wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:00 PM BST

PDB ID	:	3J8H
EMDB ID:	:	EMD-2807
Title	:	Structure of the rabbit ryanodine receptor RyR1 in complex with FKBP12 at 3.8 Angstrom resolution
Authors	:	Yan, Z.; Bai, X.; Yan, C.; Wu, J.; Scheres, S.H.W.; Shi, Y.; Yan, N.
Deposited on	:	2014-10-26
Resolution	:	3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

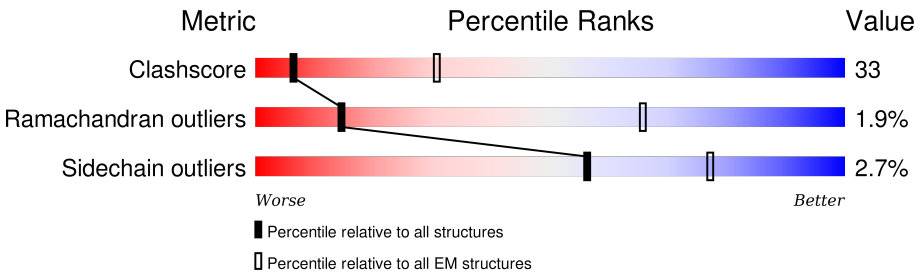
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 3.80 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	4599	48% 30% • 20%
1	C	4599	48% 30% • 20%
1	E	4599	48% 29% • 20%
1	G	4599	48% 30% • 20%
2	B	107	60% 39% •
2	D	107	62% 37% •
2	F	107	60% 39% •
2	H	107	59% 40% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	6000	-	-	X	-
3	ZN	C	6000	-	-	X	-
3	ZN	E	6000	-	-	X	-
3	ZN	G	6000	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 111160 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	3660	26957	17143	4683	4974	157	1	0
1	C	3660	26957	17143	4683	4974	157	1	0
1	E	3660	26957	17143	4683	4974	157	1	0
1	G	3660	26957	17143	4683	4974	157	1	0

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

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

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

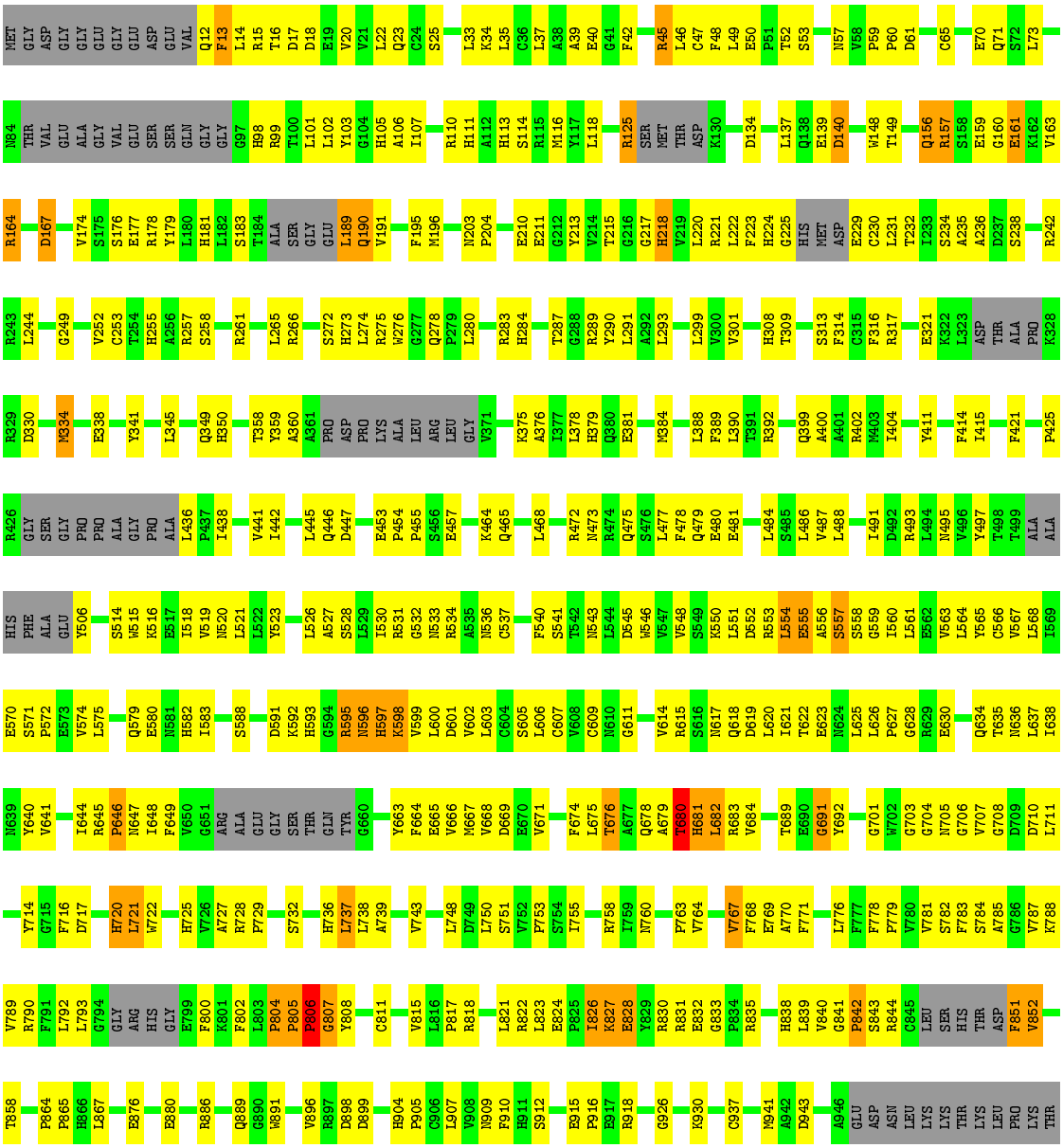
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	G	1	1	1	0
3	A	1	1	1	0
3	C	1	1	1	0
3	E	1	1	1	0

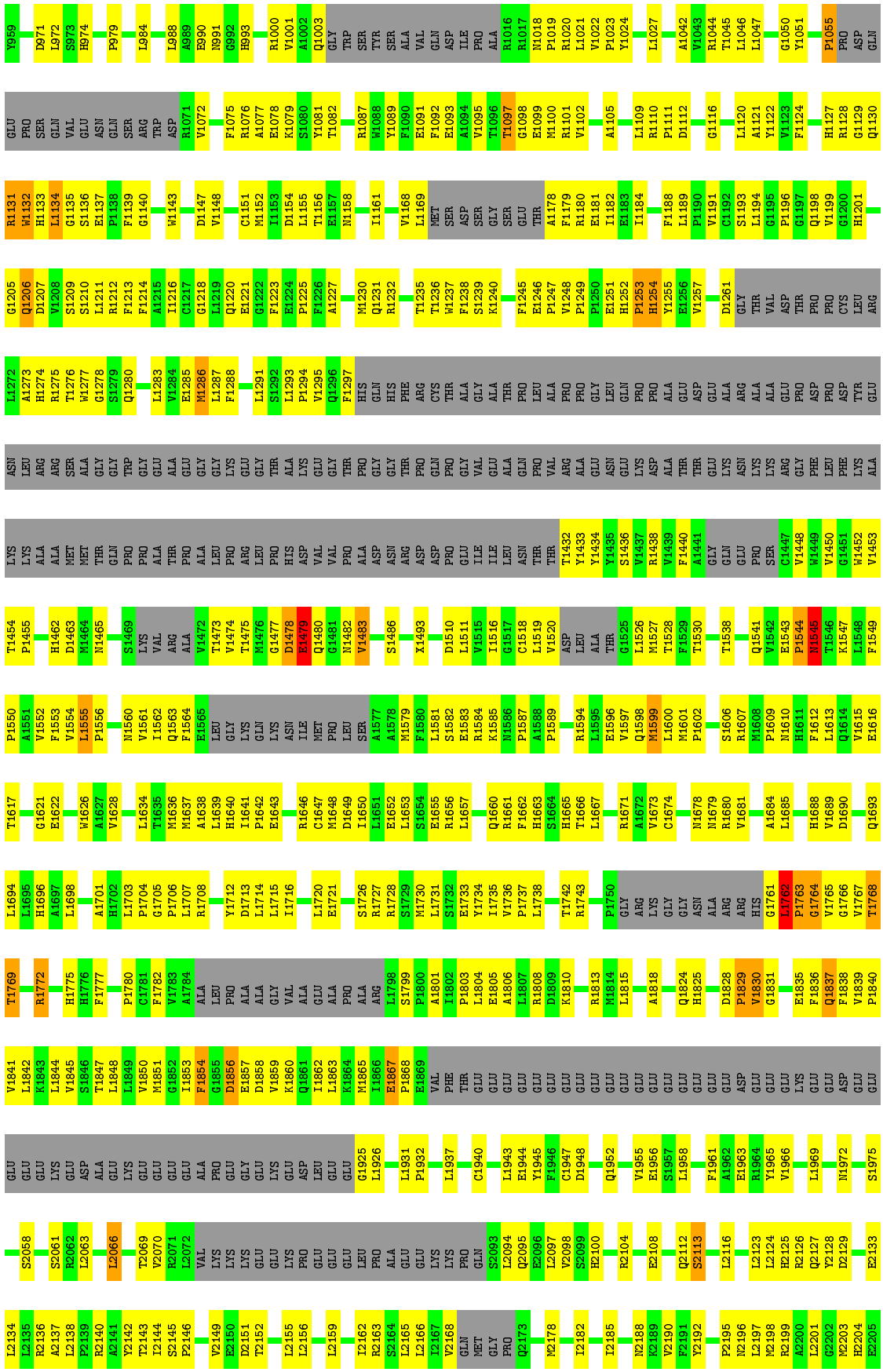
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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

Chain A: 48% 30% • 20%





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EMDataBank Unified Data Resource for 3DEM

