



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 06:07 PM UTC

PDB ID : 9E1B / pdb_00009e1b
EMDB ID : EMD-47388
Title : Structure of RyR1 in the open state in the presence of dyphylline
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 4.49 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

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

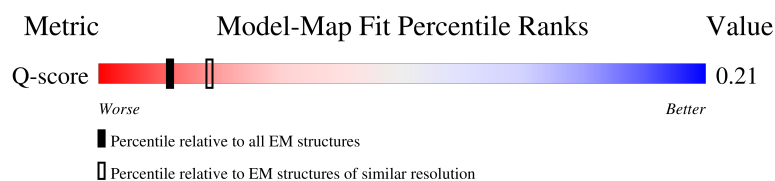
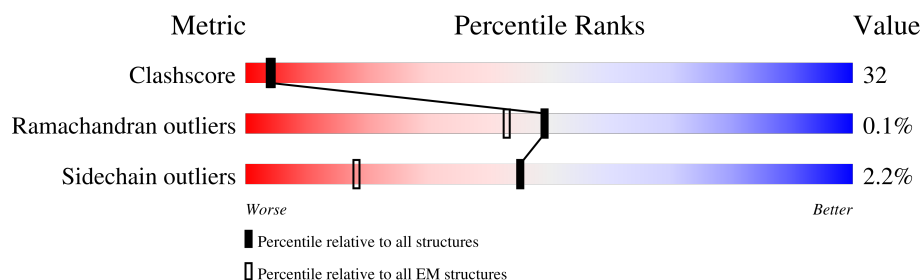
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.49 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	2913 (3.99 - 4.99)

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 $\leq 5\%$. 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	57% 39% 47% 13%
1	B	5037	57% 39% 47% 13%
1	C	5037	57% 39% 47% 13%
1	D	5037	57% 39% 47% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	97% 33% 64% ..
2	F	108	97% 38% 60% ..
2	G	108	96% 40% 57% ..
2	H	108	96% 39% 56% . .

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
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
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: C₁₀H₁₆N₅O₁₃P₃).



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

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

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

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

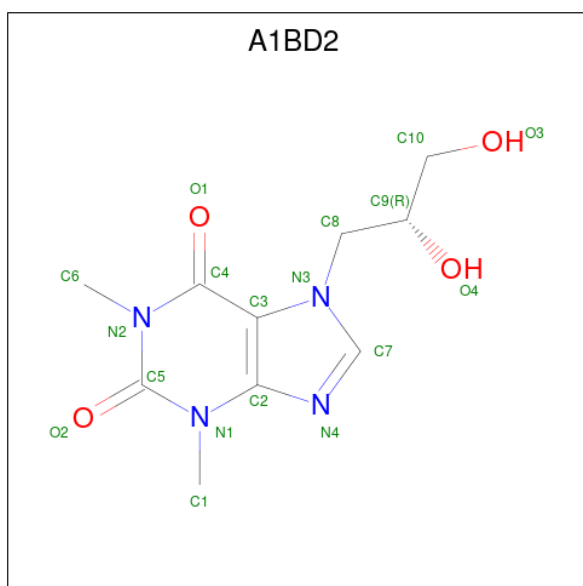
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0

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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: C₁₀H₁₄N₄O₄) (labeled as "Ligand of Interest" by depositor).

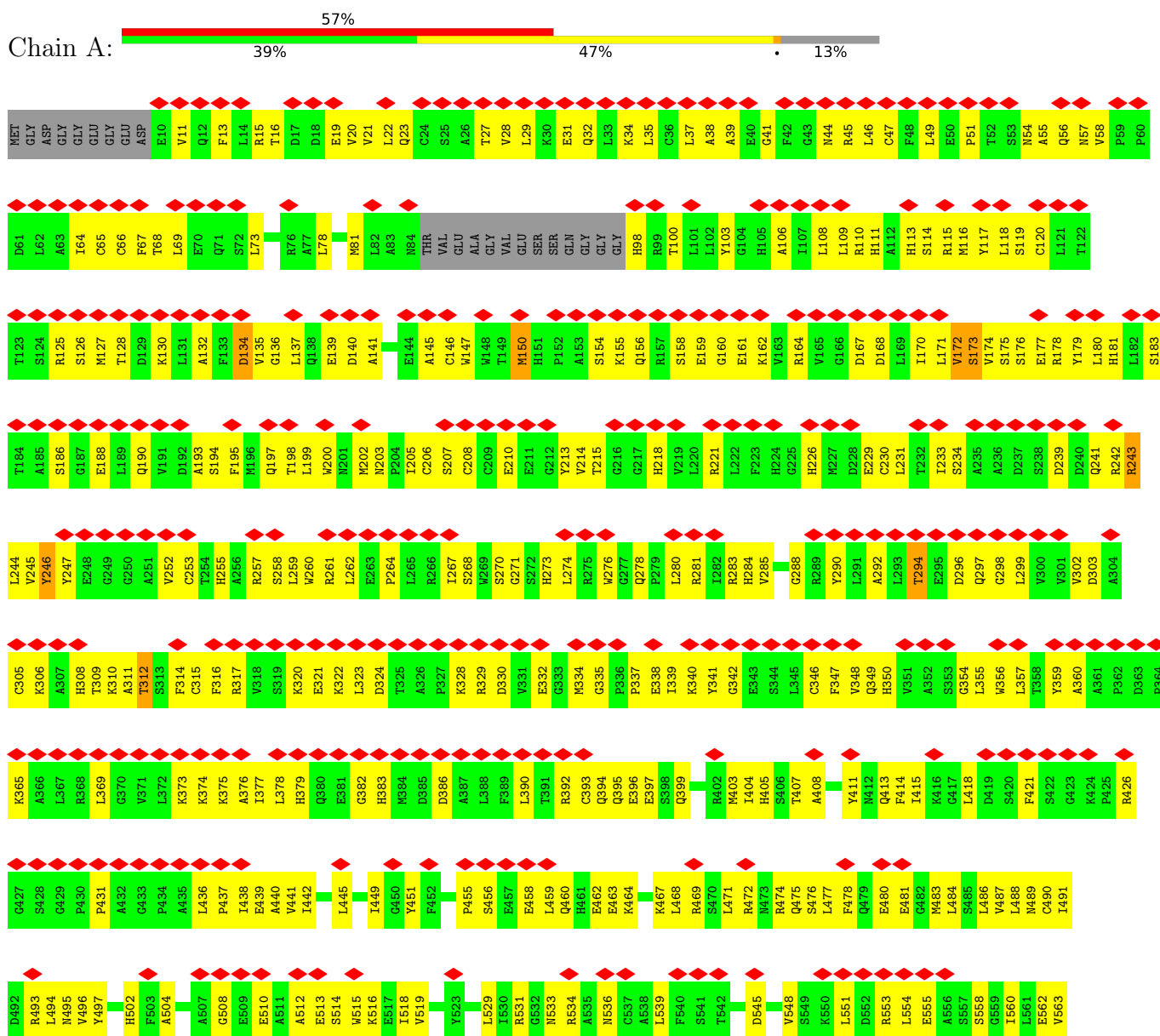


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			18	10	4	4	
6	B	1	Total	C	N	O	0
			18	10	4	4	
6	D	1	Total	C	N	O	0
			18	10	4	4	
6	C	1	Total	C	N	O	0
			18	10	4	4	

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



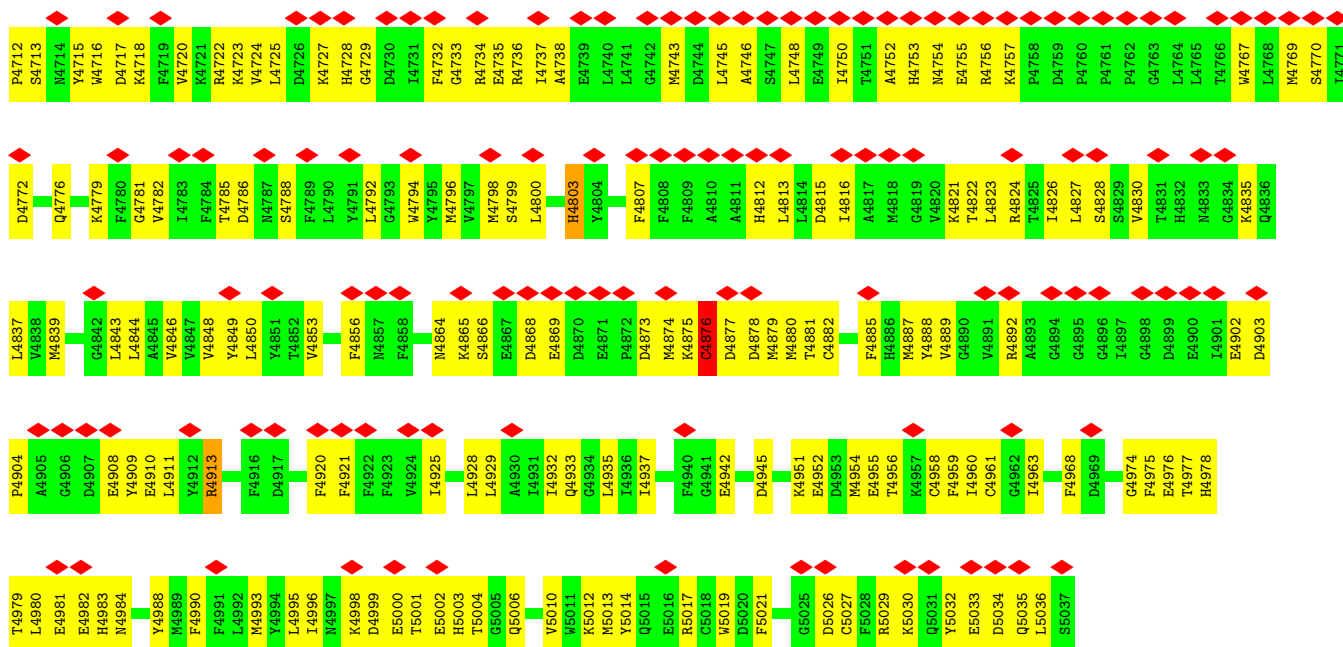




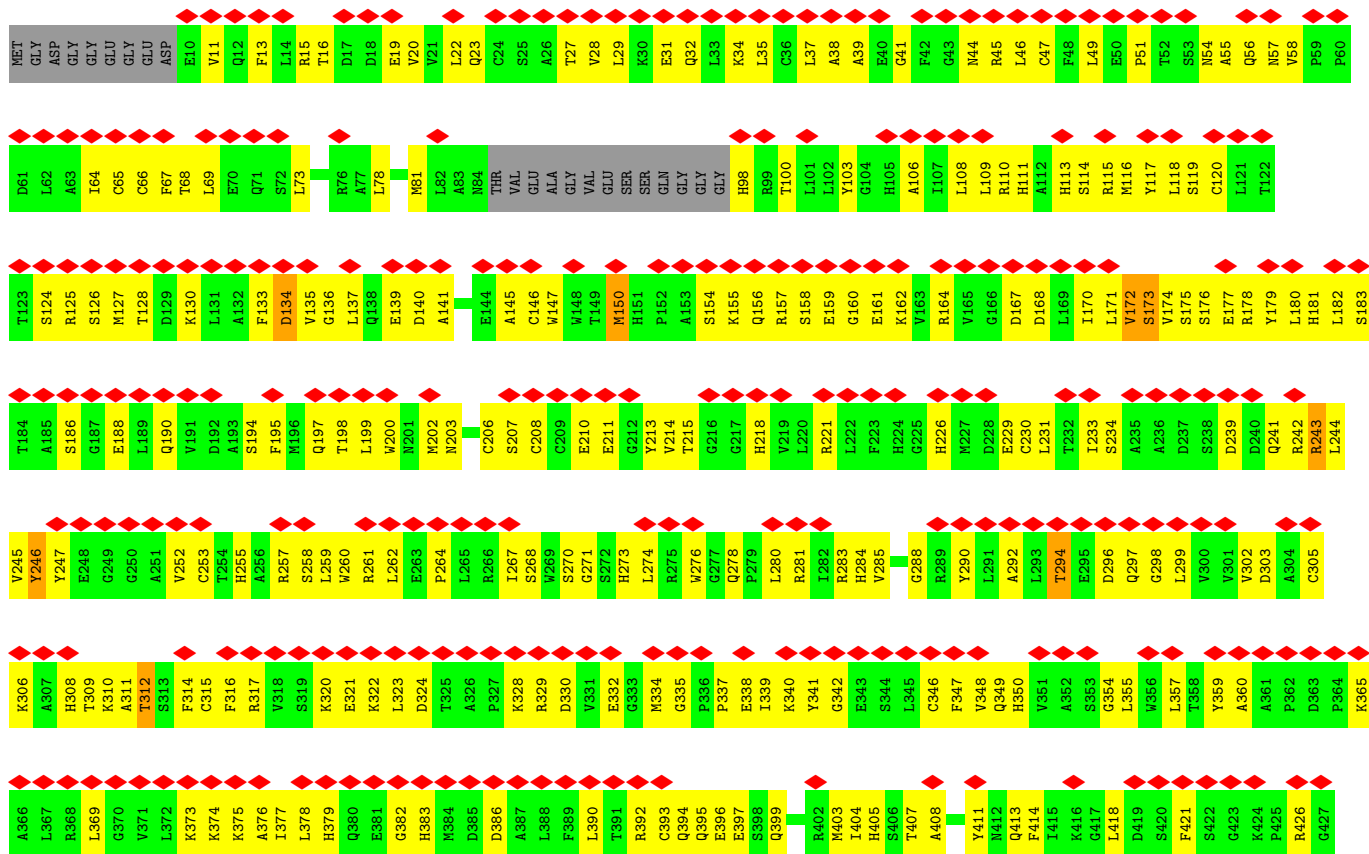
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L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	K2921	E2922	A2923	Q2924	E2925	E2926	L2927	L2928	K2929	F2930	L2931	M2932	N2933	G2934	Y2935	A2936	V2937	F2938	R2939	GLY	LEU	L3000	L3001	L3002	L3003	L3004	L3005	L3006	R3007	O3008	F3009	F3010	T3011	R3012	H3013	C3014	L3015	F3016	F3017	F2985	A2966	F2967	G2968	F2969	S3010	T3020	F3021	K3022	K3023	V3024														
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G2605	C2606	L2607	M2608	A2609	L2610	C2611	R2612	Y2613	I2614	R2615	P2616	S2617	M2618	L2619	Q2620	H2621	L2622	L2623	R2624	R2625	L2626	V2627	F2628	D2629	Y2630	P2631	L2632	L2633	N2634	E2635	F2636	A2637	K2638	M2639	P2640	L2641	K2642	L2643	L2644	T2645	N2646	H2647	Y2648	E2649	R2650	C2651	W2652	K2653	Y2654	Y2655	C2656	L2657	P2658	T2659	G2660	W2661	A2662	N2663	F2664																				
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L2785	K2786	T2787	H2																																																																												

