PRO	PRO		R1087	R1087	P1023	P1023	C894	G841	A770	T499	L606	T499	E397
ALA	ALA		W1088	W1088	Y1024	Y1024	S896	S843	F771	N610	L606	T499	E397
ALA	ALA		E1093	E1093	L1026	L1026	S896	S843	N772	N610	L606	T499	E397
GLU	GLU		E1099	E1099	L1027	L1027	S897	S843	N772	N610	L606	T499	E397
THR	THR		M100	M100			S897	S843	N772	N610	L606	T499	E397
							S898	S843	N772	N610	L606	T499	E397
							D898	S843	N772	N610	L606	T499	E397
							D899	S843	N772	N610	L606	T499	E397
							N900	S843	N772	N610	L606	T499	E397
							K901	S843	N772	N610	L606	T499	E397
							R902	S843	N772	N610	L606	T499	E397
							L903	S843	N772	N610	L606	T499	E397
							H904	S843	N772	N610	L606	T499	E397



T3133	R3073	H3013	K2953	E2893	N2773	D2713	R2650	T2585	L2518	R2452	A2383
V3134	S3074	C3014	R2954	L2894	N2774	V2714	C2651	V2586	L2519	I2453	I2384
A3135	L3075	L3015	F2955	E2895	W2775	V2715	Y2655	R2587	H2520	R2454	R2385
L3136	D3076	Y3016	A2956	A2896	S2776	D2716	C2656	L2588	D2523	R2458	I2386
L3137	A3077	F3017	F2957	K2897	G2777	S2717	L2657	S2590	V2524	S2459	S2387
R3138	R3078	L3018	G2958	G2898	E2778	A2718	R2591	R2589	G2525	L2460	E2388
V3139	T3079	S3019	F2959	G2899	E2779	S2719	G2592	G2592	P2526	P2461	I2389
V3080	V3080	T3020	L2960	C2900	N2780	S2720	T2659	R2593	L2463	L2463	P2390
M3081	M3081	P3021	Q2961	H2901	V2781	S2721	G2660	S2594	D2464	D2464	A2391
K3082	K3082	A3022	Q2962	H2902	D2782	K2722	M2663	L2595	D2465	D2465	R2392
G3083	G3083	K3023	L2963	P2903	E2783	A2723	F2664	Q2599	M2530	L2466	D2393
G3084	G3084	V3024	L2964	L2904	E2784	E2724	G2665	Q2599	V2467	V2467	D2394
E3085	E3085	L3025	F2965	L2905	K2785	K2725	Q2599	Q2599	I2469	I2469	P2395
E3086	E3086	G3026	W2966	V2906	L2786	LYS	V2666	R2600	L2472	L2472	G2396
I3087	I3087	S3027	M2967	V2907	K2787	ALA	T2667	D2601	P2473	P2473	V2397
V3088	V3088	G3028	D2968	P2907	T2787	THR	S2668	D2602	R2474	R2474	ARG
K3089	K3089	G3029	L2969	Y2908	H2788	VAL	E2669	I2603	Q2475	Q2475	ASP
A3090	A3090	H3030	I2970	Y2909	P2789	ASP	E2670	E2604	I2476	I2476	ARG
G3091	G3091	A3031	Q2971	T2910	M2790	ALA	E2671	L2607	L2477	L2477	ARG
L3092	L3092	S3032	E2972	L2911	L2791	GLY	L2672	M2608	T2478	T2478	GLU
R3093	R3093	N3033	F2973	T2912	R2792	ALA	H2673	L2610	L2479	L2479	HIS
S3094	S3094	K3034	I2974	A2913	Y2793	F2735	L2674	L2611	G2480	G2480	PHE
F3095	F3095	E3035	A2975	K2914	Y2794	D2736	T2675	C2611	K2481	K2481	GLY
F3096	F3096	E3036	L2976	E2915	K2795	D2737	R2676	R2612	R2482	R2482	GLU
E3097	E3097	K3036	L2977	K2916	T2796	K2738	K2677	Y2613	G2483	G2483	
S3098	S3098	E3037	E2978	A2917	F2797	V2739	F2678	L2614	R2484	R2484	
A3099	A3099	M3038	A2979	R2918	S2798	V2740	W2680	P2615	R2485	R2485	
S3100	S3100	L3039	V2980	D2919	E2799	E2741	G2681	P2616	A2484	A2484	
E3101	E3101	T3040	V2981	R2920	K2800	T2742	I2682	S2617	L2486	L2486	
D3102	D3102	S3041	E2982	E2921	D2801	L2743	I2683	M2618	R2552	R2552	
I3103	I3103	L3042	S2983	K2922	K2802	L2744	F2683	L2619	L2553	L2553	
E3104	E3104	F3043	G2984	A2923	N2744	K2745	D2684	Q2620	L2554	L2554	
K3105	K3105	C3044	R2985	Q2924	V2745	V2746	S2685	H2621	C2555	C2555	
M3106	M3106	L3045	V2986	E2925	I2746	I2747	L2686	L2622	M2490	M2490	
V3107	V3107	K3046	E2987	L2926	Y2805	T2747	A2887	L2623	S2491	S2491	
E3108	E3108	A3047	K2988	L2927	W2807	F2748	H2688	R2624	A2492	A2492	
N3109	N3109	S3048	S2989	K2928	P2808	E2749	K2689	R2625	S2493	S2493	
R3110	R3110	L3049	P2990	F2929	N2809	K2750	K2690	L2626	F2494	F2494	
L3111	L3111	V3050	H2991	F2929	I2809	L2751	Y2691	D2627	P2496	P2496	
L3112	L3112	R3051	H2992	Q2931	K2810	D2752	Q2693	F2628	L2497	L2497	
G3113	G3113	H3052	E2992	M2932	E2811	S2753	E2694	D2629	L2568	L2568	
K3114	K3114	R3053	Q2993	M2933	S2812	F2754	L2695	P2631	A2566	A2566	
V3115	V3115	V3054	E2994	M2934	L2813	I2755	Y2696	L2632	P2567	P2567	
S3116	S3116	S3055	L2995	G2934	K2814	I2756	R2697	L2633	A2570	A2570	
GLN	GLN	L3056	K2996	Y2935	A2815	K2757	R2698	M2634	G2571	G2571	
ALA	ALA	L3057	F2997	A2936	W2816	I2758	M2699	E2635	M2502	M2502	
ARG	ARG	F3057	F2998	V2937	L2817	E2758	M2700	E2636	F2505	F2505	
THR	THR	G3058	A2999	T2938	A2818	A2759	P2701	F2637	R2508	R2508	
GLN	GLN	T3059	K3000	R2939	W2819	E2760	P2701	A2637	V2509	V2509	
K3123	K3123	D3060	I3001	R2939	E2820	Y2761	C2702	L2641	Y2510	Y2510	
G3124	G3124	A3061	L3002	L3002	W2821	T2762	L2703	K2642	G2511	G2511	
V3125	V3125	P3062	L3003	L3003	T2822	C2704	C2704	L2643	I2512	I2512	
K3126	K3126	A3063	P3004	P3004	E2764	I2705	I2705	L2644	N2514	N2514	
GLN	GLN	L3005	L3005	L3005	K2823	K2765	A2706	L2644	Q2515	Q2515	
N3128	N3128	V3064	I3006	I3006	E2824	W2766	A2707	H2647	D2516	D2516	
N3128	N3128	V3065	I3006	I3006	K2825	A2767	G2708	Y2648	F2517	F2517	
L3129	L3129	N3066	N3007	N3007	A2826	F2768	A2709	L2710			
L3130	L3130	C3067	Q3008	Q3008	R2827	D2769	L2710				
V3131	V3131	L3068	F3009	F3009	E2828	K2770					
T3132	T3132	H3069	T3011	T3011	E2829	I2771					
		L3070	N3012	N3012	E2830	Q2772					
		A3072			GLU						

S4052	S4053	M4054	V4055	Q4056	M4057	K4060	F4061	D4062	F4063	M4064	F4065	L4066	K4067	L4068	L4069	D4070	L4071	F4077	D4078	D4079	V4080	V4081	M4000	T4082	D4083	F4084	R4085	Q4086	K4090	Q4099	I4010	K4014	E4015	L4016	L4017	Q4020	K4021	V4024	V4025	M4026	L4027	L4028	S4029	M4037	A4041	R4042	Q4043	M4044	V4045	M4049	F4127	F4128	A4129	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	F3202	V3203	A3204	F3205	L3206	E3207	F3208	Q3209	L3210	M3211	E3212	V3213	M3214	A3215	C3216	S3217	V3218	Y3219	T3220	T3221	K3222	S3223	F3224	R3225	E3226	R3227	A3228	I3229	L3230	G3231	L3232	P3233	M3234	S3235	V3236	E3237	E3238	R3239	C3240	P3241	D3242	I3243	F3244	V3245	L3246	D3247	R3248	L3249	M3250	D3252	I3253	G3254	L3256	A3257	E3258	S3259	G3260	A3261	R3262	Y3263	T3264	E3265	M3266	P3267	V3268	I3270	E3271	I3272	T3273	L3274	P3275	M3276	L3277	C3278	S3279	Y3280	L3281	P3282	R3283	W3284	W3285	E3286	R3287	G3288	P3289	E3290	A3291	P3292	P3293	P3294	L3296	L3297	A3298	G3299	E3300	P3302	P3303	C3304	T3305	A3306	V3307	T3308	S3309	D3310	H3311	L3312	M3313	S3314	L3315	L3316	G3317	M3318	I3319	L3320	R3321	I3322	I3323	V3324	M3325	N3326	L3327	G3328	I3329	D3330	E3331	A3332	T3333	W3334	M3335	K3336	R3337	L3338	A3339	V3340	F3341	A3342	Q3343	P3344	L3345	V3346	S3347	R3348	A3349	R3350	P3351	E3352	L3353	R3354	M3355	S3356	H3357	I3358	N3359	A3360	R3361	T3362	I3363	G3364	P3365	L3366	K3367	R3368	G3369	K3370	K3371	V3372	V3373	A3374	E3375	E3376	E3377	Q3378	L3379	L3381	E3382	A3383	K3384	A3385	E3386	H3387	N3388	E3389	E3390	E3391	L3392	L3393	V3394	R3395	D3396	E3397	F3398	S3399	V3400	L3401	P3402	R3403	D3404	L3405	Y3406	A3407	L3408	Y3409	P3410	L3411	L3412	R3413	Y3414	V3415	V3416	D3417	N3418	ASP	ALA	ALA	ALA	GLN	SER	GLY	GLY	ASP	ASP	GLN	GLU	ARG	THR	LYS	L3434	F3435	R3436	M3437	G3438	G3439	I3440	F3442	I3443	Y3444	K3447	S3448	H3449	N3450	F3451	K3452	R3453	Q3456	N3457	F3458	V3459	V3460	Q3461	E3463	I3464	M3465	N3466	M3467	S3468	F3469	L3470	T3471	A3472	D3473	S3474	K3475	S3476	A3479	LYS	ALA	GLY	GLY	ASP	ALA	ALA	GLN	SER	GLY	GLY	ASP	ASP	GLN	GLU	ARG	THR	LYS	L3484	H3485	Q3486	G3487	D3488	D3489	D3490	D3491	D3492	D3493	D3494	D3495	D3496	D3497	D3498	D3499	D3500	D3501	D3502	D3503	D3504	D3505	D3506	D3507	D3508	D3509	D3510	D3511	D3512	D3513	D3514	D3515	D3516	D3517	D3518	D3519	D3520	D3521	D3522	D3523	D3524	D3525	D3526	D3527	D3528	D3529	D3530	D3531	D3532	D3533	D3534	D3535	D3536	D3537	D3538	D3539	D3540	D3541	D3542	D3543	D3544	D3545	D3546	D3547	D3548	D3549	D3550	D3551	D3552	D3553	D3554	D3555	D3556	L3494	L3495	L3496	L3497	L3498	L3499	L3500	L3501	L3502	L3503	L3504	L3505	L3506	L3507	L3508	L3509	L3510	L3511	L3512	L3513	L3514	L3515	L3516	L3517	L3518	L3519	L3520	L3521	L3522	L3523	L3524	L3525	L3526	L3527	L3528	L3529	L3530	L3531	L3532	L3533	L3534	L3535	L3536	L3537	L3538	L3539	L3540	L3541	L3542	L3543	L3544	L3545	L3546	L3547	L3548	L3549	L3550	L3551	L3552	L3553	L3554	L3555	L3556	L3557	L3558	L3559	L3560	L3561	L3562	L3563	L3564	L3565	L3566	L3567	L3568	L3569	L3570	L3571	L3572	L3573	L3574	L3575	L3576	L3577	L3578	L3579	L3580	L3581	L3582	L3583	L3584	L3585	L3586	L3587	L3588	L3589	L3590	L3591	L3592	L3593	L3594	L3595	L3596	L3597	L3598	L3599	V3602	L3603	Y3604	H3605	L3606	E3607	Q3608	T3609	E3610	H3611	V3612	P3613	K3614	S3615	K3616	K3617	A3618	V3619	W3620	H3621	R3622	L3623	L3624	S3625	K3626	S3627	R3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	M3638	T3639	P3640	L3641	Y3642	M3643	L3644	H3647	R3648	A3649	C3650	N3651	M3652	F3653	L3654	Y3657	K3658	A3659	A3660	W3661	I3662	E3665	D3666	H3667	S3668	D3671	R3672	M3673	L3677	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	V3689	M3690	E3691	D3692	K3693	D3696	P3697	L3698	H3699	Q3700	L3701	V3702	L3703	H3704	F3705	T3708	S3714	K3715	L3716	D3717	E3718	Q3719	Y3720	M3723	A3724	Y3725	I3728	M3729	A3730	K3731	S3732	C3733	H3734	L3735	E3736	GLU	GLY	GLY	GLU	ASN	GLY	GLU	GLU	ALA	ALA	GLU	GLU	GLU	GLU	V3749	E3750	R3762	S3768	R3769	L3770	H3771	T3772	R3773	G3774	A3775	A3776	M3777	V3779	L3780	Q3781	M3782	C3786	K3787	G3788	M3793	A3797	T3797	I3802	N3809	V3812	Q3813	Q3814	K3815	D3818	Y3819	E3825	S3831	I3832	Q3833	A3834	Q3837	T3838	L3842	D3843	L3844	R3849	Q3850	M3851	K3852	A3853	E3854	G3855	L3856	G3857	M3868	V3869	N3870	G3871	E3872	K3873	V3874	M3875	D3877	D3878	R3886	D3888	F3889	R3904	T3905	Q3906	T3912	L3924	Q3927	I3930	S3931	D3932	F3933	Y3937	K3940	D3941	Q3946	R3949	N3950	F3951	S3952	K3953	A3954	M3955	S3956	V3957	V3961	T3966	L3967	L3968	L3969	L3970	L3971	L3972	L3973	L3974	L3975	L3976	L3977	L3978	L3979	L3980	L3981	L3982	L3983	L3984	L3985	L3986	L3987	L3988	L3989	L3990	L3991	L3992	V3995	F3996	M4000	M4001	K4002	L4003	S4007	S4008	Q4009	I4010	K4014	E4015	L4016	L4017	Q4020	K4021	V4024	V4025	M4026	L4027	L4028	S4029	M4037	A4041	R4042	Q4043	M4044	V4045	M4049	F4127	F4128	A4129	L3984	L3985	L3986	L3987	L3988	L3989	L3990	L3991	L3992	L3993	L3994	L3995	L3996	L3997	L3998	L3999	L4000	L4001	L4002	L4003	L4004	L4005	L4006	L4007	L4008	L4009	L4010	L4011	L4012	L4013	L4014	L4015	L4016	L4017	L4018	L4019	L4020	L4021	L4022	L4023	L4024	L4025	L4026	L4027	L4028	L4029	L4030	L4031	L4032	L4033	L4034	L4035	L4036	L4037	L4038	L4039	L4040	L4041	L4042	L4043	L4044	L4045	L4046	L4047	L4048	L4049	L4050	L4051	L4052	L4053	L4054	L4055	L4056	L4057	L4058	L4059	L4060	L4061	L4062	L4063	L4064	L4065	L4066	L4067	L4068	L4069	L4070	L4071	L4072	L4073	L4074	L4075	L4076	L4077	L4078	L4079	L4080	L4081	L4082	L4083	L4084	L4085	L4086	L4087	L4088	L4089	L4090	L4091	L4092	L4093	L4094	L4095	L4096	L4097	L4098	L4099	L4100	L4101	L4102	L4103	L4104	L4105	L4106	L4107	L4108	L4109	L4110	L4111	L4112	L4113	L4114	L4115	L4116	L4117	L4118	L4119	L4120	L4121	L4122	L4123	L4124	L4125	L4126	L4127	L4128	L4129	L4130	L4131	L4132	L4133	L4134	L4135	L4136	L4137	L4138	L4139	L4140	L4141	L4142	L4143	L4144	L4145	L4146	L4147	L4148	L4149	L4150	L4151	L4152	L4153	L4154	L4155	L4156	L4157	L4158	L4159	L4160	L4161	L4162	L4163	L4164	L4165	L4166	L4167	L4168	L4169	L4170	L4171	L4172	L4173	L4174	L4175	L4176	L4177	L4178	L4179	L4180	L4181	L4182	L4183	L4184	L4185	L4186	L4187	L4188	L4189	L4190	L4191	L4192	L4193	L4194	L4195	L4196	L4197	L4198	L4199	L4200	L4201	L4202	L4203	L4204	L4205	L4206	L4207	L4208	L4209	L4210	L4211	L4212	L4213	L4214	L4215	L4216	L4217	L4218	L4219	L4220	L4221	L4222	L4223	L4224	L4225	L4226	L4227	L4228	L4229	L4230	L4231	L4232	L4233	L4234	L4235	L4236	L4237	L4238	L4239	L4240	L4241	L4242	L4243	L4244	L4245	L4246	L4247	L4248	L4249	L4250	L4251	L4252	L4253	L4254	L4255	L4256	L4257	L4258	L4259	L4260	L4261	L4262	L4263	L4264	L4265	L4266	L4267	L4268	L4269	L4270	L4271	L4272	L4273	L4274	L4275	L4276	L4277	L4278	L4279	L4280	L4281	L4282	L4283	L4284	L4285	L4286	L4287	L4288	L4289	L4290	L4291	L4292	L4293	L4294	L4295	L4296	L4297	L4298	L4299	L4300	L4301	L4302	L4303	L4304	L4305	L4306	L4307	L4308	L4309	L4310	L4311	L4312	L4313	L4314	L4315	L4316	L4317	L4318	L4319	L4320	L4321	L4322	L4323	L4324	L4325	L4326	L4327	L4328	L4329	L4330	L4331	L4332	L4333	L4334	L4335	L4336	L4337	L4338	L4339	L4340	L4341	L4342	L4343	L4344	L4345	L4346	L4347	L4348	L4349	L4350	L4351	L4352	L4353	L4354	L4355	L4356	L4357	L4358	L4359	L4360	L4361	L4362	L4363	L4364	L4365	L4366	L4367	L4368	L4369	L4370	L4371	L4372	L4373	L4374	L4375	L4376	L4377	L4378	L4379	L4380	L4381	L4382	L4383	L4384	L4385	L4386	L4387	L4388	L4389	L4390	L4391	L4392	L4393	L4394	L4395	L4396	L4397	L4398	L4399	L4400	L4401	L4402	L4403	L4404	L4405	L4406	L4407	L4408	L4409	L4410	L4411	L4412	L4413	L4414	L4415	L4416	L4417	L4418	L4419	L4420	L4421	L4422	L4423	L4424	L4425	L4426	L4427	L4428	L4429	L4430	L4431	L4432	L4433	L4434	L4435	L4436	L4437	L4438	L4439	L4440	L4441	L4442	L4443	L4444	L4445	L4446	L4447	L4448	L4449	L4450	L4451	L4452	L4453	L4454	L4455	L4456	L4457	L4458	L4459	L4460	L4461	L4462	L4463	L4464	L4465	L4466	L4467	L4468	L4469	L4470	L4471	L4472	L4473	L4474	L4475	L4476	L4477	L4478	L4479	L4480	L4481	L4482	L4483	L4484	L4485	L4486	L4487	L4488	L4489	L4490	L4491	L4492	L4493	L4494	L4495	L4496	L4497	L4498	L4499	L4500	L4501	L4502	L4503	L4504	L4505	L4506	L4507	L4508	L4509	L4510	L4511	L4512	L4513	L4514	L4515	L4516	L4517	L4518	L4519	L4520	L4521	L4522	L4523	L4524	L4525	L4526	L4527	L4528	L4529	L4530	L4531	L4532	L4533	L4534	L4535	L4536	L4537	L4538	L4539	L4540	L4541	L4542	L4543	L4544	L4545	L4546	L4547	L4548	L4549	L4550	L4551	L4552	L4553	L4554	L4555	L4556	L4557</
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	---------