ARG	ALA		V4072	S4007	W3935	VAL		D3696	P2903	E2799	THR		E2362	S2279	T2206
ARG	ASP	E4172	G4073	S4008	Y3936	ILE	K3787		L2904		ALA	G2434	CYS	V2280	V2207
LEU	GLU		S4074	Q4009	Y3937	ASN	G3788	H3699	L2905	K2802	THR	R2435	PHE	I2281	M2208
THR	ASP	R4175		I4010	S3938	ARG	E3789	Q3700	V2906		PHE	C2436	GLY	D2282	E2209
ALA	GLU		F4077	E4011	G3939	GLN	T3790	L3701	P2907	R2806	SER	A2437	PRO	N2283	V2210
ARG	GLY	L4178		L4012	K3940	ASN		V3702			THR	PRO	ALA	N2284	M2211
GLU	MET	G4179	D4083	L4013	D3941	GLY	M3793		T2910	I2809	T2544	GLU	LEU	E2285	V2212
ALA	GLY	R4180	P4084		V3942	GLU	V3794	F3705				MET	ARG	L2286	N2213
ALA	GLU	I4181		L4017	I3943	LYS	S3795		D2919	S2812	A2547	HIS	GLY		V2214
THR	ALA	E4182	L4087	D4018		VAL	S3796	T3708		L2813		LEU	GLU	V2299	L2215
ALA	ALA		I4088	L4019	F3951	MET	T3797	A3709	L2927	K2814	L2550	ILE	GLY	S2300	G2216
LEU	ALA	S4187		Q4020		ALA	L3798		K2928		N2551	GLN	GLY	Y2301	GLY
ALA	GLU	R4188	Q4100	K4021	A3954	D3877	K3799	E3712	F2929	A2818	R2552	ALA	SER		GLY
ALA	GLY	R4189	LYS		M3955	D3878		K3713	L2930	W2819	Y2553	GLY	G2375	L2307	GLU
LEU	ALA	I4190	Q4102	V4024	S3956	E3879	I3802	S3714		E2820	L2554	LYS	L2376	GLN	THR
LEU	GLU	E4191		V4025	V3957	F3880		K3715	N2933	W2821	C2555	GLY	L2377	SER	LYS
TRP	GLU	R4192	P4106	M4026	A3958	T3881	L3805			T2822	L2556	E2449		CYS	GLU
ALA	GLY	I4193	E4107	L4027		Q3882	N3806	Y3722	V2937		A2557		I2380	PRO	ILE
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VAL	ALA	F4195	Q4109	S4029	F3962	L3884	N3809	A3724	R2939		L2559	I2453	A2383	LEU	PHE
ALA	GLY	E4196	F4110	L4030	N3963	F3885		Y3725		E2830	P2560	R2454	I2384	LEU	P2226
ARG	ALA	I4197	L4111	L4031		R3886	Q3813	A3726	H3647	GLU		A2455	R2385	ALA	K2227
ALA	GLU		L4112	E4032	T3966	F3887		D3727	R3648	GLU	X2591	I2456	I2386	LYS	
GLY	GLY	P4208	S4113		E3967	L3888	L3817	I3728	A3649	ARG		L2457	SER	GLY	T2230
ALA	ALA			V4035	Y3968	Q3889			C3650	THR	X2595	R2458	GLU	TYR	
ALA	ALA	K4214	N4120	V4036	I3969	L3890	L3820	K3731	N3651	GLU			ASP	PRO	R2234
GLY	GLY			N4037	Q3970	L3891		S3732		LYS	X2625	X2465	PRO	ASP	
ALA	THR	F4217	I4123	G4038	G3971	C3892	V3826	C3733	Y3657	LYS		X2466	ALA	ILE	C2237
GLY	VAL	I4218		M4039	P3972	E3893	G3827	HIS		LYS	T2742	X2467	ARG	GLY	Y2238
ALA	ALA	F4219	R4131	I4040	C3973		F3828	LEU	I3662	THR			ASP	TRP	F2239
ALA	ALA	D4220	PHE	A4041	T3974	N3897	F3829	GLU		ARG	V2745	P2496	GLY	ASN	C2240
ALA	GLY	V4221	GLN	R4042	G3975	D3898	Q3830	GLU	H3667	LYS		D2497	PRO	P2325	R2241
GLY	ALA	V4222	GLU	Q4043	N3976	F3899	S3831	GLY	S3668	ILE	P2748	H2498	GLY	C2326	I2242
ALA	THR	N4223	P4135	M4044	Q3977	Q3900		GLY	F3669	SER		K2499	VAL		
LEU	ALA	E4224				N3901	L3835	GLU	E3670	GLN	L2751	A2500	ARG	E2329	Q2245
ARG	ARG	G4225	D4138	M4047	L3980	Y3902	M3836	ASN	D3671	THR	D2752	S2501	ARG	R2330	N2246
LEU	LEU	G4226		L4048		L3903	Q3837	GLY	R3672	ALA	S2753	M2502	ASP	Y2331	Q2247
LEU	ALA	E4227	F4141	V4049	S3983	R3904	T3838	GLU	M3673	GLN	F2754	V2503	ARG		R2248
TRP	ALA	A4228	N4142	E4050	R3984	T3905	C3839	ALA	I3674	THR	I2755	L2504	ARG	F2337	S2249
GLY	ALA			S4051	L3985	Q3906	S3840	GLU	D3675	Y2849	N2756	F2505	ARG	A2338	
SER	ALA	F4234	V4145	S4052		T3907	V3841	GLU	D3676		K2757		GLU	V2339	Y2256
LEU	ALA	V4235	L4146	S4053	A3988	G3908	L3842	GLU	L3677	R2852	F2758	Y2510	HIS	F2340	L2257
PHE	ARG		L4147	N4054	V3989	N3909	D3843	GLU	S3678	E2853	A2759	GLY	PHE	V2341	L2258
GLY	ALA	C4238	T4148	V4055	V3990		L3844	VAL	K3679	G2854	E2760	ILE	GLY	N2342	E2259
GLY	LEU	E4239	N4149	E4056	G3991	I3915		E3750	A3680	Y2855	Y2761	GLU	GLU	G2343	N2260
GLY	ARG		L4150	M4057	F3992	I3916	R3849		GLY	N2856	T2762	N2514	GLU		
LEU	GLY	I4242		I4058	L3993			Q3766	GLU	P2857	H2763		PRO	V2346	I2263
VAL	LEU	F4243	V4154	L4059	H3994	T3919	K3852	Q3767	GLN		E2764	F2517	PRO		GLY
GLU	SER		P4155	K4060	V3995	V3920	ALA	S3768	GLU	L2862			GLU	N2349	LEU
GLY	TYR	I4247	H4156	F4061	F3996		GLU	R3769	GLU		K2770	V2521	GLU	A2350	GLY
ALA	ARG		D4157	F4062	A3997	L3924	GLY		GLU	E2870		L2522	ASN	N2351	MET
LYS	SER	I4251	P4158	D4063	H3998	R3925	LEU	R3773	GLU		N2773	ASP	ARG		GLN
LYS	LEU	SER	R4159	M4064	M3999	L3926	GLY	G3774	GLU	Q2877	N2774	V2525	VAL	V2354	GLY
VAL	ARG	GLU	L4160	PHE	M4000	Q3927	MET	A3775	GLU		W2775		HIS	R2355	SER
THR	ARG	PRO	R4161	LEU	M4001	E3928	VAL		VAL	N2881		P2529	LEU	L2356	T2271
VAL	ARG	GLU		LYS	K4002	S3929	ASN	M3778	GLU	Y2882	H2788		G2419	L2357	
THR	VAL	GLY	L4164	LEU	L4003	I3930	GLU	V3779	GLU		P2789	A2533		I2358	V2275
GLU	ARG	GLU		LYS	A4004		ASP	L3780	LYS	G2900			M2423	R2359	A2276
LEU	ARG	PRO	A4167	ASP	Q4005	F3933	GLY	Q3781	K3694	T2901	Y2794	L2537		K2360	A2277
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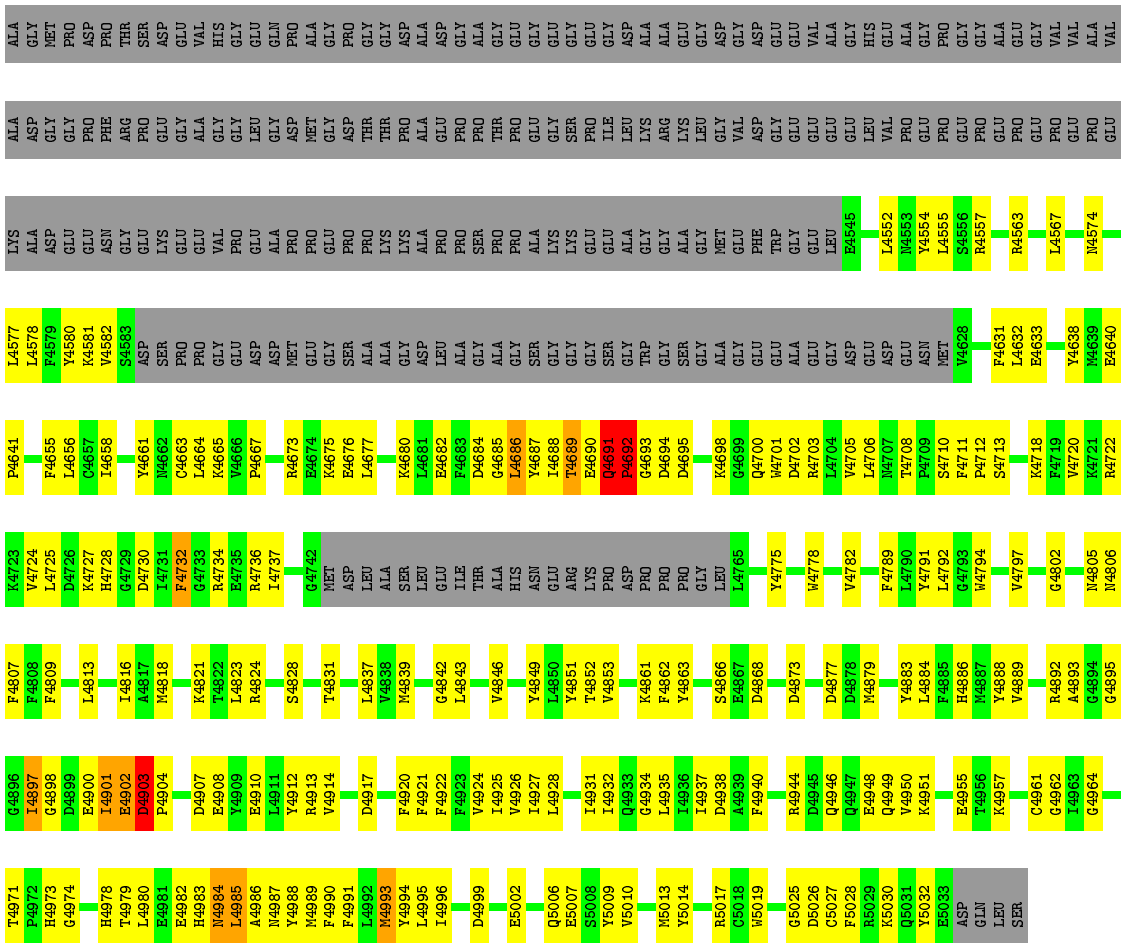
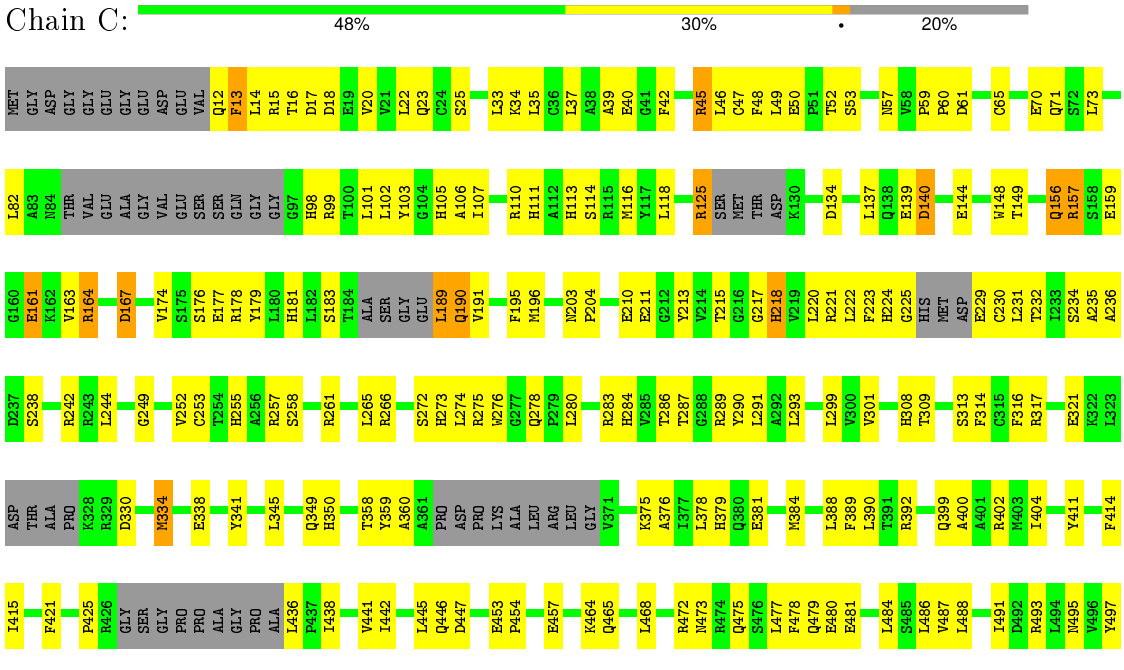


