



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 10:01 AM JST

PDB ID : 5GKY
EMDB ID : EMD-9518
Title : Structure of RyR1 in a closed state (C1 conformer)
Authors : Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-07
Resolution : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

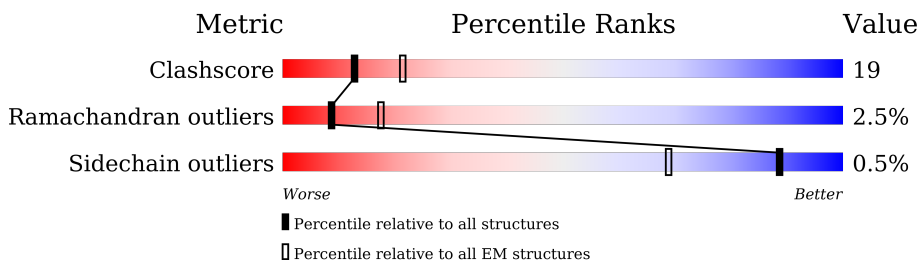
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>18%</div> <div>46%</div> <div>26%</div> <div>27%</div> </div>
1	C	5037	<div> <div>18%</div> <div>46%</div> <div>26%</div> <div>27%</div> </div>
1	E	5037	<div> <div>18%</div> <div>46%</div> <div>26%</div> <div>27%</div> </div>
1	G	5037	<div> <div>18%</div> <div>46%</div> <div>25%</div> <div>27%</div> </div>
2	B	108	<div> <div>16%</div> <div>56%</div> <div>43%</div> </div>
2	D	108	<div> <div>17%</div> <div>56%</div> <div>43%</div> </div>
2	F	108	<div> <div>17%</div> <div>56%</div> <div>43%</div> </div>
2	H	108	<div> <div>16%</div> <div>56%</div> <div>43%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 111036 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	3660	Total	C	N	O	S	1	0
			26926	17112	4683	4974	157		
1	C	3660	Total	C	N	O	S	1	0
			26926	17112	4683	4974	157		
1	E	3660	Total	C	N	O	S	1	0
			26926	17112	4683	4974	157		
1	G	3660	Total	C	N	O	S	1	0
			26926	17112	4683	4974	157		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	D	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	F	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	H	107	Total	C	N	O	S	0	0
			832	527	146	155	4		

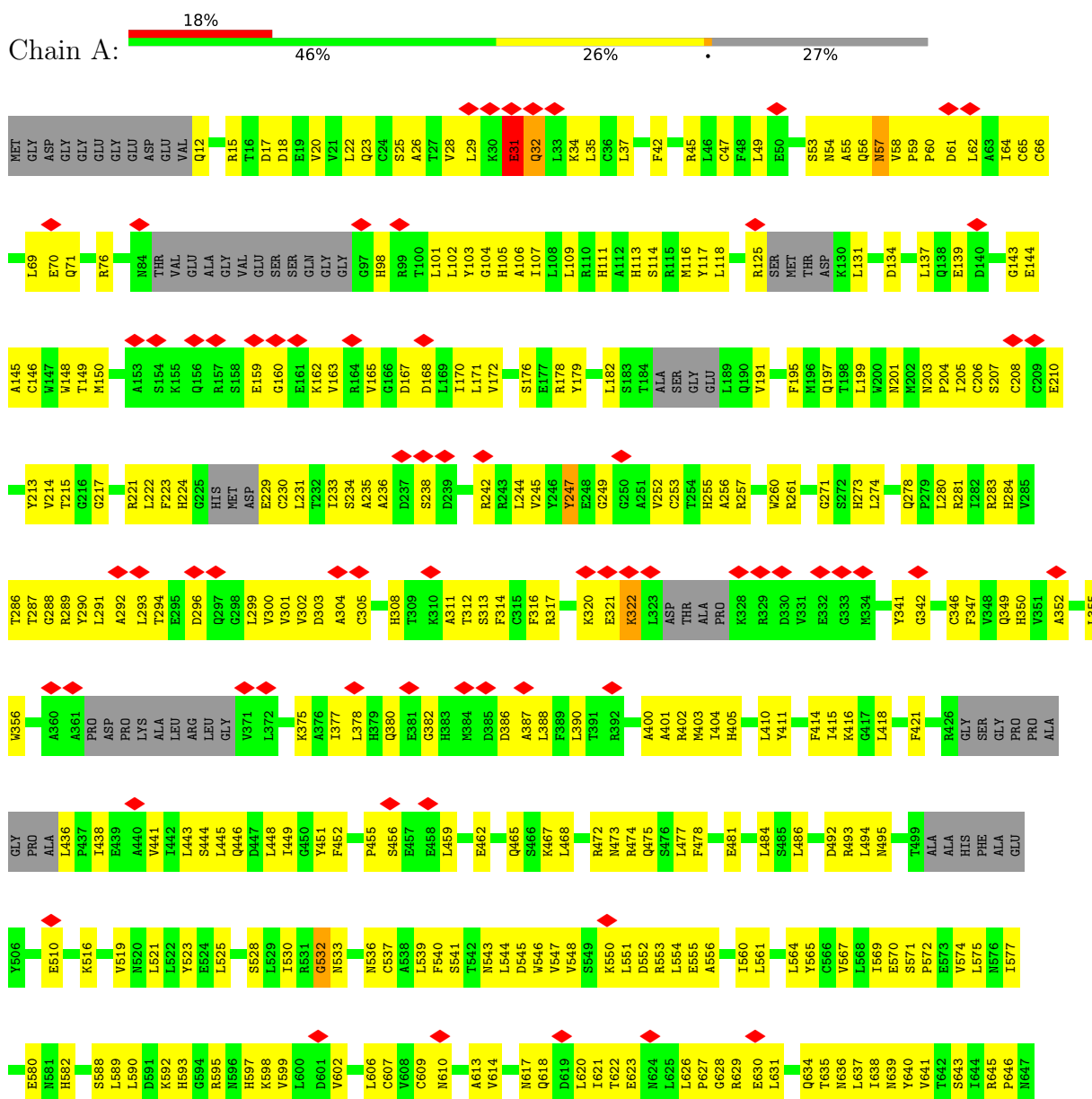
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

