



## wwPDB EM Validation Summary Report ⓘ

Mar 19, 2024 – 10:49 PM JST

PDB ID : 6JV2  
EMDB ID : EMD-9889  
Title : Structure of RyR2 (P/L-Ca<sup>2+</sup>/Ca<sup>2+</sup>-CaM dataset)  
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.  
Deposited on : 2019-04-15  
Resolution : 4.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

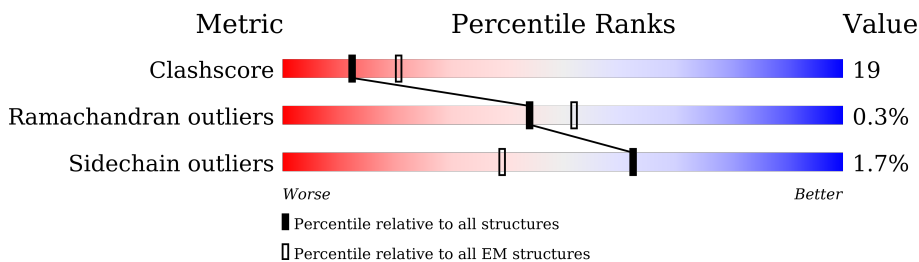
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4968	7% (Poor fit), 42% (0 outliers), 27% (1 outlier), 24% (2 outliers), 2% (3+ outliers), 2% (Not modelled)
1	C	4968	7% (Poor fit), 42% (0 outliers), 28% (1 outlier), 23% (2 outliers), 2% (3+ outliers), 2% (Not modelled)
1	E	4968	7% (Poor fit), 42% (0 outliers), 27% (1 outlier), 24% (2 outliers), 2% (3+ outliers), 2% (Not modelled)
1	G	4968	7% (Poor fit), 42% (0 outliers), 28% (1 outlier), 23% (2 outliers), 2% (3+ outliers), 2% (Not modelled)
2	B	149	55% (Poor fit), 58% (0 outliers), 30% (1 outlier), 11% (2+ outliers), 6% (Not modelled)
2	D	149	55% (Poor fit), 59% (0 outliers), 30% (1 outlier), 11% (2+ outliers), 6% (Not modelled)
2	F	149	55% (Poor fit), 61% (0 outliers), 28% (1 outlier), 11% (2+ outliers), 6% (Not modelled)
2	H	149	55% (Poor fit), 59% (0 outliers), 30% (1 outlier), 11% (2+ outliers), 6% (Not modelled)

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 111080 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3509	26722	17028	4575	4961	158	0	0
1	C	3509	26722	17028	4575	4961	158	0	0
1	E	3509	26722	17028	4575	4961	158	0	0
1	G	3509	26722	17028	4575	4961	158	0	0

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	132	1042	643	169	221	9	0	0
2	D	132	1042	643	169	221	9	0	0
2	F	132	1042	643	169	221	9	0	0
2	H	132	1042	643	169	221	9	0	0