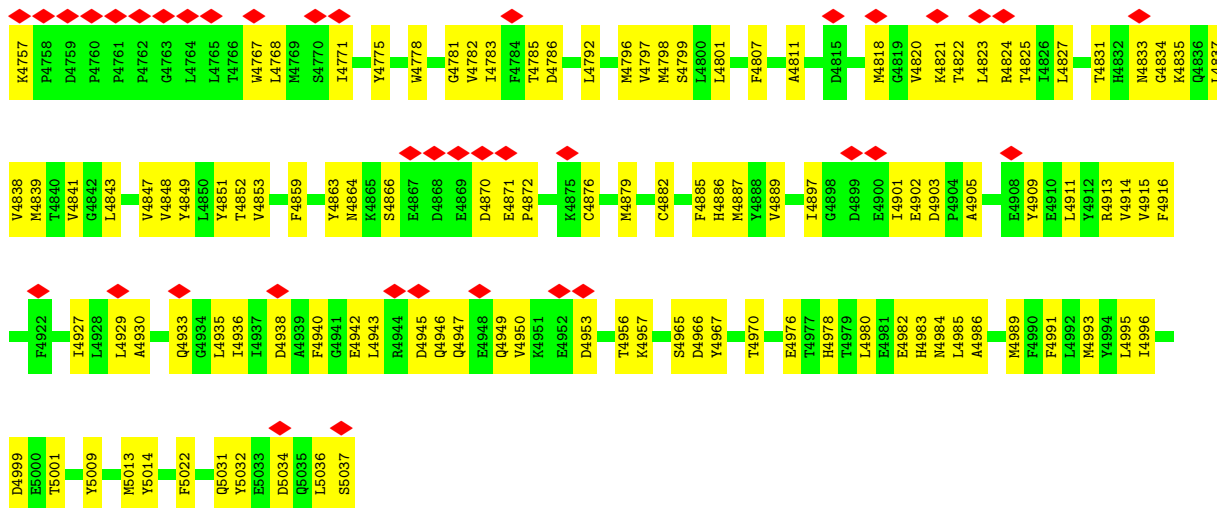




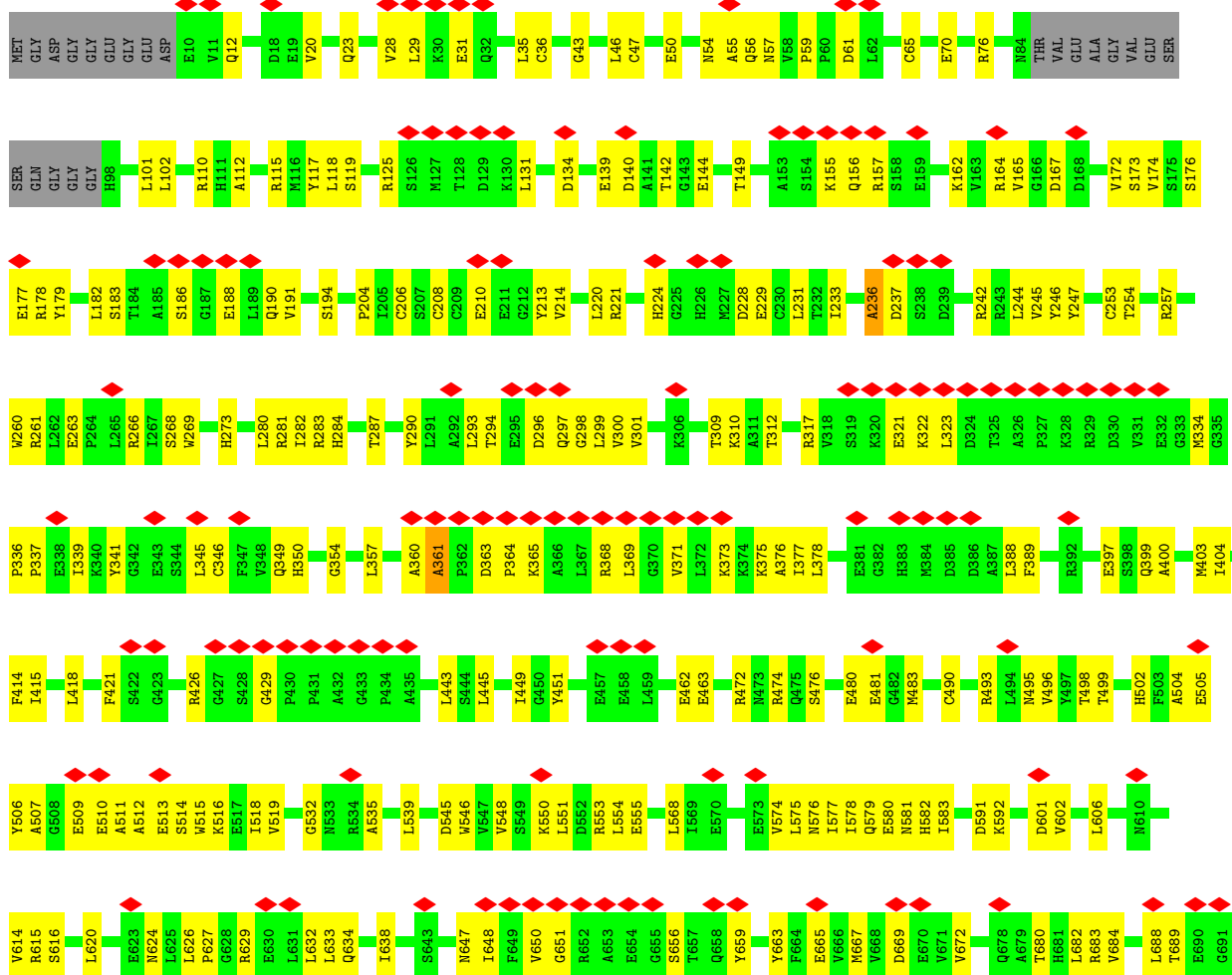


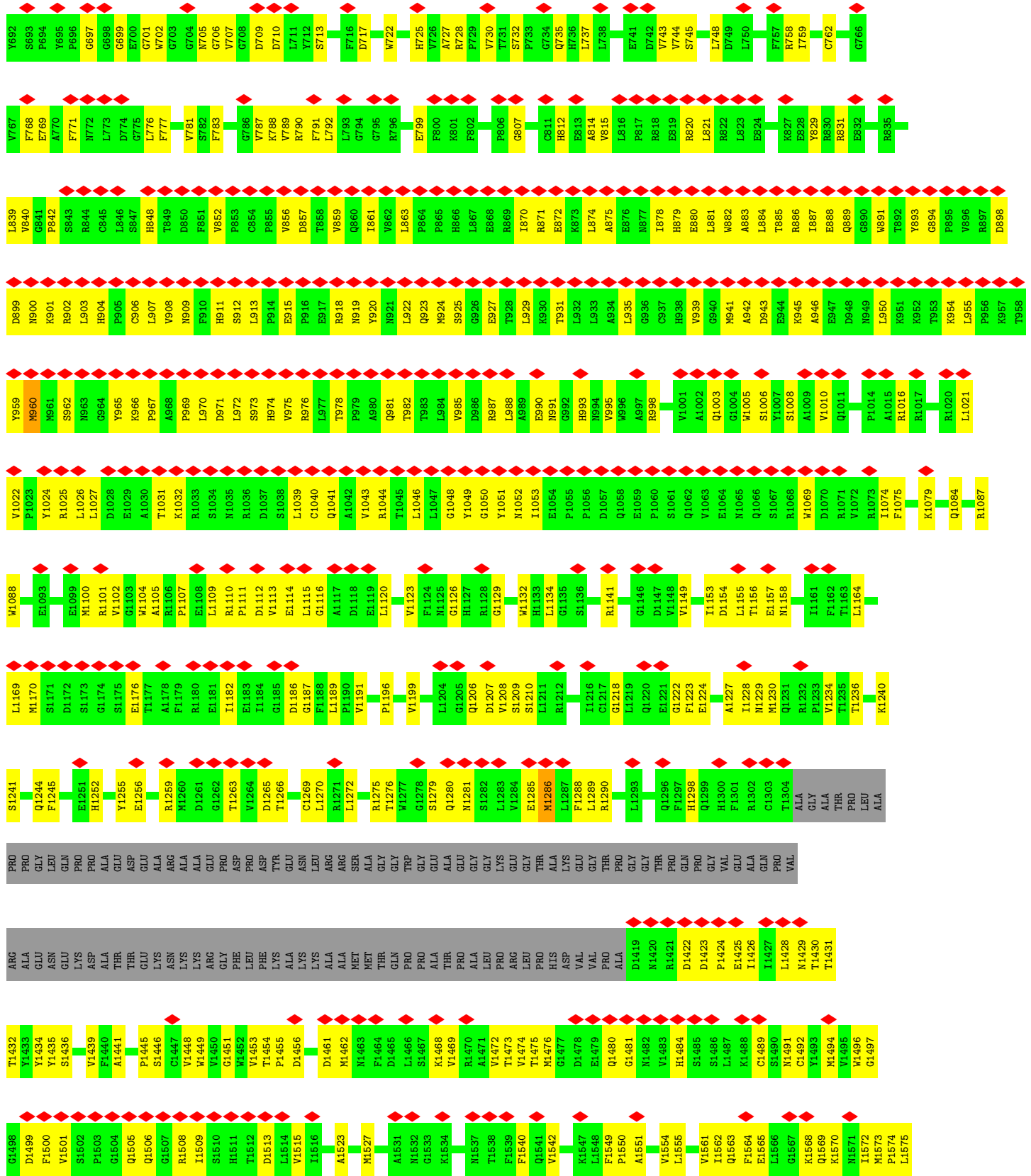
E2893	R2953	H3013	R3073	T3133	L3194	G3254	S3314	A3374	F3435	LYS	H3558	Y3619
L2894	R2954	C3014	S3074	V3134	A3195	G3255	L3315	E3375	R3436	R3498	L3559	W3620
E2895	F2955	L3015	L3075	A3135	R3196	L2256	L3316	E3376	M3437	R3499	Q3560	H3621
A2896	F2956	Y3016	D3076	L3136	L3197	A3257	G3317	E3377	Y3438	G3500	R3561	X3622
K2897	F2957	F3017	A3077	N3318	N3318	E2258	I3319	Q3378	G3439	D3501	R3562	L3623
G2898	G2958	L3018	R3078	L3137	A3198	S2259	L3319	L3379	E3440	R3502	V3563	L3624
G2899	F2959	S3019	T3079	F3138	A3200	A3200	L3320	R3380	F3441	Y3503	E3564	S3625
G2900	L2960	T3020	V3080	V3139	A3201	A3261	R3321	R3381	F3442	S3504	G3565	K3626
T2901	Q2961	P3021	M3081	L3140	M3201	R3262	I3322	L3381	I3443	V3505	S3566	R3627
T2902	Q2962	A3022	K3082	T3141	F3202	Y3263	F3203	A3382	Y3444	Q3506	P3567	R3628
F2903	L2963	K3023	S3083	T3142	A3204	T3264	V3324	K3384	K3447	T3507	S3568	R3629
L2904	L2964	V3024	G3084	L3143	F3205	F3265	N3325	A3385	S3448	S3508	L3569	R3630
L2905	W2966	K3025	F3085	Q3145	L3206	M3266	N3326	E3386	H3449	L3509	R3570	A3631
V2906	M2967	G3026	E3086	H3146	F3207	F3267	L3327	A3387	H3450	L3510	W3571	V3632
P2907	M2968	S3027	I3087	L3147	F3208	H3268	G3328	E3388	F3451	V3511	K3572	V3633
Y2908	I2969	G3028	V3088	A3148	F3209	V3269	I3329	E3389	K3452	A3512	A3574	A3634
D2909	S2970	S3029	K3089	Q3149	Q3209	I3270	D3330	G3390	Q3456	L3513	L3575	C3635
T2910	Q2971	H3030	A3090	H3150	N3210	E3271	E3331	E3391	N3457	L3514	Y3576	F3636
L2911	E2972	A3031	G3091	Q3151	N3211	I3272	A3332	L3392	M3457	K3515	R3577	R3637
T2912	F2973	S3032	L3092	F3152	E3212	T3273	T3333	L3393	F3458	K3516	G3578	M3638
A2913	I2974	N3033	R3093	G3153	Y3213	L3274	V3334	L3394	V3459	M3517	L3579	T3639
K2914	A2975	K3034	S3094	D3154	N3214	P3275	M3335	R3395	V3460	V3460	P3580	F3640
E2915	H2976	E3035	F3095	D3155	C3216	M3276	K3336	D3396	Q3461	Q3461	G3581	L3641
K2916	L2977	K3036	F3096	I3157	S3217	L3277	A3337	E3397	F3462	N3462	R3582	Y3642
A2917	E2978	E3037	S3098	L3158	Y3218	C3278	L3338	F3398	E3463	E3463	E3583	L3644
R2918	A2979	M3038	A3099	D3159	Y3219	S3279	A3339	S3399	M3464	M3464	E3584	P3645
D2919	V2980	I3039	S3100	Q3160	T3220	L3281	V3340	V3400	N3465	N3465	D3585	R3646
R2920	V2981	T3040	E3101	V3161	T3221	P3282	F3341	L3401	M3466	M3466	A3586	A3649
E2921	S2982	S3041	D3102	Q3162	K3222	R3283	A3342	C3402	K3467	S3468	F3587	C3650
K2922	S2983	L3042	T3103	W3163	S3223	W3284	Q3343	R3403	F3469	F3469	R3588	N3651
A2923	G2984	F3043	E3104	S3164	F3224	W3285	P3344	E3404	L3470	L3470	D3589	F3652
Q2924	R2985	C3044	K3105	C3165	R3225	E3286	L3345	D3404	L3471	L3471	E3590	L3654
E2925	V2986	K3045	M3106	Y3166	E3226	G3288	V3346	Y3406	T3471	T3471	K3591	Y3657
L2926	E2987	R3046	V3107	R3167	R3227	G3289	S3347	A3407	A3472	A3472	V3592	K3658
L2927	K2988	A3047	E3108	T3168	A3228	P3289	R3348	L3408	D3473	D3473	R3593	A3659
K2928	S2989	A3048	N3109	L3169	I3229	E3290	A3349	Y3409	S3474	S3474	R3594	A3660
F2929	P2990	L3049	V3050	L3170	G3230	A3291	R3350	P3410	S3476	S3476	V3595	W3661
L2930	H2991	R3051	R3111	I3172	C3231	P3292	F3352	L3411	K3477	K3477	Q3597	L3662
Q2931	E2992	H3052	L3112	S3173	L3232	P3293	L3353	E3413	M3478	A3479	E3598	E3665
M2932	Q2993	K3053	G3113	S3174	P3233	A3294	H3354	R3414	LYS	ALA	L3603	D3671
M2933	E2994	R3053	K3114	L3175	N3234	G3295	H3355	Y3415	ALA	ALA	Y3604	R3672
G2934	I2995	V3054	V3115	G3176	S3235	L3296	S3356	V3416	ALA	GLY	L3605	L3673
Y2935	K2996	S3055	V3116	T3177	Y3236	P3297	H3357	D3417	GLY	GLY	E3607	E3680
A2936	F2997	L3056	GLN	R3178	E3237	A3298	F3358	R3420	ASP	ASP	G3608	G3681
W2937	F2998	F3057	ALA	K3179	E3238	A3299	I3359	R3421	ALA	ALA	T3609	E3682
T2938	A2999	R3058	ARG	N3180	H3239	G3299	L3360	A3421	GLN	GLN	E3610	E3683
R2939	K3000	T3059	THR	T3181	H3239	H3239	T3361	H3422	SER	SER	R3611	E3684
GLY	I3001	D3060	GLN	F3182	C3240	P3301	I3362	W3423	GLY	GLY	P3612	R3685
LEU	L3002	A3061	VAL	V3183	P3241	P3302	G3363	N3428	GLY	GLY	K3614	E3686
LYS	L3002	P3062	K3123	E3184	D3242	P3303	G3364	N3429	ASP	ASP	S3615	S3615
ASP	L3003	A3063	G3124	E3185	L3243	C3304	R3365	A3429	GLU	GLU	K3616	K3616
MET	P3004	A3063	V3125	K3185	P3244	T3305	R3366	E3427	GLU	GLU	K3617	K3617
GLU	L3005	V3064	Q3126	L3186	V3245	A3306	K3367	N3428	ARG	ARG	A3618	A3618
L2946	I3006	V3065	Q3127	R3187	L3246	V3307	R3368	A3429	THR	THR	E3661	E3661
D2947	N3007	V3066	N3128	P3188	D3247	T3308	A3369	A3429	LYS	LYS	E3662	E3662
T2948	Q3008	C3067	L3129	A3189	R3248	S3309	G3370	A3431	LYS	LYS	E3663	E3663
S2949	F3009	L3068	T3130	L3190	L3249	H3311	K3371	E3432	LYS	LYS	E3664	E3664