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E3757	V3690	Q3627	P3567	T3507	A3387	L3327	P3267	E3207	I3147	I3087	S3027
E3759	E3691	R3628	S3568	S3508	E3388	Q3328	H3268	P3208	A3148	V3088	G3028
K3760	E3692	R3629	L3569	L3509	E3389	G3329	V3269	Q3209	Q3149	K3089	G3029
Q3761	K3693	R3630	R3570	L3510	G3390	D3330	I3270	L3210	H3150	A3090	H3030
K3762	K3694	A3631	W3571	V3511	E3391	E3331	E3271	N3211	Q3151	G3091	A3031
L3763	P3695	V3632	Q3572	A3512	L3392	A3332	I3272	E3212	F3152	L3092	S3032
Q3766	L3698	V3633	A3574	T3513	L3393	T3333	T3273	Y3213	G3153	R3093	N3033
Q3767	L3701	A3634	L3575	L3514	V3394	W3334	L3274	N3214	D3154	S3094	K3034
Q3768	V3702	C3635	Y3576	K3515	R3395	W3335	P3275	A3215	D3155	F3095	E3035
R3769	F3636	F3636	Y3577	K3516	D3396	K3336	M3276	C3216	V3156	F3096	K3036
H3771	R3637	M3638	R3577	M3517	E3397	R3337	L3277	S3217	I3157	E3097	E3037
L3772	R3707	R3638	G3578	L3518	F3398	L3338	C3278	V3218	L3158	S3098	K3038
R3773	L3710	T3639	P3580	P3519	S3399	A3339	S3279	Y3219	D3159	A3099	I3039
G3774	T3711	P3640	Q3581	I3520	V3400	V3340	Y3280	T3220	D3160	S3100	T3040
A3775	K3712	L3641	R3582	G3521	L3401	F3341	L3281	T3221	V3161	E3101	S3041
E3777	K3713	Y3642	E3583	L3522	C3402	A3342	R3282	K3222	Q3162	D3102	L3042
V3779	S3714	N3643	E3584	N3523	R3403	Q3343	R3283	S3223	V3163	I3103	F3043
L3780	K3715	L3644	E3585	M3524	D3404	P3344	W3284	P3224	G3164	E3104	C3044
Q3781	L3716	H3647	D3586	C3525	L3405	V3345	W3285	R3225	C3165	K3105	K3045
K3782	D3717	R3648	A3587	A3526	Y3406	V3346	E3286	E3226	Y3166	M3106	L3046
L3783	E3718	A3649	D3588	P3527	A3407	S3347	R3287	R3227	R3167	V3107	A3047
A3785	D3719	C3650	P3589	T3528	L3408	R3348	G3288	A3228	T3168	E3108	A3048
K3786	K3720	N3651	K3589	K3529	F3469	A3349	P3289	I3229	L3169	N3109	L3049
K3787	L3721	K3652	E3590	Q3530	L3470	R3350	E3290	L3230	G3170	L3110	V3050
V3789	V3722	F3653	K3591	D3531	T3471	P3351	A3291	G3231	S3171	R3111	R3051
G3788	K3723	L3654	I3592	L3532	A3472	E3352	P3292	L3232	Y3173	L3112	H3052
E3789	A3724	E3655	V3593	T3533	D3473	L3353	P3293	P3233	G3174	G3113	R3053
T3790	Y3725	E3656	R3594	I3534	S3474	L3354	P3294	N3234	K3174	K3114	V3054
K3793	I3728	A3659	R3595	M3534	R3414	H3355	A3295	S3235	L3175	V3115	S3055
S3796	M3729	A3660	V3596	L3535	Y3415	S3356	P3297	V3236	G3176	S3116	L3056
T3797	A3730	W3661	Q3597	A3536	V3416	H3357	P3297	E3237	T3177	GLN	F3057
L3798	K3731	I3662	E3598	K3537	D3417	F3358	A3298	E3238	T3178	ALA	G3058
K3799	S3732	L3663	S3599	T3538	N3418	I3359	G3299	M3239	K3179	THR	T3059
L3800	C3733	T3664	S3600	R3539	R3419	P3360	A3300	C3240	N3180	GLN	D3060
G3801	H3734	E3665	A3601	Y3540	A3421	T3361	P3301	P3241	T3181	VAL	A3061
I3802	L3735	D3666	V3602	A3541	H3422	I3362	P3302	D3242	Y3182	K3123	P3062
L3805	E3736	H3667	L3603	L3542	W3423	G3363	P3303	I3243	V3183	G3124	A3063
N3806	GLU	S3668	Y3604	K3543	L3424	R3364	C3304	P3244	E3184	V3125	V3064
Q3807	GLY	F3669	H3605	D3544	T3425	L3365	T3305	V3245	K3185	G3127	V3065
G3808	GLY	E3670	L3606	T3545	Q3426	R3366	A3306	L3246	L3186	N3128	N3066
Q3809	ASN	E3671	E3607	D3546	F3427	K3367	V3307	D3247	R3187	L3129	C3067
GLY	GLY	R3672	Q3608	E3547	ASP	ASP	T3308	R3248	P3188	L3130	L3068
GLU	ALA	K3673	T3609	E3548	N3428	R3368	T3308	L3249	A3189	T3130	H3069
GLU	GLU	L3674	L3607	E3549	A3429	A3369	S3309	L3249	Y3131	Y3131	H3069
GLU	GLU	D3675	H3611	R3550	ARG	G3370	D3310	M3250	L3190	T3132	L3071
GLU	GLU	D3676	P3612	R3551	THR	K3371	H3311	A3251	G3191	T3133	L3071
GLU	GLU	K3679	Y3613	F3552	LYS	V3372	L3312	D3252	E3192	V3134	A3072
Y3819	V3749	A3680	K3614	L3553	E3433	V3373	N3313	I3253	C3193	V3134	K3073
Q3812	E3750	G3681	S3615	Q3554	L3434	A3374	S3314	G3254	L3194	A3136	S3074
Q3813	V3751	E3682	K3616	N3555	F3435	E3375	L3315	G3255	A3195	L3137	L3075
Q3814	S3752	Q3683	K3617	N3556	R3436	E3376	L3316	L3256	L3196	P3138	D3076
F3753	F3753	K3684	A3618	L3557	M3437	E3377	G3317	A3257	L3197	V3139	K3077
E3754	E3754	E3685	V3619	H3558	Q3438	Q3378	N3318	E3258	A3198	V3139	A3078
		E3686	W3620	L3559	G3439	L3379	I3319	S3259	A3199	L3140	T3079
		E3687	H3621	Q3560	E3440	R3380	I3320	G3260	A3199	T3141	V3080
			K3622	G3561	I3441	L3381	R3321	A3261	K3201	T3142	K3081
			L3623	K3562	F3442	E3382	I3322	K3262	P3202	L3143	K3082
			L3624	V3563	I3443	A3383	I3323	Y3263	V3203	F3144	S3083
				E3564	Y3444	K3384	V3324	T3264	A3204		G3084





• Molecule 1: Ryanodine receptor 1



M1170	R1110	G1050	E990	K930	I870	A809	D749	L688	G628	Y565	R493	S428
S1171	P1111	Y1051	N991	T931	R871	P810	L750	T689	R629	C566	L494	G429
D1172	D1112	M1052	G992	L932	E872	C811	S751	E690	E630	V567	N495	P430
S1173	V1113	I1053	H993	L933	K873	E813	V752	G891	L631	L569	V496	P431
G1174	E1114	E1054	N994	A934	L874	E814	P753	Y692	L632	S754	H502	A432
S1175	L1115	P1055	W996	L935	A875	W815	I755	S693	L633	S571	F503	G433
E1176	G1116	P1056	A997	G936	E876	L816	S756	P694	T635	P572	A504	P434
T1177	A1117	D1057	R998	C937	N877	P817	F757	Y695	N636	E573	A435	A436
L1178	D1118	Q1058	D999	H938	R878	R818	R758	P696	L637	V574	A507	L436
F1179	E1119	E1059	R1000	V939	H879	E819	N759	G697	I638	L575	G508	P437
E1180	L1120	P1060	V1001	G940	E880	R820	N760	G698	E509	N576	E509	I438
E1181	A1121	S1061	A1002	W941	L881	L821	G761	G699	N639	I577	E510	A440
I1182	Y1122	Q1062	Q1003	A942	W882	R822	C762	E700	Y640	I578	A511	V441
E1183	F1123	V1063	G1004	D943	A883	R823	P763	G701	V641	Q579	A512	I442
F1124	F1124	E1064	W1005	E944	L884	L823	W764	W702	T642	E580	E513	
N1125	N1125	Q1065	S1006	K945	T885	E824	Q765	G703	S643	N581	S514	
G1185	G1126	Q1066	Y1007	A946	R886	P825	G766	G704	I644	I583	W515	L445
D1186	H1127	Q1067	Y1007	E947	T887	K827	V767	G706	R645	K584	K516	
G1187	R1128	S1067	S1008	E947	T887	R826	F768	G706	P646	S585	E517	
F1188	Q1129	A1068	A1009	D948	E888	E828	E769	W707	N647	I518	I518	
L1189	Q1130	W1069	W1010	W949	Q889	Y829	A770	G708	T648	I587	V519	F452
P1190	R1131	D1070	Q1011	L950	G890	R830	E771	D709	F649	S588	Y523	
V1191	W1132	R1071	D1012	K951	H891	R831	W772	D710	V650	L589		P455
C1192	H1133	V1072	I1013	K952	T892	E832	L773	L711	G651	I590	L529	S456
S1193	L1134	R1073	P1014	T953	Y893	G833	D774	Y712	R652	K592	I530	E457
L1194	G1135	I1074	A1015	K954	G894	P834	G775	S713	A653	H593	R531	E458
G1195	S1136	F1075	R1016	L955	P895	R835	L776	E654	G594	N533	G532	L459
P1196	E1137	R1076	R1017	P956	W896	H838	L777	R564	G655	R595	N534	Q460
G1197	F1138	A1077	N1018	K957	R897	W840	F777	F716	S656	H461	A535	E462
Q1198	A1077	E1078	P1019	T958	D898	L839	F778	D717	T657	K598	E463	E462
V1199	K1079	K1079	R1020	K958	D899	W840	W779	G718	Q658	V599	K464	K464
G1200	L1021	S1080	L1021	Y959	N900	P842	V781	L719	Y659	A538	L539	K467
H1201	W1143	Y1081	V1022	M960	K901	S843	S782	H720	D601	L539	L539	L468
L1202	Q1144	T1082	P1023	N961	R902	R844	F783	L721	G660	V602	F540	R469
N1203	S1145	Y1083	Y1024	S962	L903	C845	W722	W722	N662	L603	S541	S470
G1205	Q1084	Q1084	R1025	N963	L903	C845	S784	T723	Y663	C604	T542	
Q1206	D1147	S1085	L1026	G964	H904	L846	A785	G724	F664	S605		L471
D1207	V1148	G1086	L1027	Y965	P905	S847	G786	W725	E665	L606	D545	R472
V1208	L1149	R1087	D1028	K966	C906	H848	W787	W726	V666	C607		N473
S1209	G1150	W1088	E1029	P967	L907	T849	K788	A727	N667			R474
S1210	C1151	Y1089	Y908	A968	Y908	D850	W789	R728	V668	K610	V548	Q475
L1211	M1152	F1090	A1030	P969	N909	P851	R790	P729	D669	S549	K550	S476
R1212	I1153	E1091	T1031	L970	F910	W851	F791	V730	E570	L551	L551	L477
F1213	D1154	F1092	K1032	D971	H911	P853	L792	T731	V671	D552		F478
F1214	L1155	E1093	R1033	L972	S912	C854	L793	S732	V672	R553		Q479
A1215	T1156	A1094	N1035	S973	L913	P855	G794	P733	P673	L554		E481
I1216	E1157	V1095	R1036	H974	P914	W856	G795	G734	F674	E555		G482
C1217	T1159	T1096	D1037	V975	E915	D857	R796	Q735	I621	A556		M483
G1218	I1160	T1097	S1038	R976	P916	T858	H797	T736	T622	S557		S485
L1219	L1219	G1098	L1039	L977	E917	W859	G798	L737	E676	S558		L486
Q1220	F1162	E1099	C1040	T978	R918	Q860	E799	L738	Q678	G559		V487
E1221	T1163	M1100	Q1041	P979	N919	T861	F800	A739	N624	L561		L488
G1222	L1164	R1101	A1042	A980	Y920	W862	P802	P740	A679	L626		N489
F1223	N1165	V1102	I1043	Q981	N921	L863	P804	E741	T680	L626		C490
E1224	G1166	G1103	T982	T982	L922	P864	P804	D742	H681	P627		
F1225	E1167	W1104	Q923	T983	Q923	P865	P805	W743	R683			
F1226	V1168	A1105	L1045	N984	R924	H866	P806	S745	V684			
A1227	L1106	R1106	L1046	Y985	S925	L867	G807		G685			
I1228	P1107	P1107	G1047	P986	G926	E868	Y808		N686			
N1229	E1108	E1108	L1048	R987	E927	R869		L748	A687			
	L1109	L1109	Y1049	L989	T928							