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

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

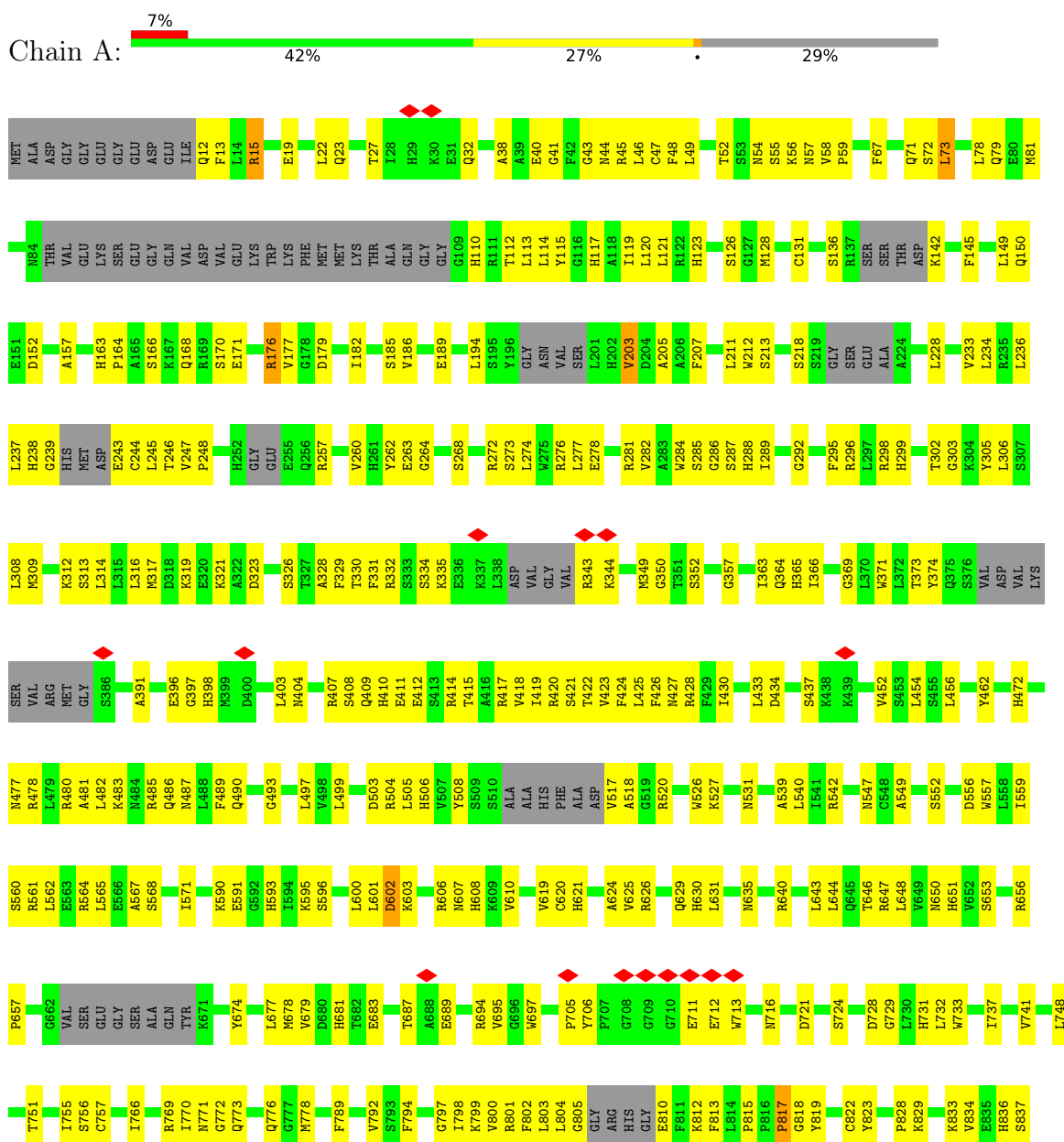
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Ca 1	0
4	B	4	Total 4	Ca 4	0
4	C	1	Total 1	Ca 1	0
4	D	4	Total 4	Ca 4	0
4	E	1	Total 1	Ca 1	0
4	F	4	Total 4	Ca 4	0
4	G	1	Total 1	Ca 1	0
4	H	4	Total 4	Ca 4	0