S2950	F3010	H3069	Y3131	G3191	M3250	H3312	V3372	E3433	LYS	LYS	E3665	E3665
T2951	N3011	L3070	T3132	E3192	D3252	N3313	V3373	L3434	LYS	LYS	E3666	E3666
E2952	N3012	A3072	A3072	C3193	I3253							





• Molecule 1: Ryanodine receptor 1



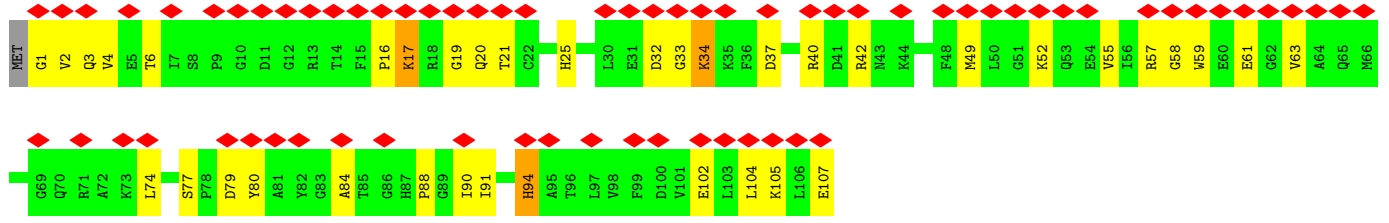




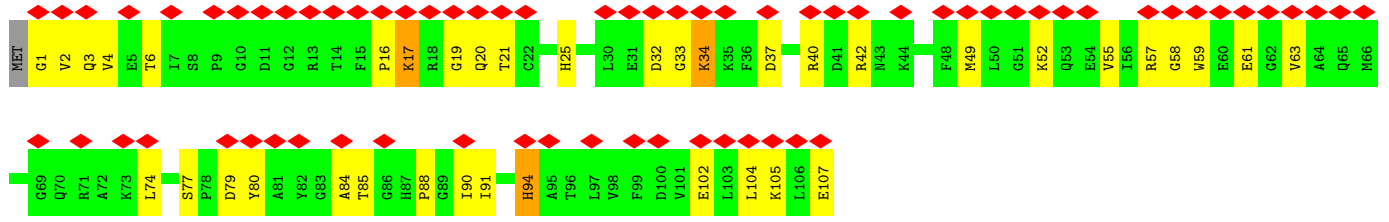
A3300	A3301	P3301	P3302	P3303	P3304	C3304	T3305	A3306	T3307	T3308	S3309	D3310	H3311	L3312	N3313	S3314	L3315	L3316	G3317	N3318	T3319	L3320	R3321	L3322	L3323	V3324	N3325	N3326	N3327	G3328	L3329	D3330	A3331	A3332	T3333	N3334	N3335	K3336	R3337	L3338	L3339	V3340	F3341	A3342	O3343	F3344	I3345	V3346	R3347	R3348	A3349	R3350	F3351	E3352	L3353	L3354	H3355	S3356	F3357	F3358	I3359					
G3240	P3241	D3242	I3243	P3244	V3245	L3246	D3247	R3248	L3249	M3250	A3251	D3252	I3253	G3254	G3255	L3256	A3257	E3258	S3259	G3260	A3261	R3262	F3263	T3264	E3265	M3266	K3267	H3268	V3269	I3270	N3271	I3272	T3273	T3274	N3275	N3276	K3277	L3278	S3279	G3280	R3281	S3282	T3283	T3284	N3285	E3286	R3287	G3288	P3289	E3290	A3291	P3292	P3293	P3294	L3295	L3296	P3297	A3298	G3299							
N3180	T3181	Y3182	V3183	E3184	K3185	L3186	R3187	P3188	A3189	L3190	G3191	E3192	C3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	Y3213	N3214	A3215	C3216	S3217	V3218	Y3219	T3220	K3221	K3222	S3223	P3224	R3225	E3226	R3227	A3228	L3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3238	M3239								
ARG	THR	GLN	VAL	K3123	G3124	V3125	Q3127	N3128	L3129	T3130	Y3131	T3132	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140	T3141	T3142	L3143	F3144	Q3145	H3146	I3147	A3148	Q3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	I3157	L3158	D3159	D3160	V3161	C3162	V3163	S3164	C3165	R3166	T3167	L3168	L3169	I3172	Y3173	S3174	L3175	G3176	T3177	L3178	K3179	ALA								
T3059	D3060	A3061	P3062	A3063	V3064	V3065	N3066	C3067	L3068	H3069	I3070	L3071	A3072	R3073	S3074	L3075	D3076	A3077	R3078	T3079	V3080	M3081	K3082	S3083	G3084	F3085	E3086	I3087	V3088	K3089	A3090	G3091	L3092	R3093	D3094	S3095	F3096	F3097	S3098	A3099	S3100	E3101	D3102	T3103	E3104	K3105	M3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA							
A2999	K3000	T3001	L3002	L3003	P3004	L3005	T3006	N3007	Q3008	Y3009	F3010	T3011	N3012	H3013	C3014	L3015	Y3016	F3017	L3018	S3019	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	A3031	S3032	N3033	K3034	E3035	K3036	E3037	M3038	L3039	T3040	S3041	L3042	F3043	C3044	K3045	L3046	A3047	A3048	L3049	V3050	R3051	H3052	Q3053	R3054	S3055	L3056	F3057	G3058							
R2939	GLY	L3940	D2947	T2948	S2949	S2950	I2951	E2952	K2953	R2954	F2955	A2956	F2957	G2958	F2959	L2960	Q2961	Q2962	L2963	L2964	R2965	V2966	M2967	I2968	L2969	S2970	Q2971	E2972	F2973	I2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	P2989	E2992	H2991	E2993	E2994	L2995	K2996	F2997	F2998	T2998												
A2879	E2880	N2881	Y2882	H2883	N2884	T2885	K2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	K2897	G2898	G2899	Q2901	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	Y2909	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	K2927	A2928	P2929	H2929	E2932	Q2931	N2932	N2933	G2934	Y2935	V2937	T2938						
W2819	E2820	W2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	THR	GLU	THR	L3958	L3959	L3960	L3961	L3962	L3963	L3964	R3965	V3966	M3967	I3968	L3969	S3970	Q3971	E3972	F3973	I3974	A3975	H3976	L3977	E3978	A3979	V3980	V3981	S3982	S3983	G3984	R3985	V3986	E3987	K3988	P3989	E3992	H3991	E3993	E3994	L3995	K3996	F3997	F3998	T3998									
A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	Q2771	Q2772	N2773	W2774	W2775	A2776	Y2777	G2778	G2779	E2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	N2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	L2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	T2817	A2818							
L2633	N2634	E2635	F2636	A2637	L2641	K2642	L2643	L2644	H2647	Y2648	E2649	R2650	C2651	Y2655	C2656	L2657	P2658	T2659	G2660	N2663	F2664	G2665	V2666	T2667	S2668	E2669	E2670	E2671	L2672	H2673	L2674	T2675	R2676	K2677	L2678	F2679	V2680	G2681	I2682	F2683	D2684	S2685	L2686	A2687	H2688	K2689	K2690	Y2691	D2692	Q2693	E2694	L2695	Y2696	R2697	M2698											
A2689	M2700	P2701	C2702	L2703	C2704	A2705	L2706	A2707	G2708	L2710	P2711	D2712	D2713	Y2714	V2715	D2716	A2717	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	L3958	L3959	L3960	L3961	L3962	L3963	L3964	R3965	V3966	M3967	I3968	L3969	S3970	Q3971	E3972	F3973	I3974	A3975	H3976	L3977	E3978	A3979	V3980	V3981	S3982	S3983	G3984	R3985	V3986	E3987	K3988	P3989	E3992	H3991	E3993	E3994	L3995	K3996	F3997	F3998	T3998