S3568	S3448	G3328	H3268	P3208	A3148	V3088	G3028	D2968	Y2908	THR
L3569	H3449	I3329	V3269	Q3209	Q3149	K3089	G3029	I2969	D2909	TTR
I3610	N3450	D3330	I3270	L3210	H3150	A3090	H3030	S2970	T2910	ASP
V3611	F3451	E3331	E3271	N3211	Q3151	G3091	A3031	Q2971	L2911	PRO
T3612	K3452	L3332	I3272	E3212	F3152	L3092	S3032	E2972	T2912	ARG
L3613	L3393	T3333	T3273	Y3213	G3153	R3093	N3033	F2973	A2913	GLY
L3614	V3394	W3334	L3274	N3214	D3154	S3094	K3034	I2974	K2914	
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P3619	S3399	A3339	S3279	Y3219	D3159	A3099	I3039	A2979	D2919	
I3620	V3400	F3340	Y3280	T3220	D3160	S3100	T3040	V2980	R2920	
G3621	L3401	V3341	L3281	T3221	V3161	E3101	S3041	V2981	E2921	
L3622	C3402	A3342	P3282	K3222	Q3162	D3102	L3042	S2982	K2922	
N3623	R3403	Q3343	R3283	S3223	V3163	I3103	F3043	S2983	A2923	
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C3625	L3405	I3345	W3285	R3225	C3165	K3105	K3045	R2985	E2925	
A3626	V3406	V3346	E3286	E3226	Y3166	M3106	L3046	V2986	L2926	
P3627	A3407	R3347	R3287	R3227	R3167	V3107	A3047	E2987	L2927	
L3628	L3408	S3348	C3288	A3228	T3168	E3108	A3048	K2988	K2928	
F3629	Y3409	A3349	P3289	I3229	L3169	N3109	L3049	S2989	F2929	
Q3630	P3410	R3350	E3290	L3230	C3170	L3110	V3050	P2990	L2930	
D3631	L3411	P3351	A3291	G3231	S3171	R3111	R3051	H2991	Q2931	
L3632	L3412	E3352	P3292	L3232	I3172	L3112	H3052	E2992	M2932	
I3633	I3413	L3353	P3293	R3233	Y3173	G3113	R3053	Q2993	N2933	
M3634	R3414	L3354	P3294	N3234	S3174	K3114	V3054	E2994	G2934	
L3635	Y3415	H3355	A3295	S3235	L3175	P3115	S3055	I2995	Y2935	
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K3637	D3417	H3357	P3297	E3237	T3177	GLN	F3057	F2997	V2937	
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R3639	N3419	I3359	G3299	M3239	K3179	ARG	T3059	F2999	T2939	
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A3641	A3421	T3361	P3301	G3241	T3181	VAL	A3061	I3001	LEU	
L3642	H3422	I3362	P3302	D3242	Y3182	K3123	P3062	L3002	LYS	
K3643	W3423	G3363	P3303	I3243	V3183	G3124	A3063	L3003	ASP	
D3644	L3424	R3364	C3304	R3244	E3184	V3125	V3064	P3004	MET	
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D3646	E3426	R3366	A3306	L3246	L3186	Q3127	N3066	I3006	W2886	
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R3648	N3428	R3368	T3308	R3248	P3188	L3129	C3067	Q3008	K2889	
V3649	A3429	A3369	S3309	L3249	A3189	T3130	H3069	Y3009	K2890	
R3650	N3430	G3370	D3310	M3250	L3190	Y3131	I3070	F3010	I2951	
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F3652	E3432	V3372	L3312	D3252	E3192	T3133	A3072	N3012	K2953	
L3653	L3434	A3374	N3313	G3254	L3194	V3134	R3073	H3013	L2894	
Q3654	F3435	E3375	S3314	G3255	A3195	L3136	S3074	C3014	E2895	
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L3656	R3437	E3377	G3317	L3256	R3197	L3137	D3076	Y3016	A2956	
H3658	V3438	Q3378	N3318	A3257	L3197	P3138	A3077	F3017	F2957	
L3659	G3439	L3379	I3319	S3259	L3197	V3139	R3078	G2958	G2958	
S3604	E3440	R3380	T3320	G3260	A3199	L3140	T3079	F2959	F2959	
V3605	I3441	L3381	R3321	A3261	A3200	T3141	V3080	L3018	Q2960	
Q3606	F3442	L3381	R3321	G3261	K3201	T3142	M3081	S3019	Q2961	
L3623	I3443	E3382	I3322	R3262	P3202	T3143	K3082	T3021	Q2962	
L3624	Y3444	A3383	L3323	Y3263	V3203	F3144	S3083	A3022	L2963	
S3625	W3445	K3384	V3324	T3264	A3204	Q3145	G3084	K3023	L2964	
K3626	S3446	A3385	N3325	E3265	F3205	H3146	G3085	V3024	R2965	
S3666	K3447	E3386	N3326	M3266	L3206	I3147	E3086	L3025	W2966	
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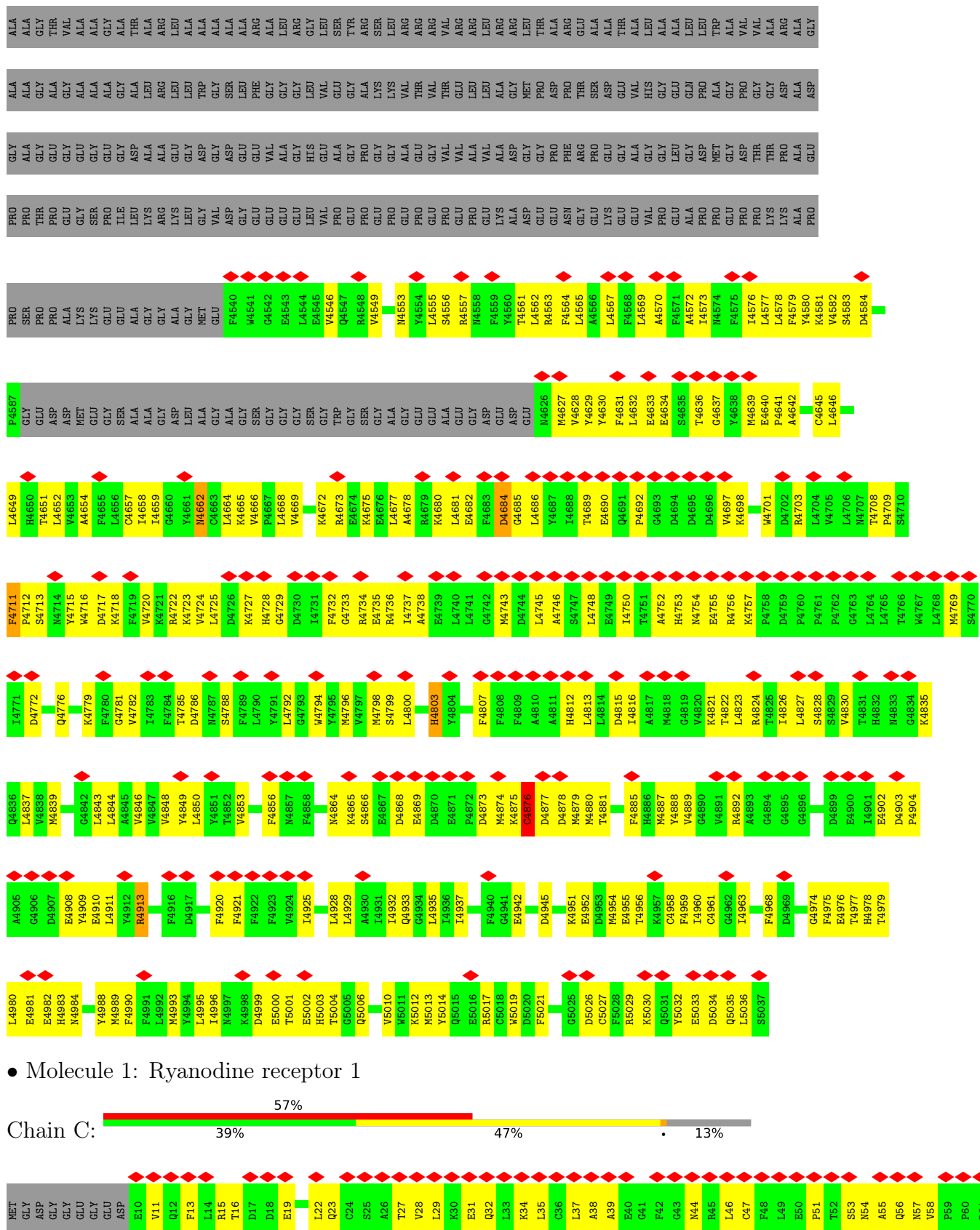
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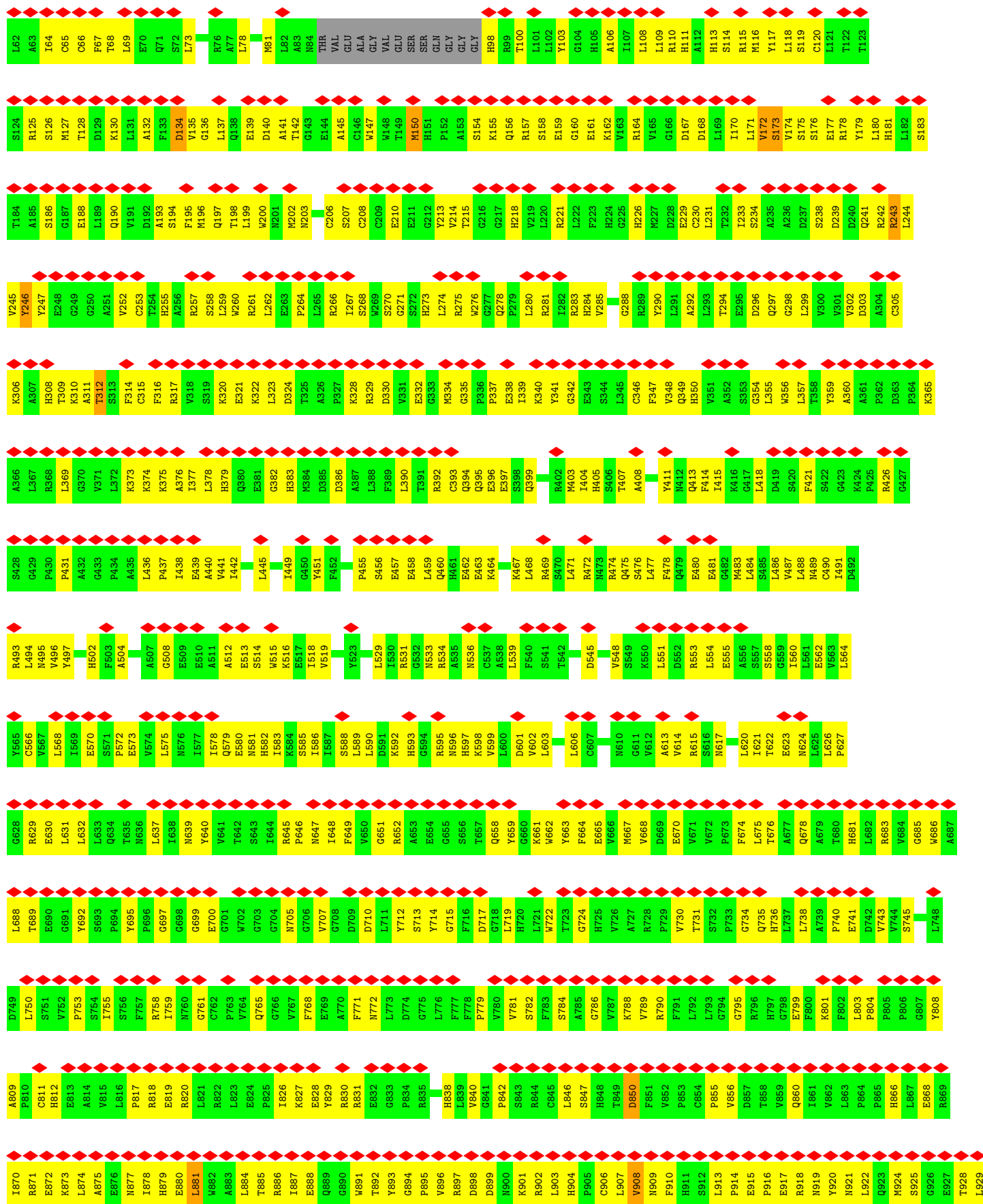
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VAL	ASP	ALA	PRO	GLU	GLY	N2734	F2735	D2736	P2737	Q2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	F2768	D2769	K2770	I2771	Q2772	N2773	D2774	W2775	L2776	Y2777	G2778	E2779	ARG	LYS	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	
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T2810	L2811	T2812	A2813	K2814	E2815	E2816	P2817	R2818	D2819	R2820	E2821	K2822	A2823	Q2824	E2825	L2826	L2827	S2828	R2829	E2830	L2831	Q2832	A2833	M2834	A2835	E2836	Q2837	L2838	A2839	E2840	W2841	E2842	Y2843	H2844	N2845	T2846	G2847	R2848	K2849	S2850	L2851	E2852	K2853	R2854	F2855	A2856	K2857	G2858	G2859	Q2860	T2861	H2862	P2863	L2864	L2865	W2866	M2867	D2868				
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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	Q2934	Y2935	A2936	V2937	T2938	R2939	GLY	LYS	ASP	MET	GLU	L2946	D2947	T2948	S2949	S2950	L2951	E2952	K2953	R2954	F2955	A2956	P2957	G2958	P2959	L2960	Q2961	L2963	R2964	R2965	W2966	M2967	D2968					
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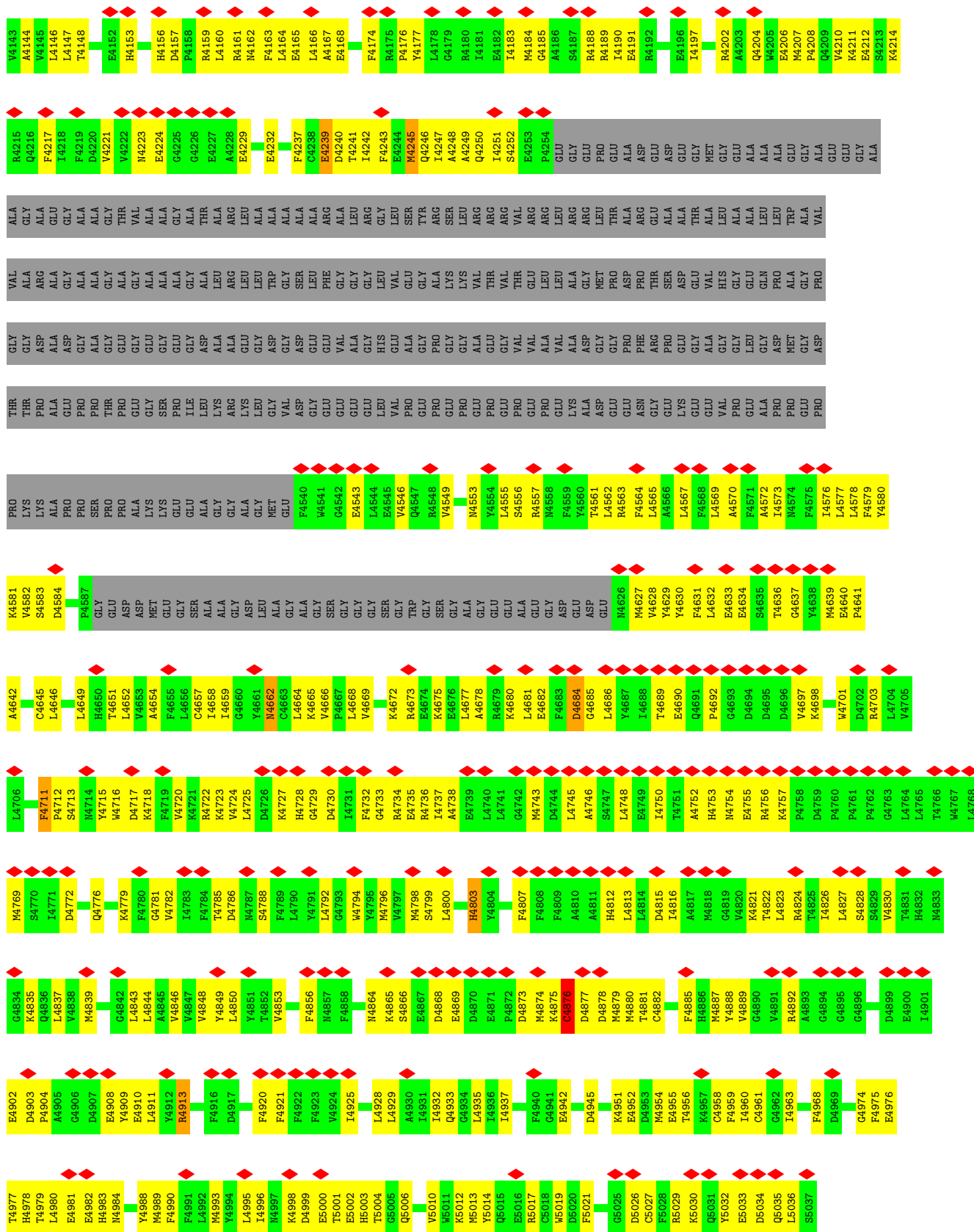


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V1597	S1536	E1596	S1536	G1477	P1284	VAL	GLY	P1284	R1232	D1172	D1112	N1052	G992	L932
L1598	M1537	V1597	M1537	D1478	V1286	PRO	THR	V1286	P1233	S1173	V1113	I1053	H993	L933
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E1617	M1494	E1617	M1494	E1479	Q1286	ALA	GLN	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
T1617	Y1435	T1617	Y1435	E1479	Q1286	ALA	GLN	Q1286	Y1255	V1191	W1132	R1071	D1012	K951
R1618	S1436	R1618	S1436	E1479	Q1286	THR	THR	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
A1619	V1437	A1619	V1437	E1479	Q1286	THR	THR	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
R1620	V1438	R1620	V1438	E1479	Q1286	GLY	GLY	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
A1620	V1438	A1620	V1438	E1479	Q1286	GLY	GLY	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
G1621	F1440	G1621	F1440	E1479	Q1286	LYS	LYS	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
E1622	A1441	E1622	A1441	E1479	Q1286	LYS	LYS	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
L1623	G1442	L1623	G1442	E1479	Q1286	ARG	ARG	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
L1624	Q1443	L1624	Q1443	E1479	Q1286	ALA	ALA	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
G1625	E1444	G1625	E1444	E1479	Q1286	PHE	PHE	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
W1626	G1504	W1626	G1504	E1479	Q1286	LEU	LEU	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
F1627	G1505	F1627	G1505	E1479	Q1286	PHE	PHE	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
V1628	Q1506	V1628	Q1506	E1479	Q1286	LYS	LYS	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
G1629	Q1507	G1629	Q1507	E1479	Q1286	LYS	LYS	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
K1629	R1508	K1629	R1508	E1479	Q1286	ALA	ALA	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
Q1630	Q1509	Q1630	Q1509	E1479	Q1286	ALA	ALA	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
G1631	K1570	G1631	K1570	E1479	Q1286	MET	MET	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
D1632	S1510	D1632	S1510	E1479	Q1286	MET	MET	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
P1633	H1511	P1633	H1511	E1479	Q1286	THR	THR	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
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A1638	V1515	A1638	V1515	E1479	Q1286	THR	THR	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
L1639	I1516	L1639	I1516	E1479	Q1286	GLY	GLY	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
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H1640	C1518	H1640	C1518	E1479	Q1286	ALA	ALA	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
I1641	L1519	I1641	L1519	E1479	Q1286	PRO	PRO	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
P1642	V1520	P1642	V1520	E1479	Q1286	ARG	ARG	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
E1643	D1521	E1643	D1521	E1479	Q1286	LEU	LEU	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
E1644	L1522	E1644	L1522	E1479	Q1286	LYS	LYS	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
R1645	A1523	R1645	A1523	E1479	Q1286	GLY	GLY	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
R1646	T1524	R1646	T1524	E1479	Q1286	THR	THR	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
C1647	L1466	C1647	L1466	E1479	Q1286	ALA	ALA	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
M1648	K1585	M1648	K1585	E1479	Q1286	LYS	LYS	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
D1649	L1526	D1649	L1526	E1479	Q1286	ARG	ARG	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
E1652	M1527	E1652	M1527	E1479	Q1286	LEU	LEU	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
L1653	T1528	L1653	T1528	E1479	Q1286	PRO	PRO	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
S1654	F1529	S1654	F1529	E1479	Q1286	GLY	GLY	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
E1655	R1588	E1655	R1588	E1479	Q1286	THR	THR	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
P1592	P1589	P1592	P1589	E1479	Q1286	ALA	ALA	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
C1591	Q1590	C1591	Q1590	E1479	Q1286	VAL	VAL	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
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E1656	G1533	E1656	G1533	E1479	Q1286	ALA	ALA	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
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D1658	L1657	D1658	L1657	E1479	Q1286	THR	THR	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
L1659	D1658	L1659	D1658	E1479	Q1286	ALA	ALA	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
Q1660	T1659	Q1660	T1659	E1479	Q1286	PRO	PRO	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
M1661	F1660	M1661	F1660	E1479	Q1286	ALA	ALA	Q1286	Y1255	G1190	W1132	R1071	D1012	K951
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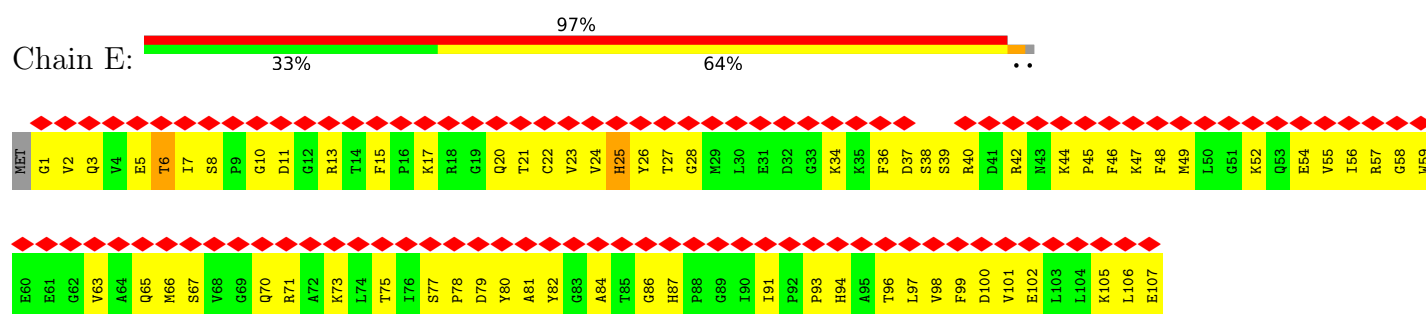
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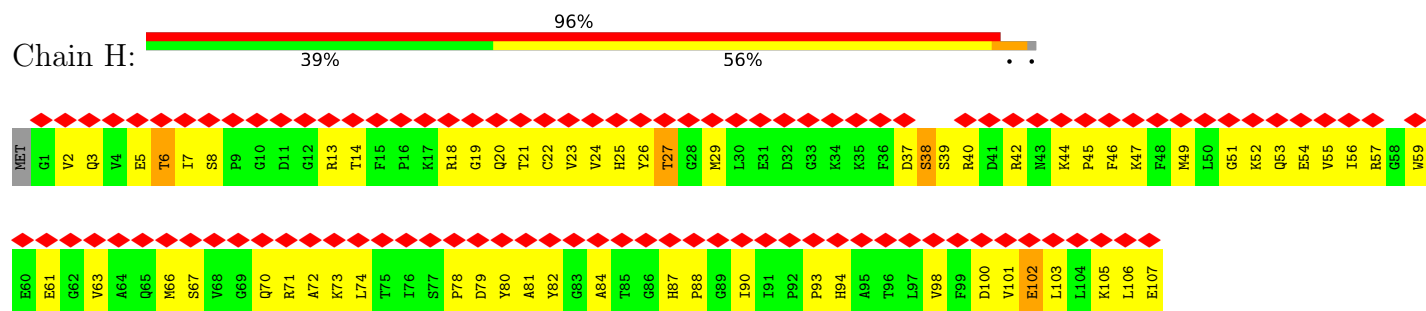
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K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	E3397	F3398	S3399	V3400	L3401	C3402	R3403	D3404	L3405	Y3406	A3407	L3408	Y3409	P3410	L3411	L3412	I3413	R3414	Y3415	V3416	D3417	N3418	N3419	R3420	A3421	H3422	W3423	L3424	T3425	L3426	E3427	P3427	N3428	A3429	N3430	A3431	E3432	E3433	L3434	F3435	R3436	M3437	V3438	E3439	E3440	I3441	F3442	I3443
Y3444	W3445	S3446	K3447	S3448	H3449	N3450	F3451	K3452	R3453	E3454	E3455	K3456	N3457	F3458	V3459	V3460	Q3461	N3462	E3463	I3464	N3465	N3466	M3467	S3468	F3469	L3470	T3471	A3472	D3473	S3474	K3475	K3477	M3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	SER	ASP	GLN	GLU	A3429	THR	ARG	LYS	LYS	LYS	R3498	R3499	G3500	D3501	R3502	Y3503	
S3504	V3505	Q3506	T3507	S3508	L3509	T3510	V3511	Q3512	T3513	L3514	K3515	K3516	N3517	L3518	P3519	L3520	G3521	L3522	N3523	M3524	A3525	A3526	P3527	T3528	D3529	Q3530	D3531	L3532	L3533	M3534	L3535	A3536	K3537	T3538	R3539	Y3540	A3541	L3542	K3543	D3544	T3545	D3546	E3547	E3548	V3549	R3550	E3551	F3552	L3553	Q3554	N3555	N3556	L3557	H3558	L3559	Q3560	K3562	V3563		
E3564	G3565	S3566	P3567	S3568	L3569	R3570	W3571	Q3572	M3573	A3574	L3575	Y3576	R3577	G3578	L3579	P3580	Q3581	R3582	E3583	E3584	D3585	A3586	D3587	S3588	P3589	K3590	K3591	I3592	R3593	R3594	R3595	V3596	Q3597	E3598	V3599	S3600	A3601	V3602	L3603	Y3604	H3605	L3606	E3607	Q3608	T3609	E3610	H3611	P3612	Y3613	K3614	K3615	K3616	K3617	A3618	V3619	W3620	H3621	K3622	L3623	
L3624	S3625	K3626	Q3627	R3628	R3629	K3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	M3638	T3639	P3640	L3641	Y3642	N3643	L3644	H3647	K3648	L3649	K3650	N3651	K3652	F3653	L3654	E3655	K3658	W3661	T3662	L3663	T3664	E3665	D3666	H3667	S3668	F3669	E3670	D3671	K3672	K3673	T3674	D3675	L3676	K3679	A3680	Q3681	E3682	Q3683	E3684	E3685	E3686	E3687					
E3688	E3689	V3690	E3691	E3692	K3693	K3694	P3695	L3698	L3701	V3702	L3703	H3704	R3707	L3710	T3711	E3712	K3713	S3714	K3715	L3716	D3717	F3718	D3719	Y3720	L3721	Y3722	M3723	A3724	Y3725	I3728	M3729	A3730	K3731	S3732	C3733	H3734	L3735	E3736	GLU	GLY	GLY	GLU	ASN	GLY	GLU	GLU	ALA	GLU	GLU	GLU	V3749	E3750	V3751	S3752						
F3753	E3754	E3755	K3756	E3757	M3758	E3759	K3760	R3761	L3763	Q3766	Q3767	S3768	L3769	L3770	H3771	T3772	R3773	G3774	A3775	A3776	E3777	M3778	L3780	Q3781	K3782	L3783	S3784	A3785	C3786	K3787	G3788	E3789	T3790	M3793	S3796	T3797	L3798	K3799	L3800	G3801	L3802	L3803	L3804	L3805	N3806	G3807	G3808	E3811	V3812	Q3813	Q3814	K3815	M3816							
Y3819	L3820	K3821	D3822	D3823	K3824	E3825	V3826	F3827	F3828	F3829	Q3830	S3831	L3832	Q3833	A3834	L3835	K3836	Q3837	T3838	C3839	S3840	V3841	L3842	D3843	L3844	F3847	N3848	R3849	Q3850	E3854	G3855	L3856	G3857	M3858	V3859	N3860	E3861	D3862	G3863	T3864	V3865	L3866	N3867	R3868	Q3869	N3870	G3871	E3872	K3873	V3874	M3875	A3876	D3877	E3878	E3879	F3880				
T3881	Q3882	F3885	F3886	F3887	L3888	Q3889	L3890	L3891	C3892	E3893	G3894	H3895	S3896	N3897	D3898	F3899	Q3900	N3901	Y3902	L3903	R3904	T3905	Q3906	T3910	T3911	T3912	N3913	N3914	I3915	I3916	T3917	T3918	V3919	D3920	Y3921	Y3922	L3923	L3924	R3925	L3926	Q3927	E3928	S3929	D3932	F3933	Y3934	W3935	Y3936	Y3937	Y3938	G3939	K3940	D3941	Y3942	I3943					
Q3946	G3947	K3948	R3949	N3950	F3951	K3952	K3953	A3954	M3955	V3956	K3958	K3959	L3965	T3966	E3967	V3968	T3969	Q3970	G3971	C3972	N3973	Q3977	L3980	A3981	H3982	S3983	R3984	I3985	V3986	A3987	V3989	V3990	G3991	L3992	H3993	H3994	V3995	F3996	A3997	H3998	M3999	M4000	M4001	K4002	L4003	A4004	Q4005	D4006	S4007	S4008	Q4009	I4010	E4011							
L4012	E4015	L4016	L4017	D4018	L4019	M4023	V4024	V4025	M4026	L4027	L4028	S4029	L4030	L4031	E4032	V4036	M4037	G4038	M4039	I4040	A4041	R4042	Q4043	M4044	V4045	D4046	M4047	L4048	V4049	E4050	S4053	E4056	L4059	K4060	F4061	F4062	D4063	M4064	F4065	L4066	K4067	L4068	K4069	D4070	I4071	V4072	G4073	S4074	E4075	A4076	F4077	Q4078	D4079							