### 3 Residue-property plots i

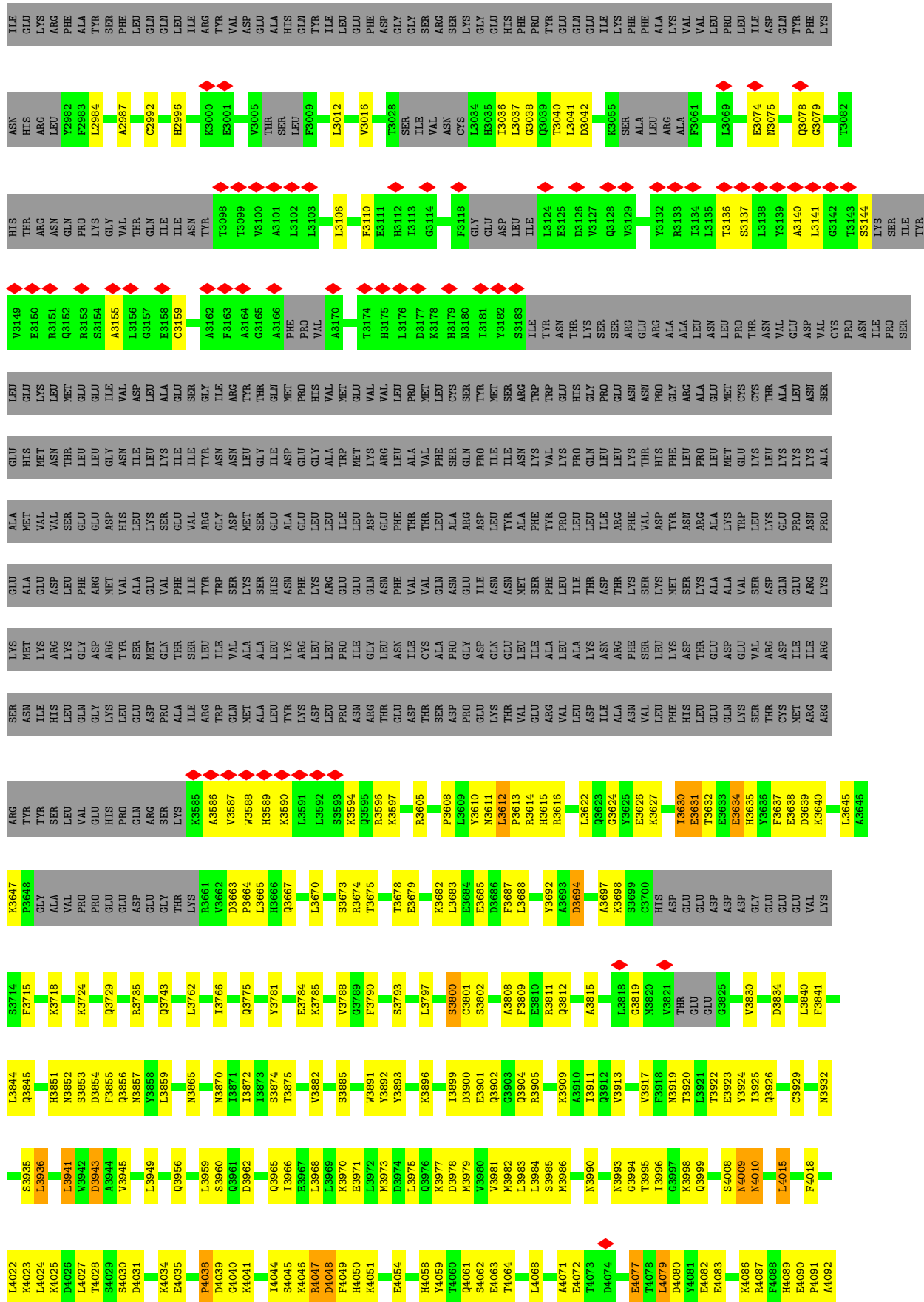
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: RyR2