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

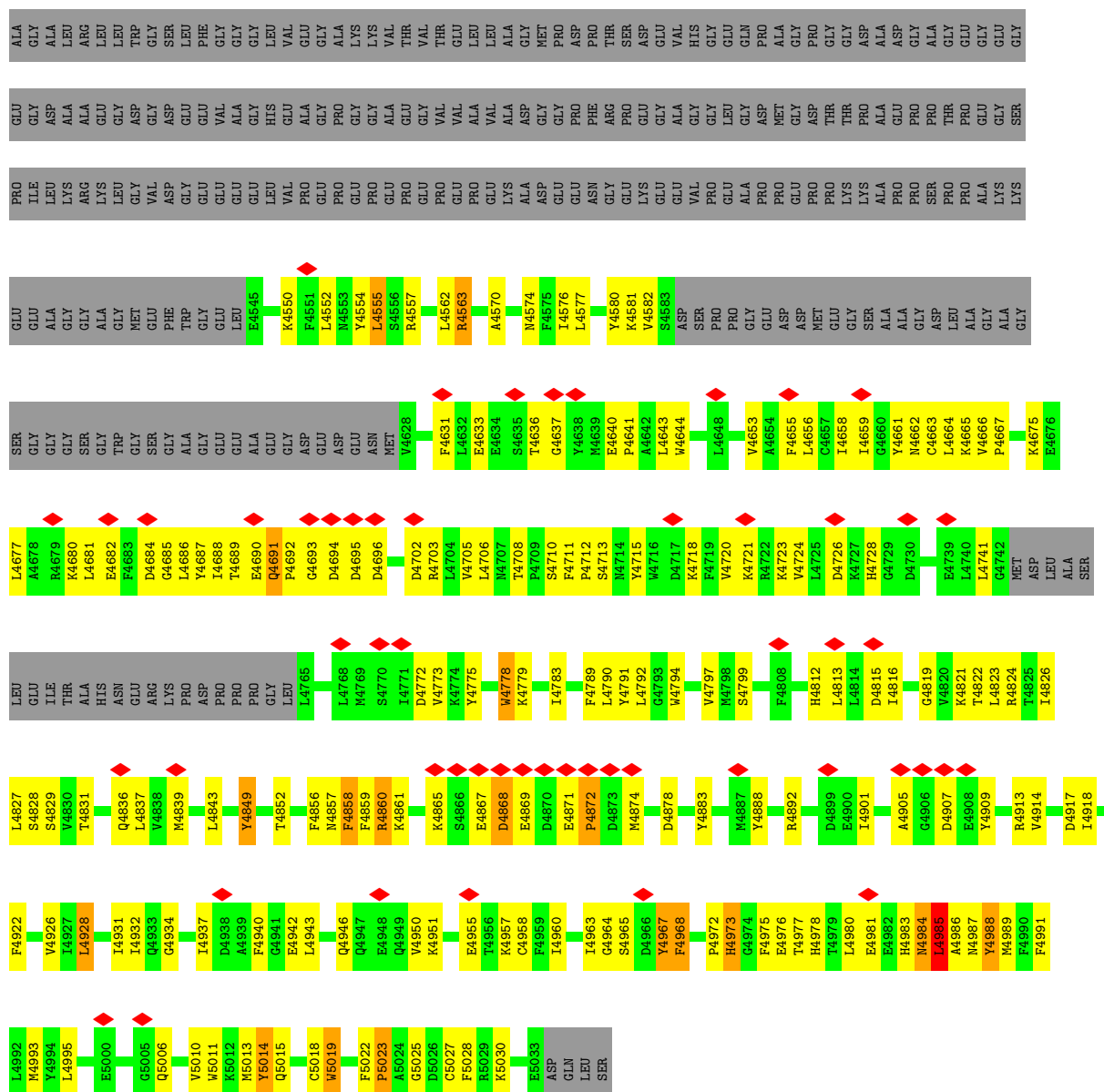




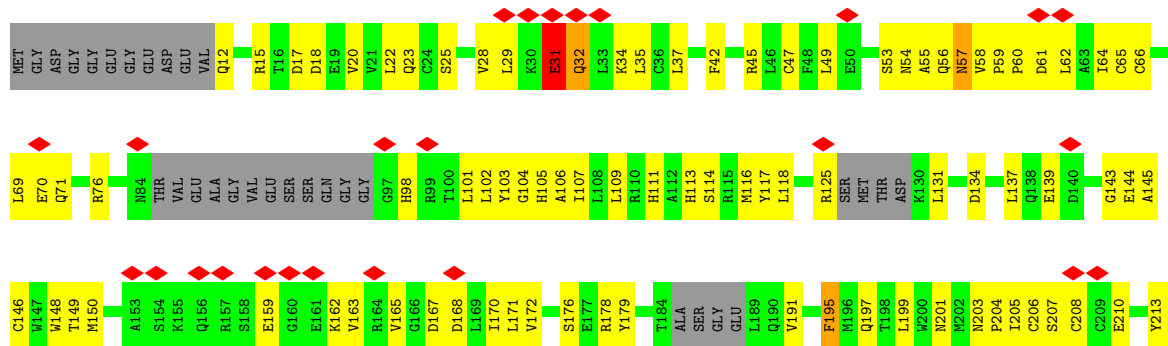


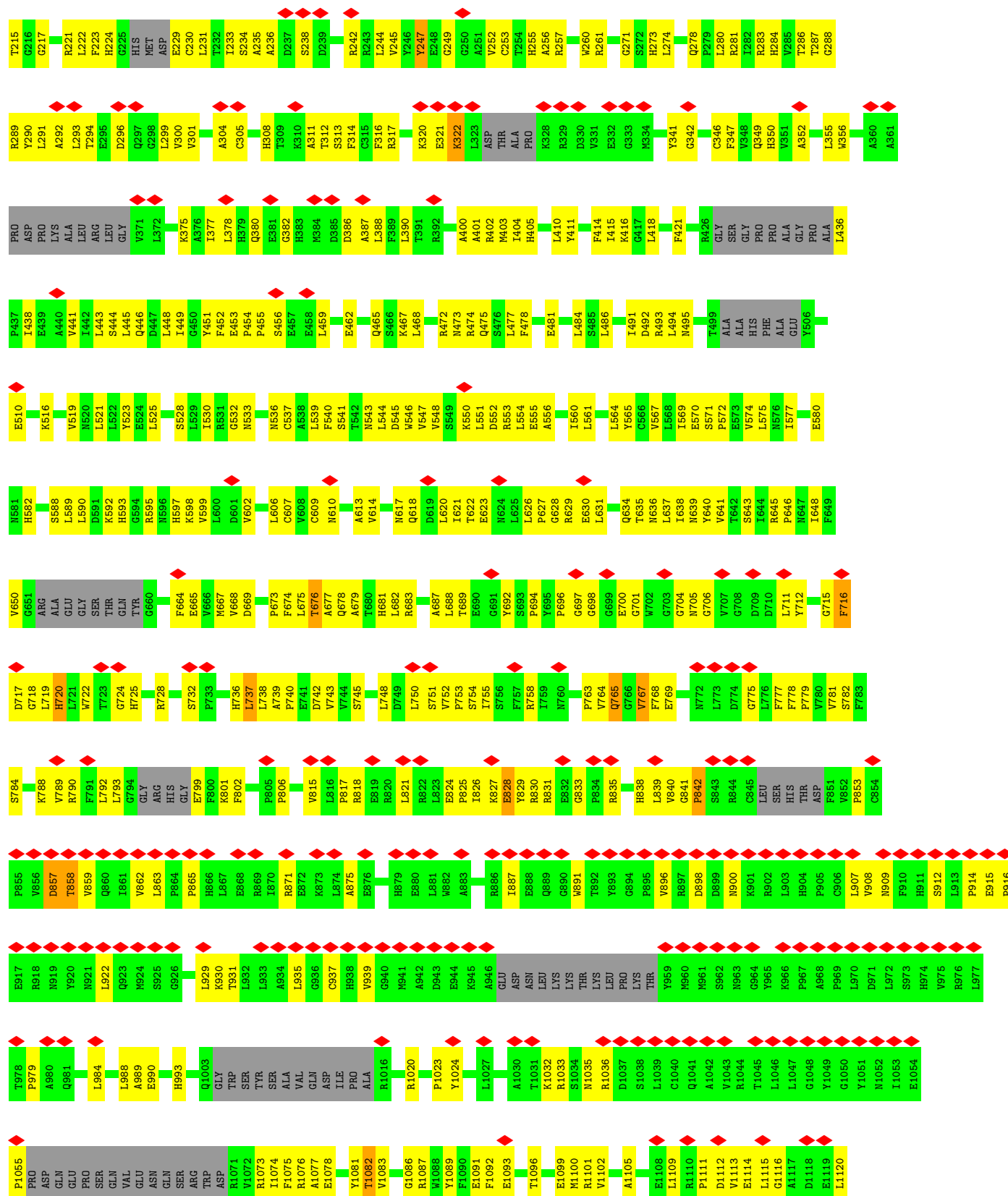


GLY	A3421	D3490	Q3554	VAL	F3753	K3852	R3921	K3999	I4071	F4141	G4225	GLY
ALA	H3422	Q3491	N3555	TRP	E3754	ALA	Y3922	K4002	V4072	M4142	G4226	ALA
THR	V3423	GLU	L3559	HIS	E3755	GLY	L3923	L4003	Q4073	V4145	E4227	THR
LEU	L3424	ARG	E3564	LEU	Q3767	GLY	L3926	L4012	A4076	L4146	A4228	ALA
ALA	THR	GLU	E3565	LEU	S3768	MET	Q3927	L4013	F4077	L4147	A4229	ALA
ALA	GLU	GLU	E3566	SER	R3769	VAL	S3928	L4017	V4081	M4148	A4230	ALA
ALA	GLU	GLU	E3567	LEU	L3770	ASN	S3929	L4018	T4082	M4149	F4234	ALA
ALA	GLU	GLU	P3567	ARG	H3771	GLU	D3932	D4018	V4083	M4150	V4235	ALA
ALA	GLU	GLU	E3568	ARG	T3772	ASP	D3936	L4019	Q4083	H4153	A4238	ALA
ALA	GLU	GLU	L3569	ARG	G3773	THR	Y3936	Q4020	P4084	V4154	E4239	ALA
ALA	GLU	GLU	R3498	ARG	A3775	VAL	Y3937	D4022	R4085	R4159	E4240	LEU
ALA	GLU	GLU	E3570	ALA	K3694	ILE	D3941	M4024	G4086	F4163	T4241	ALA
ALA	GLU	GLU	W3571	ALA	P3695	ASN	Y3941	V4025	L4087	L4164	T4242	ALA
ALA	GLU	GLU	E3572	ALA	D3696	ARG	Q3946	M4026	K4090	E4165	M4245	ALA
ALA	GLU	GLU	E3573	ALA	F3697	GLN	G3947	L4027	K4091	L4166	A4249	ALA
ALA	GLU	GLU	E3574	ALA	H3699	GLN	K3948	L4028	D4092	A4167	Q4250	ALA
ALA	GLU	GLU	E3575	ALA	Q3700	ASN	R3949	S4029	F4093	E4168	I4251	ALA
ALA	GLU	GLU	E3576	ALA	L3701	GLY	N3950	L4030	Q4094	F4171	SER	ALA
ALA	GLU	GLU	E3577	ALA	F3705	GLY	S3952	L4031	K4095	E4172	PRO	ALA
ALA	GLU	GLU	E3578	ALA	E3711	ALA	K3953	E4032	A4096	R4175	GLU	ALA
ALA	GLU	GLU	E3579	ALA	K3713	D3877	A3954	M4034	M4097	GLU	GLU	ALA
ALA	GLU	GLU	E3580	ALA	S3714	D3878	M3955	V4035	D4098	ALA	GLY	ALA
ALA	GLU	GLU	E3581	ALA	K3715	E3879	S3956	V4036	M4099	R4180	ARG	ALA
ALA	GLU	GLU	E3582	ALA	R3716	F3880	V3957	Q4037	S4099	I4181	LEU	ALA
ALA	GLU	GLU	E3583	ALA	H3648	T3881	A3958	Q4038	Q1000	G4185	GLY	ALA
ALA	GLU	GLU	E3584	ALA	R3648	Q3882	K3959	M4039	Q1001	A4186	ASP	ALA
ALA	GLU	GLU	E3585	ALA	N3651	D3883	Q3960	I4040	LYS	A4187	GLY	ALA
ALA	GLU	GLU	E3586	ALA	E3718	L3884	S3961	A4041	Q4102	S4187	THR	ALA
ALA	GLU	GLU	E3587	ALA	L3721	F3885	F3962	R4042	F4103	R4188	ALA	ALA
ALA	GLU	GLU	E3588	ALA	K3723	R3886	S3963	Q4043	T4104	R4189	GLY	ALA
ALA	GLU	GLU	E3589	ALA	Y3657	F3887	S3964	M4044	E4107	R4192	GLY	ALA
ALA	GLU	GLU	E3590	ALA	K3658	Q3888	L3965	V4045	I4108	I4193	GLY	ALA
ALA	GLU	GLU	E3591	ALA	E3661	L3889	T3966	M4046	E4109	I4194	GLY	ALA
ALA	GLU	GLU	E3592	ALA	W3661	L3891	E3967	M4047	F4195	F4196	GLY	ALA
ALA	GLU	GLU	E3593	ALA	L3728	C3892	Y3968	L4048	L4111	E4199	GLY	ALA
ALA	GLU	GLU	E3594	ALA	C3733	E3893	I3969	E4050	C4114	R4202	GLY	ALA
ALA	GLU	GLU	E3595	ALA	HIS	N3896	Q3977	S4051	S4115	A4203	GLY	ALA
ALA	GLU	GLU	E3596	ALA	LEU	N3897	L3980	S4052	E4116	Q4204	GLY	ALA
ALA	GLU	GLU	E3597	ALA	D3666	D3898	R3984	M4054	A4117	D4118	GLY	ALA
ALA	GLU	GLU	E3598	ALA	H3667	F3899	L3985	V4055	E4119	E4119	GLY	ALA
ALA	GLU	GLU	E3599	ALA	S3668	Q3900	L3986	E4056	M4120	M4120	GLY	ALA
ALA	GLU	GLU	E3600	ALA	F3669	N3901	V3986	M4057	E4121	E4121	GLY	ALA
ALA	GLU	GLU	E3601	ALA	E3670	Y3902	D3987	L4058	M4122	M4122	GLY	ALA
ALA	GLU	GLU	E3602	ALA	D3671	L3903	A3888	L4059	I4123	I4123	GLY	ALA
ALA	GLU	GLU	E3603	ALA	R3672	R3904	V3989	K4060	M4124	M4124	GLY	ALA
ALA	GLU	GLU	E3604	ALA	H3673	T3905	F3992	P4064	F4125	F4125	GLY	ALA
ALA	GLU	GLU	E3605	ALA	Q3674	Q3906	H3994	LEU	E4126	E4126	GLY	ALA
ALA	GLU	GLU	E3606	ALA	T3674	I3915	V3995	LYS	E4127	E4127	GLY	ALA
ALA	GLU	GLU	E3607	ALA	L3677	I3916	F3996	LYS	F4128	F4128	GLY	ALA
ALA	GLU	GLU	E3608	ALA	A3680	T3919	H3997	ASP	R4131	PHE	GLY	ALA
ALA	GLU	GLU	E3609	ALA	GLY	V3920	H3998	ASP	GLN	GLN	GLY	ALA
ALA	GLU	GLU	E3610	ALA	GLN	E3750	E3752	ASP	GLU	GLU	GLY	ALA
ALA	GLU	GLU	E3611	ALA	GLN	V3751	S3752	ASP	P4135	P4135	GLY	ALA
ALA	GLU	GLU	E3612	ALA	GLN	E3752	S3752	ASP	D4138	D4138	GLY	ALA
ALA	GLU	GLU	E3613	ALA	GLN	E3752	S3752	ASP	D4138	D4138	GLY	ALA