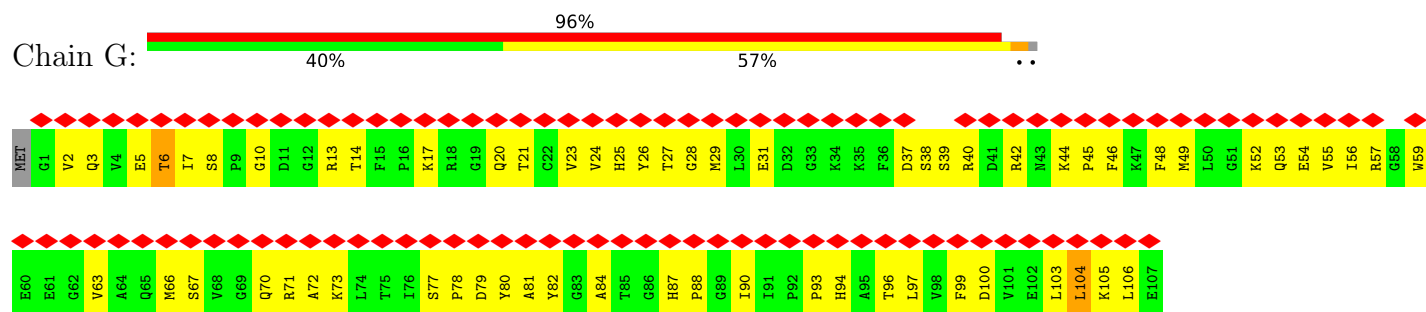
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



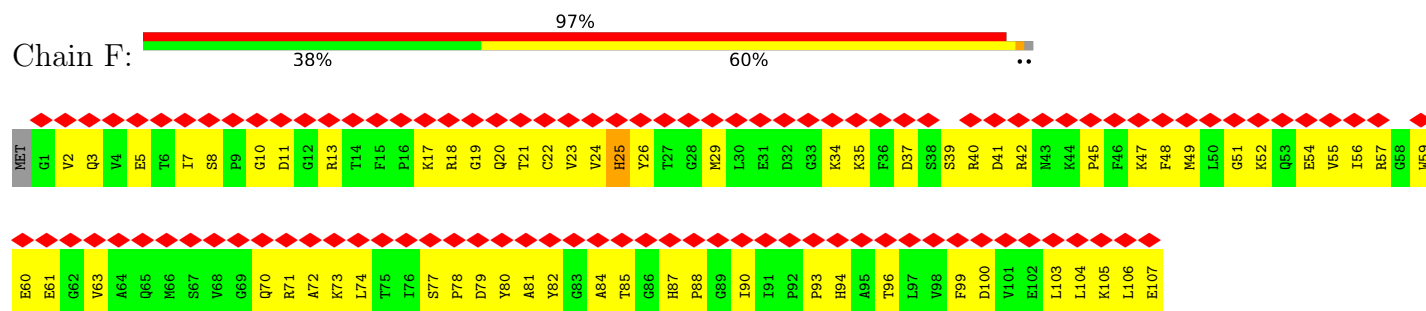
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- 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	17284	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	0.224	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	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

5.1 Standard geometry

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

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	0.19	0/35977	0.51	6/48726 (0.0%)
1	B	0.20	0/35977	0.51	6/48726 (0.0%)
1	C	0.20	0/35977	0.51	6/48726 (0.0%)
1	D	0.20	0/35977	0.51	6/48726 (0.0%)
2	E	0.21	0/850	0.60	0/1146
2	F	0.20	0/850	0.57	0/1146
2	G	0.18	0/850	0.51	0/1146
2	H	0.19	0/850	0.59	0/1146
All	All	0.20	0/147308	0.51	24/199488 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4876	CYS	CA-CB-SG	7.38	131.37	114.40
1	A	4876	CYS	CA-CB-SG	7.37	131.34	114.40
1	B	4876	CYS	CA-CB-SG	7.35	131.31	114.40
1	D	4876	CYS	CA-CB-SG	7.35	131.30	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2481	LYS	CA-C-N	7.10	135.10	121.54

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1671	ARG	Sidechain
1	A	4876	CYS	Peptide
1	B	1671	ARG	Sidechain
1	B	4876	CYS	Peptide
1	D	1671	ARG	Sidechain

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	35150	0	34793	2264	0
1	B	35150	0	34793	2262	0
1	C	35150	0	34793	2299	0
1	D	35150	0	34793	2289	0
2	E	831	0	831	73	0
2	F	831	0	830	68	0
2	G	831	0	831	76	0
2	H	831	0	831	81	0
3	A	31	0	12	1	0
3	B	31	0	12	2	0
3	C	31	0	12	2	0
3	D	31	0	12	2	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
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	18	0	0	1	0
6	C	18	0	0	1	0
6	D	18	0	0	1	0
All	All	144128	0	142543	9179	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 32.

The worst 5 of 9179 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:40:ARG:NH2	1:B:674:PHE:CE2	1.90	1.19
1:D:1220:GLN:HB3	1:C:3522:LEU:HD13	1.12	1.12
1:A:3522:LEU:HD13	1:B:1220:GLN:HB3	1.09	1.07
1:B:3522:LEU:HD13	1:C:1220:GLN:HB3	1.11	1.07
1:A:1220:GLN:HB3	1:D:3522:LEU:HD13	1.06	1.06

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%)	4250 (97%)	129 (3%)	6 (0%)	48	83
1	B	4385/5037 (87%)	4250 (97%)	129 (3%)	6 (0%)	48	83
1	C	4385/5037 (87%)	4249 (97%)	130 (3%)	6 (0%)	48	83
1	D	4385/5037 (87%)	4250 (97%)	129 (3%)	6 (0%)	48	83
2	E	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
All	All	17960/20580 (87%)	17404 (97%)	532 (3%)	24 (0%)	49	83

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	908	VAL
1	A	3300	ALA
1	A	4711	PHE
1	B	908	VAL
1	B	3300	ALA

5.3.2 Protein sidechains ⓘ

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%)	3747 (98%)	89 (2%)	44	63
1	B	3836/4276 (90%)	3748 (98%)	88 (2%)	44	63
1	C	3836/4276 (90%)	3750 (98%)	86 (2%)	45	64
1	D	3836/4276 (90%)	3748 (98%)	88 (2%)	44	63
2	E	89/90 (99%)	87 (98%)	2 (2%)	45	64
2	F	89/90 (99%)	85 (96%)	4 (4%)	24	46
2	G	89/90 (99%)	85 (96%)	4 (4%)	24	46
2	H	89/90 (99%)	83 (93%)	6 (7%)	15	37
All	All	15700/17464 (90%)	15333 (98%)	367 (2%)	45	63

5 of 367 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2268[A]	GLN
1	C	243	ARG
1	D	2461	VAL
1	D	3232	LEU

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Mol	Chain	Res	Type
1	C	1231[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 275 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1837	GLN
1	C	2180	GLN
1	C	3734	HIS
1	B	1837	GLN
1	B	1631	GLN

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	$\# Z > 2$
6	A1BD2	C	5304	-	19,19,19	0.34	0	28,28,28	0.47	0
6	A1BD2	B	5304	-	19,19,19	0.34	0	28,28,28	0.49	0
3	ATP	D	5301	-	32,33,33	0.37	0	48,52,52	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	5301	-	32,33,33	0.37	0	48,52,52	0.40	0
3	ATP	A	5301	-	32,33,33	0.36	0	48,52,52	0.40	0
3	ATP	C	5301	-	32,33,33	0.37	0	48,52,52	0.40	0
6	A1BD2	A	5304	-	19,19,19	0.34	0	28,28,28	0.48	0
6	A1BD2	D	5304	-	19,19,19	0.34	0	28,28,28	0.48	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
6	A1BD2	C	5304	-	-	0/6/6/6	0/2/2/2
6	A1BD2	B	5304	-	-	0/6/6/6	0/2/2/2
3	ATP	D	5301	-	-	6/22/38/38	0/3/3/3
3	ATP	B	5301	-	-	6/22/38/38	0/3/3/3
3	ATP	A	5301	-	-	6/22/38/38	0/3/3/3
3	ATP	C	5301	-	-	6/22/38/38	0/3/3/3
6	A1BD2	A	5304	-	-	0/6/6/6	0/2/2/2
6	A1BD2	D	5304	-	-	0/6/6/6	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	5301	ATP	O4'-C4'-C5'-O5'
3	A	5301	ATP	O4'-C4'-C5'-O5'
3	B	5301	ATP	O4'-C4'-C5'-O5'
3	C	5301	ATP	O4'-C4'-C5'-O5'
3	A	5301	ATP	PG-O3B-PB-O3A

There are no ring outliers.