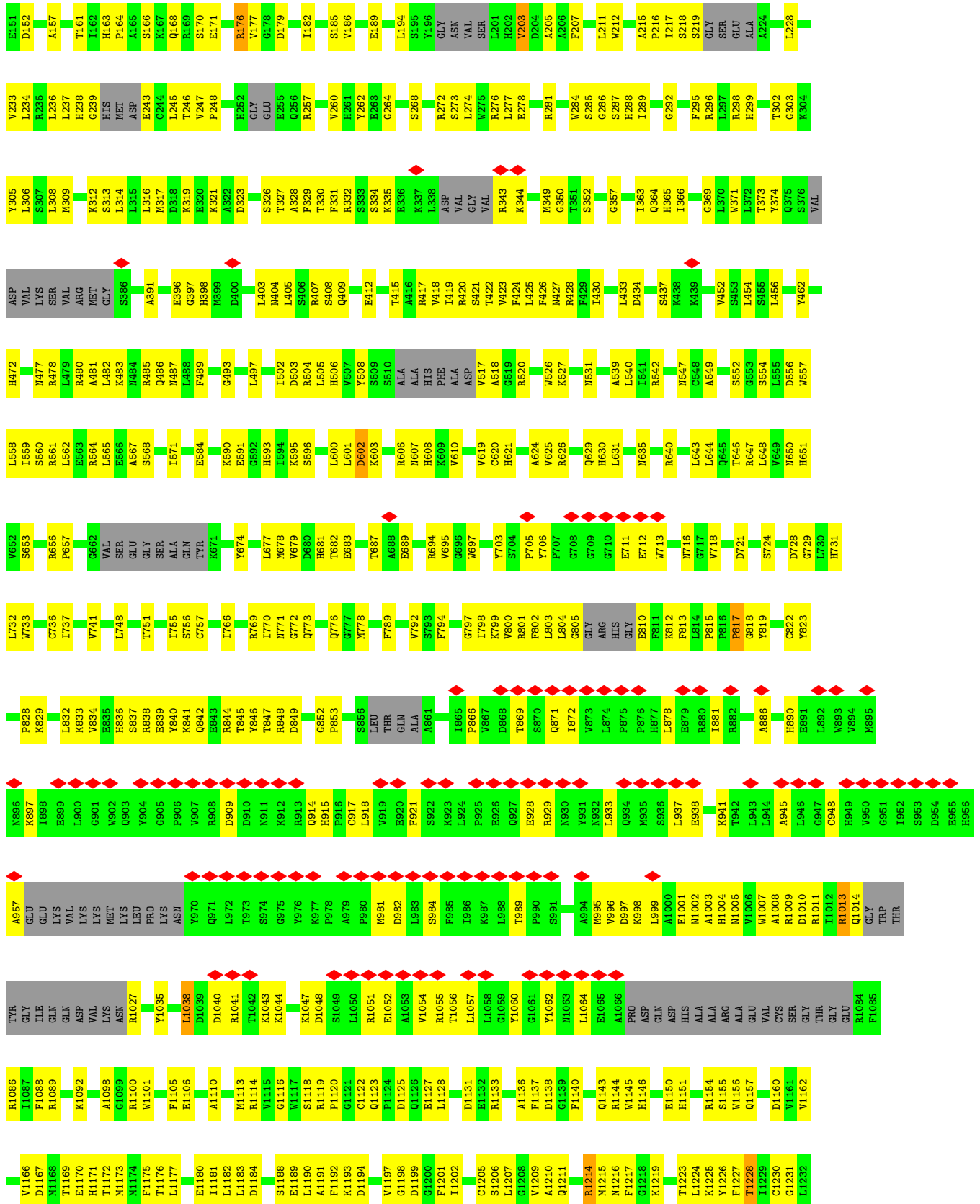
L1658	R1659	F1590	G1516	G1444	W1250	E1180	F1105	Y1035	LYS	ASN	V907	R838
L1667	H1592	L1591	F1520	W1445	L1251	I1161	E1106	L1035	ALA	ASN	R908	E839
G1668	H1593	T1521	T1447	L1446	S1252	L1182	L1038	D1039	SER	Y970	R909	Y840
N1669	V1594	S1448	L1448	T1447	K1253	L1183	M1113	D1040	PHE	Q971	D910	K841
H1670	L1595	M1522	L1449	L1448	L1254	D1184	R1114	T1041	GLY	L972	N911	Q842
R1671	G1524	F1450	F1450	F1450	P1256	S1188	G1115	T1042	PRO	T973	K912	R844
S1672	K1525	H1451	H1451	H1451	Q1257	L1189	W1117	K1043	LYS	S974	R913	T845
D1673	L1452	Q1452	Q1452	Q1452	W1260	L1190	S1118	K1044	ASN	G975	H914	Y846
C1677	S1528	L1459	L1459	L1459	V1261	L1191	R1119	K1044	LEU	Y976	H915	T847
V1680	Y1530	ASP	ASP	ASP	E1269	K1193	P1120	K1047	PRO	K977	P916	R848
D1681	Y1531	ARG	ARG	ARG	R1272	D1194	C1122	D1048	TYR	P978	C917	D849
P1683	Q1532	VAL	VAL	VAL	T1273	G1197	Q1123	S1049	ASP	A979	L918	G852
Q1684	P1535	THR	THR	THR	I1273	G1198	P1124	L1050	ASP	P980	V919	P853
L1685	K1538	SER	SER	SER	D1274	D1199	D1125	R1051	ASP	M981	E920	S856
L1686	L1539	ALA	ALA	ALA	THR	G1200	Q1126	E1052	SER	D982	S922	LEU
Y1687	L1540	ARG	ARG	ARG	ILE	I1202	L1128	A1053	PHE	L983	R921	THR
A1688	F1541	THR	THR	THR	LEU	C1205	D1131	V1054	GLY	S984	K923	GLN
I1689	A1542	LEU	LEU	LEU	SER	E1206	E1132	R1055	SER	F985	L924	ALA
G1696	V1543	GLU	GLU	GLU	PRO	L1207	R1133	L1057	MET	T1056	P925	A861
R1697	F1544	ASP	ASP	ASP	CYS	G1208	L1145	L1061	LYS	K987	E926	I865
R1699	T1548	VAL	VAL	VAL	LEU	V1209	A1136	L1058	THR	L988	Q927	D868
A1700	S1549	ALA	ALA	ALA	LYS	A1210	F1137	G1059	ALA	T989	R928	T869
D1704	Q1554	ASP	ASP	ASP	LYS	Q1211	D1138	Y1060	HIS	P990	R929	S870
I1707	F1555	ASP	ASP	ASP	GLY	T1286	Q1143	G1062	ASP	S991	N930	I871
K1788	E1556	CYS	CYS	CYS	PRO	Q1287	R1144	M1063	HIS	A994	M932	Q870
A1789	LEU	TYR	TYR	TYR	ASP	M1216	W1145	L1064	VAL	V996	L933	I872