• Molecule 1: Ryanodine receptor 1



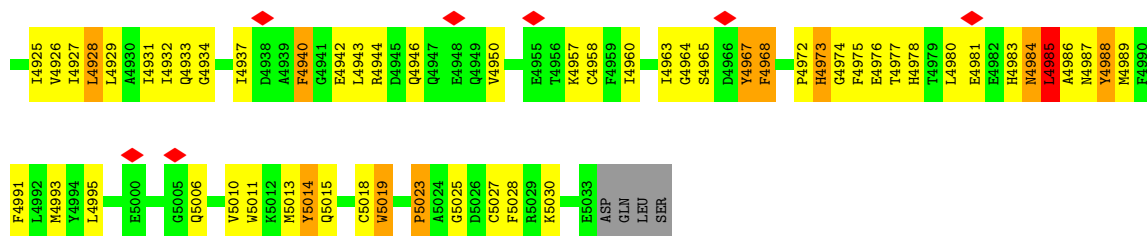




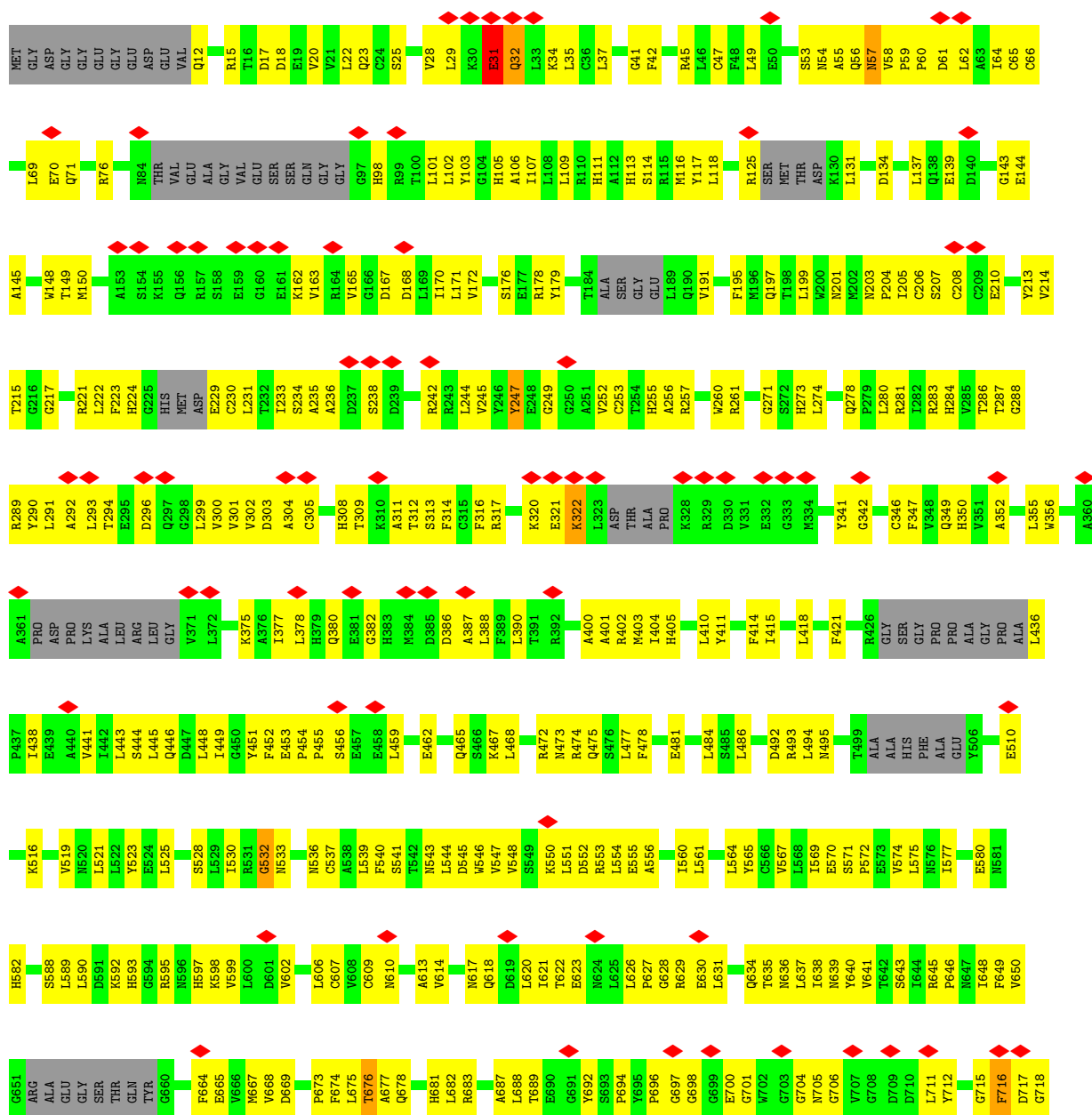








• Molecule 1: Ryanodine receptor 1

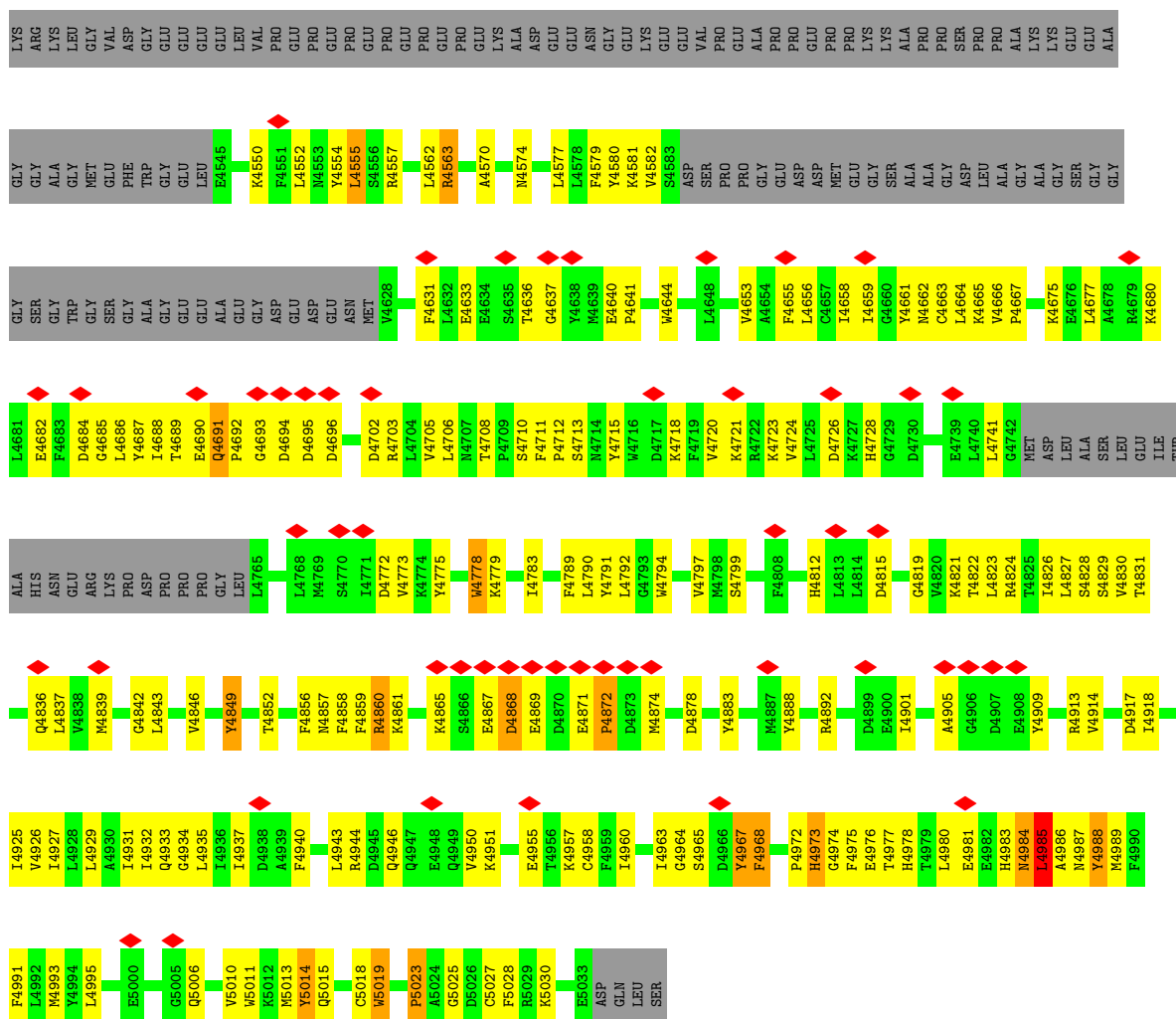




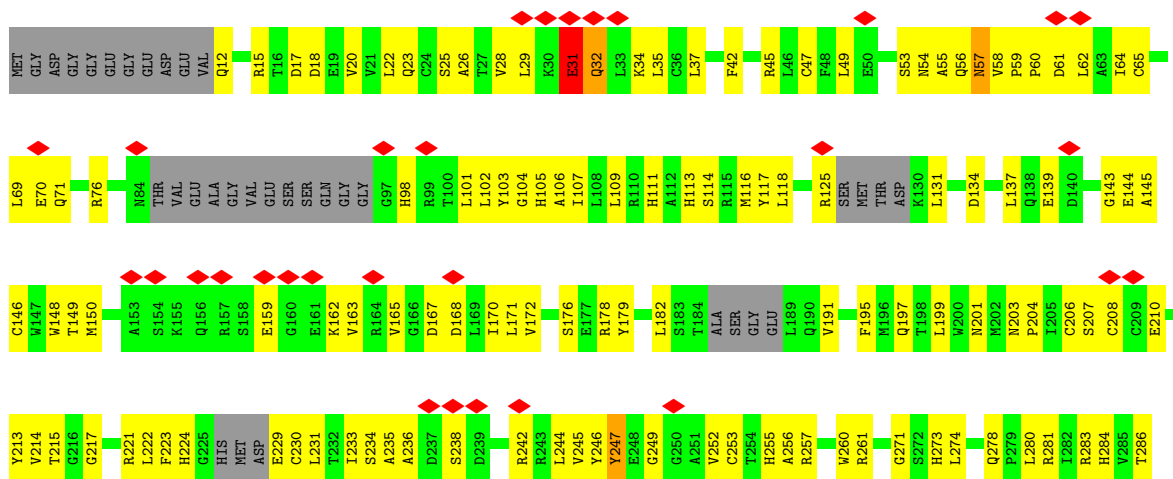








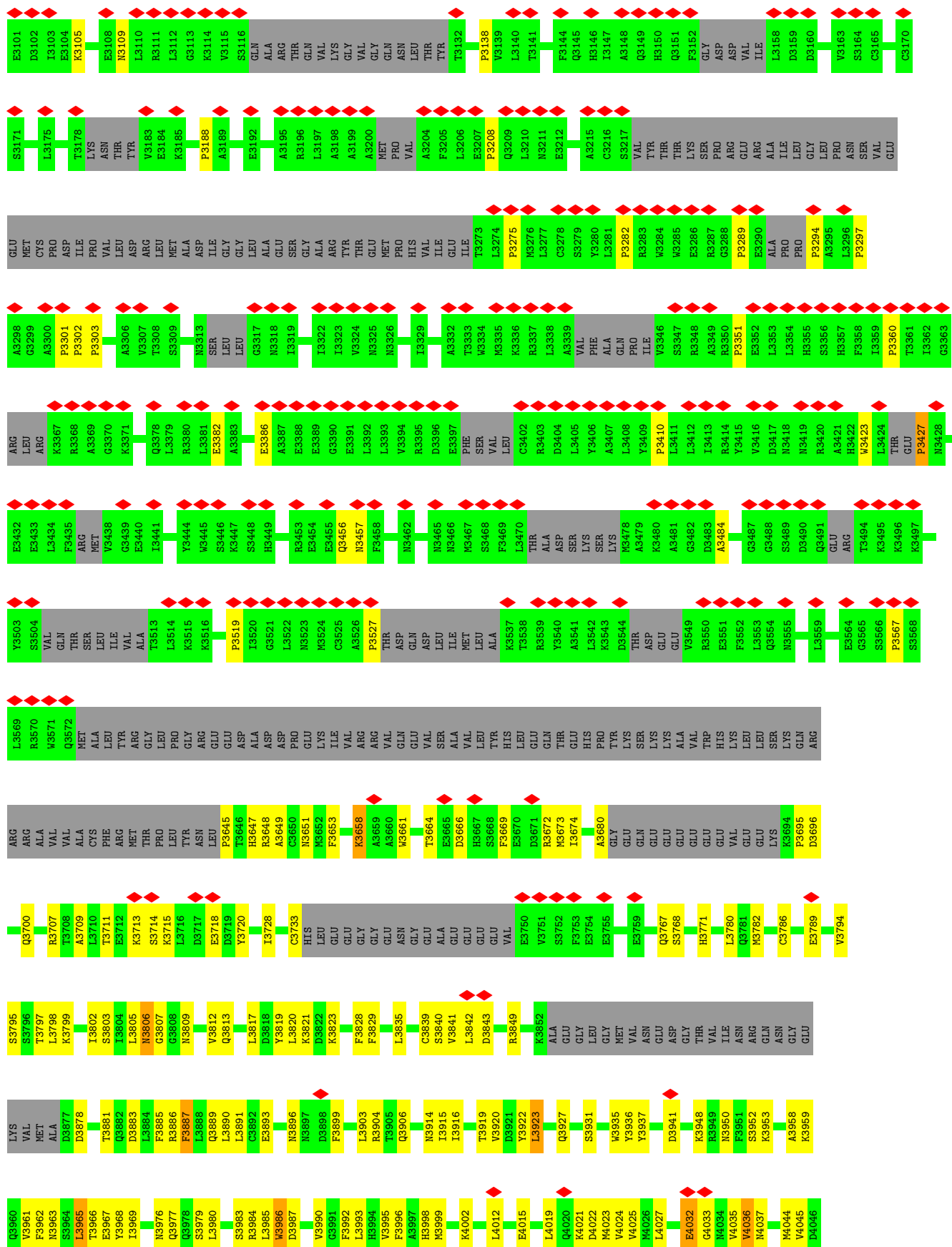
• Molecule 1: Ryanodine receptor 1

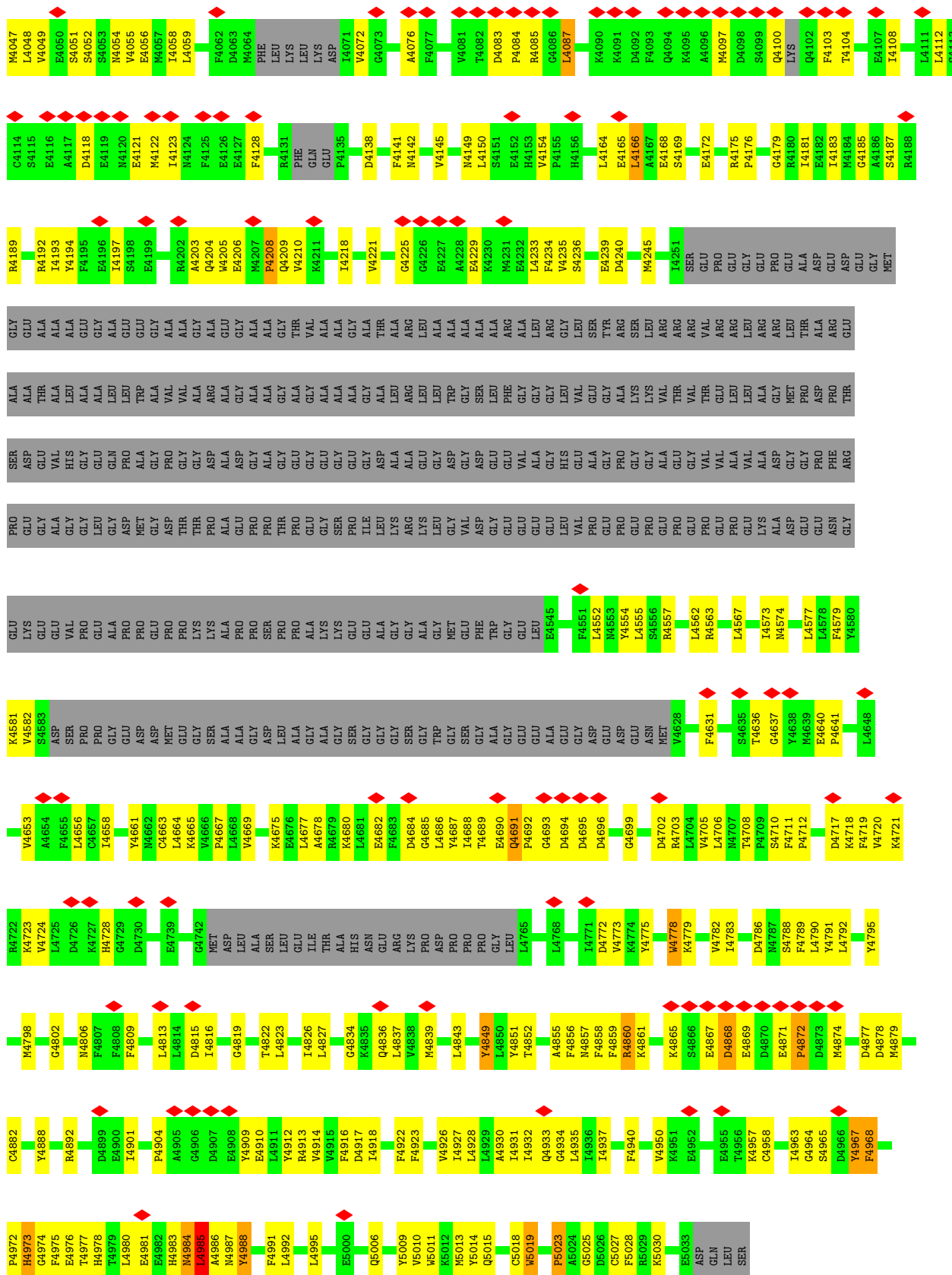


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E1054	P1055	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	ARG	TRP	ASP	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	Y1081	T1082	V1083	G1086	R1087	W1088	Y1089	F1090	E1091	F1092	E1093	T1096	E1099	M1100	R1101	GLY	SER	GLU	GLU	THR															
L977	T978	P979	A980	Q981	L984	L988	A989	E990	H993	Q1003	GLY	TRP	SER	TYR	ALA	VAL	GLN	ASP	ILE	PRO	ALA	R1016	R1020	P1023	Y1024	L1027	A1030	T1031	K1032	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	G1050	Y1051	N1052	I1053										
P916	E917	R918	N919	Y920	N921	L922	Q923	N924	S925	Q926	L929	K930	T931	L932	R933	A934	L935	G936	C937	H938	V939	G940	H941	A942	D943	E944	K945	A946	GLU	ASP	ASN	LEU	LYS	LYS	LYS	THR	LEU	PRO	LYS	W896	D898	N899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915
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F783	S794	W788	V789	R790	W791	W792	T793	L792	L793	G794	GLY	ARG	HIS	GLY	E799	F800	R801	F802	P805	P806	V815	L816	R817	R818	A875	E876	H879	E880	L881	L882	R883	E887	G891	E892	Y893	R894	R895	R896	R897	D899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915		
C854	P855	V856	D857	T858	V859	Q860	T861	V862	L863	P864	P865	H866	L867	E868	I870	R871	E872	K873	L874	A875	E876	H879	E880	L881	L882	R883	E887	G891	E892	Y893	R894	R895	R896	R897	D899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915							
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L977	T978	P979	A980	Q981	L984	L988	A989	E990	H993	Q1003	GLY	TRP	SER	TYR	ALA	VAL	GLN	ASP	ILE	PRO	ALA	R1016	R1020	P1023	Y1024	L1027	A1030	T1031	K1032	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	G1050	Y1051	N1052	I1053										
E1054	P1055	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	ARG	TRP	ASP	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	Y1081	T1082	V1083	G1086	R1087	W1088	Y1089	F1090	E1091	F1092	E1093	T1096	E1099	M1100	R1101	GLY	SER	GLU	GLU	THR															