• Molecule 1: Ryanodine receptor 1

Chain C:



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N1610	E1543	C1447	ARG	GLU	ASP	P1196	V1123	G1050	THR	HIS	S784	V707	T635	C566	T498
H1611	P1544	V1448	GLY	PRO	THR	G1197	F1124	Y1051	LYS	THR	A785	G708	N636	V567	T499
F1612	N1545	W1449	PHE	ASP	PRO	Q1198			LEU	ASP	G786	D709	L637	L568	ALA
L1613	T1546	V1450	LEU	PRO	PRO	V1199	H1127	P1055	PRO	F851	V787	D710	I638	I569	ALA
Q1614	K1547	G1451	PHE	ASP	CYS	G1200	R1128	PRO	LYS	V852	K788	L711	N639	E570	HIS
V1615	L1548	W1452	LYS	TYR	LEU	H1201	G1129	ASP	THR		V789		Y640	S571	PHE
E1616	F1549	V1453	ALA	GLU	ARG		Q1130	GLN	Y959	T858	R790	Y714	V641	P572	ALA
T1617	P1550	T1454	LYS	ASN	L1272	G1205	R1131	GLU			F791	G715		E573	GLU
	A1551	P1455	LYS	LEU	A1273	Q1206	W1132	PRO	D971	P864	L792	F716	I644	V574	Y506
G1621	V1552		ALA	ARG	H1274	D1207	H1133	SER	L972	P865	L793	D717	R645	L575	
E1622	F1553	H1462	ALA	ARG	R1275	V1208	L1134	GLN	S973	H866	G794		P646		S514
	V1554	D1463	MET	SER	T1276	S1209	G1135	VAL	H974	L867	GLY	H720	N647	Q579	W515
W1626	L1555	M1464	MET	ALA	W1277	S1210	S1136	GLU	V975		ARG	L721	I648	E580	K516
A1627	P1556	N1465	THR	GLY	G1278	L1211	E1137	ASN		E876	HIS	W722	F649	N581	E517
V1628			GLN	GLY	S1279	R1212	P1138	GLN	P979		GLY		V650	H582	I518
	N1560	S1469	PRO	TRP	Q1280	F1213	F1139	SER		E880	E799	H725	G651	I583	V519
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M1636	Q1563	ARG	THR	ALA	V1284	I1216	W1143	ASP	L988		F802	R728	GLU		L522
M1637	F1564	ALA	PRO	GLU	E1285	C1217		R1071	A989	Q889	L803	F729	GLY	D591	Y523
A1638	E1565	V1472	ALA	GLY	M1286	G1218	D1147	V1072	E990	G890	P804		SER	K592	
L1639	LEU	T1473	LEU	GLY	L1287	L1219	V1148		N991	W891	P805	S732	THR	H593	L526
H1640	GLY	V1474	PRO	LYS	F1288	Q1220		F1075	G992		P806		GLN	G594	A527
I1641	LYS	T1475	ARG	GLU		E1221	C1151	R1076	H993	V896	G807	H736	TYR	R595	S528
P1642	GLN	M1476	LEU	GLY	L1291	G1222	M1152	A1077		R897	Y808	L737	G660	N596	L529
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D1649	LEU	N1482	PRO	THR	F1297		N1158		TRP	C906	L816	L748	V666	V602	A535
I1650	SER	V1483	ALA	PRO	HIS	M1230		R1087	SER	L907	P817	D749	M667	L603	N536
L1651	A1577		ASP	GLY	GLN	Q1231	I1161	W1088	TYR	V908	R818	L750	V668	C604	C537
E1652	A1578	S1486	ASN	GLY	HIS	R1232		Y1089	SER	N909		S751	D669	S605	
L1653	M1579		ARG	THR	PHE		V1168	F1090	ALA	F910	L821	V752	E670	L606	F540
S1654	F1580	X1493	ASP	PRO	ARG	T1235	L1169	E1091	VAL	H911	R822	P753	V671	C607	S541
E1655	L1581		ASP	GLN	CYS	T1236	MET	F1092	GLN	S912	L823	S754		V608	T542
R1656	S1582	D1510	PRO	PRO	THR	W1237	SER	E1093	ASP		E824	I755	F674	C609	N543
L1657	E1583	L1511	GLU	GLY	ALA	F1238	ASP	A1094	ILE	E915	P825		L675	N610	L544
	R1584	V1515	ILE	VAL	GLY	S1239	SER	V1095	PRO	P916	I826	R758	T676	G611	D545
Q1660	K1585	I1516	ILE	GLU	ALA	K1240	GLY	T1096	ALA	E917	K827	I759	A677		W546
R1661	N1586	G1517	LEU	ALA	THR		SER	T1097	R1016	R918	E828	N760	Q678	V614	V547
F1662	P1587	C1518	ASN	GLN	PRO	F1245	GLU	G1098	R1017		Y829		A679	R615	V548
	A1588	L1519	THR	PRO	LEU	E1246	THR	E1099	N1018	G926	R830	P763	T680	S616	S549
H1665	P1589	V1520	THR	VAL	ALA	P1247	A1178	M1100	P1019		R831	V764	H681	N617	K550
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L1667	R1594	LEU	Y1433	ALA	PRO	P1249	R1180	V1102	L1021		G833	V767	R683	D619	D552
	L1595	ALA	Y1434	GLU	GLY	P1250	E1181		V1022	C937	P834	F768	V684	L620	R553
R1671	E1596	THR	Y1435	ASN	LEU	E1251	I1182	A1105	P1023		R835	E769		I621	L554
A1672	V1597	G1525	S1436	GLU	GLN	H1252	E1183		Y1024	M941		A770	T689	T622	E555
V1673	Q1598	L1526	V1437	LYS	PRO	P1253	I1184	L1109		A942	H838	F771	E690	E623	A556
C1674	M1599	M1527	R1438	ASP	PRO	H1254		R1110	L1027	D943	L839		G691	N624	S557
	L1600	T1528	V1439	ALA	ALA	Y1255	F1188	P1111			V840	L776	Y692	L625	S558
N1678	M1601	F1529	F1440	THR	GLU	E1256	L1189	D1112	A1042	A946	G841	F777		L626	G559
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	R1607		GLU	ASN	ARG	GLY	S1193	L1120	L1046	LEU	C845	V781	G704	E630	V563
A1684	M1608	Q1541	PRO	LYS	ALA	THR	L1194	A1121	L1047	LYS	LEU	S782	N705		L564
L1685	P1609	V1542	SER	LYS	ALA	VAL	G1195	Y1122		LYS	SER	F783	G706	Q634	Y565