K1790	H1487	TYR	TYR	TYR	ASP	G1218	H1146	E1065	ALA	K995	Q934	V873
M1794	A1490	TYR	TYR	TYR	ARG	K1219	E1150	A1066	PRO	V997	Q935	L874
L1795	GLY	TYR	TYR	TYR	VAL	I1299	H1151	PR0	GLN	D997	M935	P875
T1716	GLU	LEU	LEU	LEU	VAL	M1300	R1154	ASP	ASP	K998	Q936	L876
R1717	GLN	GLN	GLN	GLN	LYS	F1301	S1156	GLN	ASP	L999	L937	P876
A1798	SER	THR	THR	THR	ASP	Y1302	W1156	HIS	HIS	A1000	E938	H877
V1799	MET	SER	MET	MET	LYS	L1304	Q1157	ASP	ASP	E1001	K941	L878
Q1800	LEU	SER	LEU	SER	GLU	F1227	A1158	ALA	ALA	N1002	T942	E879
E1801	PRO	PRO	PRO	PRO	ALA	T1228	A1158	ALA	ALA	A1003	L943	R880
G1802	SER	GLY	GLY	GLY	THR	I1229	G1159	ARG	ARG	H1004	L944	I881
S1803	GLN	GLN	GLN	GLN	P1307	C1230	D1160	ALA	ALA	N1005	A945	R882
E1724	G1569	Y1426	Y1427	Y1428	F1306	G1231	V1161	GLU	GLU	V1006	A945	A886
I1726	F1571	V1430	S1429	S1429	E1309	V1162	V1162	VAL	VAL	W1007	L946	H890
M1729	K1572	N1501	R1431	R1431	ALA	V1166	D1167	VAL	CYS	A1008	L946	H890
E1731	H1575	N1502	I1432	I1432	GLU	E1234	E1170	SER	SER	R1009	G947	G891
E1732	K1576	G1504	F1433	F1433	VAL	Y1236	M1168	THR	THR	D1010	C948	L892
K1733	V1579	T1507	GLY	GLY	PHE	E1237	T1169	GLY	GLY	I1012	H949	W893
K1734	P1580	G1508	GLN	GLN	ASP	P1238	H1171	GLU	GLU	R1013	V950	W894
S1735	R1585	C1509	PRO	PRO	LYS	F1239	H1172	F1085	THR	Q1014	G951	M895
L1821	L1586	V1511	ALA	ALA	ALA	V1241	M1173	R1086	ALA	THR	S953	N896
I1822	L1587	ASP	N1440	N1440	GLY	R1245	F1175	I1087	THR	GLY	E954	K897
K1823	W1588	ALA	W1441	W1441	ILE	T1248	L1176	R1088	LYS	T97	E955	I898
Y1826	Q1589	SER	V1443	V1443	PRO	T1248	L1177	R1089	GLN	ILE	H956	E999
					ARG			K1092	GLN	GLN	A957	L900
								A1098	ASP	ASP	GLU	G901
								G1099	VAL	VAL	GLU	W902
								W1101	LYS	LYS	VAL	Q903
									ASN	ASN	LYS	Y904
									LYS	LYS	LYS	G905
									ASN	ASN	MET	P906
									LYS	LYS	LEU	
									PRO	PRO	PRO	