L1120	A1121	N1125	G1126	H1127	R1128	R1131	H1132	H1133	L1134	E1137	W1143	Q1144	D1147	V1148	V1149	M1152	I1153	D1154	L1155	T1156	E1157	N1158	T1159	L1160	I1161	F1162	L1163	L1164	V1168	L1169	W1178	F1179	R1180	E1181	G1187	F1188	L1189	P1190	V1191	C1192	S1193	L1194	G1195															
E1054	P1055	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	ARG	TRP	ASP	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	Y1081	T1082	V1083	G1086	R1087	W1088	Y1089	F1090	E1091	F1092	E1093	T1096	E1099	M1100	R1101	GLY	SER	GLU	GLU	THR															
L977	T978	P979	A980	Q981	L984	L988	A989	E990	H993	Q1003	GLY	TRP	SER	TYR	ALA	VAL	GLN	ASP	ILE	PRO	ALA	R1016	R1020	P1023	Y1024	L1027	A1030	T1031	K1032	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	G1050	Y1051	N1052	I1053										
P916	E917	R918	N919	Y920	N921	L922	Q923	N924	S925	Q926	L929	K930	T931	L932	R933	A934	L935	G936	C937	H938	V939	G940	H941	A942	D943	E944	K945	A946	GLU	ASP	ASN	LEU	LYS	LYS	LYS	THR	LEU	PRO	LYS	W896	D898	N899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915
C854	P855	V856	D857	T858	V859	Q860	T861	V862	L863	P864	P865	H866	L867	E868	I870	R871	E872	K873	L874	A875	E876	H879	E880	L881	L882	R883	E887	G891	E892	Y893	R894	R895	R896	R897	D899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915							
F716	D717	G718	L719	H720	L721	W722	T723	G724	GLN	TYR	G660	F664	E665	V666	M667	V668	D669	P673	F674	L675	T676	A677	Q678	A679	T680	H681	L682	R683	A687	L688	G691	Y692	S693	P694	T695	P696	G697	G698	G699	G701	W702	G703	G704	N705	G706	V707	G708	D709	L710	L711	Y712	G715						
F783	S794	W788	V789	R790	W791	W792	T793	L792	L793	G794	GLY	ARG	HIS	GLY	E799	F800	R801	F802	P805	P806	V815	L816	R817	R818	A875	E876	H879	E880	L881	L882	R883	E887	G891	E892	Y893	R894	R895	R896	R897	D899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915		
C854	P855	V856	D857	T858	V859	Q860	T861	V862	L863	P864	P865	H866	L867	E868	I870	R871	E872	K873	L874	A875	E876	H879	E880	L881	L882	R883	E887	G891	E892	Y893	R894	R895	R896	R897	D899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915							
P916	E917	R918	N919	Y920	N921	L922	Q923	N924	S925	Q926	L929	K930	T931	L932	R933	A934	L935	G936	C937	H938	V939	G940	H941	A942	D943	E944	K945	A946	GLU	ASP	ASN	LEU	LYS	LYS	LYS	THR	LEU	PRO	LYS	W896	D898	N899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915
C854	P855	V856	D857	T858	V859	Q860	T861	V862	L863	P864	P865	H866	L867	E868	I870	R871	E872	K873	L874	A875	E876	H879	E880	L881	L882	R883	E887	G891	E892	Y893	R894	R895	R896	R897	D899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915							