ASN	A3775	GLU	Q2877	H2788	A2533		I2358	V2275	G2202	Y2128		LYS	E1835	G1764	
GLU		GLU		P2789		M2423	R2359	A2276	M2203	D2129	N1972	GLU	F1836	V1765	H1688
ASP	M3778	VAL	N2881		L2537		K2360	A2277	H2204			GLU	Q1837	G1766	V1689
GLY	V3779	GLU	Y2882	P2793	ASP	D2431	P2361	A2278	E2205	E2133	S1975	ASP	F1838	V1767	D1690
THR	L3780	GLU		Y2794	THR		E2362	S2279	T2206	L2134		GLU	V1839	T1768	
VAL	Q3781	LYS	G2900	K2795	ALA	G2434	CYS	V2280	V2207	L2135	S2058	GLU	P1840	T1769	Q1693
ILE	M3782	K3694	T2901	T2796	THR	R2435	PHE	I2281	M2208	R2136		GLU	V1841		L1694
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ASN	E3789	H3699	L2905	K2802	T2544	GLU	LEU	E2285	V2212	R2140		GLU	V1845	H1775	A1701
GLY	T3790	Q3700	V2906			MET	ARG	L2286	N2213	A2141	L2066	ASP	S1846	H1776	H1702
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LYS	M3793	V3702				LEU	GLU	V2299	L2215	T2143	T2069	GLU	L1848		P1704
VAL	V3794		T2910	I2809	L2550	ILE	GLY	S2300	G2216	I2144	V2070	LYS	L1849	P1780	G1705
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ALA	S3796		D2919	S2812	R2552	ALA	SER		GLY	P2146	L2072	GLU	M1851	F1782	L1707
D3877	T3797	T3708		L2813	Y2553	GLY	G2375	L2307	GLU		VAL	GLU	G1852	V1783	R1708
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E3893	G3827	S3732	N3651	GLU	T2742		ASP	TRP	F2239	I2167	LYS	P1932	P1868	S1799	L1731
	F3828	C3733		LYS		P2496	GLY	ASN	C2240	V2168	LYS		E1869	P1800	S1732
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	L3844	GLU	D3676		E2760	GLU	GLU	G2343	N2260	K2189	E2108	E1956	GLU	L1815	ARG
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	GLU	Q3767	GLU	P2857	K2770	L2522	ASN	N2351	MET	N2196		E1963	GLU		ARG
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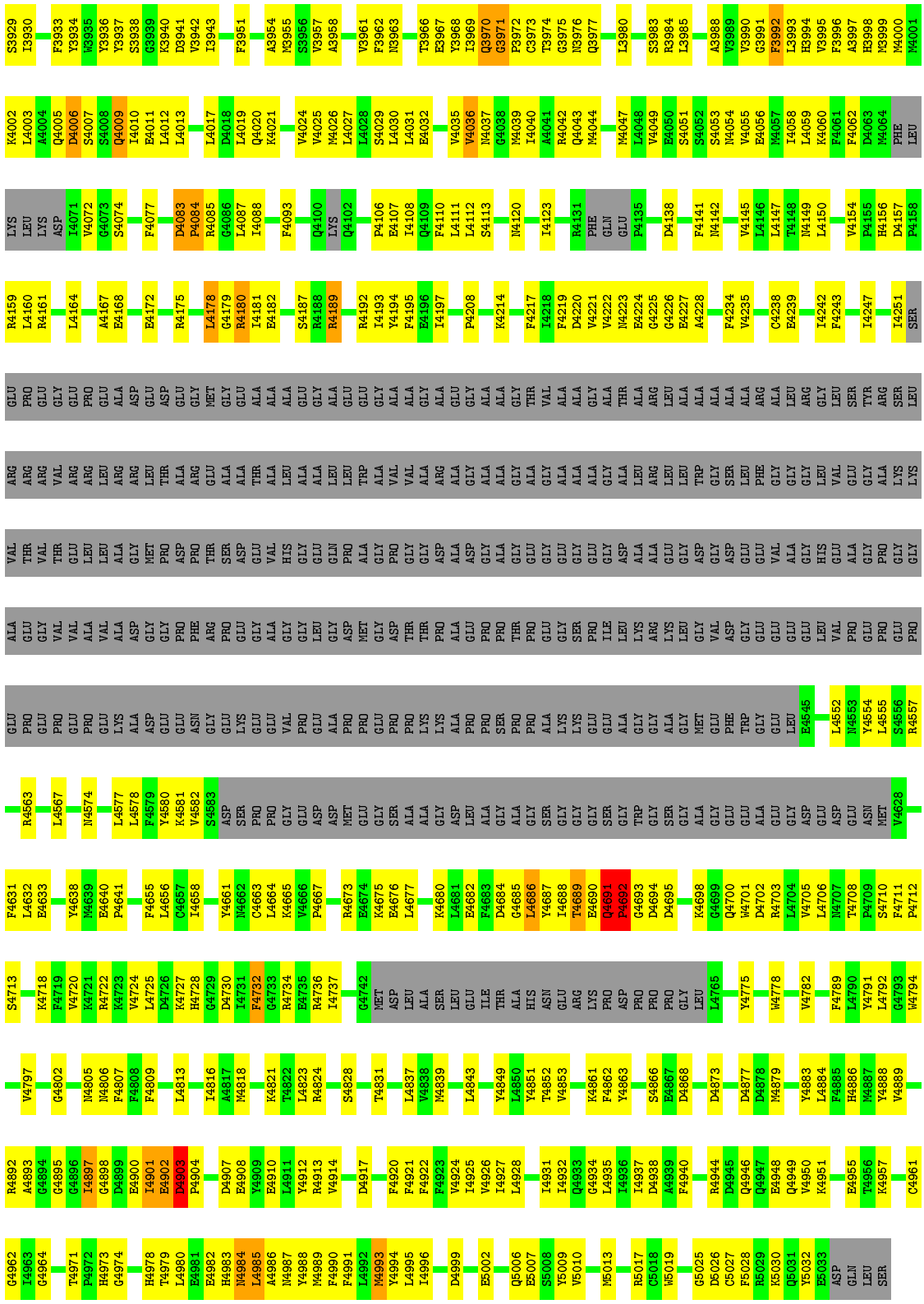
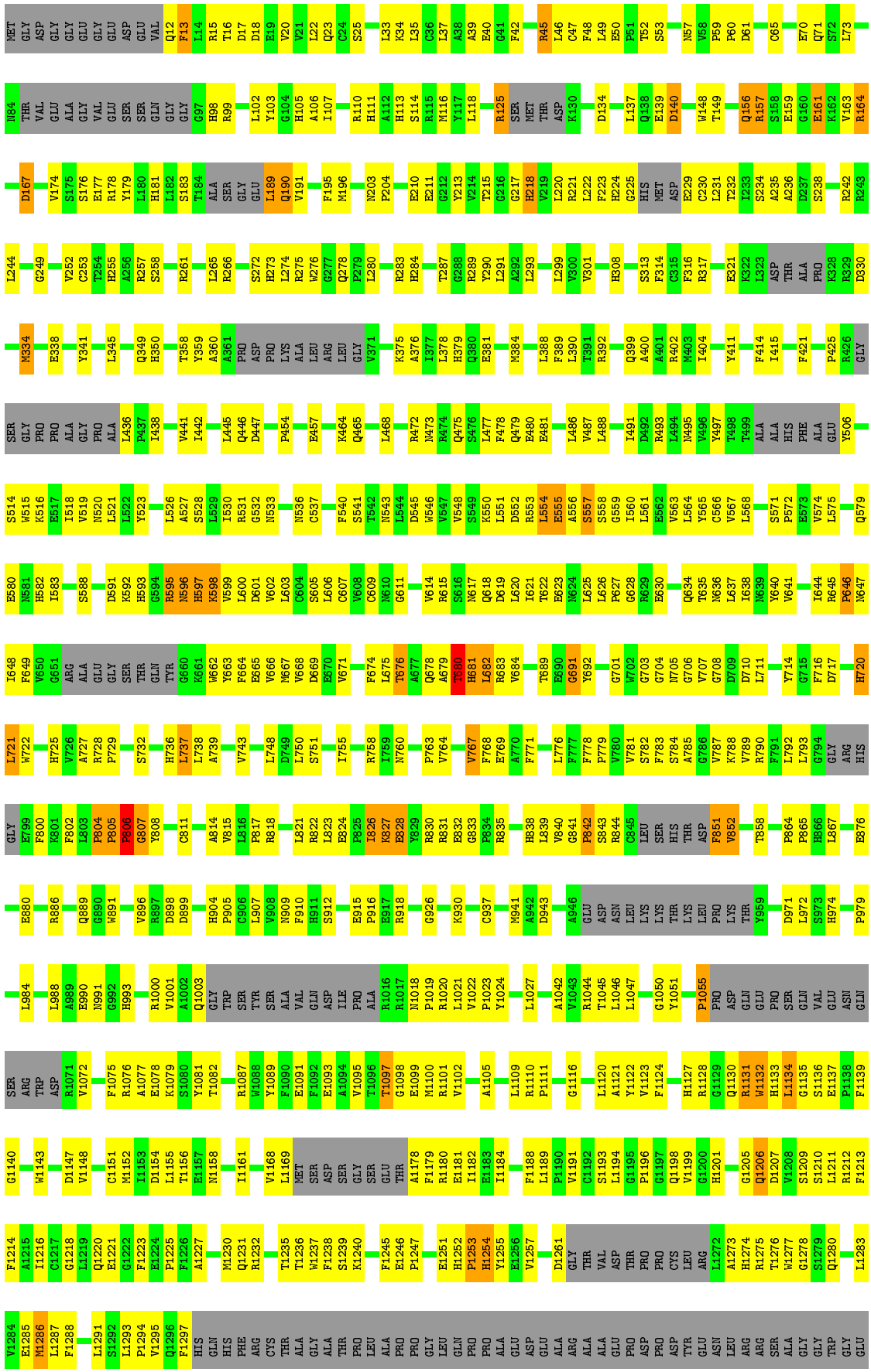


- Molecule 1: Ryanodine receptor 1

Chain E: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HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ARG SER ALA GLY GLY TRP GLY GLU
F1214 A1215 I1216 C1217 G1218 L1219 Q1220 E1221 G1222 F1223 E1224 P1225 F1226 A1227 M1230 Q1231 R1232 T1235 T1236 W1237 F1238 S1239 K1240 F1245 E1246 P1247 E1251 H1252 P1253 H1254 Y1255 E1256 V1257 D1261 GLY THR VAL ASP THR PRO PRO CYS LEU ARG L1272 A1273 H1274 R1275 T1276 W1277 G1278 S1279 Q1280 L1283
G1140 W1143 D1147 V1148 C1151 M1152 I1153 D1154 L1155 T1156 E1157 N1158 I1161 V1168 L1169 MET SER ASP SER GLY SER GLU THR A1178 F1179 R1180 E1181 I1182 E1183 I1184 F1188 L1189 P1190 V1191 C1192 S1193 L1194 G1195 P1196 G1197 Q1198 V1199 G1200 H1201 G1205 Q1206 D1207 V1208 S1209 S1210 L1211 R1212 F1213
SER ARG TRP ASP R1071 V1072 F1075 R1076 A1077 E1078 K1079 S1080 Y1081 T1082 R1087 W1088 Y1089 F1090 E1091 F1092 E1093 A1094 V1095 T1096 T1097 G1098 E1099 N1100 R1101 V1102 A1105 L1109 R1110 P1111 G1116 C1120 A1121 Y1122 V1123 F1124 H1127 R1128 G1129 Q1130 R1131 W1132 H1133 L1134 G1135 S1136 E1137 P1138 F1139
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GLY E799 F800 K801 F802 L803 P804 P805 P806 G807 Y808 C811 A814 V815 L816 P817 R818 L821 R822 L823 E824 P825 I826 K827 E828 Y829 R830 R831 E832 G833 P834 R835 H838 L839 V840 G841 P842 S843 R844 G845 LEU SER HIS THR ASP F851 V852 T858 P864 P865 H866 L867 E876
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D167 V174 S175 S176 E177 R178 Y179 L180 H181 L182 S183 T184 ALA SER GLY GLU L189 Q190 V191 F195 M196 N203 P204 E210 E211 G212 Y213 V214 T215 G216 G217 H218 V219 L220 R221 L222 F223 H224 G225 HIS MET ASP E229 C230 L231 T232 I233 S234 A235 A236 D237 S238 R242 R243
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MET GLY ASP GLY GLY GLU GLY GLU ASP GLU VAL Q12 F13 L14 R15 T16 D17 D18 E19 V20 V21 L22 Q23 C24 S25 L33 K34 L35 C36 L37 A38 A39 E40 G41 F42 R45 L46 C47 F48 L49 E50 P51 T52 S53 N57 V58 P59 P60 D61 C65 E70 Q71 S72 L73