K2858	L2859	E2860	L2861	E2862	S2863	K2864	G2865	G2866	G2867	M2868	H2869	P2870	L2871	L2872	V2873	P2874	P2875	D2876	T2877	L2878	L2879	A2880	K2881	E2882	K2883	A2884	K2885	D2886	K2887	K2888	K2889	Q2890	Q2891	D2892	L2893	L2894	K2895	F2896	L2897	L2898	L2899	N2900	G2901	Y2902	A2903	V2904	S2905	G2906	PHE	LYS	ASP	LEU	LEU	LEU	THR	PRO	SER		
L2738	A2739	N2740	G2741	N2742	I2743	Y2744	G2745	E2746	Y2747	Y2748	S2749	D2750	G2751	S2752	K2753	V2754	Q2755	P2756	M2757	L2758	K2759	P2760	Y2761	K2762	L2763	L2764	S2765	E2766	E2768	K2769	E2770	I2771	Y2772	R2773	W2774	P2775	I2776	K2777	E2778	S2779	L2780	K2781	T2782	M2783	L2784	A2785	W2786	W2788	R2789	I2790	E2791	R2792	T2793	E2795	G2796	D2797			
SER	MET	ALA	LEU	TYR	ASN	ARG	THR	ARG	ILE	GLN	THR	SER	GLN	VAL	VAL	ALA	H2819	H2820	G2821	Y2822	S2823	P2824	R2825	A2826	I2827	D2828	N2829	S2830	N2831	V2832	T2833	L2834	S2835	D2836	D2837	L2838	H2839	N2841	A2842	E2843	M2844	N2845	A2846	E2847	N2848	H2850	N2851	T2852	W2853	A2854	L2855	L2856	ASP	LEU	LEU	ASP	THR	PRO	SER
P2678	F2679	ASP	TYR	MET	GLU	SER	ASN	TVR	VAL	SER	MET	MET	GLU	GLN	LYS	THR	HIS	K2605	A2611	K2609	T2612	E2616	G2627	GLY	ASN	PHE	GLY	ALA	ALA	L2643	L2644	F2646	W2647	G2648	L2649	F2650	D2651	A2652	L2653	TYR	ARG	LEU	SER	K2558	G2559	L2562	T2563	Q2566	S2576										
ILE	CYS	GLY	GLN	LEU	L2582	L2583	V2597	K2601	HIS	ALA	LEU	SER	ALA	T2511	L2515	A2516	L2517	N2518	R2519	L2521	L2529	THR	ARG	ALA	ALA	PRO	L2535	H2541	H2542	A2543	S2544	L2545	L2546	D2547	L2550	H2551	T2552	V2553	TYR	ARG	LEU	SER	G2559	L2562	T2563	Q2566	S2576												
F2392	L2399	L2400	G2401	R2402	P2405	E2406	M2407	H2408	L2409	A2413	A2417	L2418	R2419	L2420	R2421	S2422	L2423	L2424	R2425	S2426	P2429	L2430	G2431	D2432	L2433	V2436	G2442	PRO	THR	ILE	ALA	LYS	ASP	GLY	ASN	VAL	VAL	GLU	PRO	ASP	GLY	VAL	F2461	G2462	D2464	R2475	V2476												