F716	D717	G718	L719	H720	L721	W722	T723	G724	GLN	TYR	G660	F664	E665	V666	M667	V668	D669	P673	F674	L675	T676	A677	Q678	A679	T680	H681	L682	R683	A687	L688	G691	Y692	S693	P694	T695	P696	G697	G698	G699	G701	W702	G703	G704	N705	G706	V707	G708	D709	L710	L711	Y712	G715						
F783	S794	W788	V789	R790	W791	W792	T793	L792	L793	G794	GLY	ARG	HIS	GLY	E799	F800	R801	F802	P805	P806	V815	L816	R817	R818	A875	E876	H879	E880	L881	L882	R883	E887	G891	E892	Y893	R894	R895	R896	R897	D899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915		
C854	P855	V856	D857	T858	V859	Q860	T861	V862	L863	P864	P865	H866	L867	E868	I870	R871	E872	K873	L874	A875	E876	H879	E880	L881	L882	R883	E887	G891	E892	Y893	R894	R895	R896	R897	D899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915							
P916	E917	R918	N919	Y920	N921	L922	Q923	N924	S925	Q926	L929	K930	T931	L932	R933	A934	L935	G936	C937	H938	V939	G940	H941	A942	D943	E944	K945	A946	GLU	ASP	ASN	LEU	LYS	LYS	LYS	THR	LEU	PRO	LYS	W896	D898	N899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915
C854	P855	V856	D857	T858	V859	Q860	T861	V862	L863	P864	P865	H866	L867	E868	I870	R871	E872	K873	L874	A875	E876	H879	E880	L881	L882	R883	E887	G891	E892	Y893	R894	R895	R896	R897	D899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915							
F716	D717	G718	L719	H720	L721	W722	T723	G724	GLN	TYR	G660	F664	E665	V666	M667	V668	D669	P673	F674	L675	T676	A677	Q678	A679	T680	H681	L682	R683	A687	L688	G691	Y692	S693	P694	T695	P696	G697	G698	G699	G701	W702	G703	G704	N705	G706	V707	G708	D709	L710	L711	Y712	G715						
F783	S794	W788	V789	R790	W791	W792	T793	L792	L793	G794	GLY	ARG	HIS	GLY	E799	F800	R801	F802	P805	P806	V815	L816	R817	R818	A875	E876	H879	E880	L881	L882	R883	E887	G891	E892	Y893	R894	R895	R896	R897	D899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915		
C854	P855	V856	D857	T858	V859	Q860	T861	V862	L863	P864	P865	H866	L867	E868	I870	R871	E872	K873	L874	A875	E876	H879	E880	L881	L882	R883	E887	G891	E892	Y893	R894	R895	R896	R897	D899	N900	K901	R902	L903	H904	P905	C906	L907	Y908	N909	F910	H911	S912	L913	P914	E915							
P																																																										

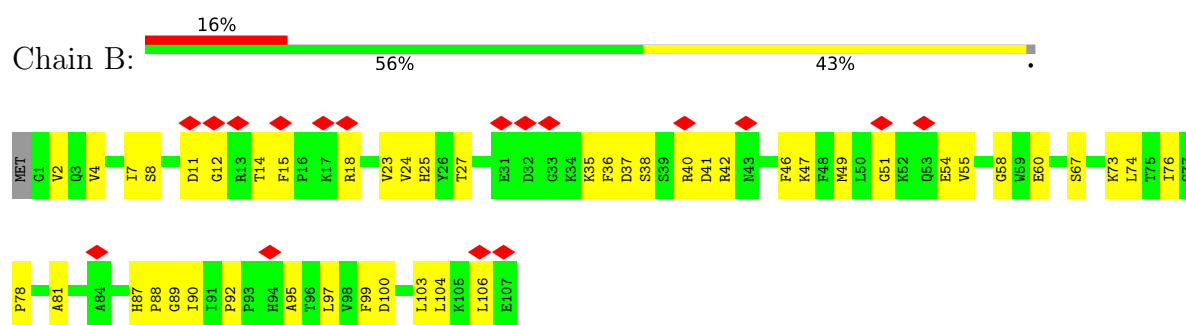




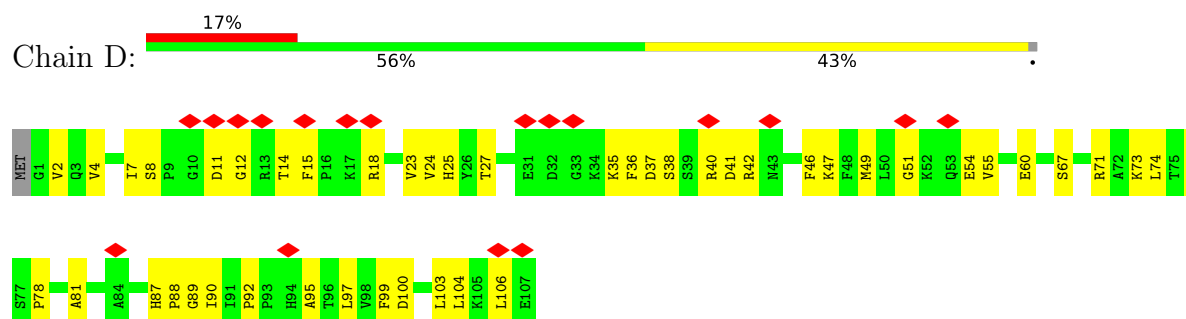




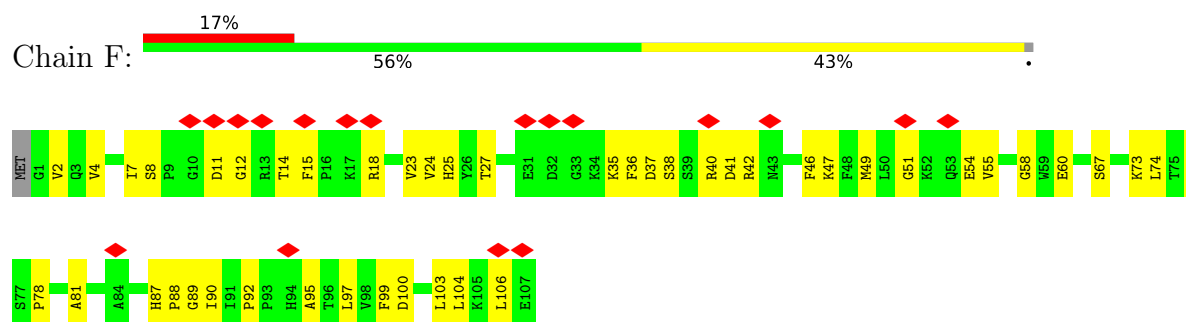
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