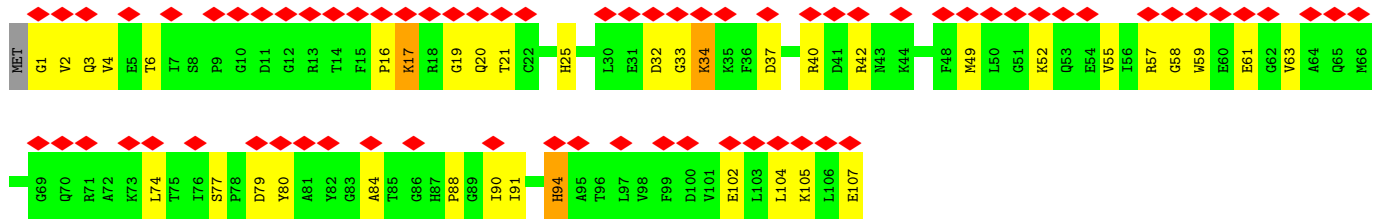




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113183	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 ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.268	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	427.008, 427.008, 427.008	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, ATP, A1BD2

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	0.21	1/35977 (0.0%)	0.47	27/48726 (0.1%)
1	B	0.21	1/35977 (0.0%)	0.47	27/48726 (0.1%)
1	C	0.21	1/35977 (0.0%)	0.47	26/48726 (0.1%)
1	D	0.21	1/35977 (0.0%)	0.47	27/48726 (0.1%)
2	E	0.32	0/850	0.81	6/1146 (0.5%)
2	F	0.32	0/850	0.81	6/1146 (0.5%)
2	G	0.32	0/850	0.81	6/1146 (0.5%)
2	H	0.32	0/850	0.81	6/1146 (0.5%)
All	All	0.22	4/147308 (0.0%)	0.48	131/199488 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	6
1	D	0	6
All	All	0	24

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2440	MET	SD-CE	5.18	1.92	1.79
1	C	2440	MET	SD-CE	5.18	1.92	1.79
1	A	2440	MET	SD-CE	5.17	1.92	1.79
1	D	2440	MET	SD-CE	5.17	1.92	1.79

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	3622	LYS	CB-CG-CD	14.01	143.52	111.30
1	B	3622	LYS	CB-CG-CD	14.00	143.51	111.30
1	C	3622	LYS	CB-CG-CD	14.00	143.51	111.30
1	D	3622	LYS	CB-CG-CD	13.98	143.46	111.30
1	A	3622	LYS	CG-CD-CE	13.35	142.01	111.30

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1025	ARG	Sidechain
1	A	2702	CYS	Peptide
1	A	3196	ARG	Sidechain
1	A	3366	ARG	Sidechain
1	A	3436	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35150	0	34795	1578	0
1	B	35150	0	34795	1574	0
1	C	35150	0	34795	1594	0
1	D	35150	0	34795	1595	0
2	E	831	0	831	45	0
2	F	831	0	831	43	0
2	G	831	0	831	44	0
2	H	831	0	831	43	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	18	0	0	3	0
6	B	18	0	0	3	0
6	C	18	0	0	3	0
6	D	18	0	0	3	0
All	All	144128	0	142552	6434	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 22.

The worst 5 of 6434 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:D:3365:LEU:HD11	1:D:3405:LEU:HD23	1.43	1.00
1:B:899:ASP:OD1	1:B:902:ARG:NH2	1.95	0.99
1:B:3308:THR:OG1	1:B:3310:ASP:OD1	1.80	0.99
1:A:899:ASP:OD1	1:A:902:ARG:NH2	1.95	0.99
1:C:899:ASP:OD1	1:C:902:ARG:NH2	1.95	0.99

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	4385/5037 (87%)	4253 (97%)	128 (3%)	4 (0%)	48	76
1	B	4385/5037 (87%)	4254 (97%)	127 (3%)	4 (0%)	48	76
1	C	4385/5037 (87%)	4253 (97%)	128 (3%)	4 (0%)	48	76
1	D	4385/5037 (87%)	4254 (97%)	127 (3%)	4 (0%)	48	76
2	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
All	All	17960/20580 (87%)	17426 (97%)	518 (3%)	16 (0%)	49	76

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3300	ALA
1	A	4711	PHE
1	B	3300	ALA
1	B	4711	PHE
1	D	3300	ALA

### 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	3836/4276 (90%)	3819 (100%)	17 (0%)	84	82
1	B	3836/4276 (90%)	3819 (100%)	17 (0%)	84	82
1	C	3836/4276 (90%)	3819 (100%)	17 (0%)	84	82
1	D	3836/4276 (90%)	3819 (100%)	17 (0%)	84	82
2	E	89/90 (99%)	87 (98%)	2 (2%)	45	63
2	F	89/90 (99%)	87 (98%)	2 (2%)	45	63
2	G	89/90 (99%)	87 (98%)	2 (2%)	45	63
2	H	89/90 (99%)	87 (98%)	2 (2%)	45	63
All	All	15700/17464 (90%)	15624 (100%)	76 (0%)	81	80

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3622	LYS

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	2870[B]	GLU
1	C	960	MET
1	C	2584[B]	HIS
1	C	3856	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 177 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3109	ASN
1	C	1298	HIS
1	D	3523	ASN
1	D	4547	GLN
1	C	1941	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
3	ATP	B	5301	-	32,33,33	0.66	0	48,52,52	0.63	0
6	A1BD2	D	5304	-	19,19,19	0.38	0	28,28,28	0.46	0
6	A1BD2	A	5304	-	19,19,19	0.39	0	28,28,28	0.46	0
6	A1BD2	B	5304	-	19,19,19	0.39	0	28,28,28	0.46	0
3	ATP	A	5301	-	32,33,33	0.67	0	48,52,52	0.63	0
3	ATP	D	5301	-	32,33,33	0.67	0	48,52,52	0.63	0
3	ATP	C	5301	-	32,33,33	0.67	0	48,52,52	0.63	0
6	A1BD2	C	5304	-	19,19,19	0.38	0	28,28,28	0.46	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5301	-	-	8/22/38/38	0/3/3/3
6	A1BD2	D	5304	-	-	2/6/6/6	0/2/2/2
6	A1BD2	A	5304	-	-	2/6/6/6	0/2/2/2
6	A1BD2	B	5304	-	-	2/6/6/6	0/2/2/2
3	ATP	A	5301	-	-	8/22/38/38	0/3/3/3
3	ATP	D	5301	-	-	8/22/38/38	0/3/3/3
3	ATP	C	5301	-	-	8/22/38/38	0/3/3/3
6	A1BD2	C	5304	-	-	2/6/6/6	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

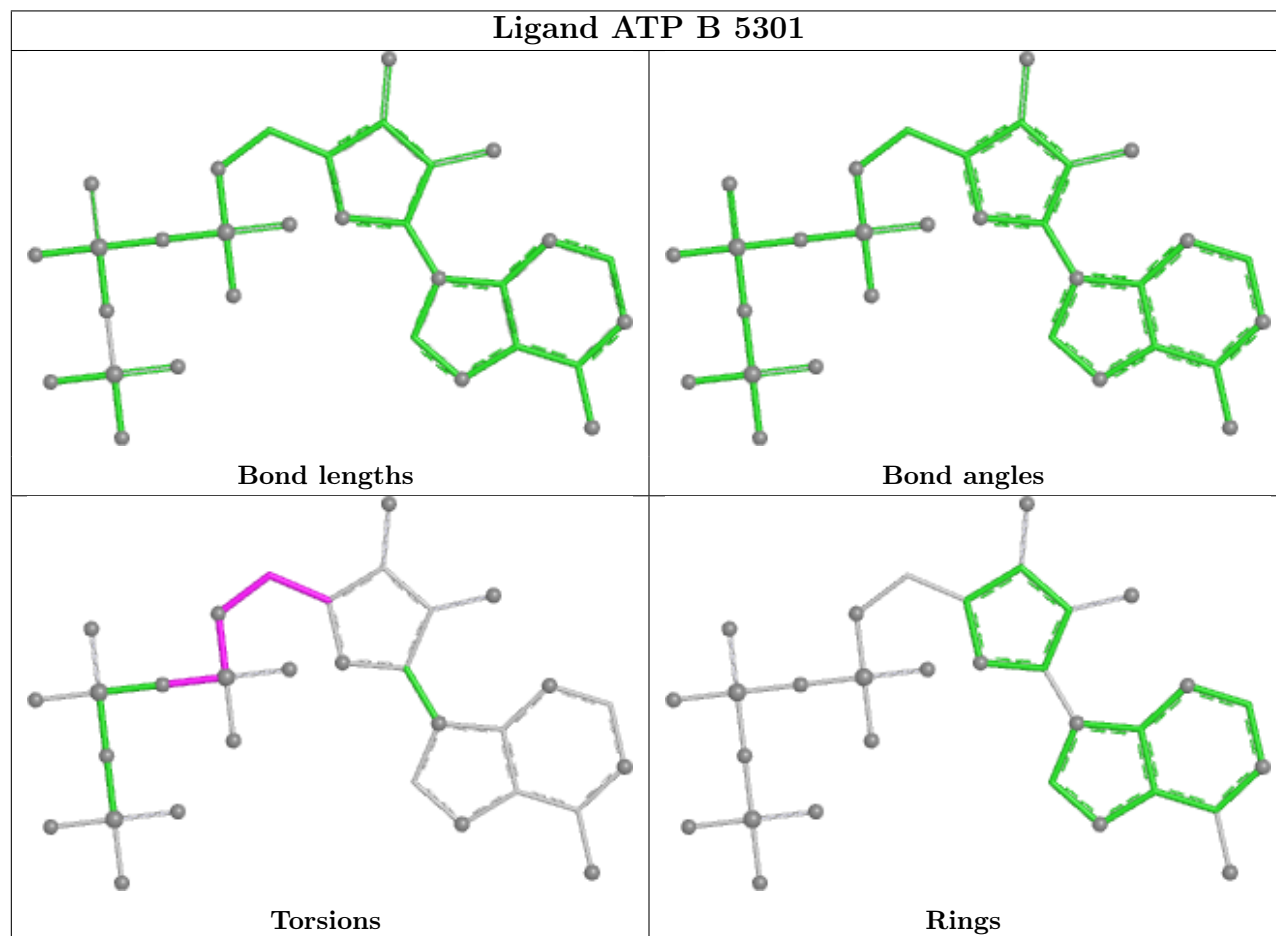
Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O2A
3	A	5301	ATP	C5'-O5'-PA-O3A
3	A	5301	ATP	C3'-C4'-C5'-O5'
3	B	5301	ATP	C5'-O5'-PA-O2A
3	B	5301	ATP	C5'-O5'-PA-O3A

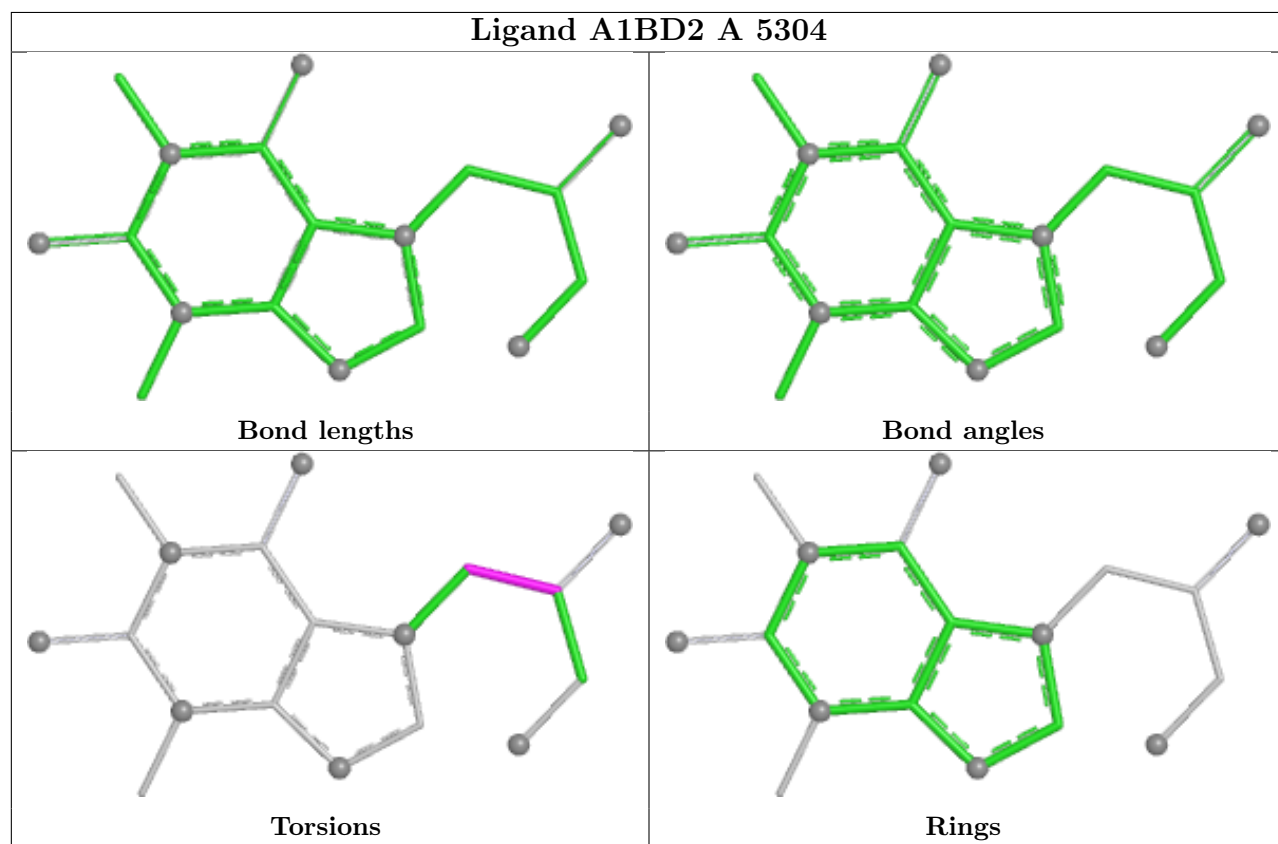
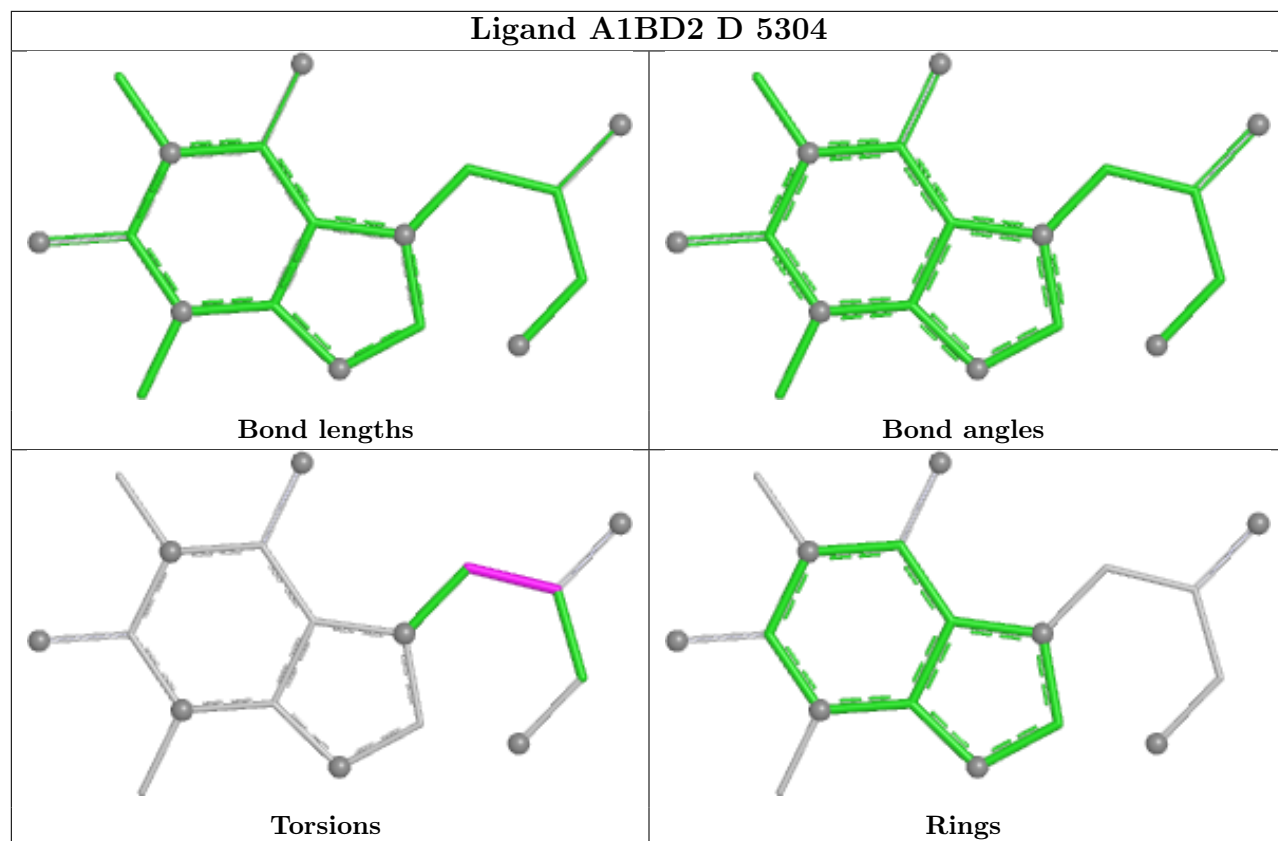
There are no ring outliers.