M2319	R2323	L2326	R2327	R2328	F2329	E2330	PHE	GLY	PRO	ALA	ARG	LEU	GLY	GLN	GLU	G2343	L2354	ALA	GLU	ASP	PRO	PRO	ARG	ASP	GLY	PRO	SER	THR	THR	ILE	LYS	THR	LYS	ASP	GLY	THR	THR	ILE	HIS	MET	G2386	H2387	L2389																
MET	ARG	GLY	SER	T2239	S2247	D2250	CYS	L2256	W2270	L2271	L2258	R2259	E2264	K2265	V2266	V2267	R2268	Y2269	L2270	A2271	L2275	GLN	SER	CYS	GLN	MET	LEU	VAL	PRO	SER	TYR	GLY	TYR	PRO	ASP	ILE	GLY	TRP	TRP	ASN	P2293	V2294	D2301	F2302	L2303	R2304	V2307	F2308	C2309	N2310	V2314	E2315	E2316	N2317	A2318				
Q2061	L2062	I2063	S2064	E2065	K2067	V2068	W2070	A2071	Q2072	V2075	I2076	P2079	E2080	L2081	V2082	R2083	F2086	W2087	L2088	L2089	Q2092	G2098	R2101	A2102	L2103	T2106	Y2107	V2114	T2117	N2118	N2119	L2120	L2124	G2125	S2129	V2133	ARG	MET	GLY	LYS	LYS	E2138	K2141	R2145															
ASN	MET	LEU	LEU	ASN	PHE	LYS	ASP	ASP	SER	P1990	R1991	P2079	E2080	L2081	V2082	R2083	F2086	W2087	L2088	L2089	Q2092	G2098	R2101	A2102	L2103	T2106	Y2107	V2114	T2117	N2118	N2119	L2120	L2124	G2125	S2129	V2133	ARG	MET	GLY	LYS	LYS	E2138	K2141	R2145															
LYS	GLU	G1893	P1900	F1834	K1904	H1836	L1905	M1907	L1914	V1919	R1920	I1923	I1926	S1930	D1931	D1932	F1933	V1934	A1935	K1936	L1937	Q1938	Q1941	R1942	F1943	R1944	Y1945	M1946	E1947	M1953	MET	LEU	SER	ALA	ALA	LYS	LYS	GLN	ALA	ALA	GLU	THR	PHE	GLU	GLU	SER	SER	PRO	GLY	GLY	GLN	GLU	PRO	ARG	ILE				
T1827	I1830	I1833	F1834	H1836	H1836	L1838	L1838	L1840	H1841	I1842	L1843	E1847	P1848	S1849	VAL	PHE	LYS	GLY	ALA	ALA	GLY	PRO	GLU	GLU	GLU	GLY	ASP	R1942	F1943	R1944	Y1945	M1946	E1947	M1953	MET	LEU	SER	ALA	ALA	LYS	LYS	GLN	ALA	ALA	GLU	THR	PHE	GLU	GLU	SER	SER	PRO	GLY	GLY	GLN	GLU	PRO	ARG	ILE