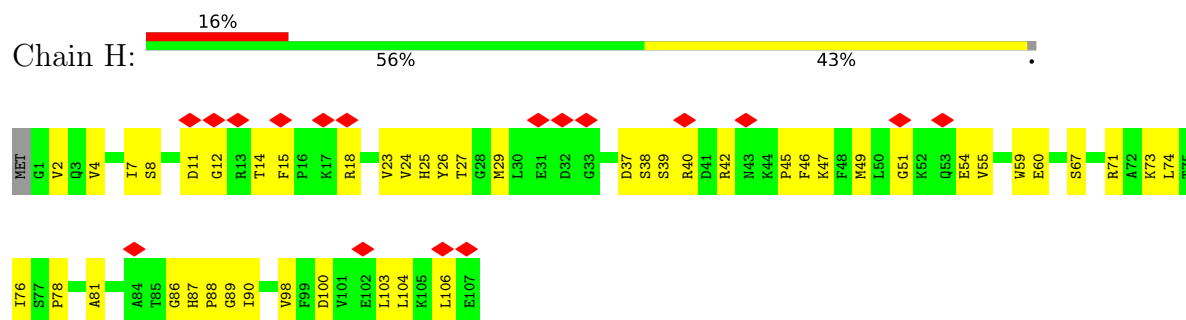
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- 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, C4	Depositor
Number of particles used	119000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.382	Depositor
Minimum map value	-0.148	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.85	25/27395 (0.1%)	0.86	68/37119 (0.2%)
1	C	0.85	27/27395 (0.1%)	0.86	64/37119 (0.2%)
1	E	0.85	24/27395 (0.1%)	0.86	63/37119 (0.2%)
1	G	0.84	26/27395 (0.1%)	0.85	59/37119 (0.2%)
2	B	0.64	0/851	0.68	0/1146
2	D	0.64	0/851	0.68	0/1146
2	F	0.64	0/851	0.68	0/1146
2	H	0.66	0/851	0.69	0/1146
All	All	0.84	102/112984 (0.1%)	0.85	254/153060 (0.2%)

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	17
1	C	0	17
1	E	0	17
1	G	0	16
All	All	0	67

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2853	GLU	CD-OE1	17.93	1.45	1.25
1	E	2853	GLU	CD-OE1	17.88	1.45	1.25
1	G	2853	GLU	CD-OE1	17.49	1.44	1.25
1	C	2853	GLU	CD-OE1	17.32	1.44	1.25
1	G	4988	TYR	CG-CD1	-9.48	1.26	1.39

The worst 5 of 254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	4032	GLU	OE1-CD-OE2	-7.83	113.91	123.30
1	G	4985	LEU	CB-CG-CD1	-7.61	98.06	111.00
1	G	2118	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	A	3773	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	G	4563	ARG	NE-CZ-NH2	7.46	124.03	120.30

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1187	GLY	Mainchain
1	A	31	GLU	Mainchain,Peptide
1	A	322	LYS	Peptide
1	A	841	GLY	Mainchain,Peptide
1	A	857	ASP	Mainchain,Peptide

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	26926	0	24467	1003	0
1	C	26926	0	24467	1022	0
1	E	26926	0	24467	1004	0
1	G	26926	0	24467	952	0
2	B	832	0	831	41	0
2	D	832	0	831	41	0
2	F	832	0	831	41	0
2	H	832	0	831	40	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	111036	0	101192	3945	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 19.

The worst 5 of 3945 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:G:1808:ARG:NH1	1:G:1858:ASP:OD2	1.79	1.16
1:E:1808:ARG:NH1	1:E:1858:ASP:OD2	1.79	1.16
1:C:1808:ARG:NH1	1:C:1858:ASP:OD2	1.79	1.15
1:A:1808:ARG:NH1	1:A:1858:ASP:OD2	1.79	1.14
1:A:1243:PRO:HD2	1:A:1458:HIS:HB3	1.20	1.10

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	3499/5037 (70%)	3211 (92%)	199 (6%)	89 (2%)	5	36
1	C	3499/5037 (70%)	3211 (92%)	201 (6%)	87 (2%)	5	36
1	E	3499/5037 (70%)	3211 (92%)	199 (6%)	89 (2%)	5	36
1	G	3499/5037 (70%)	3211 (92%)	199 (6%)	89 (2%)	5	36
2	B	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	D	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	F	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	H	105/108 (97%)	97 (92%)	7 (7%)	1 (1%)	15	52
All	All	14416/20580 (70%)	13232 (92%)	829 (6%)	355 (2%)	9	36

5 of 355 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	A	737	LEU
1	A	858	THR

Continued on next page...

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Mol	Chain	Res	Type
1	A	896	VAL
1	A	916	PRO

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	2503/4276 (58%)	2489 (99%)	14 (1%)	86	92
1	C	2504/4276 (59%)	2490 (99%)	14 (1%)	86	92
1	E	2504/4276 (59%)	2490 (99%)	14 (1%)	86	92
1	G	2502/4276 (58%)	2489 (100%)	13 (0%)	88	94
2	B	89/90 (99%)	89 (100%)	0	100	100
2	D	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	10369/17464 (59%)	10314 (100%)	55 (0%)	89	94

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	377	ILE
1	E	914	PRO
1	G	4972	PRO
1	G	979	PRO
1	E	380	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	3960	GLN
1	G	1640	HIS
1	E	4153	HIS

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Mol	Chain	Res	Type
1	G	203	ASN
1	G	1775	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

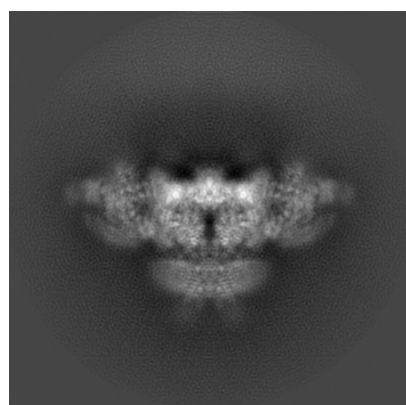
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9518. These allow visual inspection of the internal detail of the map and identification of artifacts.

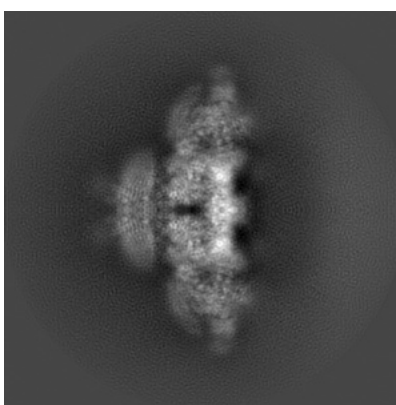
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

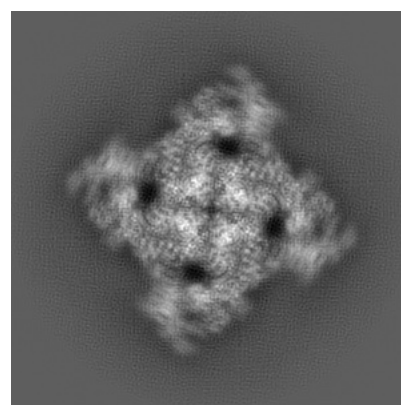
6.1.1 Primary map



X



Y

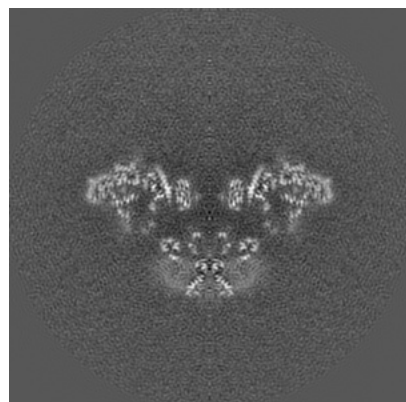


Z

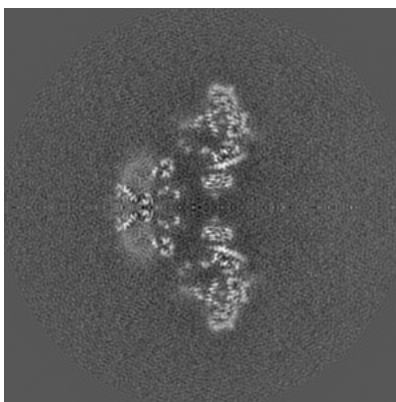
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

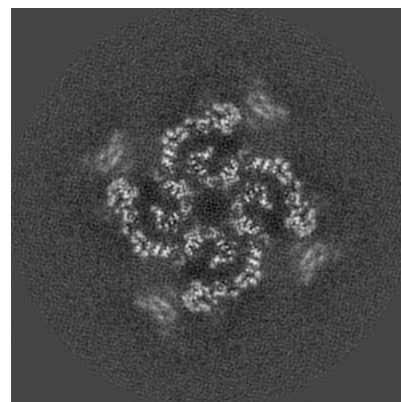
6.2.1 Primary map



X Index: 180



Y Index: 180

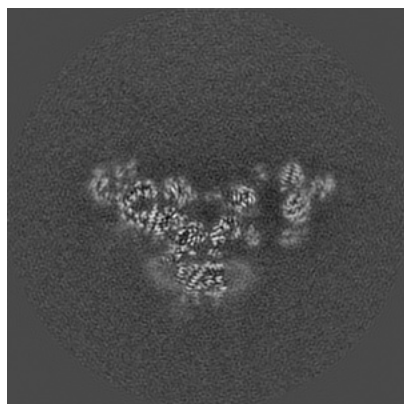


Z Index: 180

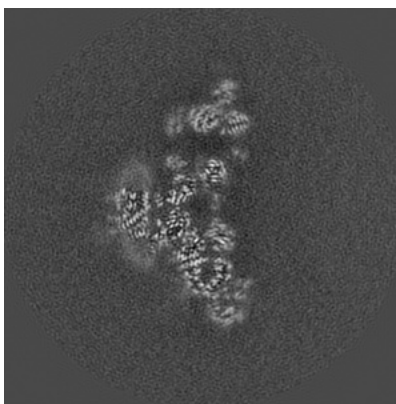
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

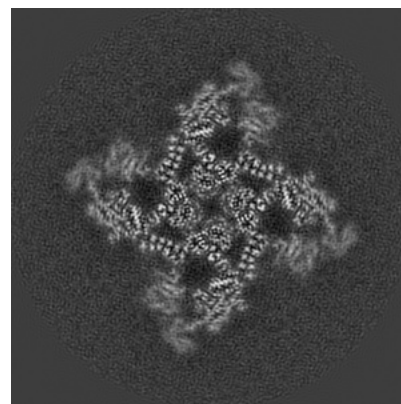
6.3.1 Primary map



X Index: 191



Y Index: 169

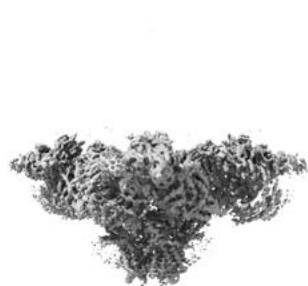


Z Index: 190

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

6.4 Orthogonal surface views [i](#)

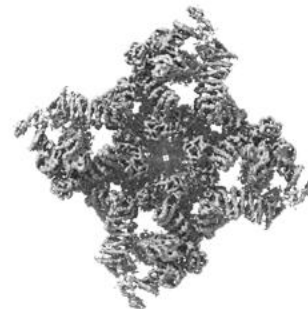
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