8 monomers are involved in 11 short contacts:

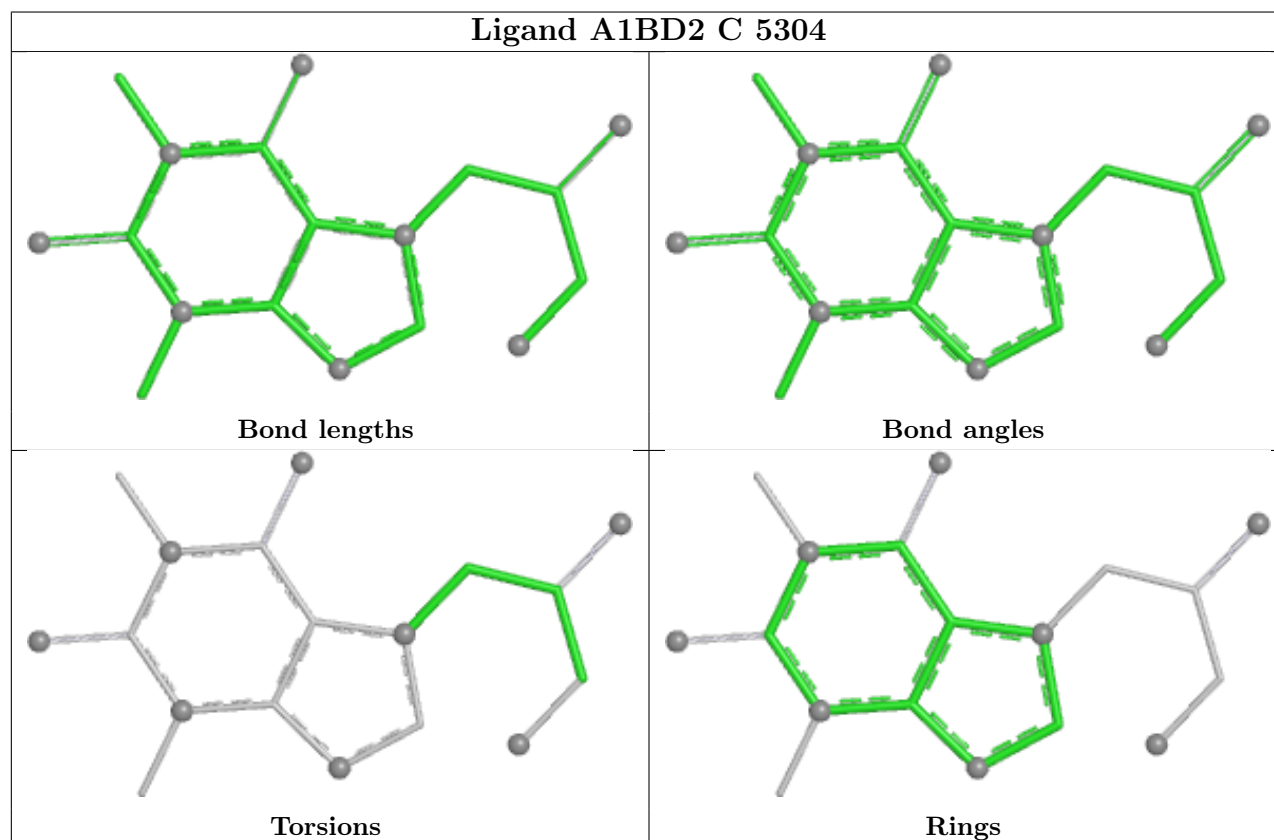
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	5304	A1BD2	1	0
6	B	5304	A1BD2	1	0
3	D	5301	ATP	2	0

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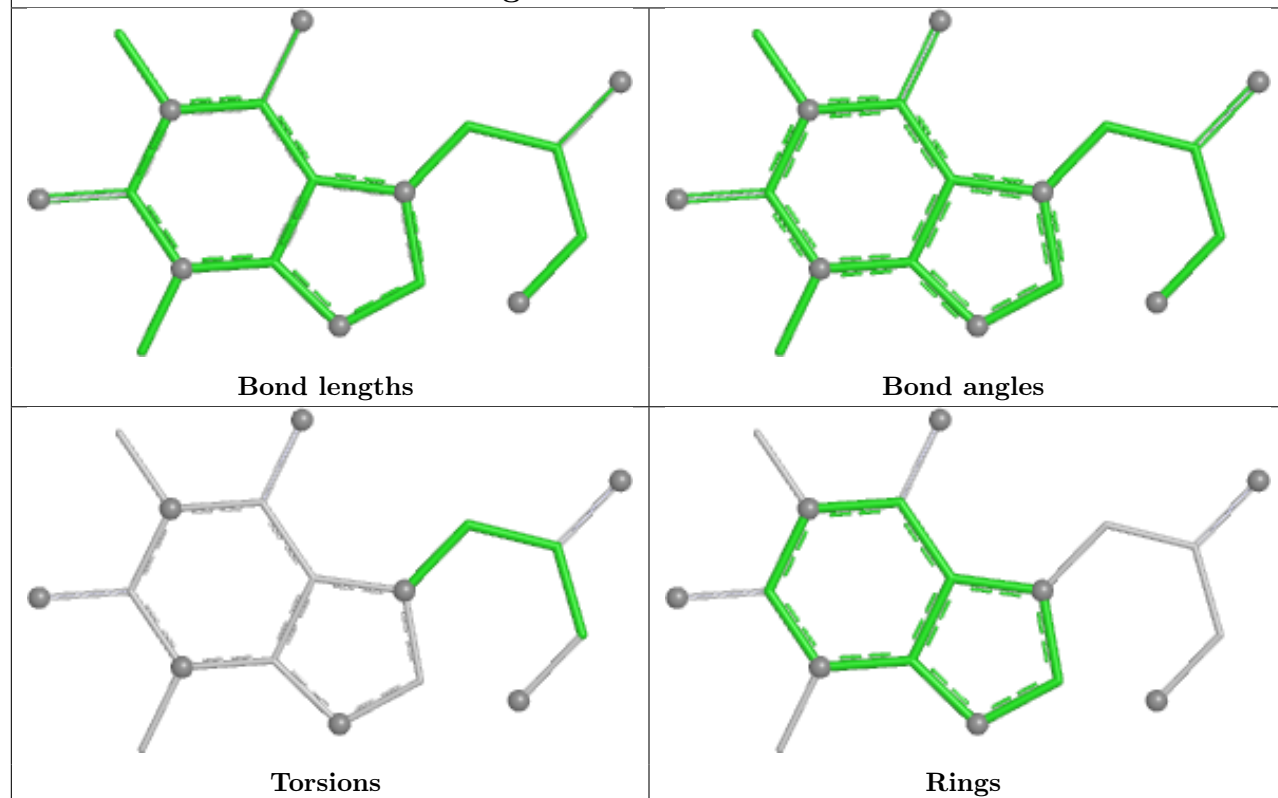
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5301	ATP	2	0
3	A	5301	ATP	1	0
3	C	5301	ATP	2	0
6	A	5304	A1BD2	1	0
6	D	5304	A1BD2	1	0

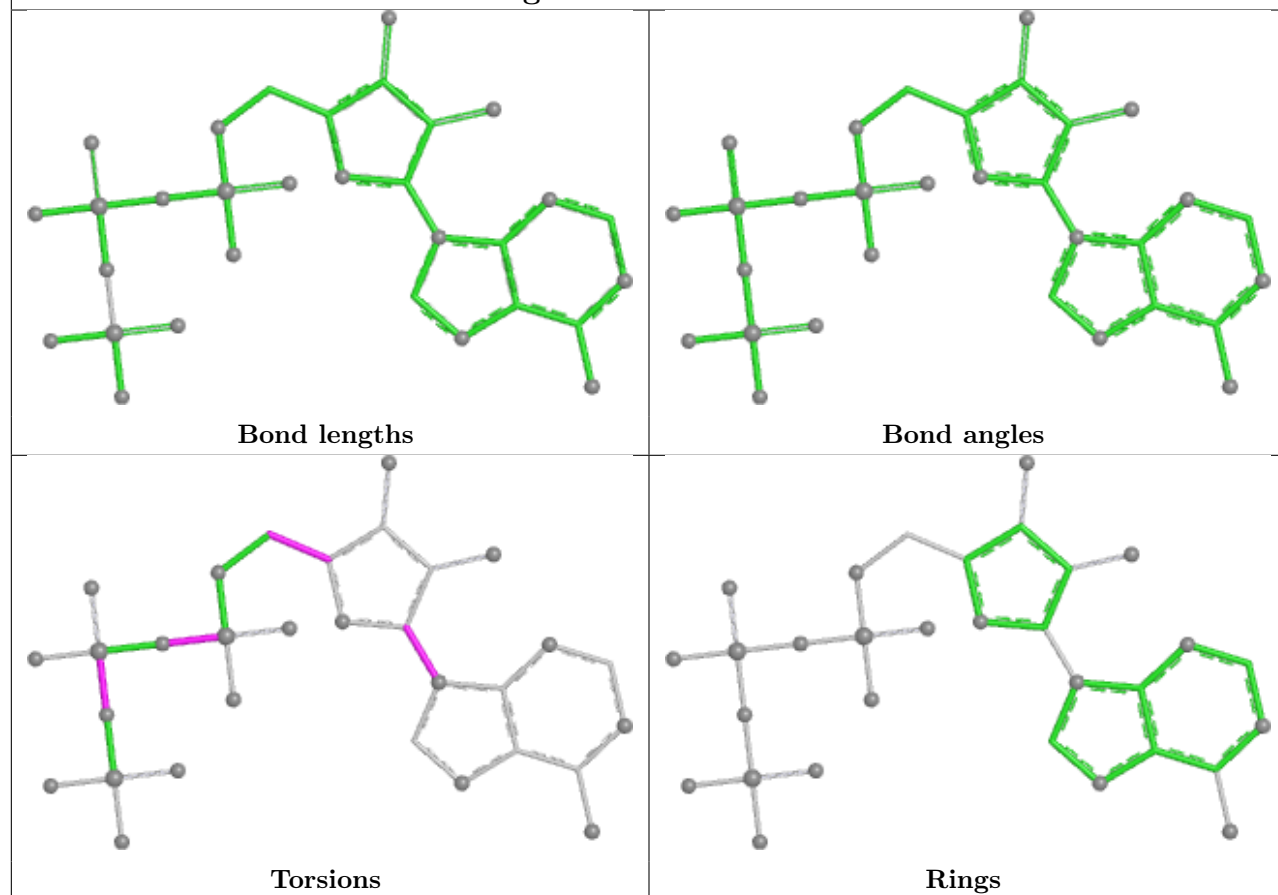
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