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A2557		I2380	PRO	ILE	T2152	GLU	GLU	G1852	V1783	R1708	M1636	I1562	VAL	PRO	GLU
V2558	R2452		MET	ARG		GLU	GLU	I1853	A1784		M1637	Q1563	ARG	ALA	GLY
L2559	I2453	A2383	LEU	PHE	L2155	LYS	ALA	F1854	ALA	Y1712	A1638	F1564	ALA	LEU	GLY
P2560	R2454	I2384	LEU	P2226	L2156	PRO	PRO	G1855	LEU	D1713	L1639	E1565	V1472	PRO	LYS
	A2455	R2385	ALA	K2227		GLU	GLU	D1856	PRO	L1714	H1640	LEU	T1473	ARG	GLU
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	L2457	SER	GLY	T2230		GLU	GLU	D1858	ALA	I1716	P1642	LYS	T1475	PRO	THR
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		ASP	PRO	R2234	R2163	PRO	GLU	K1860	VAL	L1720		LYS	G1477	ASP	LYS
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	D2497	PRO	P2325	R2241	GLN	PRO		I1866	ARG	S1729	L1651	SER	V1483	ASN	GLY
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	K2499	VAL			GLY	S2093		P1868	S1799	L1731	L1653	A1578	S1486	ASP	PRO
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F2754	V2503	ARG		R2248	M2178	L2097		THR	P1803	I1735	L1657	S1582	D1510	ILE	VAL
I2755	L2504	ARG	F2337	S2249		V2098	L1943	GLU	L1804	V1736		E1583	L1511	ILE	GLU
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	P2529	LEU	L2356	T2271	A2200	R2126	E1963	GLU		ARG	N1679	P1602	T1530	GLN	LYS
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		M2423	R2359	A2276	M2203	D2129	V1966	GLU	V1830	G1761		M1608		SER	LYS
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Y2794	THR		E2362	S2279	T2206	L2134		LYS	E1835	G1764		H1611	E1543	W1449	PHE
	ALA	G2434	CYS	V2280	V2207	L2135	N1972	GLU	F1836	V1765	H1688	F1612	P1544	V1450	LEU
R2806	THR	R2435	PHE	I2281	M2208	R2136		GLU	Q1837	G1766	V1689	L1613	N1545	G1451	PHE
	PHE	C2436	GLY	D2282	E2209	A2137	S1975	ASP	F1838	V1767	D1690	Q1614	T1546	W1452	LYS
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	THR	PRO	ALA	N2284	M2211	P2139	L2063	GLU	P1840	T1769	Q1693	E1616	L1548	T1454	LYS
S2812	T2544	GLU	LEU	E2285	V2212	R2140		GLU	V1841	S1770	L1694	T1617	F1549	P1455	LYS
L2813		MET	ARG	L2286	N2213	A2141	L2066	GLU	L1842	L1771			P1550		ALA
K2814	A2547	HIS	GLY		V2214	Y2142		GLU	K1843	R1772	L1698	G1621	A1551	H1462	ALA
		LEU	GLU	V2299	L2215	T2143	T2069	LYS	L1844			E1622	V1552	D1463	MET
A2818	L2550	ILE	GLY	S2300	G2216	I2144	V2070	GLU	V1845	H1775	A1701		F1553	M1464	MET
W2819	N2551	GLN	GLY	Y2301	GLY	S2145	R2071	ASP	S1846	H1776	H1702	W1626	V1554	N1465	THR
E2820	R2552	ALA	SER		GLY	P2146	L2072	ALA	T1847	F1777	L1703	A1627	L1555	F1466	GLN
W2821	Y2553	GLY	G2375	L2307	GLU		VAL	GLU	L1848		P1704	V1628	P1556	D1467	PRO
T2822	L2554	LYS	L2376	GLN	THR	V2149	LYS	LYS	L1849	P1780	G1705			L1468	PRO
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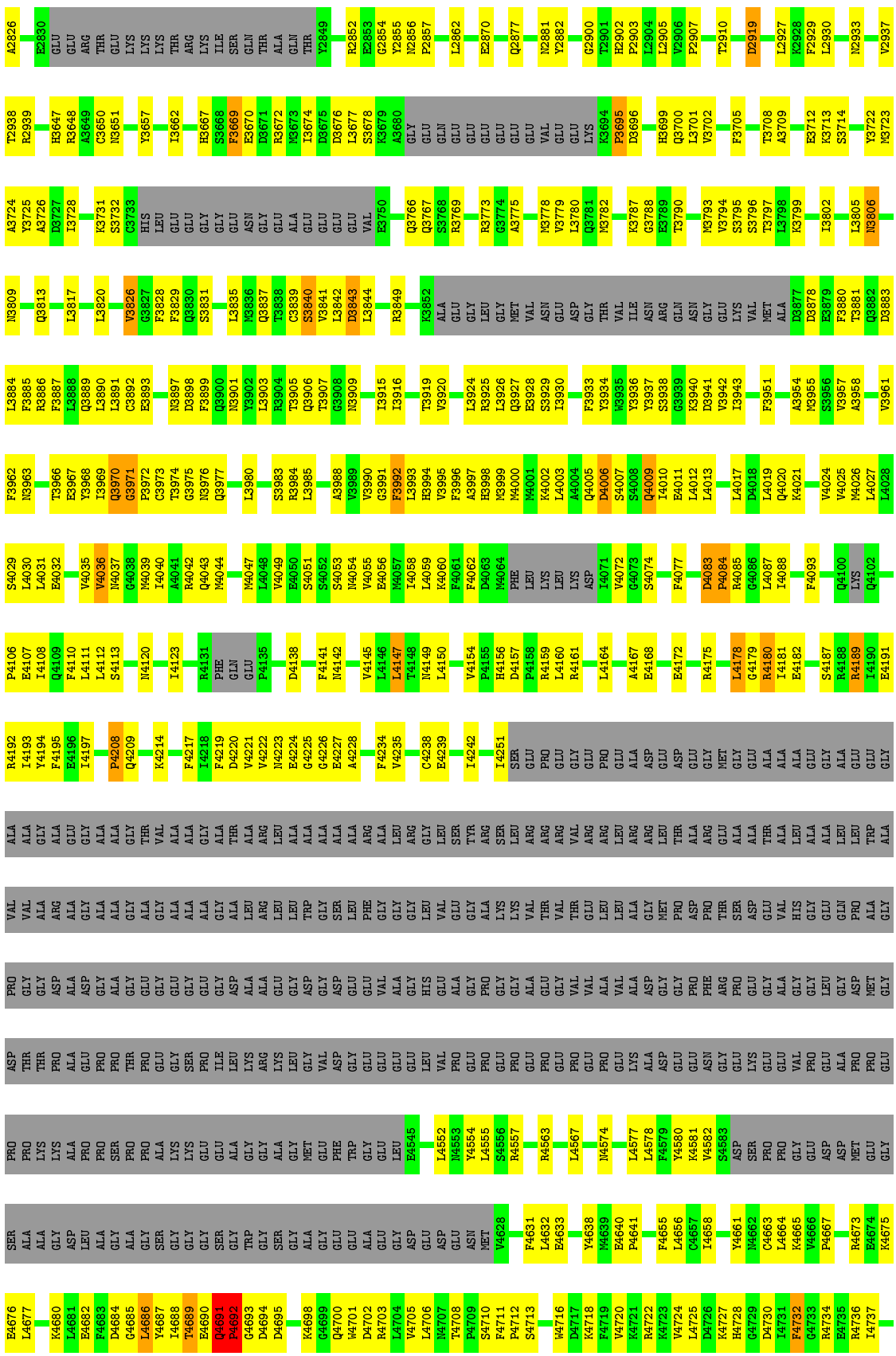
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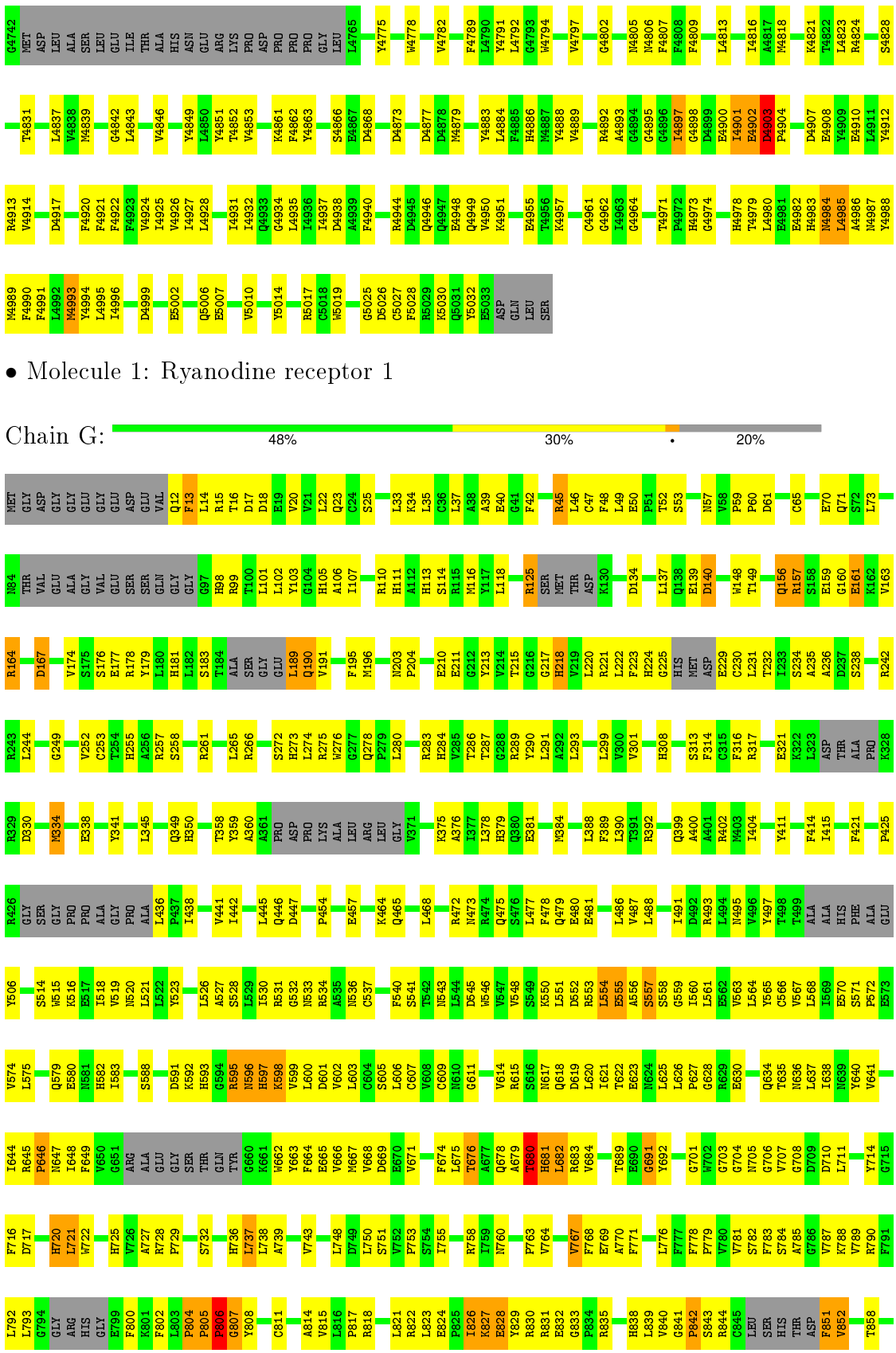
T2938 R2939 H3647 R3648 A3649 C3650 N3651 Y3657 I3662 H3667 S3668 F3669 E3670 D3671 R3672 M3673 I3674 D3675 D3676 L3677 S3678 K3679 A3680 GLY GLU GLN GLU GLU GLU GLU GLU GLU GLU GLU VAL GLU LYS K3694 P3695 D3696 H3699 Q3700 L3701 V3702 F3705 T3708 A3709 E3712 K3713 S3714 Y3722 M3723
A3724 Y3725 A3726 D3727 I3728 K3731 S3732 C3733 HIS LEU GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU GLU VAL E3750 Q3766 Q3767 S3768 R3769 R3773 G3774 A3775 M3778 V3779 L3780 Q3781 M3782 K3787 G3788 E3789 T3790 M3793 V3794 S3795 S3796 T3797 L3798 K3799 I3802 L3805 N3806
N3809 Q3813 L3817 L3820 L3890 L3891 C3892 V3826 G3827 F3828 F3829 Q3830 S3831 L3835 M3836 Q3837 T3838 C3839 S3840 V3841 L3842 D3843 L3844 R3849 K3852 ALA GLU GLY LEU GLY MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY GLU LYS VAL MET ALA D3877 D3878 E3879 F3880 T3881 Q3882 D3883
L3884 F3885 R3886 F3887 L3888 Q3889 L3890 L3891 C3892 E3893 N3897 D3898 F3899 Q3900 N3901 Y3902 L3903 R3904 T3905 Q3906 T3907 G3908 N3909 I3915 I3916 T3919 V3920 L3924 R3925 L3926 Q3927 E3928 S3929 I3930 F3933 Y3934 W3935 Y3936 Y3937 S3938 G3939 K3940 D3941 V3942 I3943 F3951 A3954 M3955 S3956 V3957 A3958 V3961
F3962 N3963 T3966 E3967 Y3968 I3969 Q3970 G3971 P3972 C3973 T3974 G3975 N3976 Q3977 L3980 S3983 R3984 L3985 A3988 V3989 V3990 G3991 F3992 L3993 H3994 L4059 K4060 F4061 F4062 D4063 M4064 PHE LEU LYS LEU LYS ASP I4071 V4072 G4073 S4074 F4077 D4083 P4084 R4085 G4086 L4087 I4088 F4093 Q4100 LYS Q4102
S4029 L4030 L4031 E4032 V4035 V4036 N4037 G4038 M4039 I4040 A4041 R4042 Q4043 M4044 M4047 L4048 V4049 E4050 S4051 S4052 S4053 N4054 V4055 E4056 M4057 I4058 L4059 K4060 F4061 F4062 D4063 M4064 M4000 M4001 K4002 L4003 A4004 Q4005 D4006 S4007 S4008 Q4009 I4010 E4011 L4012 L4013 L4017 D4018 L4019 Q4020 K4021 V4024 V4025 M4026 L4027 L4028
P4106 E4107 I4108 Q4109 F4110 L4111 L4112 S4113 N4120 I4123 R4131 PHE GLN GLU P4135 D4138 F4141 N4142 V4145 L4146 L4147 T4148 N4149 L4150 V4154 P4155 H4156 D4157 P4158 R4159 L4160 R4161 L4164 A4167 E4168 E4172 R4175 L4178 G4179 R4180 I4181 E4182 S4187 R4188 R4189 I4190 E4191
R4192 I4193 Y4194 F4195 E4196 I4197 P4208 Q4209 K4214 F4217 I4218 F4219 D4220 V4221 V4222 N4223 E4224 G4225 G4226 E4227 A4228 F4234 V4235 C4238 E4239 I4242 I4251 SER GLU PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA THR ALA ALA LEU LEU TRP ALA
ALA ALA GLY ALA GLU GLY THR VAL ALA ALA ALA GLY ALA ALA ARG LEU ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU LEU ARG ARG ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA LEU LEU ARG
VAL VAL ALA ARG ALA GLY ALA ALA ALA GLY GLY GLY ALA GLY ALA ALA ALA GLY SER LEU PHE GLY GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO GLY
PRO GLY GLY ASP ALA ASP GLY ALA ALA GLY GLU GLY GLY GLY ALA ALA GLU GLU ALA ASP GLY GLU GLU ALA ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA VAL GLU GLU VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY VAL HIS GLY GLY GLU ALA
ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU GLU PRO GLU GLU PRO GLU LYS ALA ASP GLU GLU GLU GLU GLU VAL VAL GLU GLU LEU GLU GLU ALA
PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA ALA GLY MET GLU PHE TRP GLY GLU LEU E4545 L4552 N4553 Y4554 L4555 S4556 R4557 R4563 L4567 N4574 L4577 L4578 F4579 Y4580 K4581 V4582 S4583 ASP SER PRO GLU GLY GLY PRO GLU GLY GLY GLY PRO PRO GLU GLU ASP
SER ALA ALA GLY ASP LEU ALA GLY GLY GLY ALA GLU GLU GLU ALA GLU GLY SER GLY GLY GLY ALA GLU ASN MET V4628 F4631 L4632 E4633 Y4638 M4639 E4640 P4641 F4655 L4656 C4657 I4658 Y4661 M4662 C4663 L4664 K4665 V4666 P4667 R4673 E4674 K4675
E4676 L4677 K4680 L4681 E4682 F4683 D4684 G4685 L4686 Y4687 I4688 T4689 E4690 Q4691 P4692 G4693 D4694 D4695 K4698 G4699 Q4700 W4701 D4702 R4703 L4704 V4705 L4706 W4707 T4708 P4709 S4710 F4711 P4712 S4713 W4716 D4717 K4718 F4719 V4720 K4721 R4722 K4723 V4724 L4725 D4726 K4727 H4728 G4729 D4730 I4731 F4732 G4733 R4734 E4735 R4736 I4737