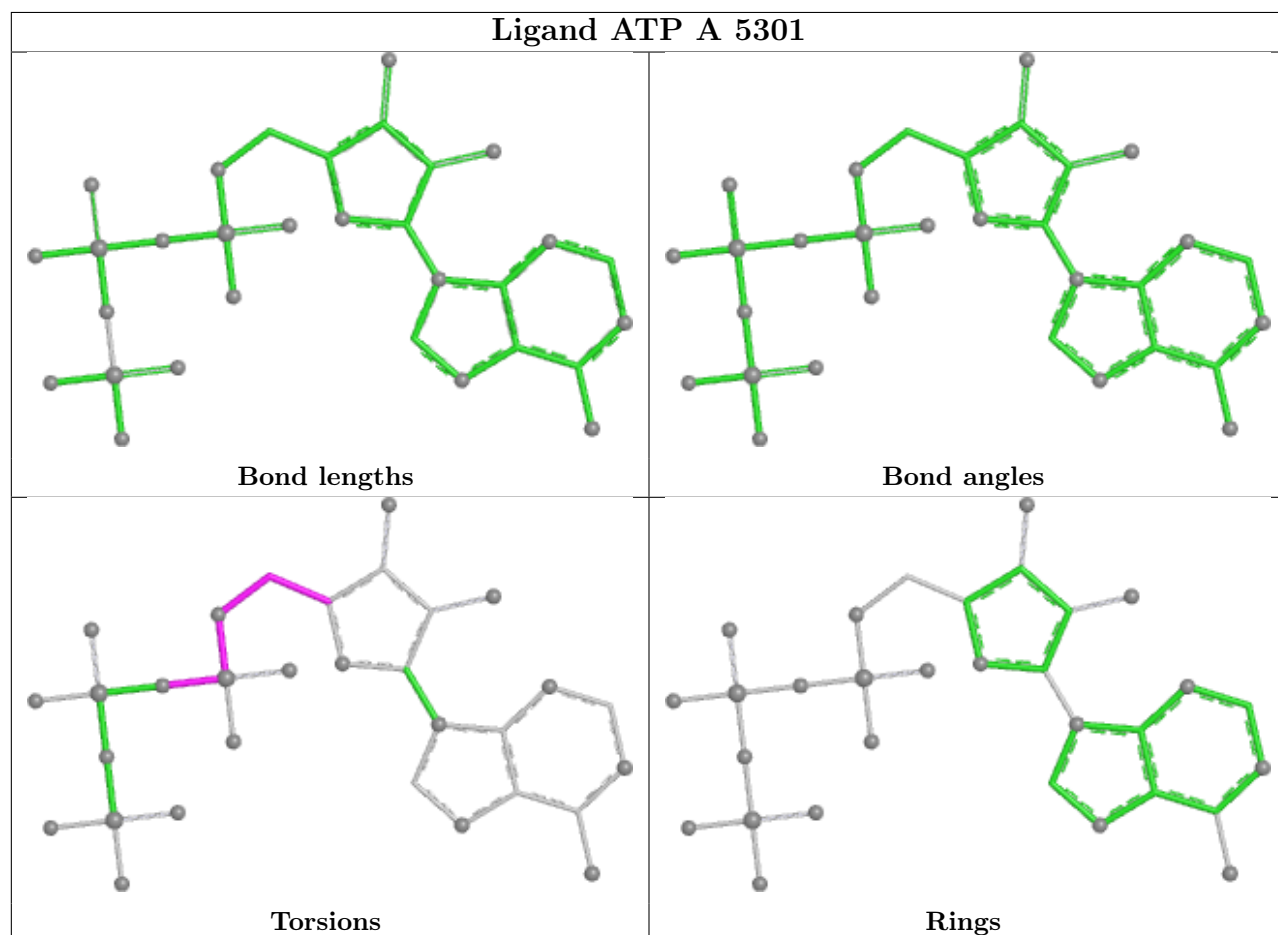
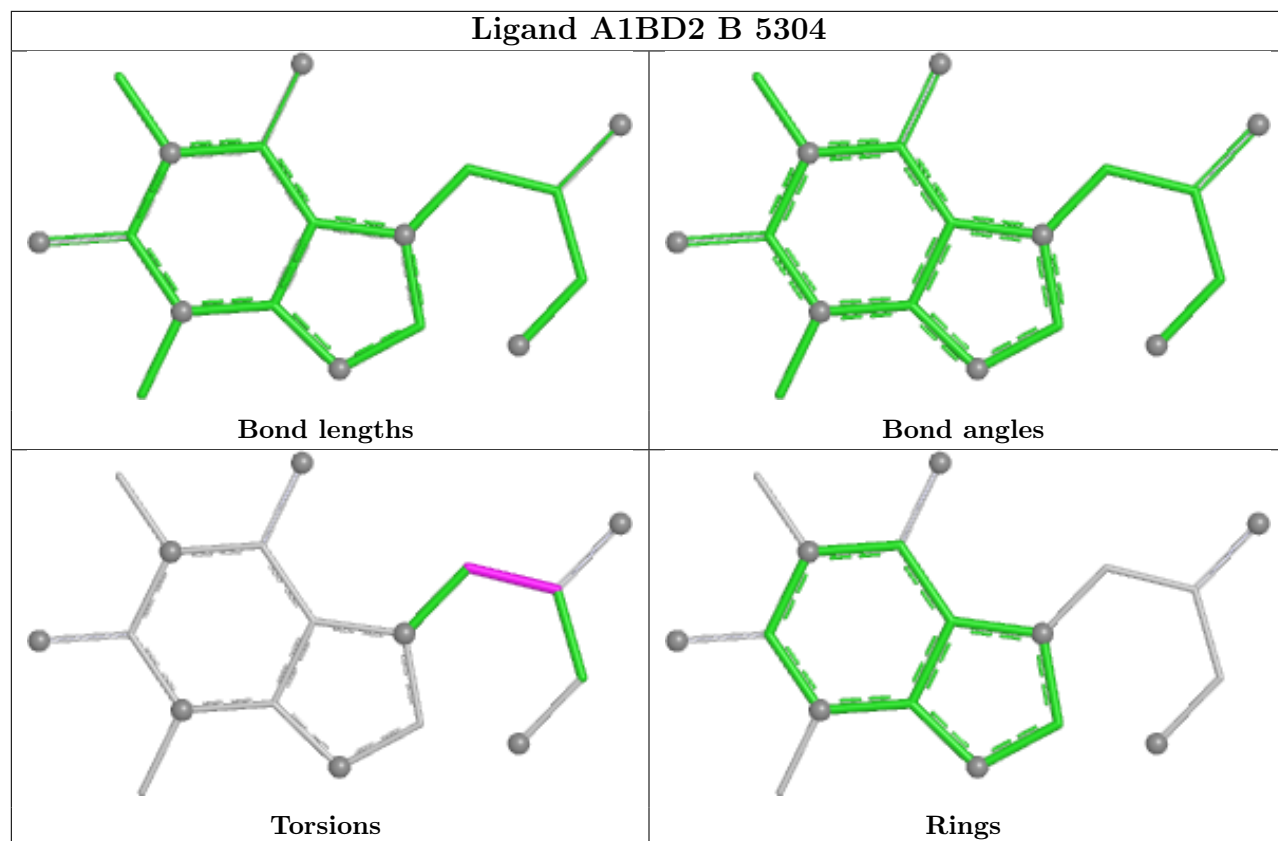
4 monomers are involved in 12 short contacts:

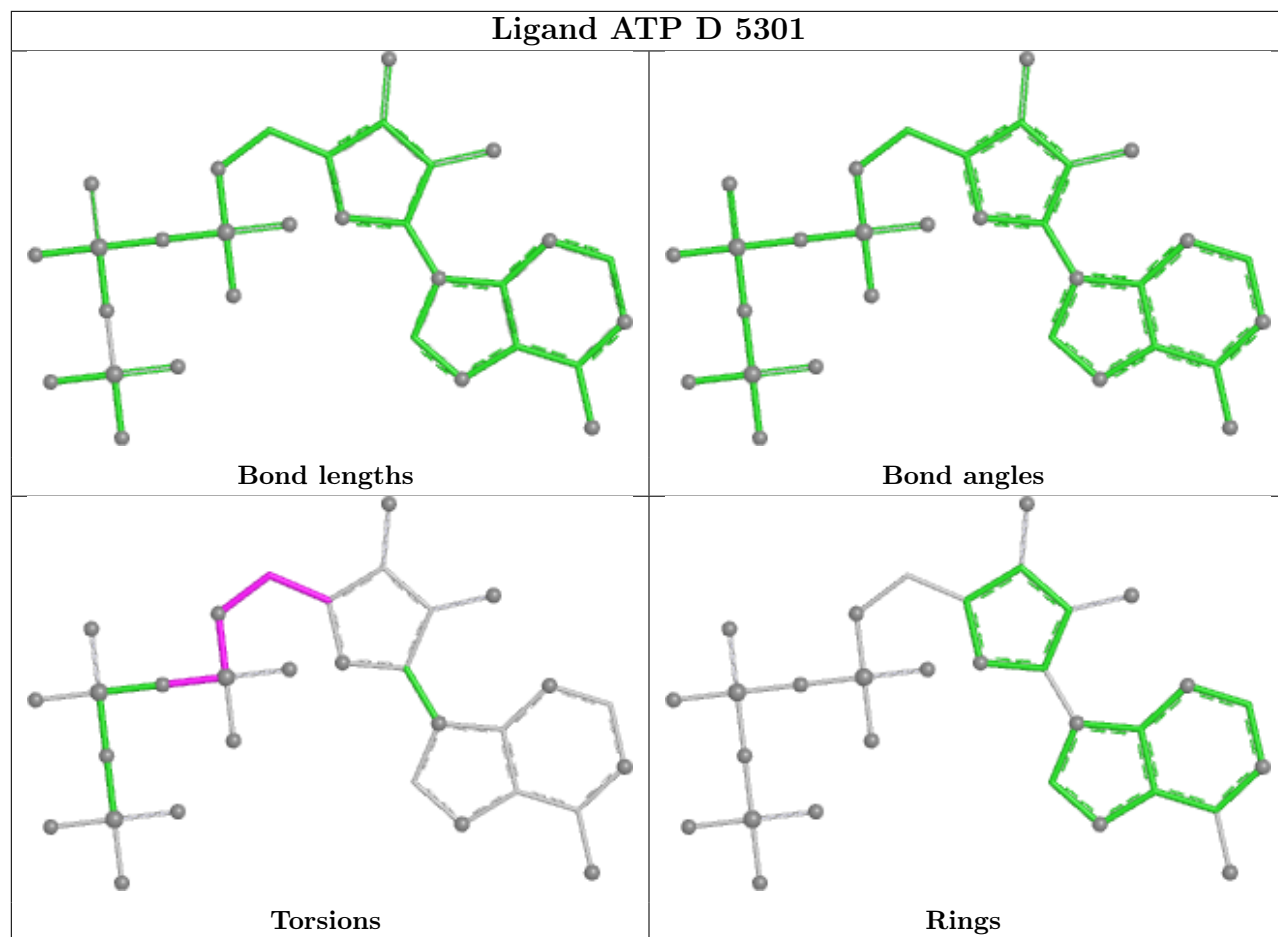
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	5304	A1BD2	3	0
6	A	5304	A1BD2	3	0
6	B	5304	A1BD2	3	0
6	C	5304	A1BD2	3	0