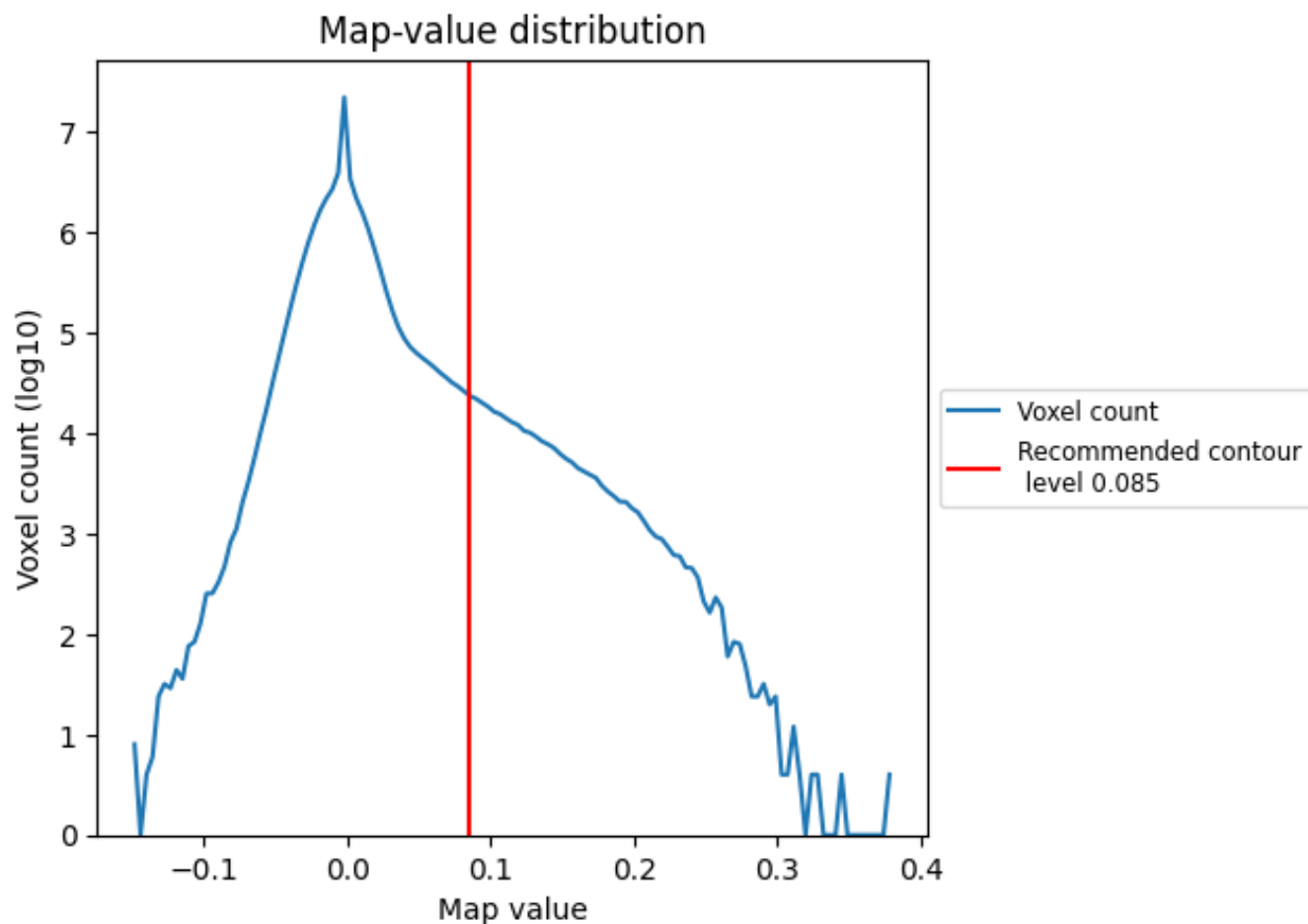
6.5 Mask visualisation

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

7 Map analysis [i](#)

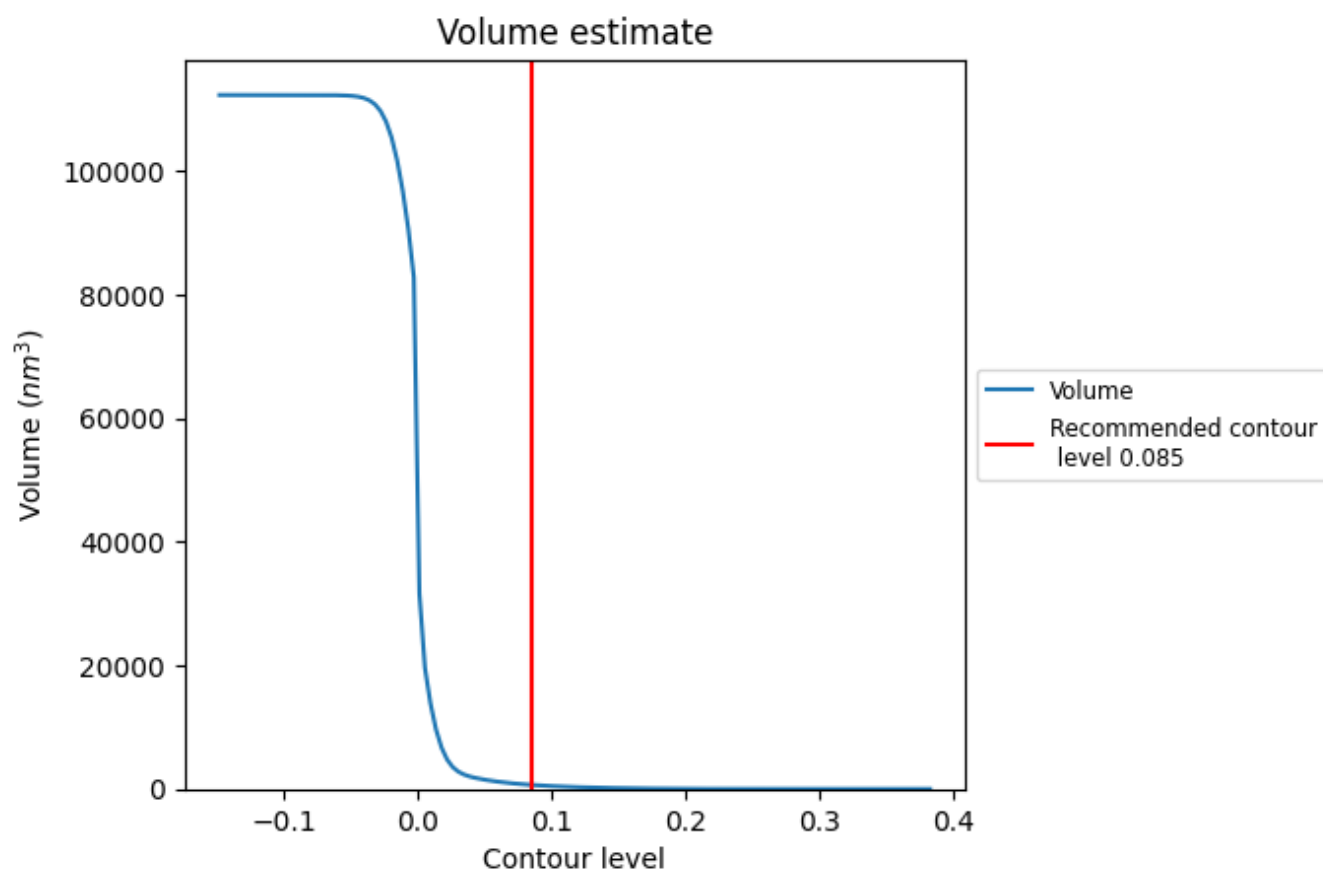
This section contains the results of statistical analysis of the map.

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.

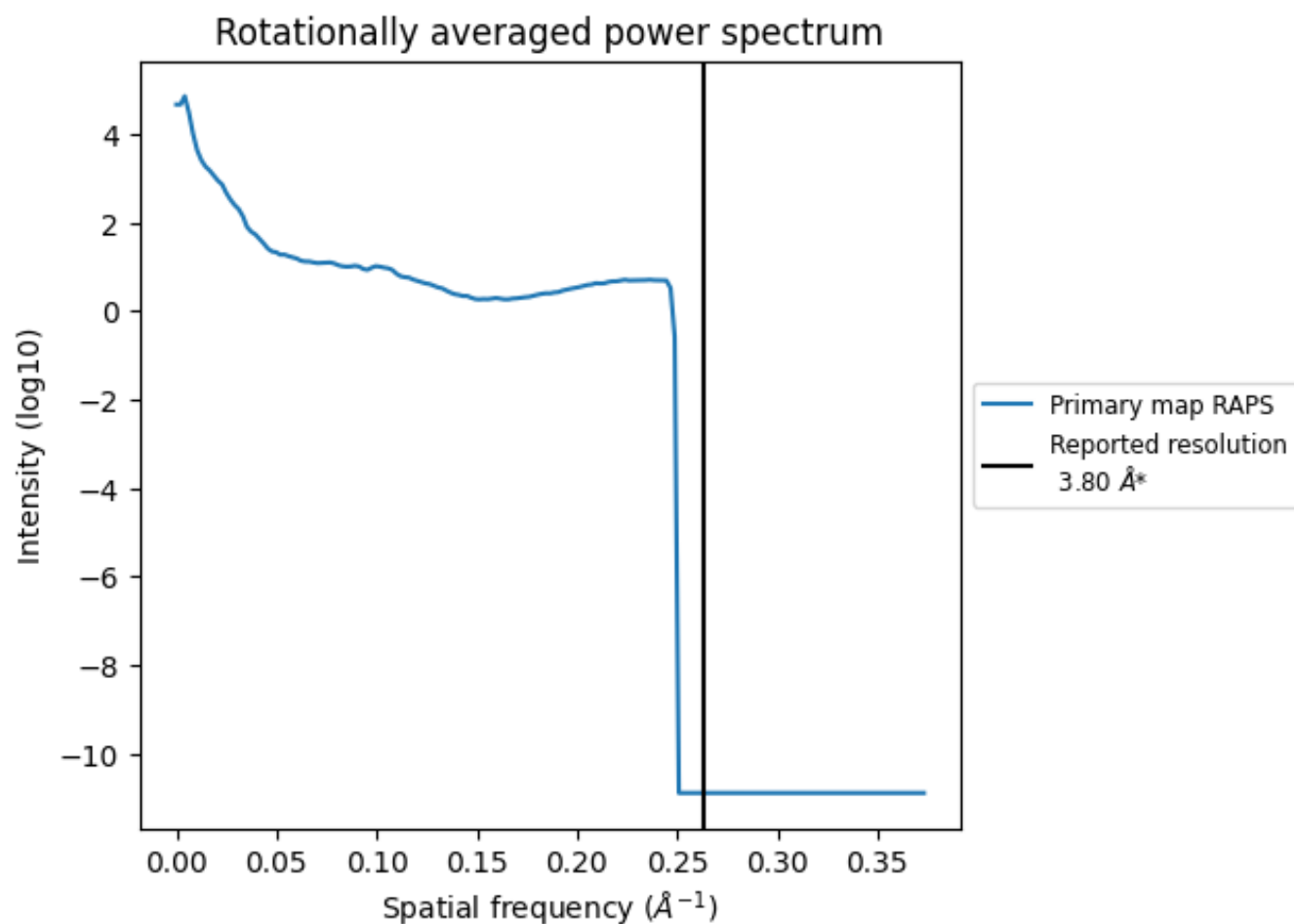
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 655 nm^3 ; this corresponds to an approximate mass of 591 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 0.263 Å⁻¹