- Molecule 1: Ryanodine receptor 1

Chain G:

WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM

L2066	ASP	S1846	P1774	A1701	A1627	L1555	F1466	GLN	GLY	S1279	S1209	L1134	SER	D971	P864
	ALA	T1847	H1775	H1702	V1628	P1556	D1467	PRO	TRP	Q1280	S1210	G1135	GLN	L972	P865
T2069	GLU	L1848	H1776	L1703			L1468	PRO	GLY		L1211	S1136	VAL	S973	H866
V2070	LYS	L1849	F1777	P1704	L1634	N1560	S1469	ALA	GLU	L1283	R1212	E1137	GLU	H974	L867
R2071	GLU	V1850		G1705	T1635	V1561	LYS	THR	ALA	V1284	F1213	P1138	ASN		
L2072	GLU	M1851	P1780	P1706	M1636	I1562	VAL	PRO	GLU	E1285	F1214	F1139	GLN	P979	E876
VAL	GLU	G1852	C1781	L1707	M1637	Q1563	ARG	ALA	GLY	M1286		G1140	SER		
LYS	GLU	I1853	F1782	R1708	A1638	F1564	ALA	LEU	GLY	L1287	G1218		ARG	L984	E880
LYS	ALA	F1854	V1783		L1639	E1565	V1472	PRO	LYS	F1288		W1143	TRP		
LYS	PRO	G1855	A1784	Y1712	H1640	LEU	T1473	ARG	GLU		E1221		ASP	L988	R886
GLU	GLU	D1856	ALA	D1713	I1641	GLY	V1474	LEU	GLY	L1291	G1222	D1147	R1071	A989	
GLU	GLY	E1857	LEU	L1714	P1642	LYS	T1475	PRO	THR	S1292	F1223	V1148	V1072	E990	Q889
LYS	GLU	D1858	PRO	L1715	E1643	GLN	M1476	HIS	ALA	L1293	E1224			N991	G890
PRO	LYS	V1859	ALA	I1716		LYS	G1477	ASP	LYS	P1294	P1225	C1151	F1075	G992	W891
GLU	GLU	K1860	ALA		R1646	ASN	D1478	VAL	GLU	V1295	F1226	M1152	R1076	H993	
GLU	ASP	Q1861	GLY	L1720	C1647	ILE	E1479	VAL	GLY	Q1296	A1227	I1153	A1077		V896
GLU	LEU	I1862	VAL	E1721	M1648	MET	Q1480	PRO	THR	F1297		D1154	E1078	R1000	R897
LEU	GLU	L1863	ALA		D1649	PRO	G1481	ALA	PRO	HIS	M1230	L1155	K1079	V1001	D898
PRO	GLU	K1864	GLU	S1726	I1650	LEU	N1482	ASP	GLY	GLN	Q1231	T1156	S1080	A1002	D899
ALA	G1925	M1865	ALA	R1727	L1651	SER	V1483	ASN	GLY	HIS	R1232	E1157	Y1081	Q1003	
GLU	L1926	I1866	PRO	R1728	E1652	A1577		ARG	THR	PHE		N1158	T1082	GLY	H904
GLU		E1867	ALA	S1729	L1653	A1578	S1486	ASP	PRO	ARG	T1235			TRP	P905
LYS	P1932	P1868	ARG	M1730	S1654	M1579		ASP	GLN	CYS	T1236	I1161	R1087	SER	C906
LYS		E1869	L1798	L1731	E1655	F1580	X1493	PRO	PRO	THR	W1237		W1088	TYR	L907
PRO	L1937	VAL	S1799	S1732	R1656	L1581		GLU	GLY	ALA	F1238	V1168	Y1089	SER	V908
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Q2095	L1943	GLU	E1805	V1736	R1661	K1585	I1516	ASN	GLN	PRO	F1245	ASP	E1093	ASP	S912
E2096	E1944	GLU	A1806	P1737	F1662	N1586	G1517	THR	PRO	LEU	E1246	SER	A1094	ILE	
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V2098	F1946	GLU	R1808	T1739	H1665	A1588	L1519	T1432	ARG	PRO	V1248	SER	T1096	ALA	P916
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	Q1952	GLU		R1743		R1594	LEU	Y1435	ASN	LEU	E1251	A1178	E1099	N1018	
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	V1955	GLU	M1814	P1750	A1672	E1596	THR	V1437	LYS	PRO	P1253	R1180	R1101	R1020	
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	S1957	GLU		ARG	C1674	Q1598	L1526	V1439	ALA	ALA	Y1255	I1182		V1022	
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S2113		GLU		GLY	N1678	L1600	T1528	A1441	THR	ASP	V1257	I1184		Y1024	
	F1961	GLU	Q1824	GLY	N1679	M1601	F1529	GLY	GLU	GLU			L1109		M941
L2116	A1962	GLU	H1825	ASN	R1680	P1602	T1530	GLN	LYS	ALA	D1261	F1188	R1110	L1027	A942
	E1963	GLU		ALA	V1681			GLU	ASN	ARG	GLY	L1189	P1111		D943
L2123	R1964	GLU	D1828	ARG		R1607	T1538	PRO	LYS	ALA	THR	P1190		A1042	
L2124	Y1965	ASP	P1829	ARG	A1684	M1608		SER	LYS	ALA	VAL	V1191	G1116	V1043	A946
H2125	V1966	GLU	V1830	HIS	L1685	P1609	Q1541	C1447	ARG	GLU	ASP	C1192		R1044	GLU
R2126		GLU	G1831	G1761		N1610	V1542	V1448	GLY	PRO	THR	S1193	L1120	T1045	ASP
Q2127	L1969	GLU		L1762	H1688	H1611	E1543	W1449	PHE	ASP	PRO	L1194	A1121	L1046	ASN
Y2128		LYS	E1835	P1763	V1689	F1612	P1544	V1450	LEU	PRO	PRO	G1195	Y1122	L1047	LEU
D2129	N1972	GLU	F1836	G1764	D1690	L1613	N1545	G1451	PHE	ASP	CYS	P1196	V1123		LYS
		GLU	Q1837	V1765		Q1614	T1546	W1452	LYS	TYR	LEU	G1197	F1124	G1050	LYS
E2133	S1975	ASP	F1838	G1766	Q1693	V1615	K1547	V1453	ALA	GLU	ARG	Q1198		Y1051	THR
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P2139	L2063	LYS	L1844	R1772	E1699		F1553	M1464	MET	ALA	W1277	Q1206	W1132	GLU	Y959
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GLU		F4077	E4011	G3939	GLN	T3790	F3705				MET	ARG	L2286	N2213	A2141
ASP	R4175		L4012	K3940	ASN			D2919	R2806	A2547	HIS	GLY		V2214	Y2142
GLU		D4083	L4013	D3941	GLY	M3793	T3708				LEU	GLU	V2299	L2215	T2143