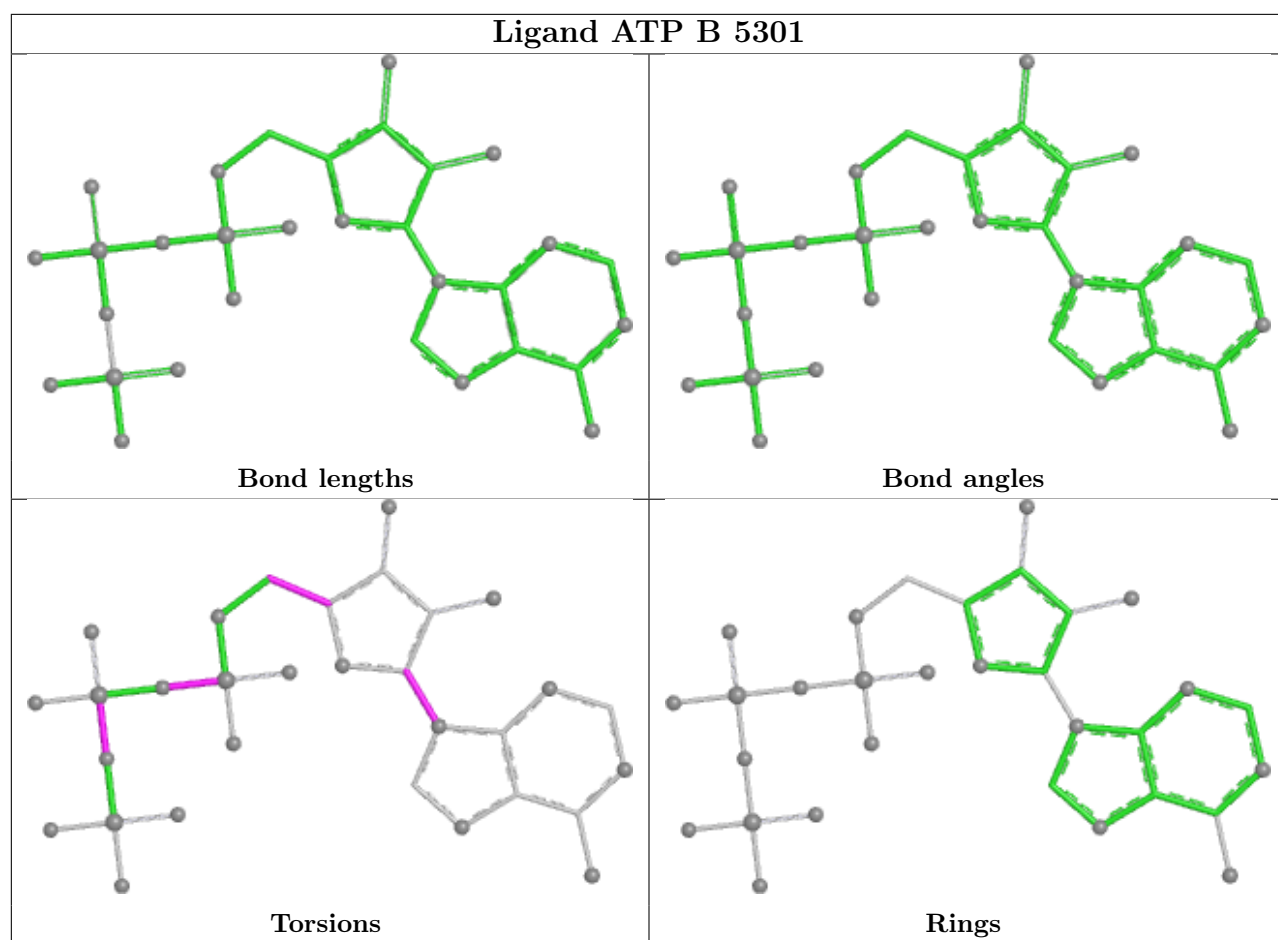


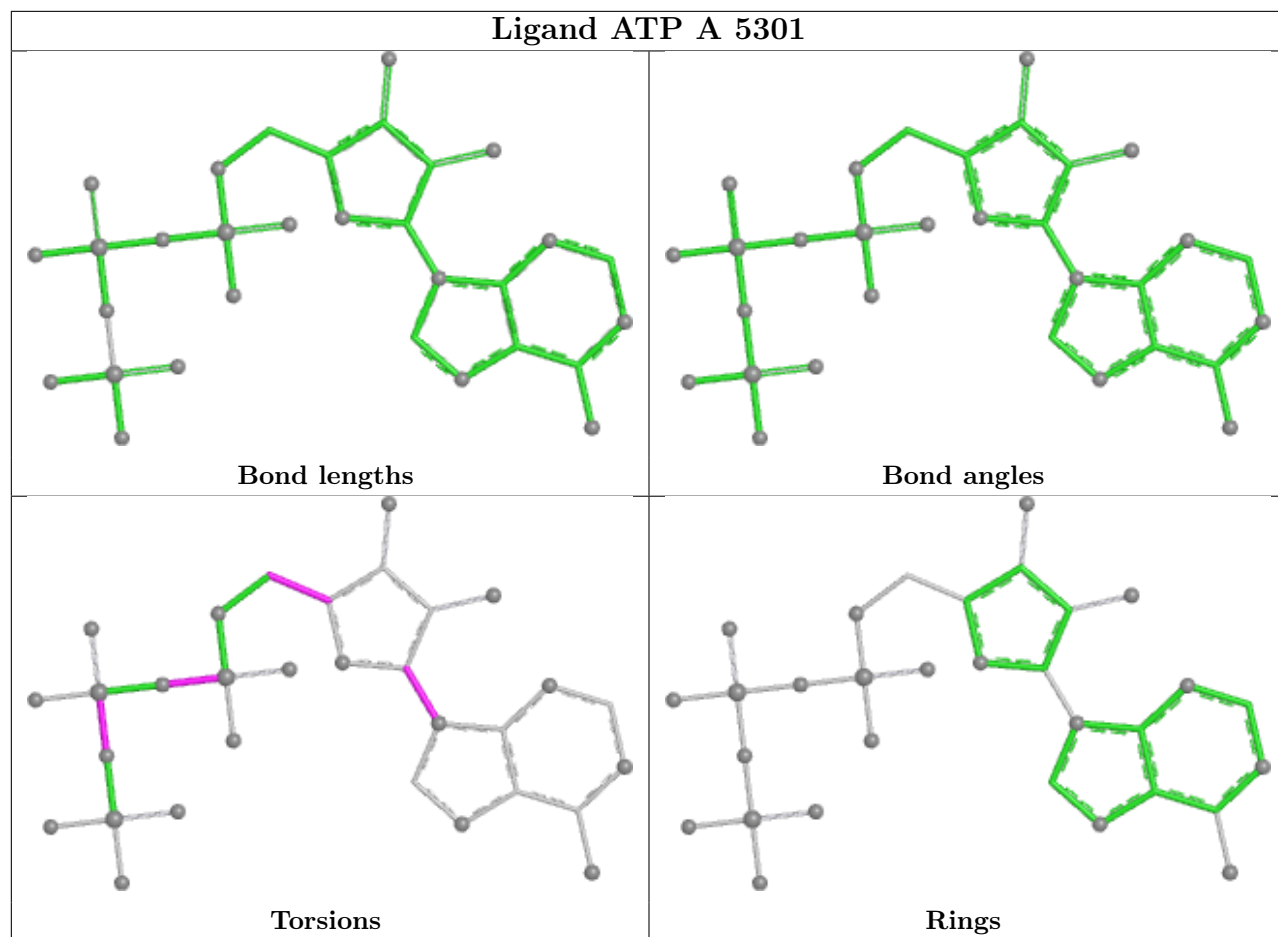
Ligand A1BD2 B 5304

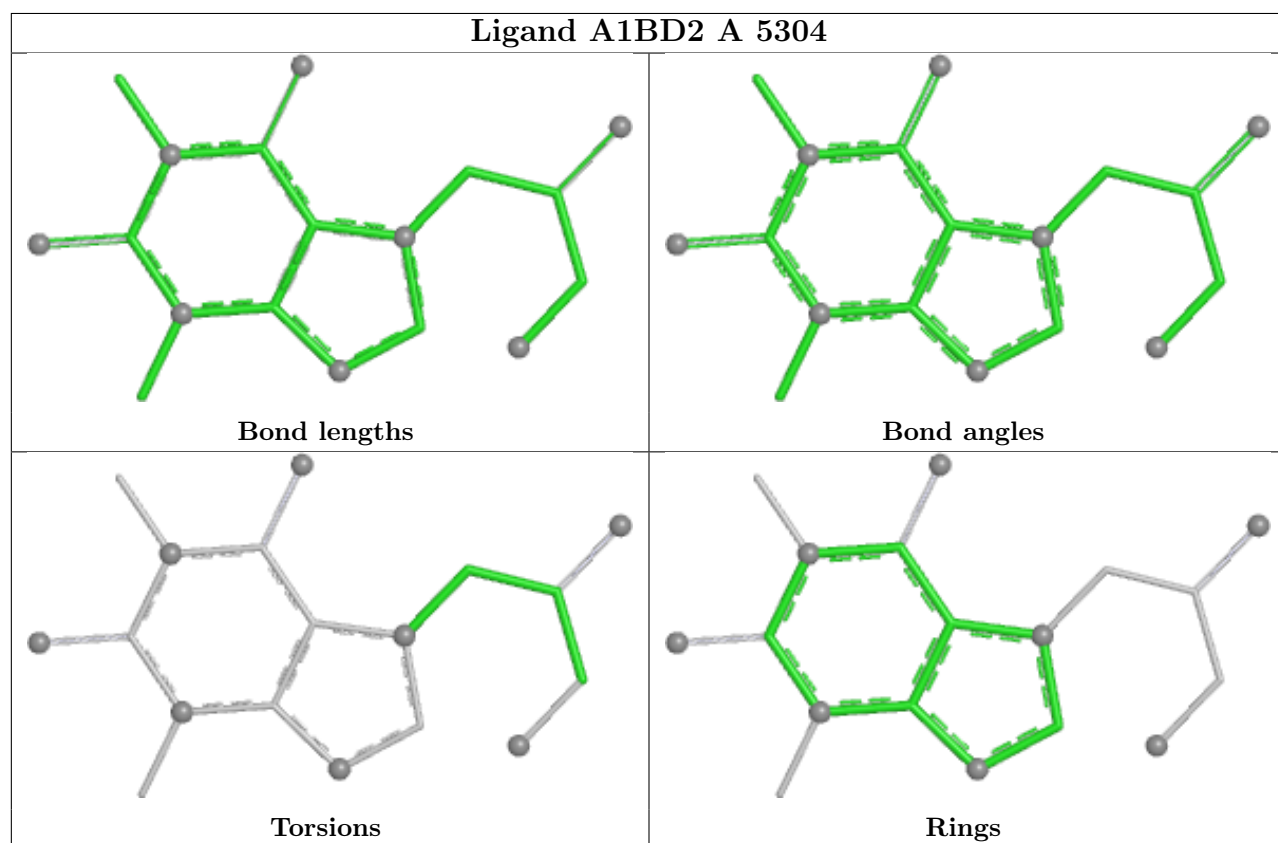
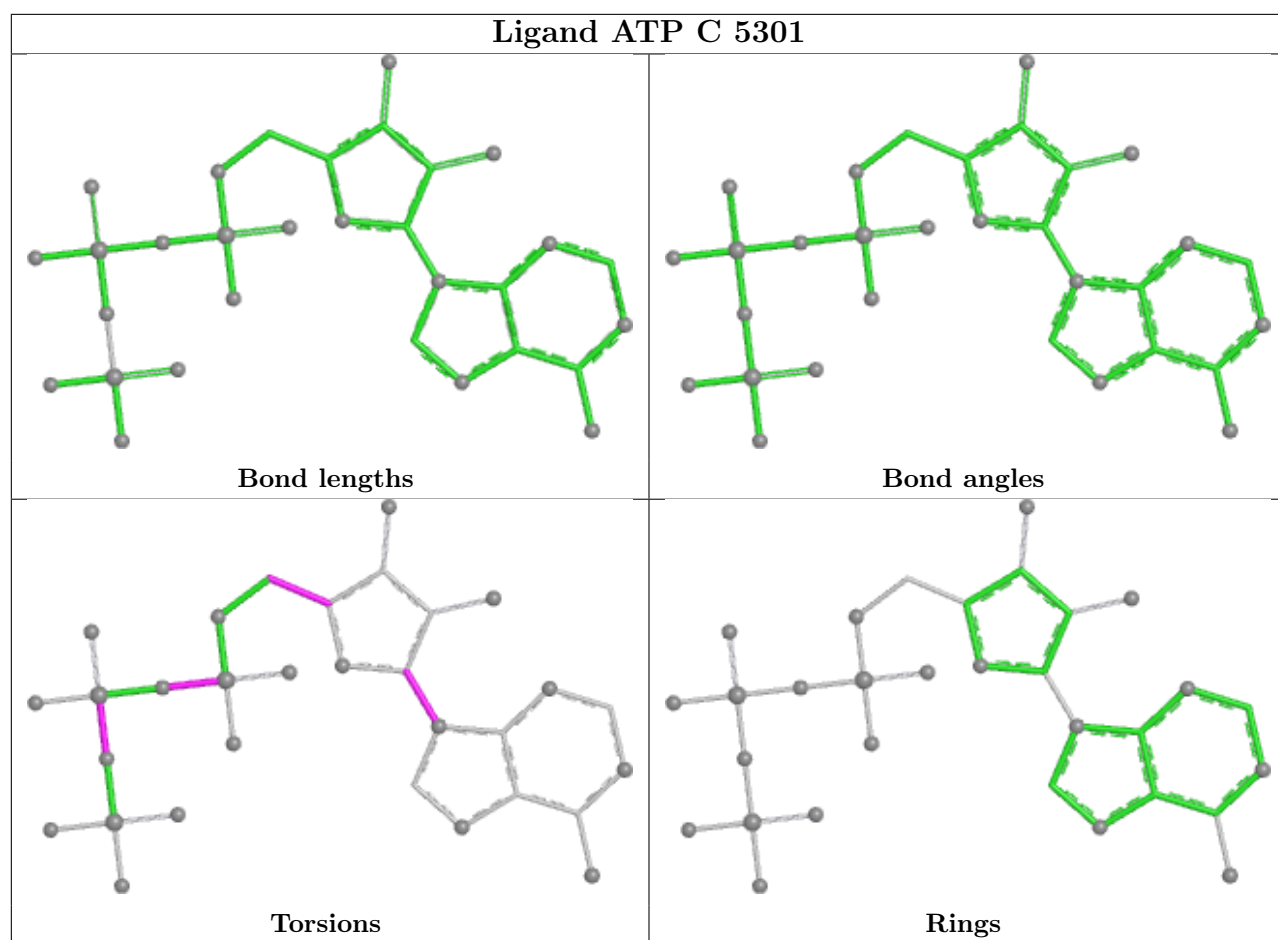


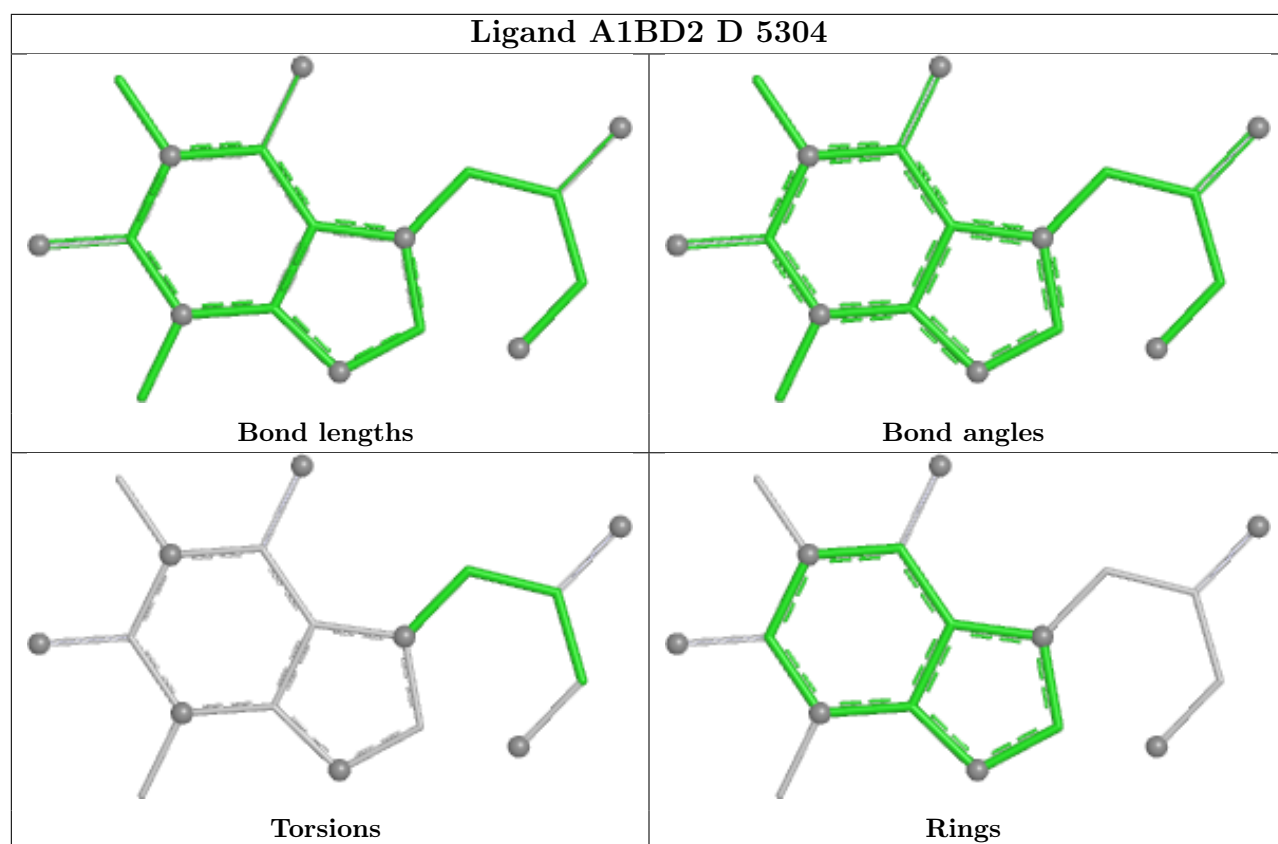
Ligand ATP D 5301











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.

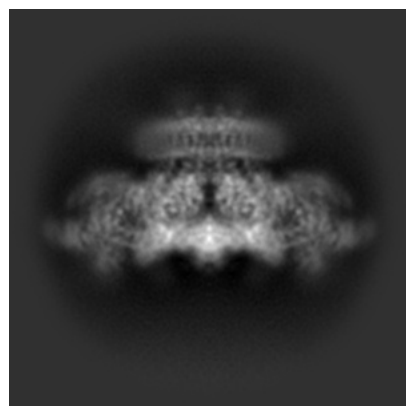
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47388. These allow visual inspection of the internal detail of the map and identification of artifacts.

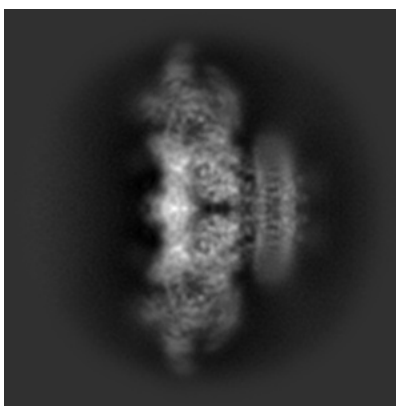
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

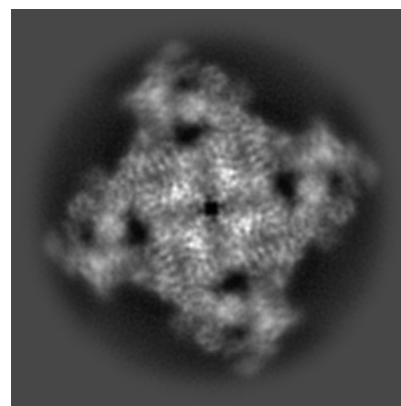
6.1.1 Primary map



X

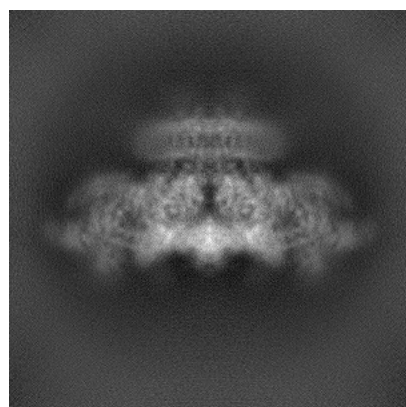


Y

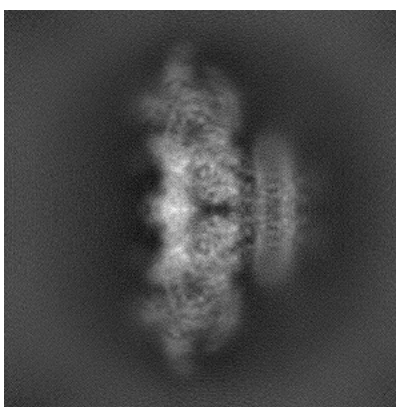


Z

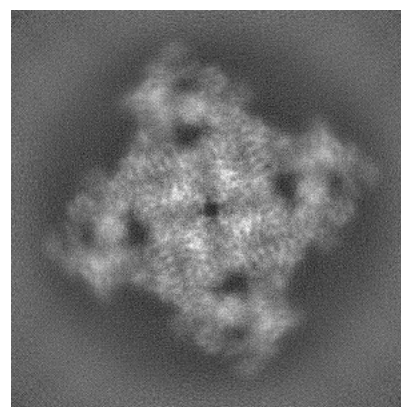
6.1.2 Raw map



X



Y

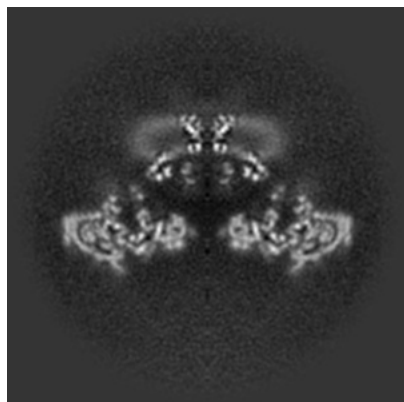


Z

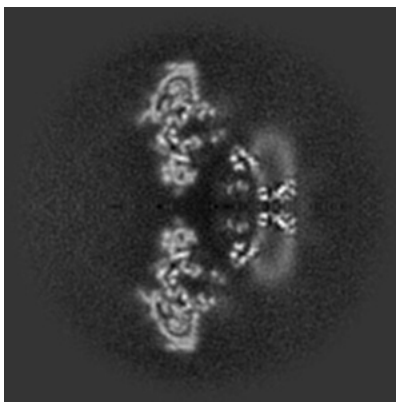
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

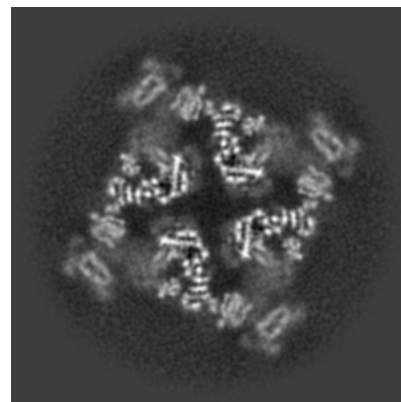
6.2.1 Primary map



X Index: 256

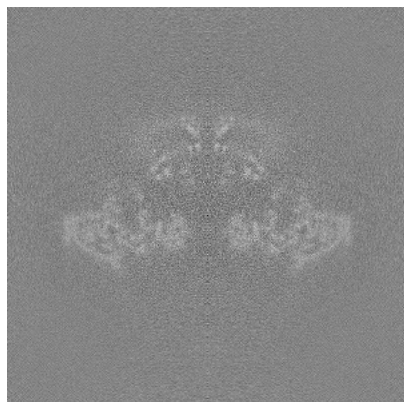


Y Index: 256

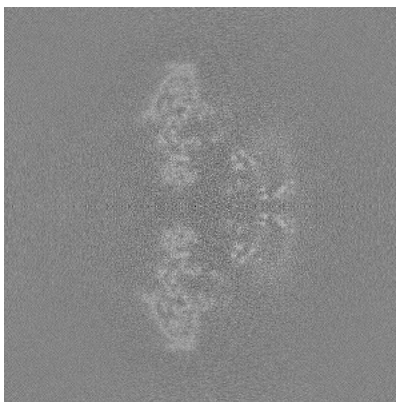


Z Index: 256

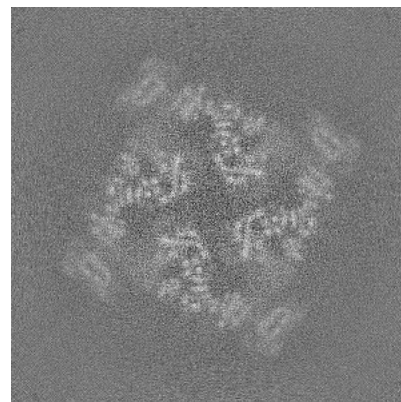
6.2.2 Raw map



X Index: 256



Y Index: 256

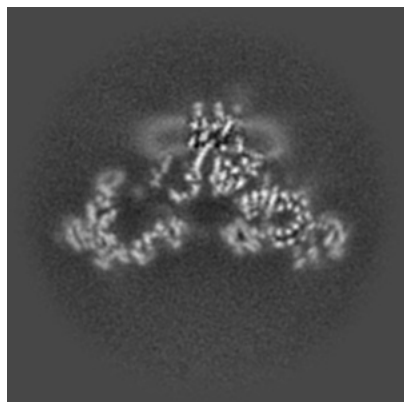


Z Index: 256

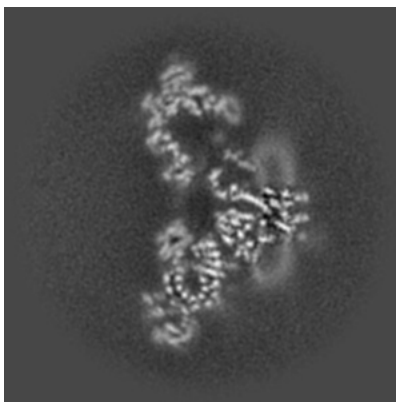
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