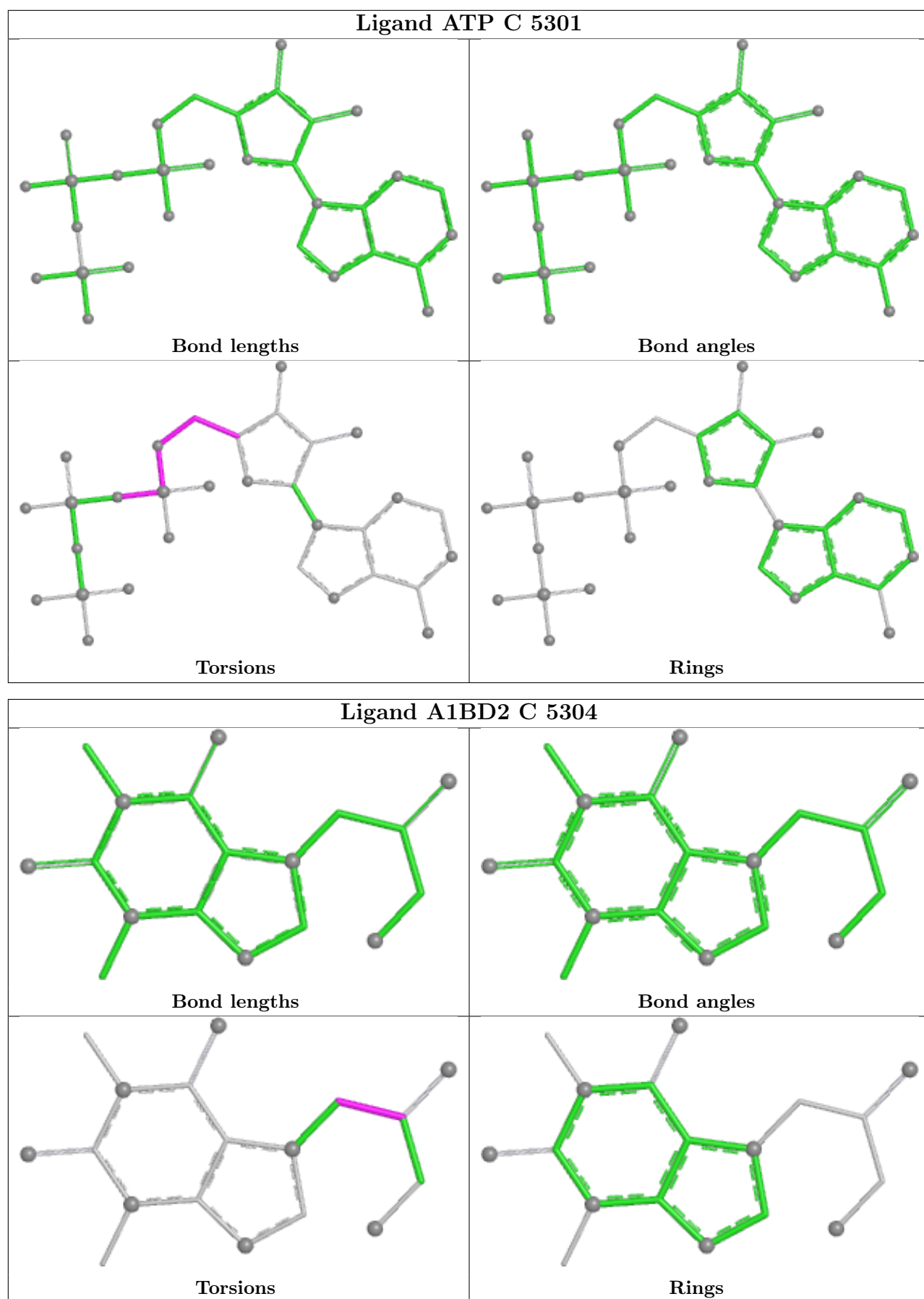
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

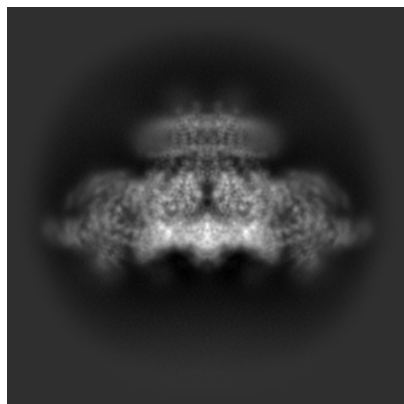
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47387. These allow visual inspection of the internal detail of the map and identification of artifacts.

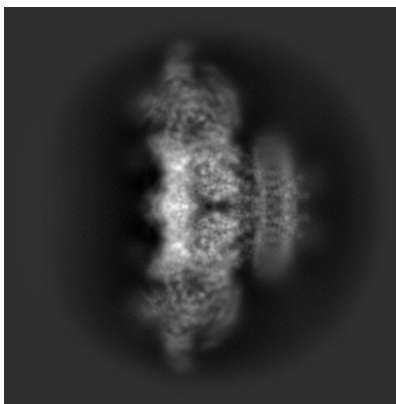
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

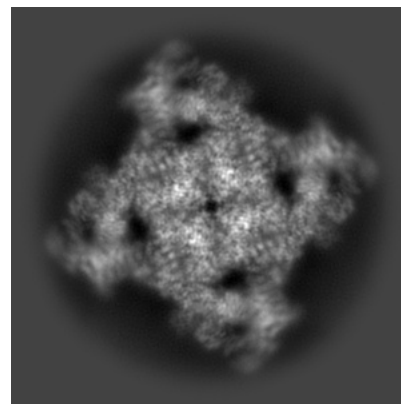
#### 6.1.1 Primary map



X

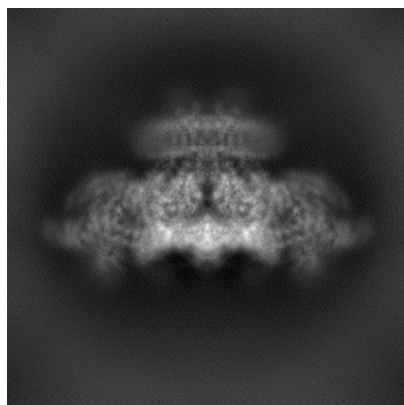


Y

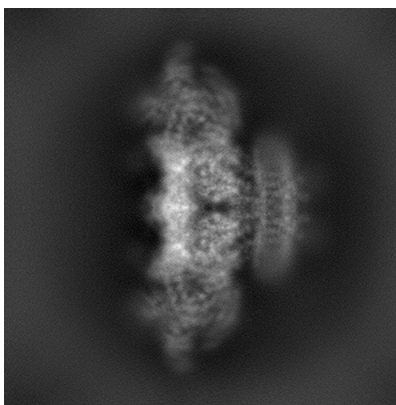


Z

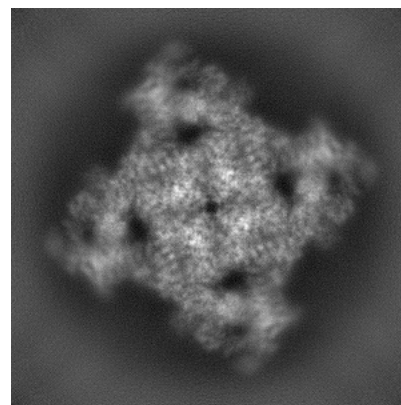
#### 6.1.2 Raw map



X



Y

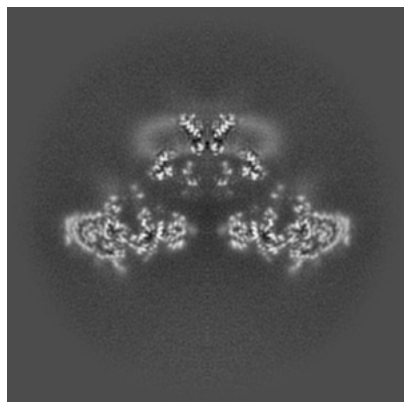


Z

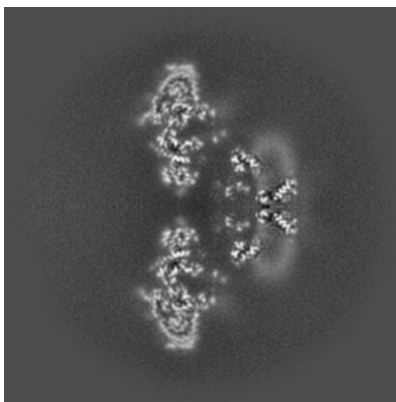
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

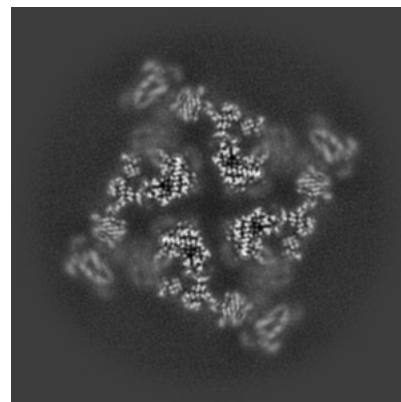
### 6.2.1 Primary map



X Index: 256

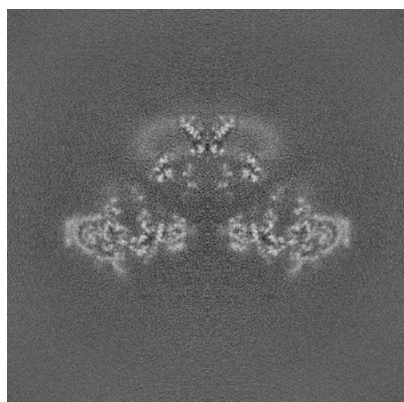


Y Index: 256

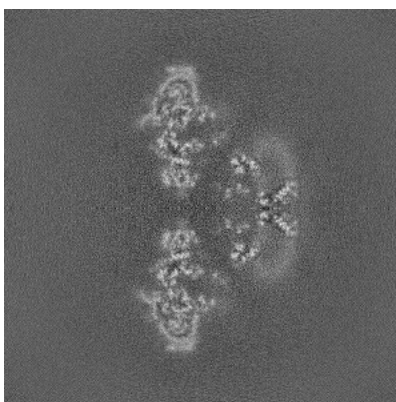


Z Index: 256

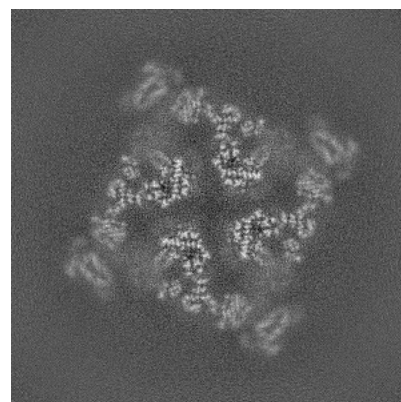
### 6.2.2 Raw map



X Index: 256



Y Index: 256

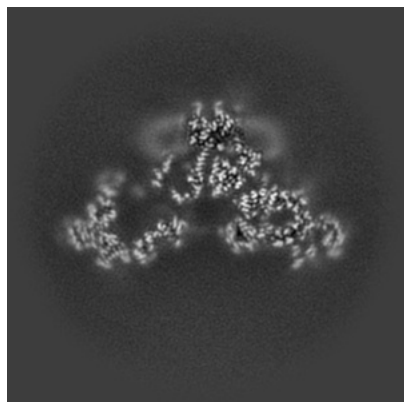


Z Index: 256

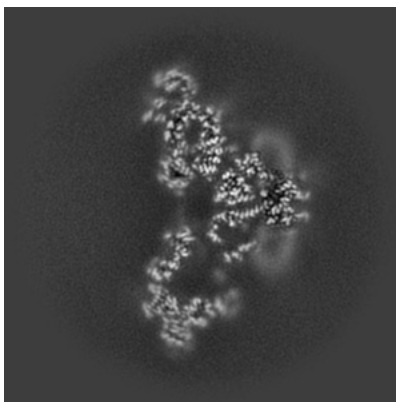
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

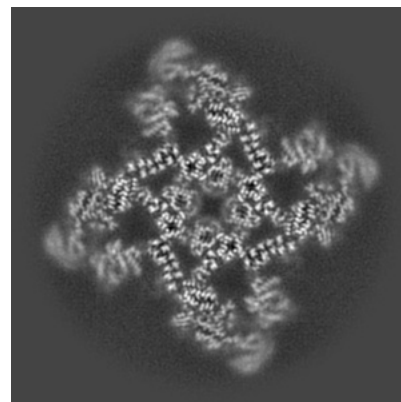
### 6.3.1 Primary map



X Index: 268

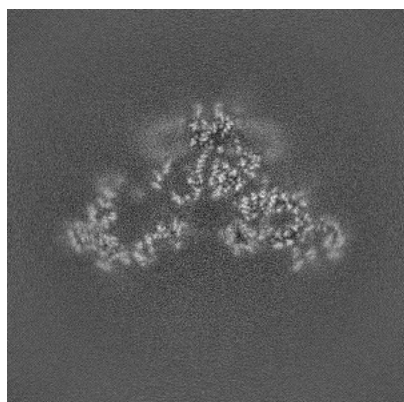


Y Index: 244

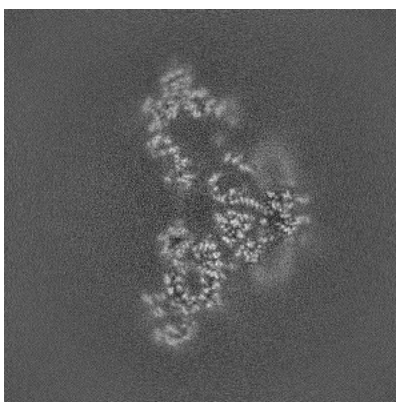


Z Index: 229

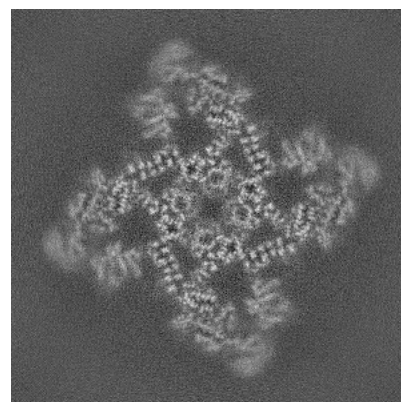
### 6.3.2 Raw map



X Index: 268



Y Index: 268

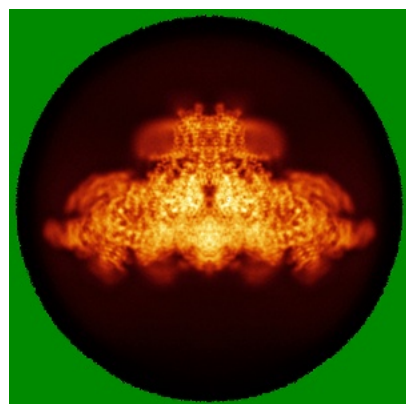


Z Index: 229

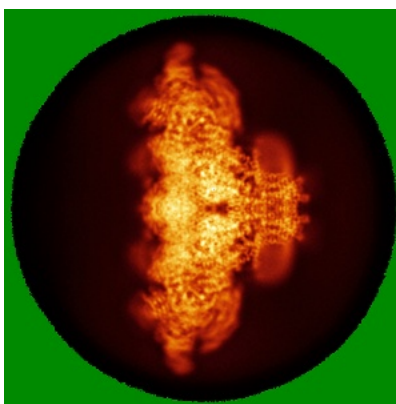
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