GLY	L4178	P4084		V3942	GLU	V3794	A3709	L2927	I2809	L2550	ILE	GLY	S2300	G2216	I2144
MET	G4179		L4017	I3943	LYS	S3795		K2928		N2551	GLN	GLY	Y2301	GLY	S2145
GLY	R4180	L4087	D4018		VAL	S3796	E3712	F2929	K2814	R2552	ALA	SER		GLY	P2146
GLU	I4181	I4088	L4019	F3951	MET	T3797	K3713	L2930		Y2553	GLY	G2375	L2307	GLU	
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ALA		F4093	K4021	A3954	D3877	K3799	K3715	N2933		C2555	GLY	L2377	SER	LYS	E2150
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GLU	R4188	Q4100	V4024	S3956	E3879	I3802		V2937	T2822	A2557		I2380	PRO	ILE	T2152
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GLU	E4191		L4027		Q3882	N3806	A3724			P2560	R2454	I2384	LEU	P2226	L2156
GLU	R4192	P4106	L4028	V3961	D3883		Y3725	H3647	E2830		A2455	R2385	ALA	K2227	
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ALA	Y4194	I4108	L4030	N3963	F3885		D3727	A3649	GLU		L2457	SER	GLY	T2230	
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GLY	E4196	F4110	E4032	T3966	F3887			N3651	THR	X2595		ASP	PRO	R2234	R2163
ALA	I4197	L4111		E3967	L3888	L3817	K3731		GLU		X2465	PRO	ASP		S2164
GLU		L4112	V4035	Y3968	Q3889		S3732	Y3657	LYS	X2625	X2466	ALA	ILE	C2237	L2165
GLY	P4208	S4113	V4036	I3969	L3890	L3820	C3733		LYS		X2467	ARG	GLY	Y2238	L2166
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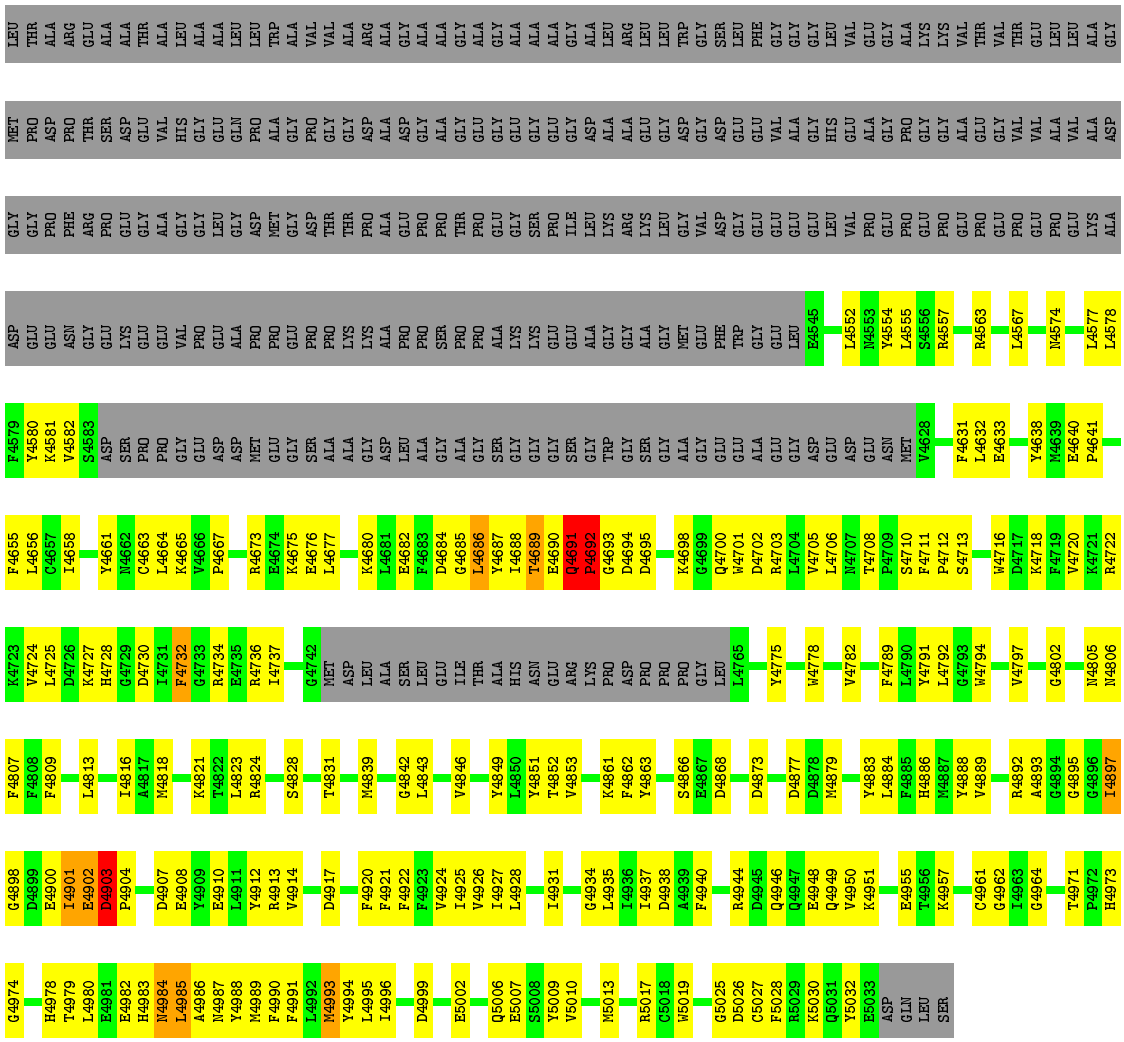
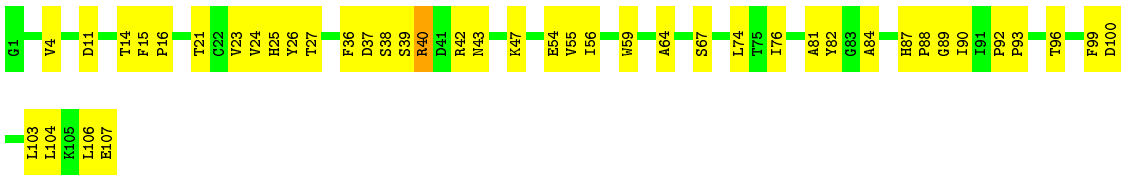
ALA	K4214	N4120	G4038	G3971	C3892	V3826	LEU		THR		P2496	GLY	ASN	C2240	V2168
GLY			M4039	P3972	E3893	G3827	GLU	H3667	ARG	V2745	D2497	PRO	P2325	R2241	GLN
THR	F4217	I4123	I4040	C3973		F3828	GLU	S3668	LYS		H2498	GLY	C2326	I2242	MET
VAL	I4218		A4041	T3974	N3897	F3829	GLY	F3669	ILE	P2748	K2499	VAL			GLY
ALA	F4219	R4131	R4042	G3975	D3898	Q3830	GLY	E3670	SER		A2500	ARG	E2329	Q2245	PRO
ALA	D4220	PHE	Q4043	N3976	F3899	S3831	GLU	D3671	GLN	L2751	S2501	ARG	R2330	N2246	Q2173
GLY	V4221	GLN	M4044	Q3977	Q3900		ASN	R3672	THR	D2752	M2502	ASP	Y2331	Q2247	
ALA	V4222	GLU			N3901	L3835	GLY	M3673	ALA	S2753	V2503	ARG		R2248	M2178
THR	N4223	P4135	M4047	L3980	Y3902	M3836	GLU	I3674	GLN	F2754	L2504	ARG	F2337	S2249	
ALA	E4224		L4048		L3903	Q3837	ALA	D3675	THR	I2755	F2505	ARG	A2338		I2182
ARG	G4225	D4138	V4049	S3983	R3904	T3838	GLU	D3676	Y2849	N2756		GLU	V2339	Y2256	
LEU	G4226		E4050	R3984	T3905	C3839	GLU	L3677		K2757	Y2510	HIS	F2340	L2257	I2185
ALA	E4227	F4141	S4051	L3985	Q3906	S3840	GLU	S3678	R2852	F2758	GLY	PHE	V2341	L2258	
ALA	A4228	N4142	S4052		T3907	V3841	GLU	K3679	E2853	A2759	ILE	GLY	N2342	E2259	N2188
ALA			S4053	A3988	G3908	L3842	VAL	A3680	G2854	E2760	GLU	GLU	G2343	N2260	K2189
ALA	F4234	V4145	N4054	V3989	N3909	D3843	E3750	GLY	Y2855	Y2761	N2514	GLU			V2190
ALA	V4235	L4146	V4055	V3990		L3844		GLU	N2856	T2762		PRO	V2346	I2263	F2191
ARG		L4147	E4056	G3991	I3915		Q3766	GLN	P2857	H2763	F2517	PRO		GLY	Y2192
ALA	C4238	T4148	M4057	F3992	I3916	R3849	Q3767	GLU		E2764		GLU	N2349	LEU	
LEU	E4239	N4149	I4058	L3993			S3768	GLU	L2862		V2521	GLU	A2350	GLY	P2195
ARG		L4150	L4059	H3994	T3919	K3852	R3769	GLU		K2770	L2522	ASN	N2351	MET	N2196
GLY	I4242		K4060	V3995	V3920	ALA		GLU	E2870		ASP	ARG		GLN	L2197
LEU	F4243	V4154	F4061	F3996		GLU	R3773	GLU		N2773	V2525	VAL	V2354	GLY	M2198
SER		P4155	F4062	A3997	L3924	GLY	G3774	GLU	Q2877	N2774		HIS	R2355	SER	R2199
TYR	I4247	H4156	D4063	H3998	R3925	LEU	A3775	VAL		W2775	P2529	LEU	L2356	T2271	A2200
ARG		D4157	M4064	M3999	L3926	GLY		GLU	Y2882			G2419	L2357		L2201
SER	I4251	P4158	PHE	M4000	Q3927	MET	M3778	GLU		H2788	A2533		I2358	V2275	G2202
LEU	SER	R4159	LEU	M4001	E3928	VAL	V3779	LYS	G2900	P2789		M2423	R2359	A2276	M2203
ARG	GLU	L4160	LYS	K4002	S3929	ASN	L3780	K3694	T2901		L2537		K2360	A2277	H2204
ARG	PRO	R4161	LEU	L4003	I3930	GLU	Q3781	P3695	H2902	P2793	ASP	D2431	P2361	A2278	E2205
ARG	GLU		LYS	A4004		ASP	M3782	D3696	P2903	Y2794	THR		E2362	S2279	T2206
VAL	GLY	L4164	ASP	Q4005	F3933	GLY			L2904	K2795	ALA	G2434	CYS	V2280	V2207
ARG	GLU		I4071	D4006	Y3934	THR	A3785	H3699	L2905	T2796	THR	R2435	PHE	I2281	M2208
ARG	PRO	A4167	V4072	S4007	W3935	VAL	C3786	Q3700	V2906		PHE	C2436	GLY	D2282	E2209
LEU	GLU	E4168	G4073	S4008	Y3936	ILE	K3787	L3701	P2907	E2799	SER	A2437	PRO	N2283	V2210
ARG	ALA		S4074	Q4009	Y3937	ASN	G3788	V3702			THR	PRO	ALA	N2284	M2211
ARG	ASP	E4172		I4010	S3938	ARG	E3789		T2910	K2802	T2544	GLU	LEU	E2285	V2212