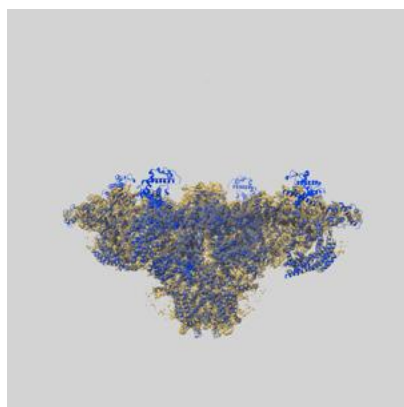
8 Fourier-Shell correlation

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

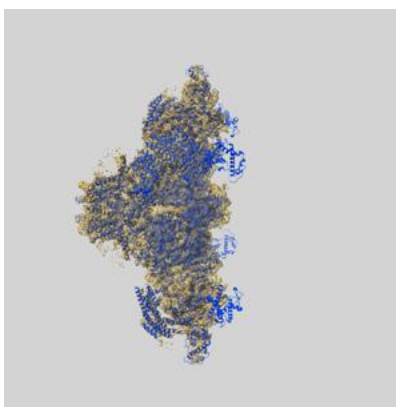
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9518 and PDB model 5GKY. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

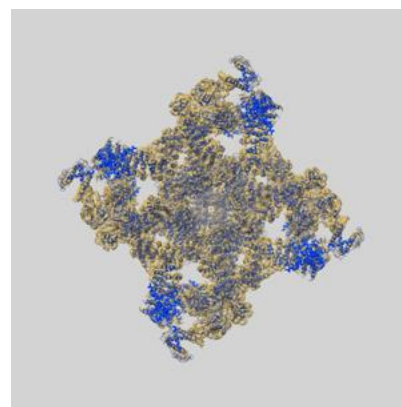
9.1 Map-model overlay [i](#)



X



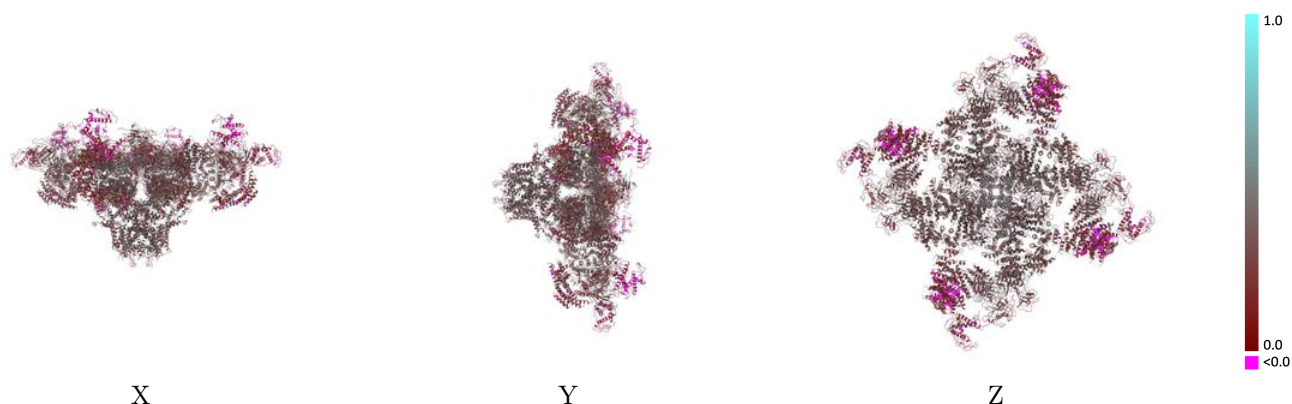
Y



Z

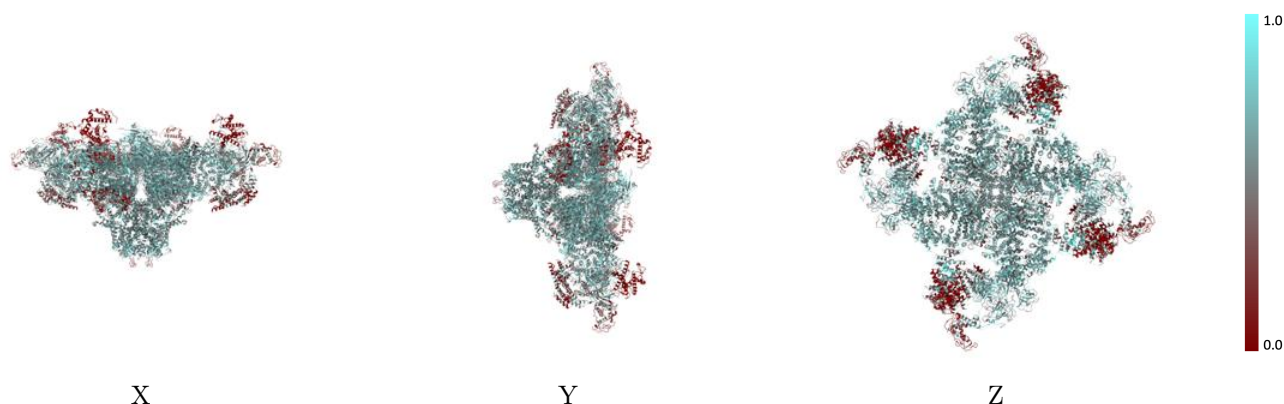
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



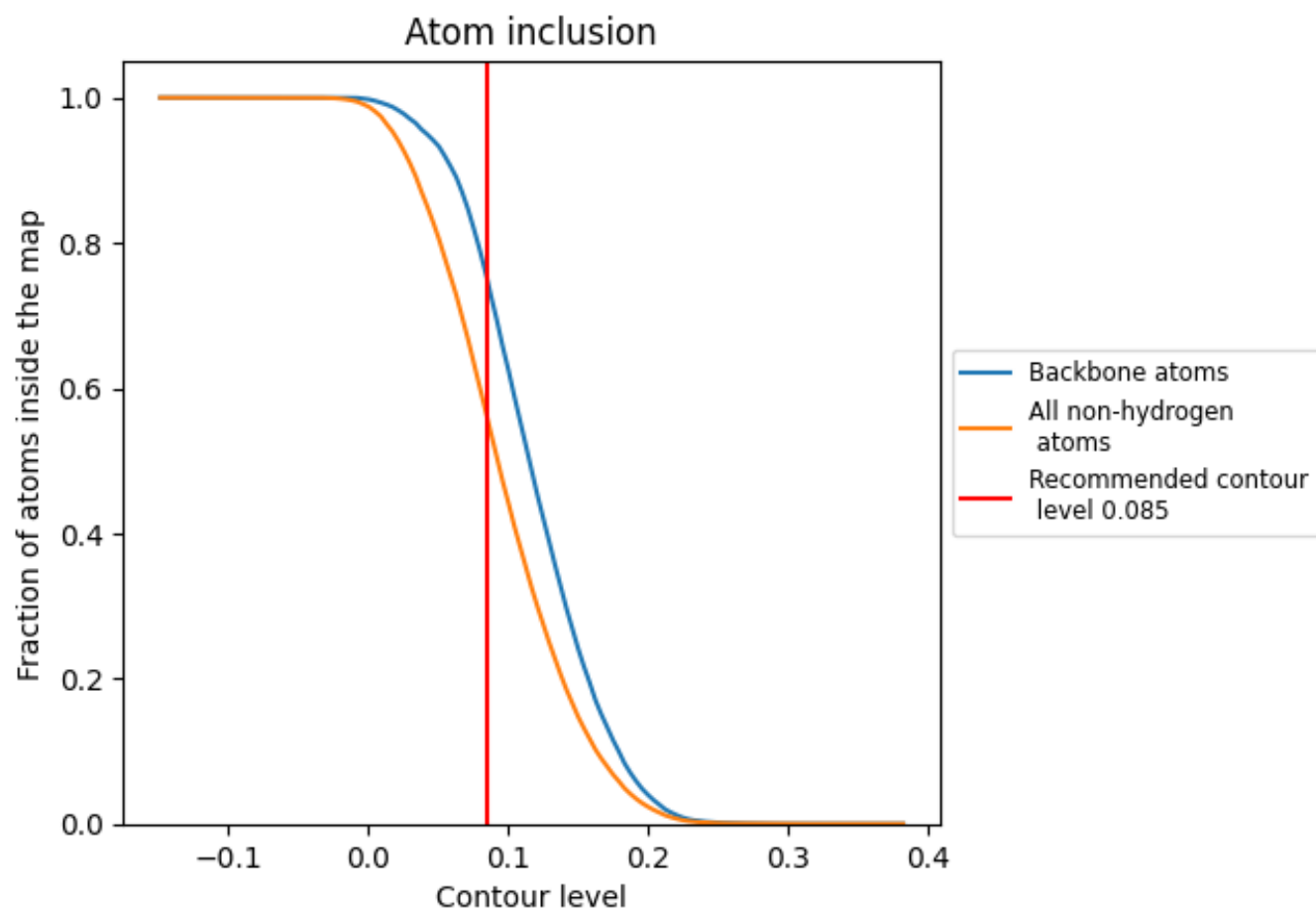
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.085).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 56% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.5631	<div><div></div></div> 0.3170
A	<div><div></div></div> 0.5629	<div><div></div></div> 0.3160
B	<div><div></div></div> 0.5760	<div><div></div></div> 0.3340
C	<div><div></div></div> 0.5627	<div><div></div></div> 0.3160
D	<div><div></div></div> 0.5760	<div><div></div></div> 0.3310
E	<div><div></div></div> 0.5628	<div><div></div></div> 0.3160
F	<div><div></div></div> 0.5735	<div><div></div></div> 0.3290
G	<div><div></div></div> 0.5626	<div><div></div></div> 0.3170
H	<div><div></div></div> 0.5735	<div><div></div></div> 0.3370

1.0

0.0

<0.0