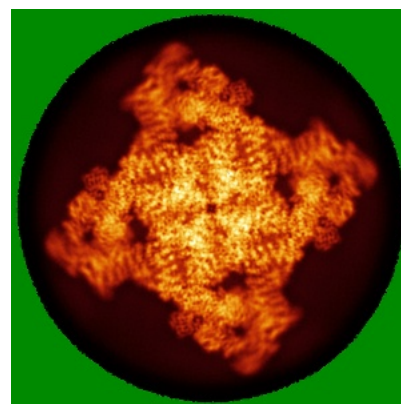
### 6.4.1 Primary map



X

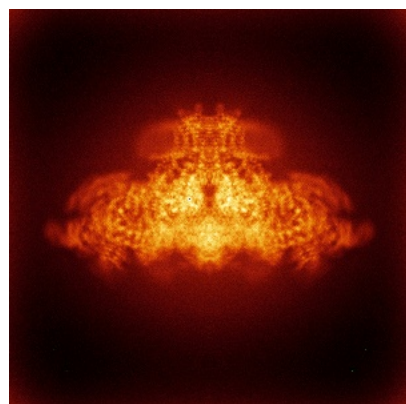


Y

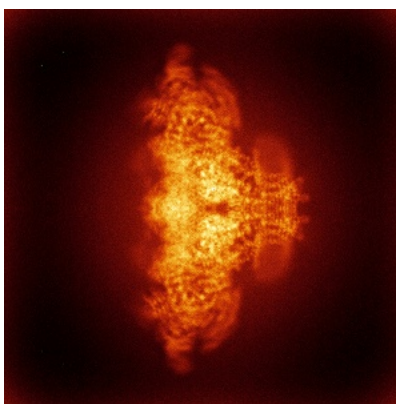


Z

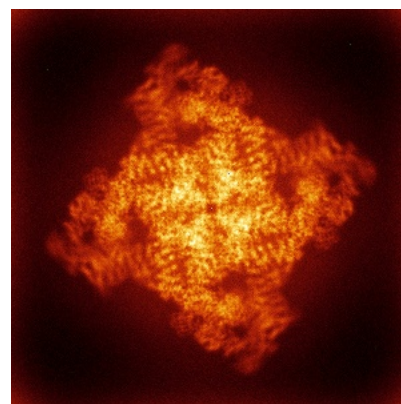
### 6.4.2 Raw map



X



Y

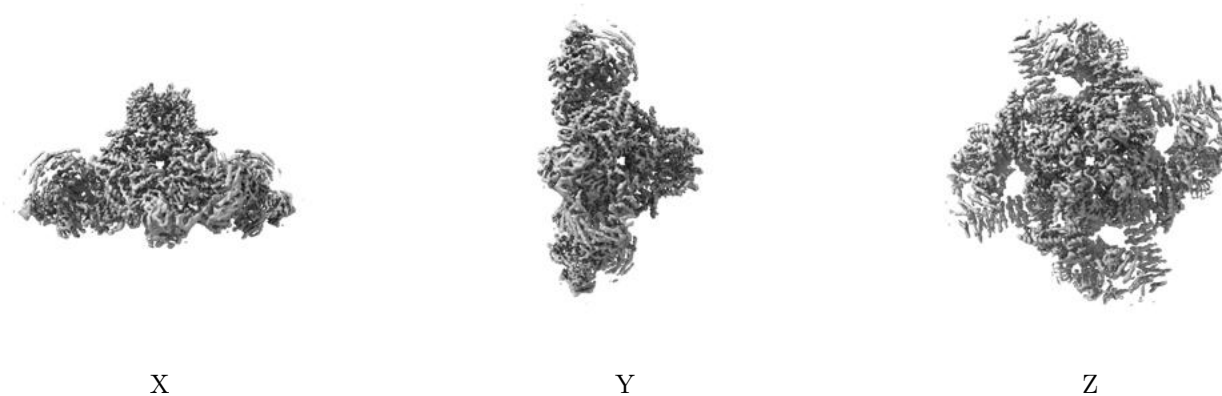


Z

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.

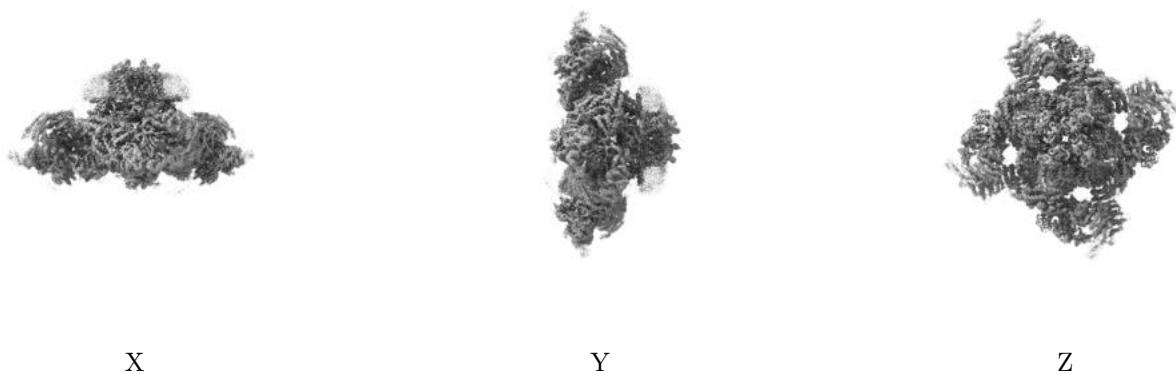
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



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

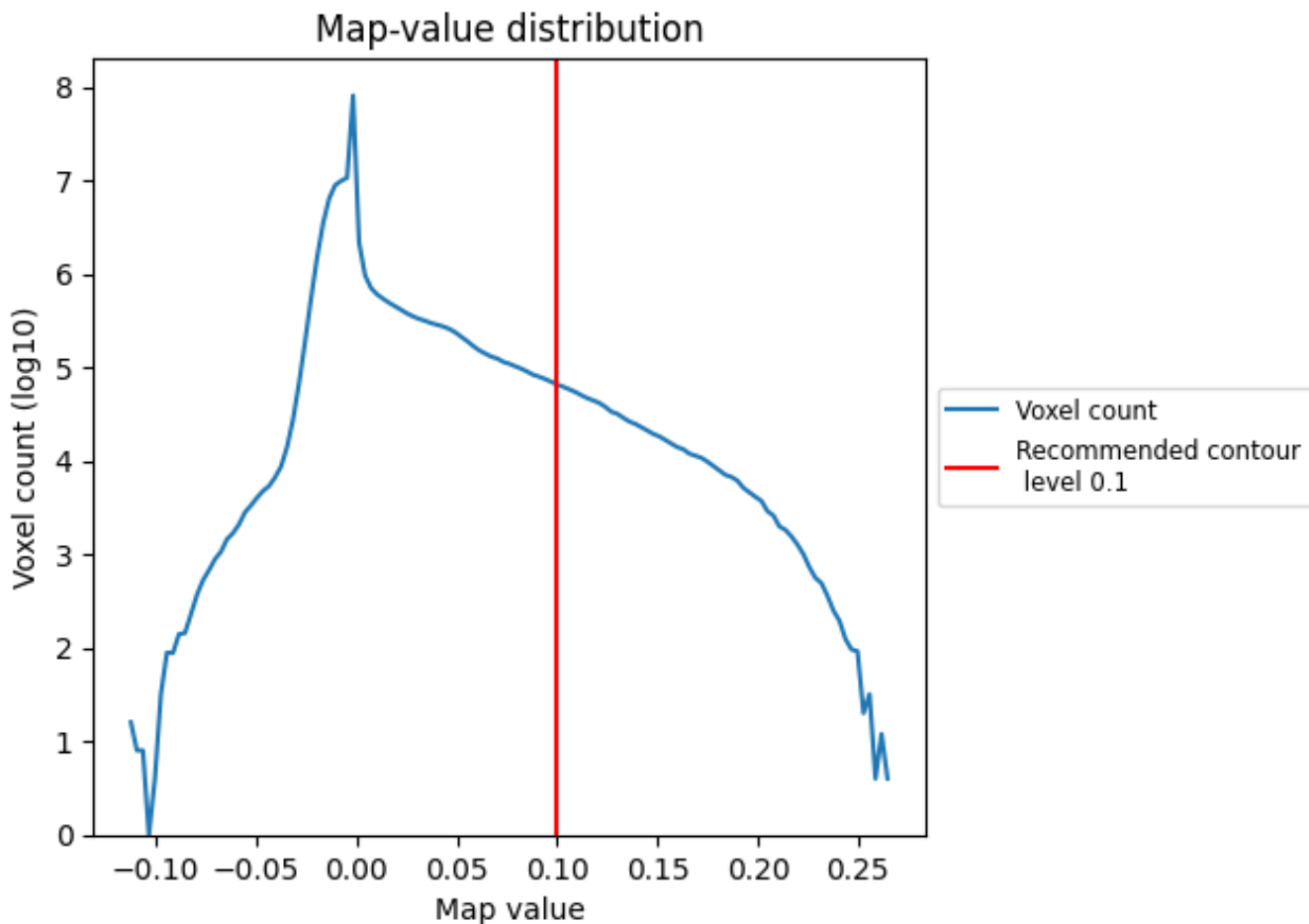
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

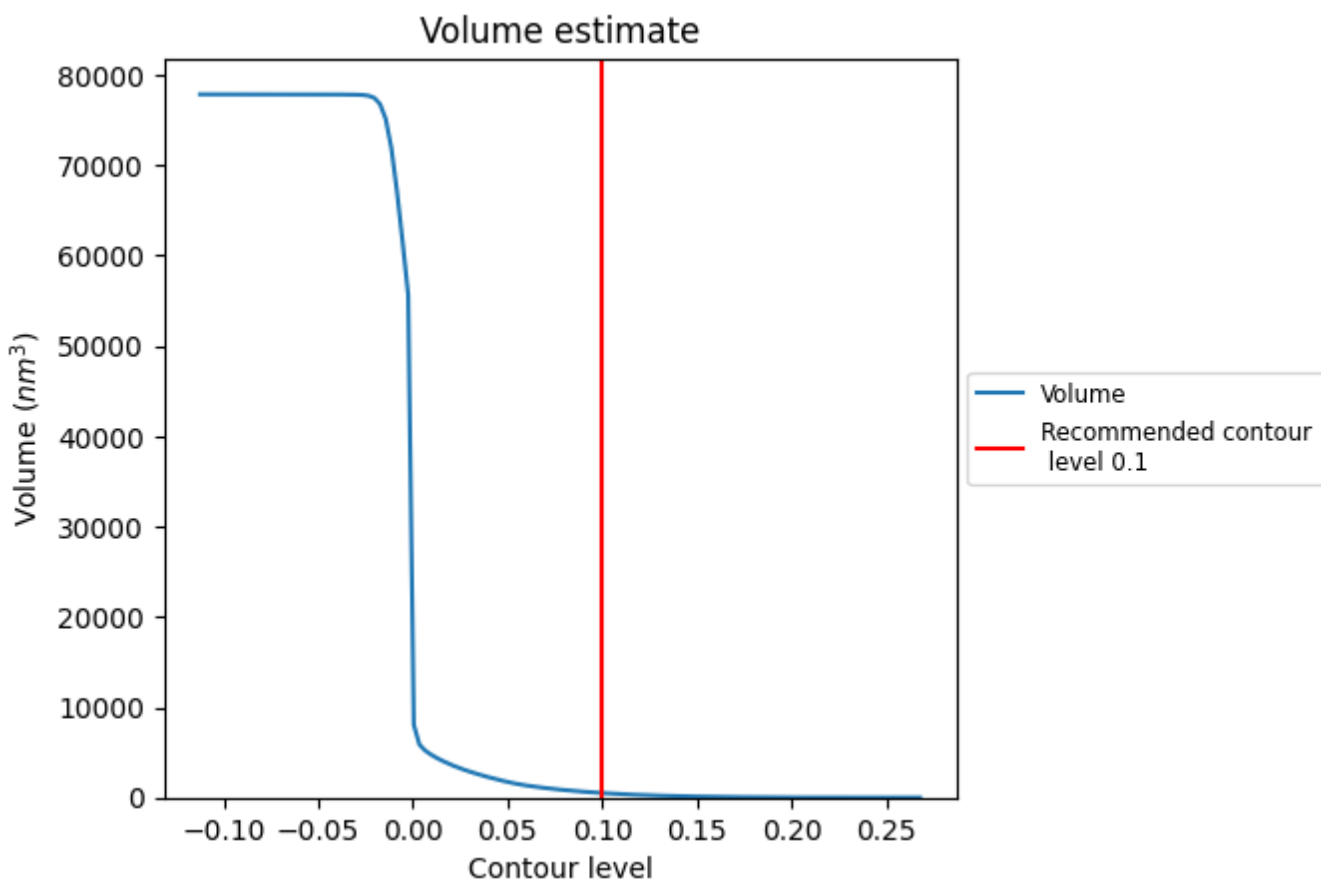
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

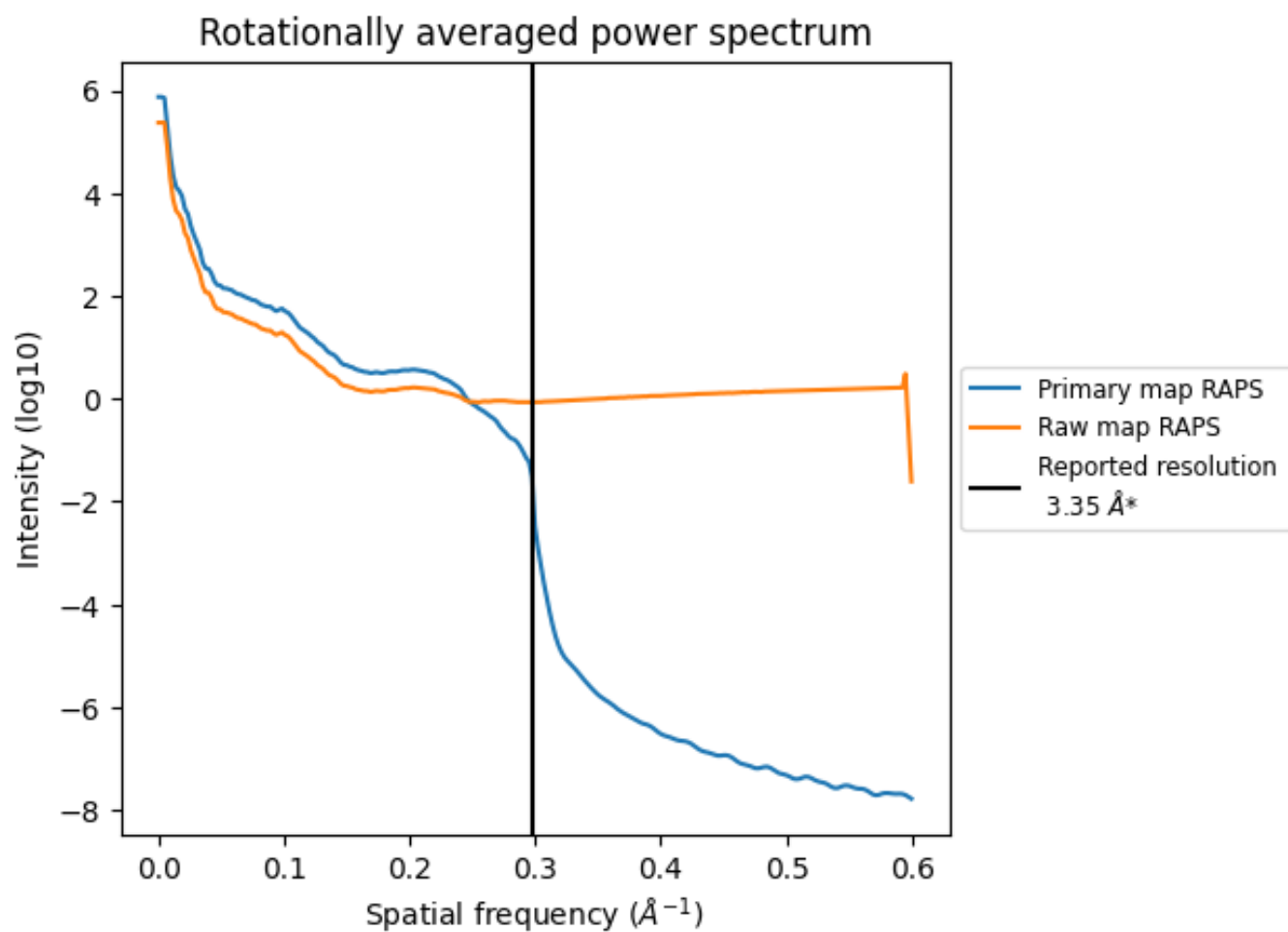
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 502 nm<sup>3</sup>; this corresponds to an approximate mass of 453 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](#)