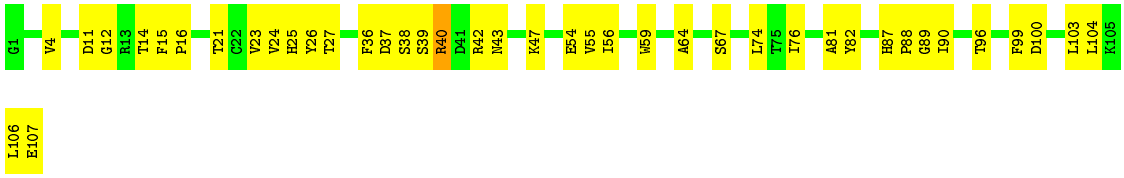
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain B:



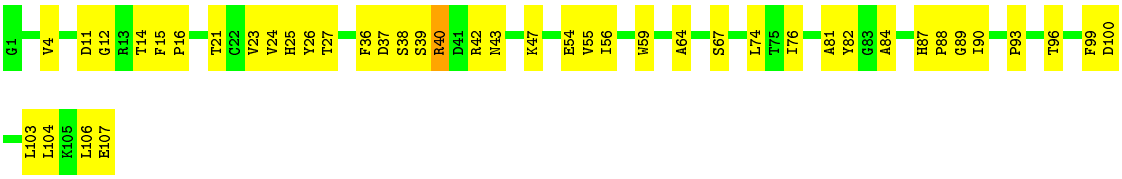
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain D:



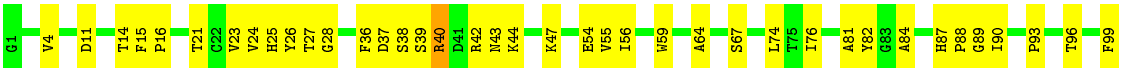
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

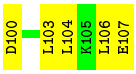
Chain F: 60% 39%



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

Chain H: 59% 40%





4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	65872	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Contrast transfer function parameters were estimated using CTFFIND3	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	5600	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4k x 4k)	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

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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.33	2/24616 (0.0%)	0.59	19/33295 (0.1%)
1	C	0.33	2/24616 (0.0%)	0.59	19/33295 (0.1%)
1	E	0.33	2/24616 (0.0%)	0.59	19/33295 (0.1%)
1	G	0.33	2/24616 (0.0%)	0.59	19/33295 (0.1%)
2	B	0.26	0/851	0.45	0/1146
2	D	0.26	0/851	0.45	0/1146
2	F	0.26	0/851	0.45	0/1146
2	H	0.26	0/851	0.45	0/1146
All	All	0.33	8/101868 (0.0%)	0.59	76/137764 (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	3
1	C	0	3
1	E	0	3
1	G	0	3
All	All	0	12

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1544	PRO	N-CD	5.20	1.55	1.47
1	C	1544	PRO	N-CD	5.20	1.55	1.47
1	E	1544	PRO	N-CD	5.20	1.55	1.47
1	G	1544	PRO	N-CD	5.20	1.55	1.47
1	A	1763	PRO	N-CD	5.05	1.54	1.47

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1764	GLY	N-CA-C	14.38	149.05	113.10
1	C	1764	GLY	N-CA-C	14.38	149.05	113.10
1	E	1764	GLY	N-CA-C	14.38	149.05	113.10
1	G	1764	GLY	N-CA-C	14.38	149.05	113.10
1	A	1765	VAL	N-CA-CB	-9.67	90.23	111.50

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1253	PRO	Peptide
1	A	1867	GLU	Peptide
1	A	646	PRO	Peptide
1	C	1253	PRO	Peptide
1	C	646	PRO	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	26957	0	23849	1705	0
1	C	26957	0	23849	1709	0
1	E	26957	0	23849	1698	0
1	G	26957	0	23849	1714	0
2	B	832	0	831	41	0
2	D	832	0	831	42	0
2	F	832	0	831	42	0
2	H	832	0	831	43	0
3	A	1	0	0	2	0
3	C	1	0	0	2	0
3	E	1	0	0	2	0
3	G	1	0	0	2	0
All	All	111160	0	98720	6845	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 33.

The worst 5 of 6845 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:E:554:LEU:HD11	1:E:593:HIS:CE1	1.12	1.64
1:G:554:LEU:HD11	1:G:593:HIS:CE1	1.12	1.63
1:A:554:LEU:HD11	1:A:593:HIS:CE1	1.12	1.62
1:C:554:LEU:HD11	1:C:593:HIS:CE1	1.12	1.61
1:G:1961:PHE:CZ	1:G:2063:LEU:HD23	1.36	1.60

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	2991/4599 (65%)	2776 (93%)	155 (5%)	60 (2%)	9	54
1	C	2991/4599 (65%)	2776 (93%)	155 (5%)	60 (2%)	9	54
1	E	2991/4599 (65%)	2776 (93%)	155 (5%)	60 (2%)	9	54
1	G	2991/4599 (65%)	2776 (93%)	155 (5%)	60 (2%)	9	54
2	B	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
2	D	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
2	F	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
2	H	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
All	All	12384/18824 (66%)	11492 (93%)	652 (5%)	240 (2%)	14	54

5 of 240 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	737	LEU
1	A	807	GLY
1	A	827	LYS

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Mol	Chain	Res	Type
1	A	852	VAL
1	A	1254	HIS

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	2507/3406 (74%)	2439 (97%)	68 (3%)	52	82
1	C	2507/3406 (74%)	2439 (97%)	68 (3%)	52	82
1	E	2507/3406 (74%)	2439 (97%)	68 (3%)	52	82
1	G	2507/3406 (74%)	2439 (97%)	68 (3%)	52	82
2	B	89/89 (100%)	88 (99%)	1 (1%)	80	92
2	D	89/89 (100%)	88 (99%)	1 (1%)	80	92
2	F	89/89 (100%)	88 (99%)	1 (1%)	80	92
2	H	89/89 (100%)	88 (99%)	1 (1%)	80	92
All	All	10384/13980 (74%)	10108 (97%)	276 (3%)	56	82

5 of 276 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4072	VAL
1	E	596	ASN
1	G	3708	THR
1	C	4180	ARG
1	E	125	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 221 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3970	GLN
1	E	533	ASN
1	G	3647	HIS

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Mol	Chain	Res	Type
1	C	4020	GLN
1	E	105	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 carbohydrates 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.