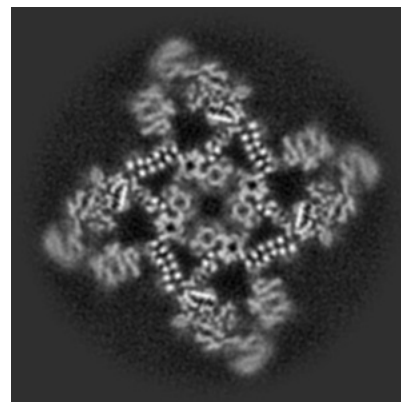
6.3.1 Primary map



X Index: 269

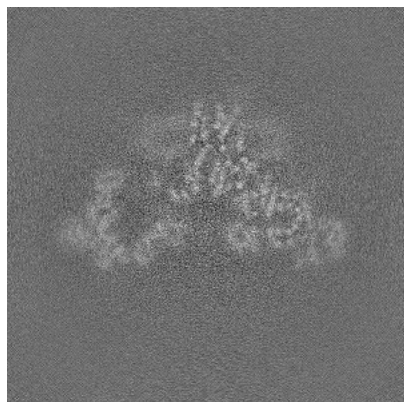


Y Index: 269

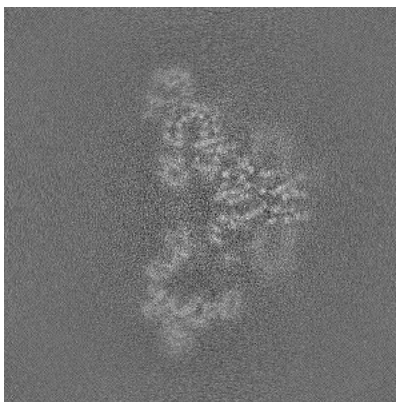


Z Index: 229

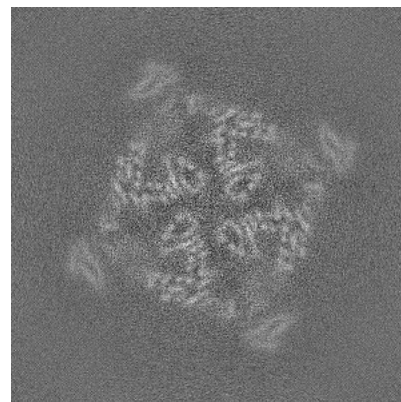
6.3.2 Raw map



X Index: 271



Y Index: 241

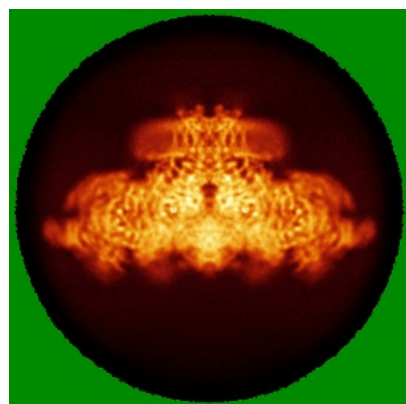


Z Index: 268

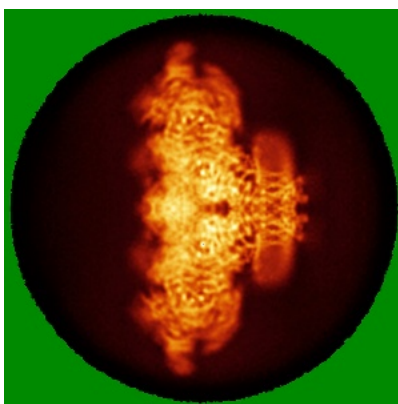
The images above show the largest variance slices of the map in three orthogonal directions.

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

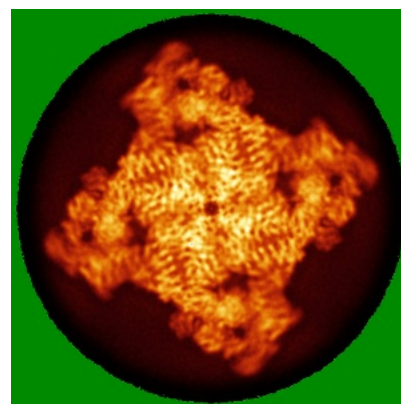
6.4.1 Primary map



X

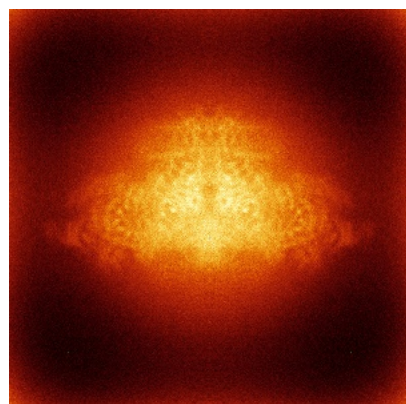


Y

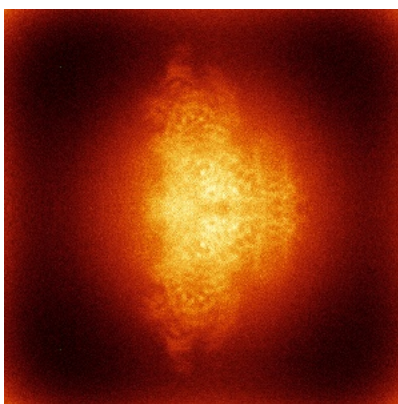


Z

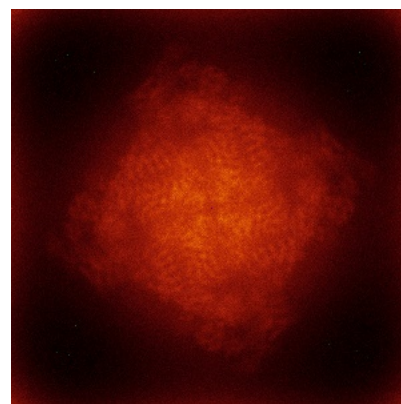
6.4.2 Raw map



X



Y

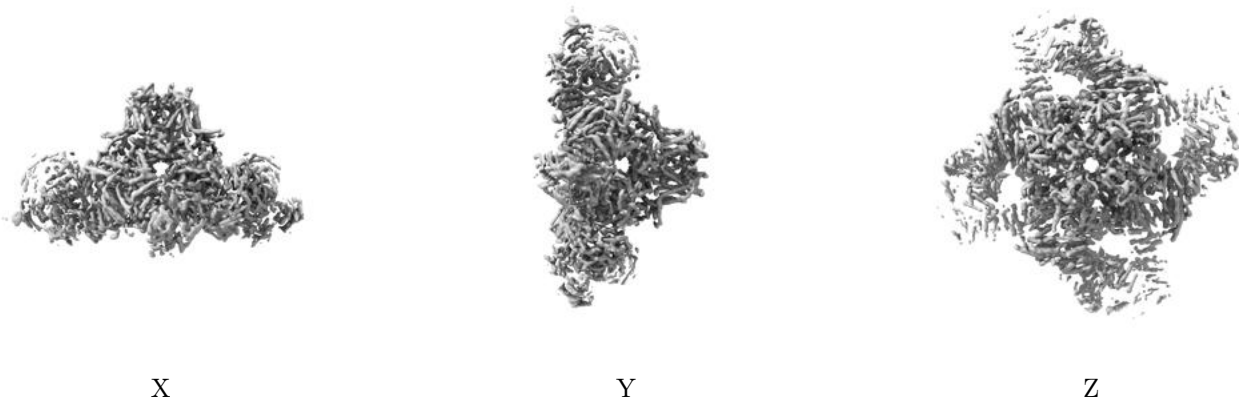


Z

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.

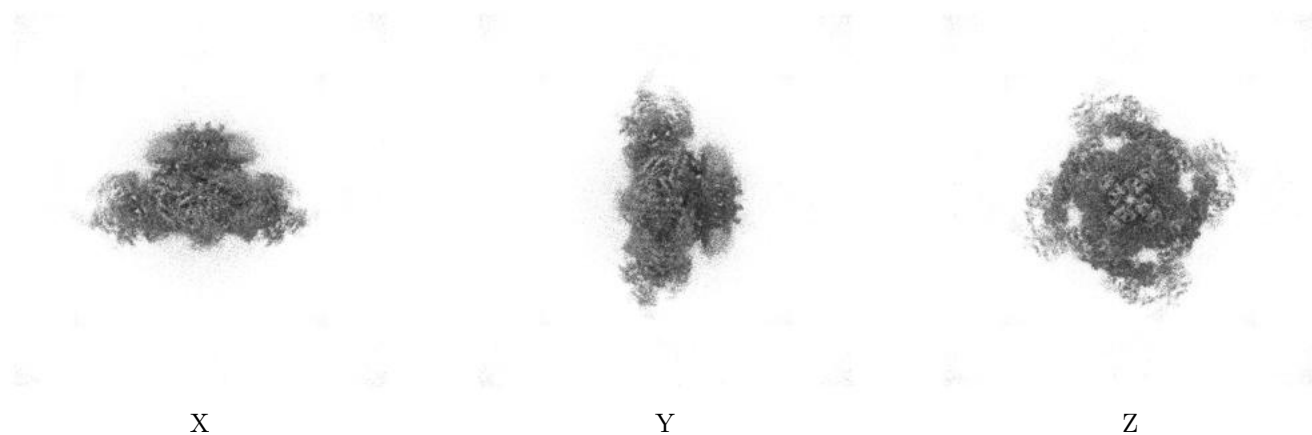
6.5 Orthogonal surface views [i](#)

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.

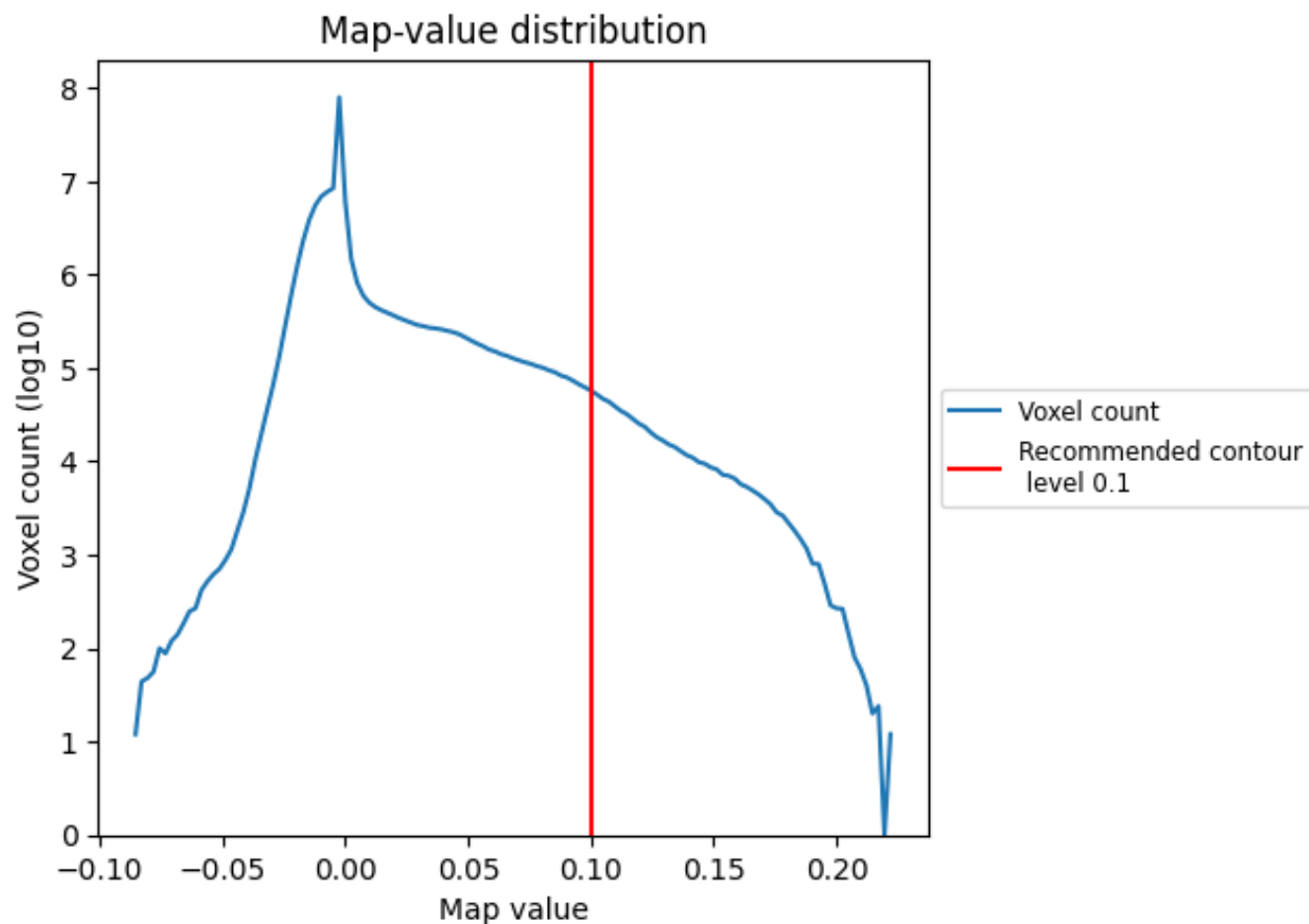
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

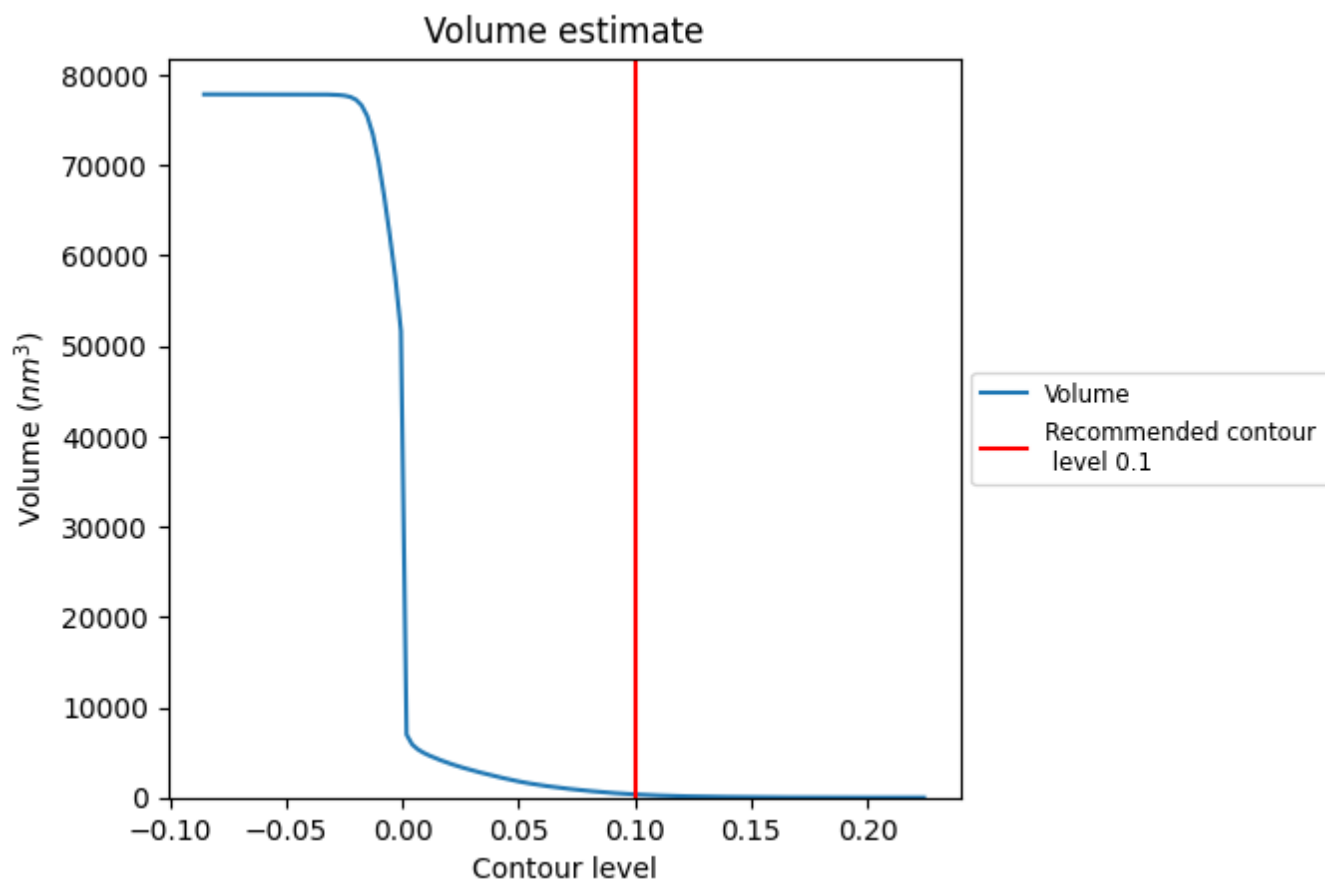
This section contains the results of statistical analysis of the map.

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.