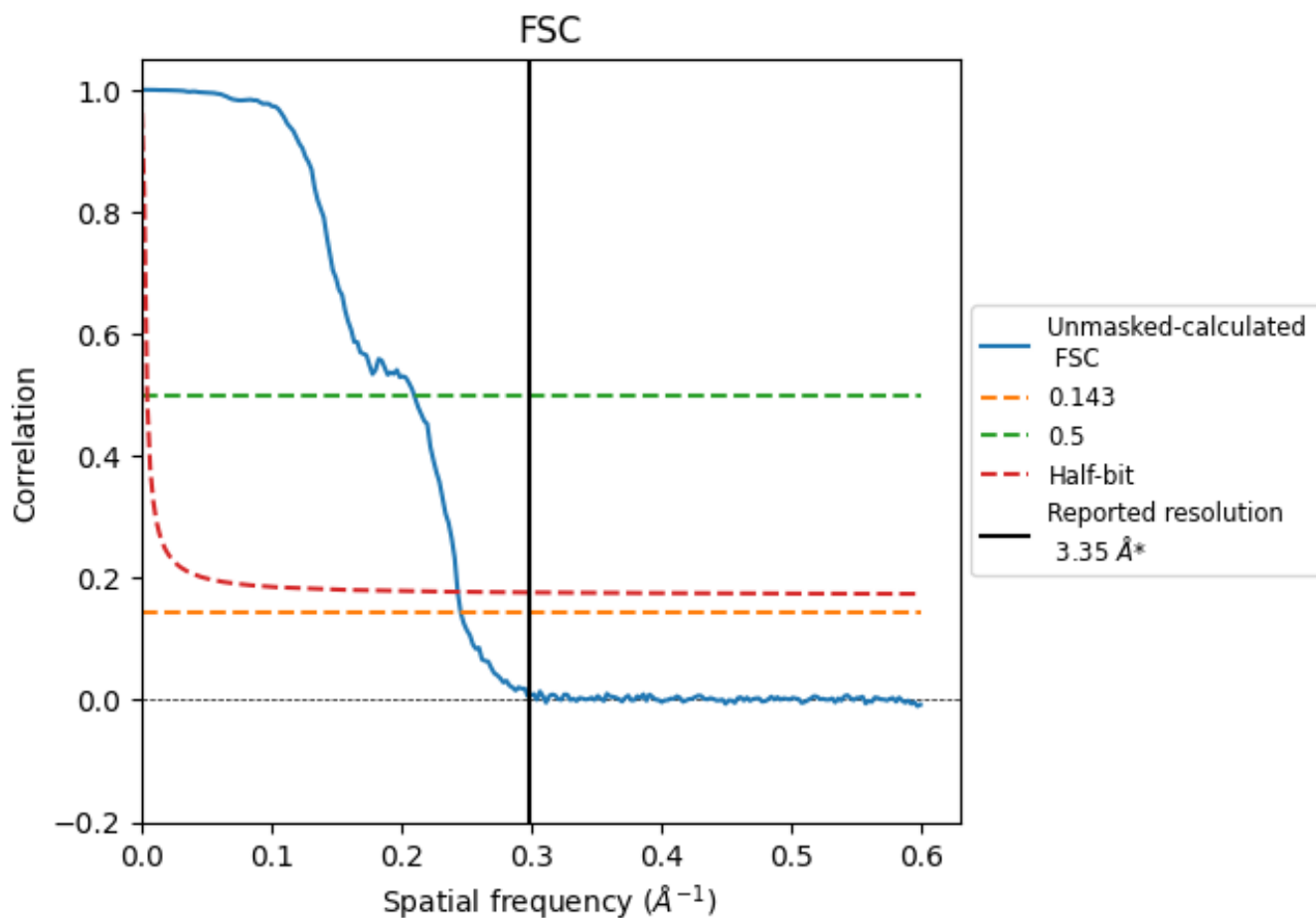


\*Reported resolution corresponds to spatial frequency of 0.299 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.299 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

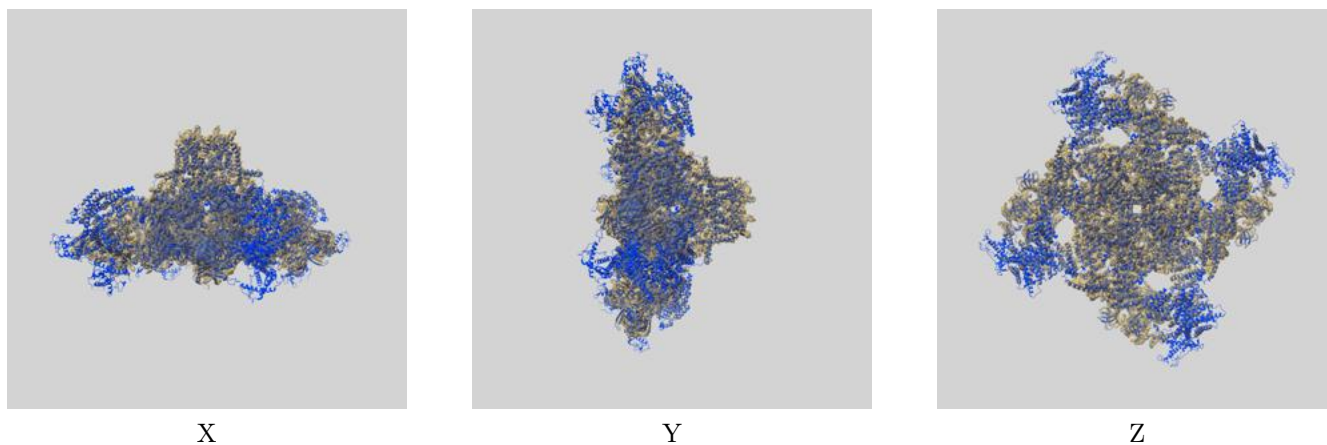
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.07	4.76	4.11

\*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 4.07 differs from the reported value 3.35 by more than 10 %

## 9 Map-model fit [i](#)

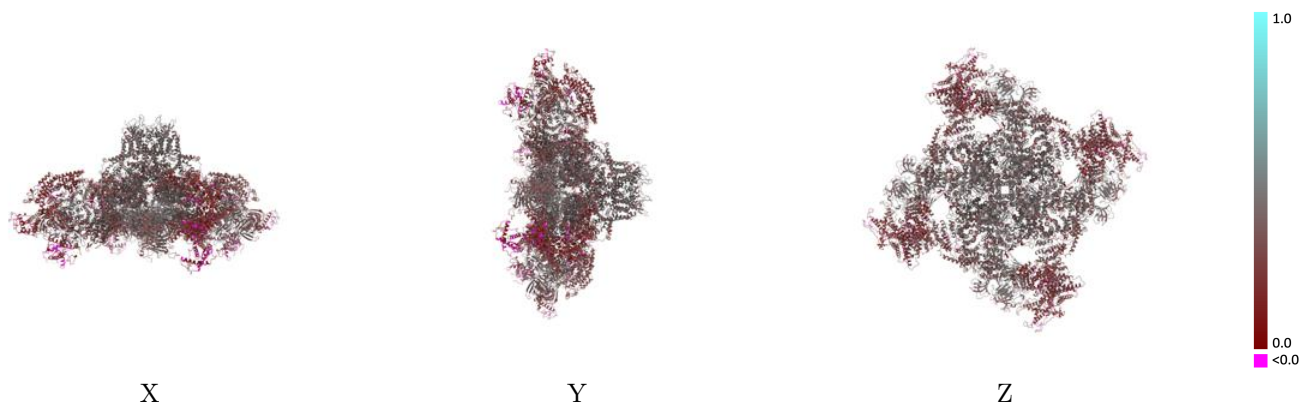
This section contains information regarding the fit between EMDB map EMD-47387 and PDB model 9E1A. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



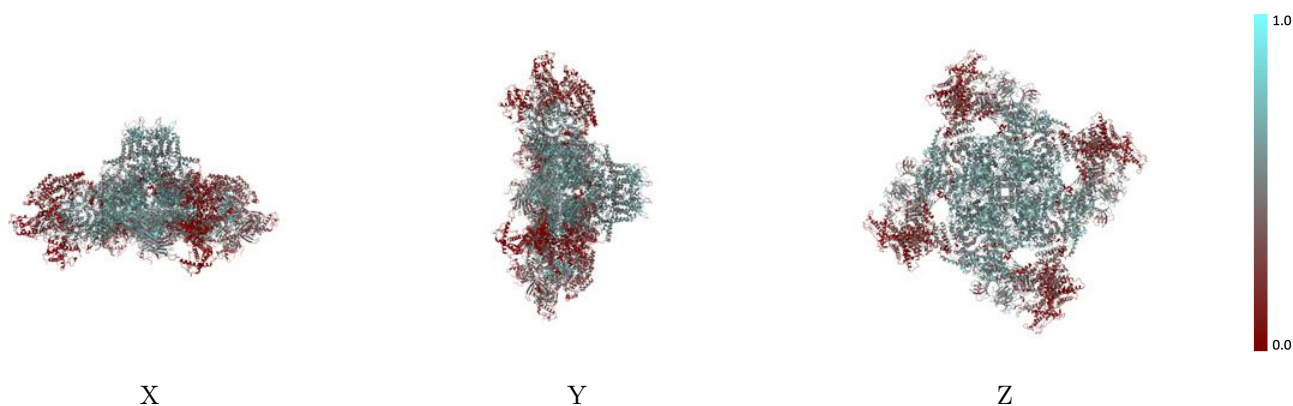
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



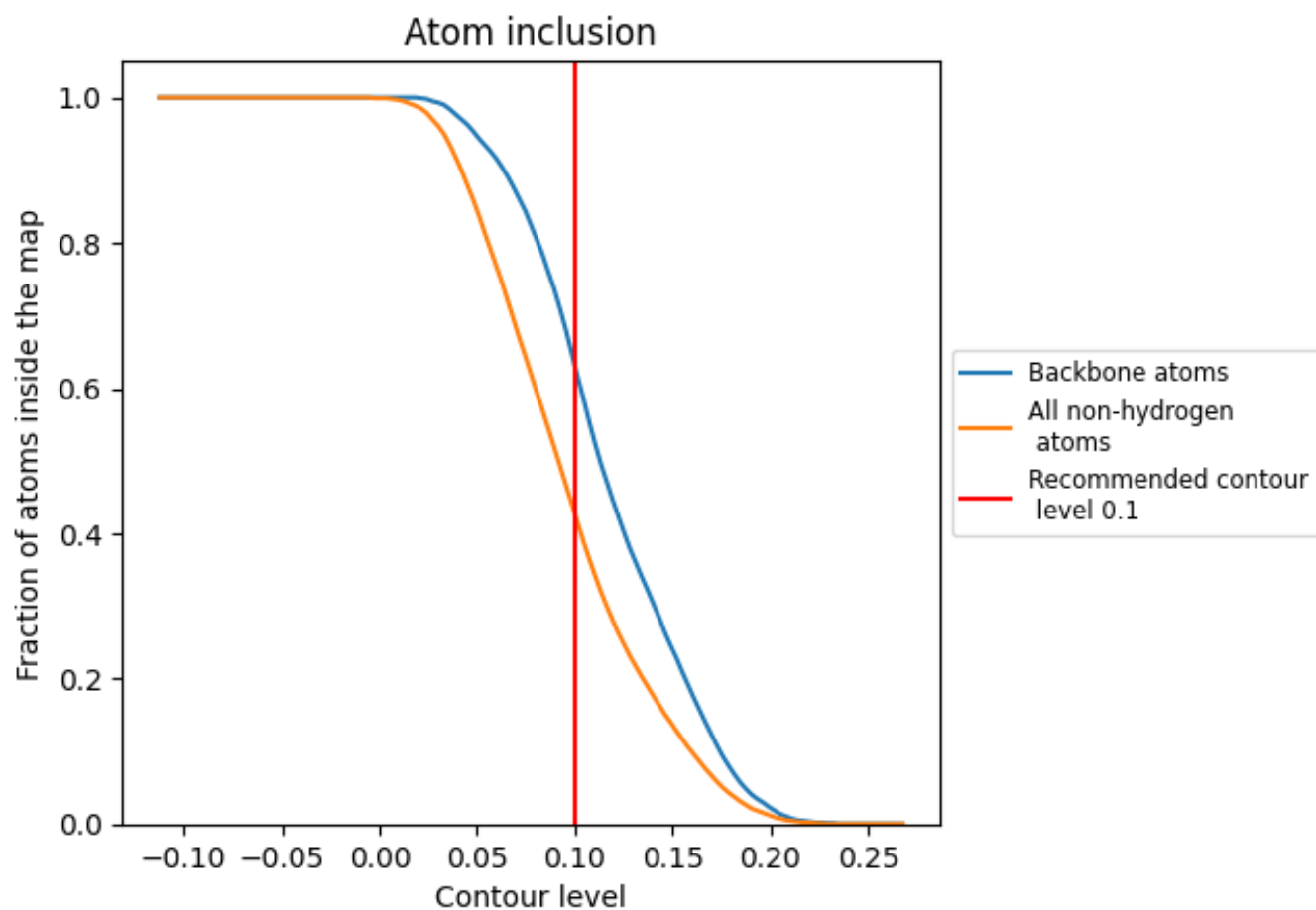
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 43% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4260	0.3280
A	0.4280	0.3280
B	0.4280	0.3270
C	0.4280	0.3270
D	0.4280	0.3270
E	0.3290	0.3760
F	0.3310	0.3770
G	0.3340	0.3760
H	0.3300	0.3750