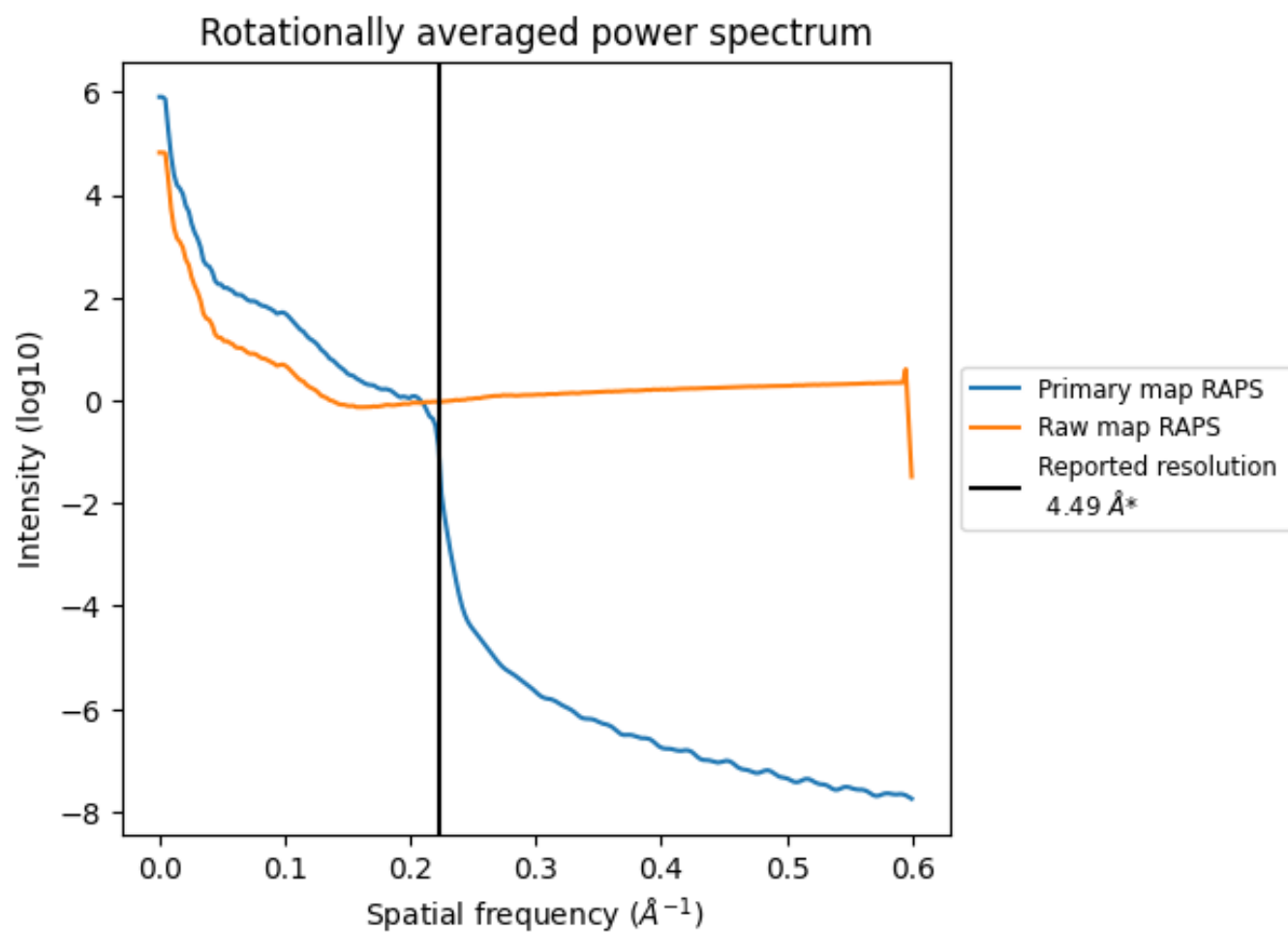
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352 nm³; this corresponds to an approximate mass of 318 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 ⓘ

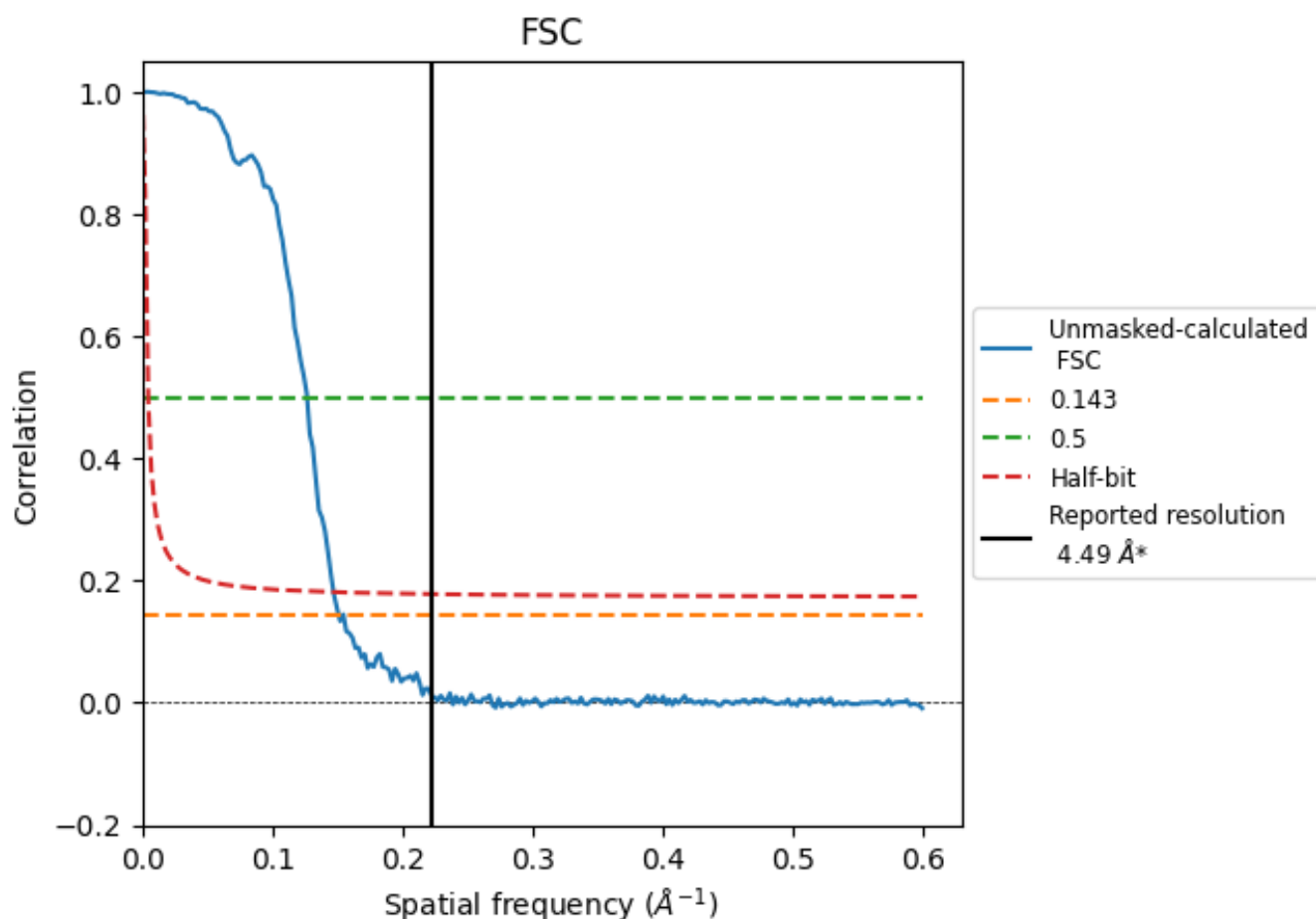


*Reported resolution corresponds to spatial frequency of 0.223 $\text{\AA}^{-1}$

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 0.223 Å⁻¹

8.2 Resolution estimates [i](#)

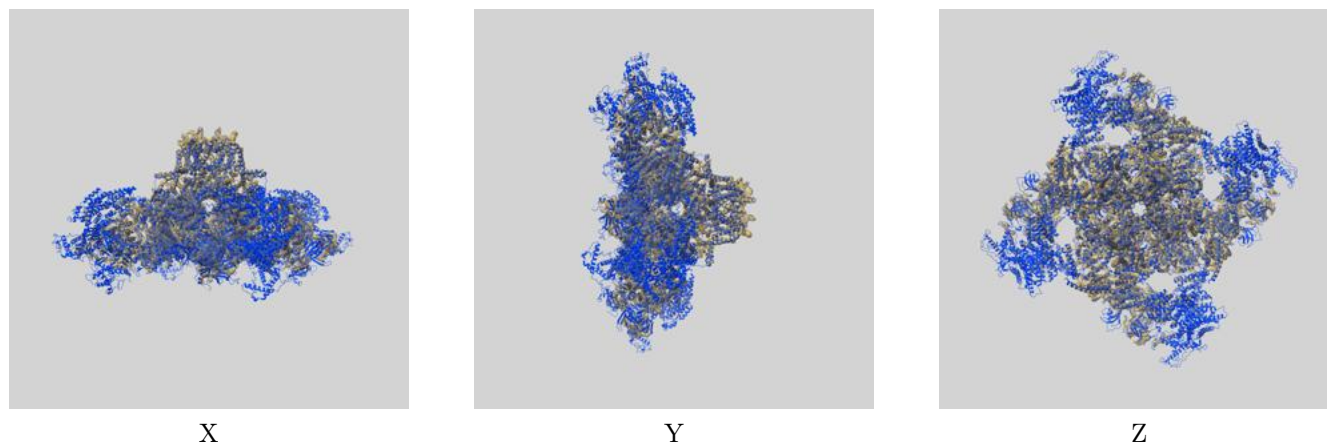
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.49	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.62	7.89	6.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.62 differs from the reported value 4.49 by more than 10 %

9 Map-model fit [i](#)

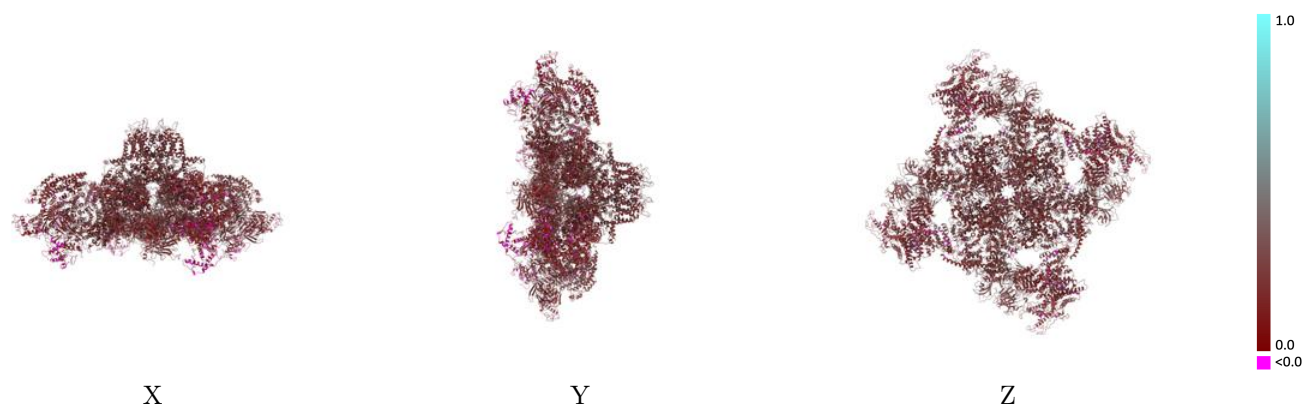
This section contains information regarding the fit between EMDB map EMD-47388 and PDB model 9E1B. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



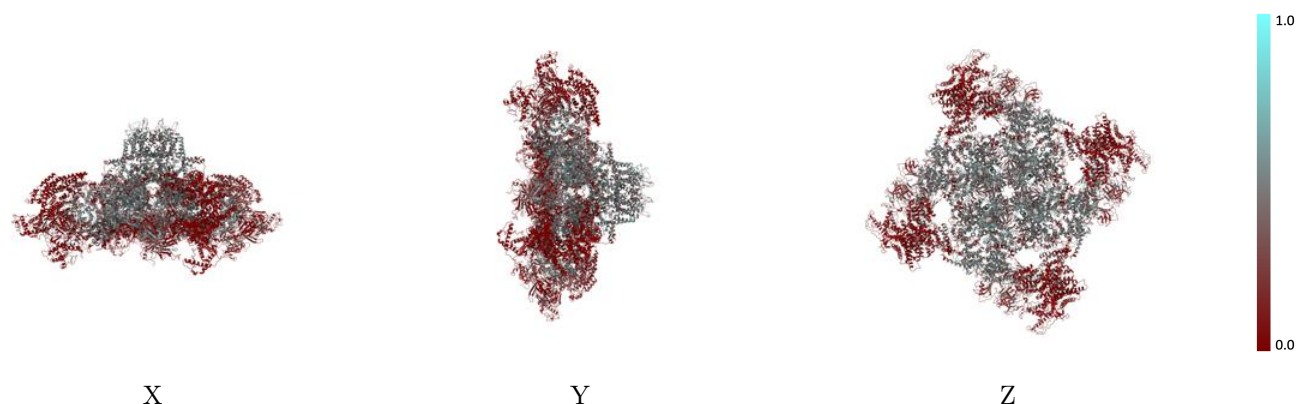
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



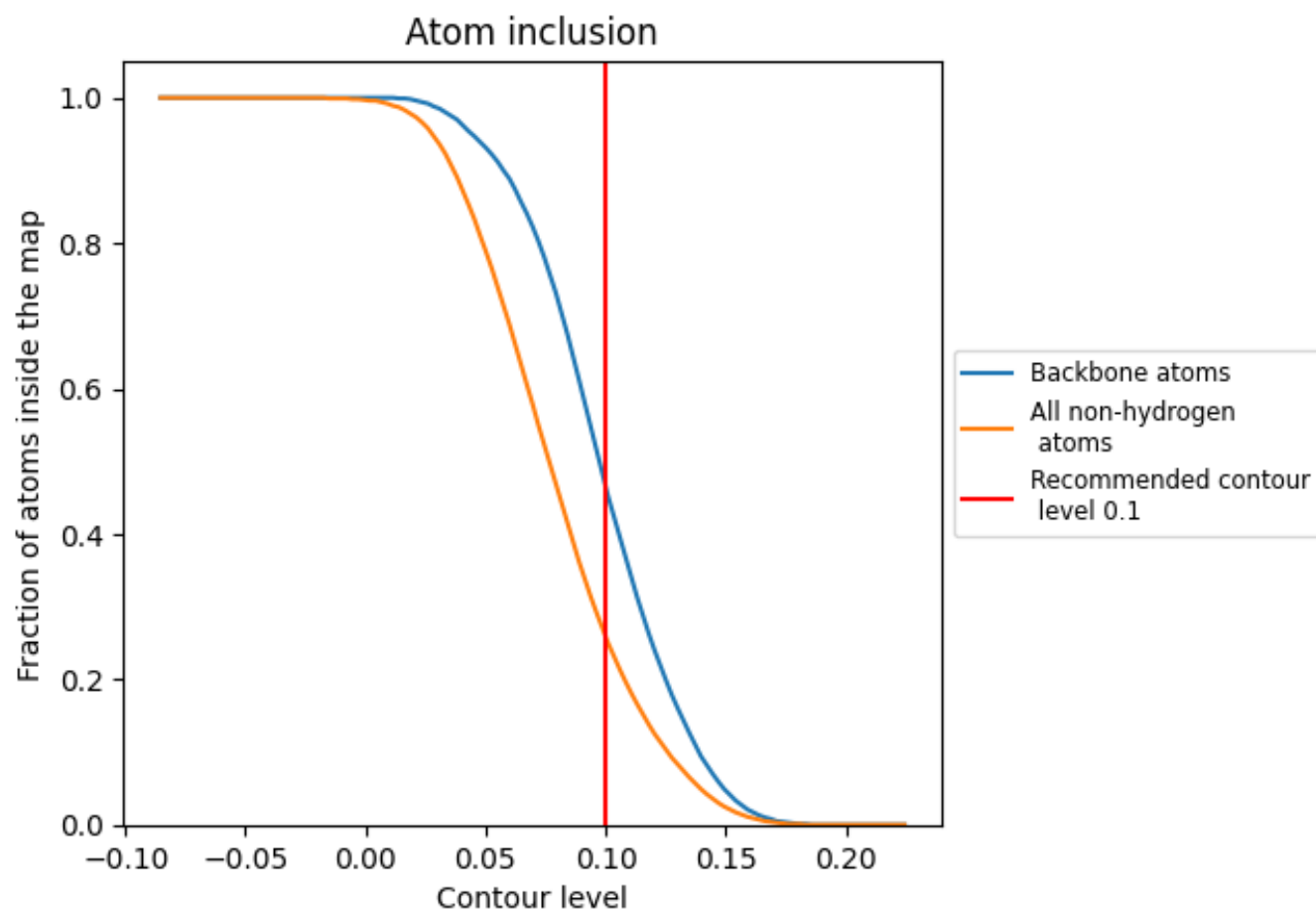
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 47% of all backbone atoms, 26% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2590	0.2100
A	0.2640	0.2100
B	0.2640	0.2090
C	0.2640	0.2090
D	0.2640	0.2090
E	0.0360	0.2600
F	0.0310	0.2560
G	0.0320	0.2630
H	0.0360	0.2580

1.0

0.0

<0.0