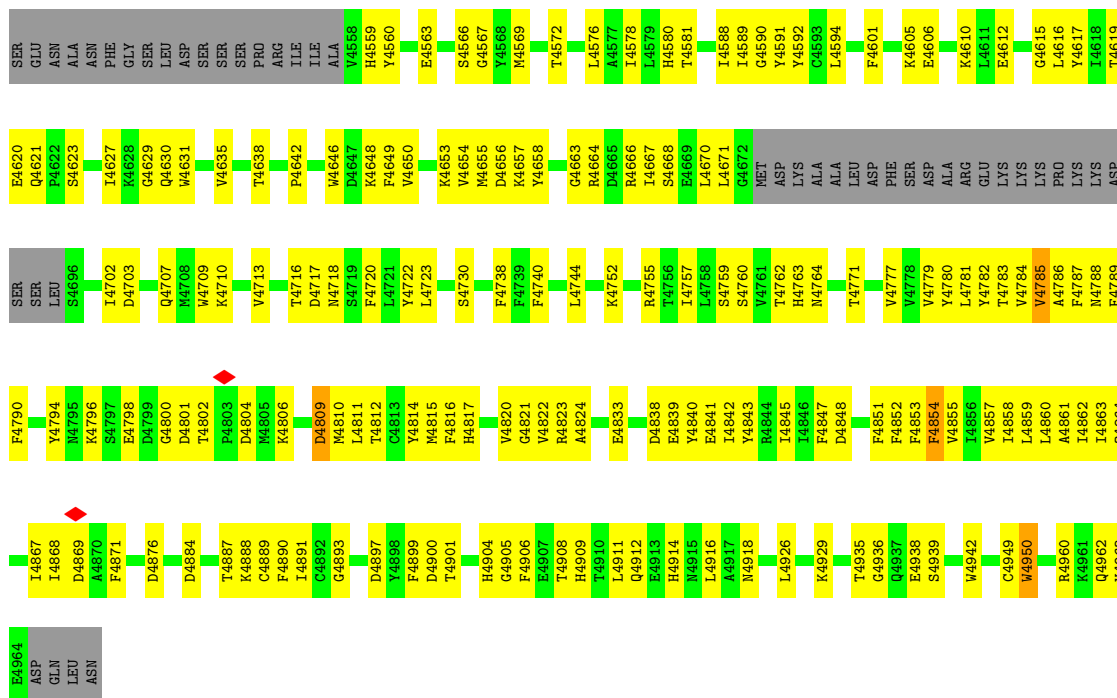




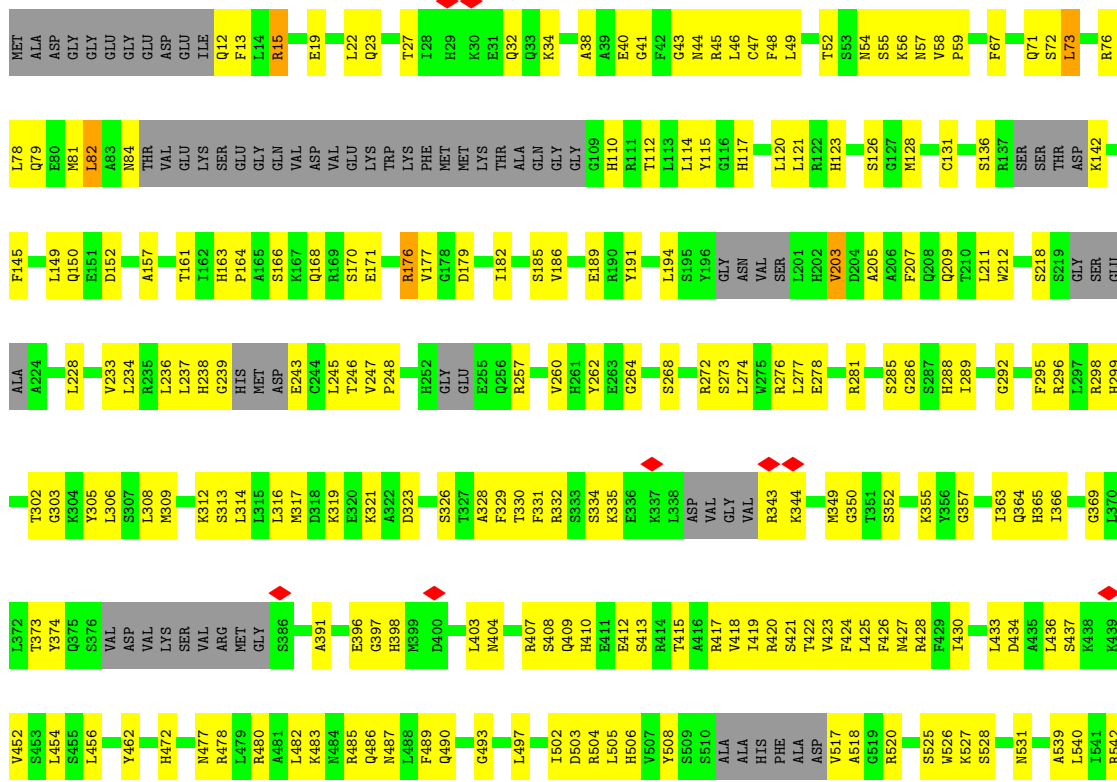
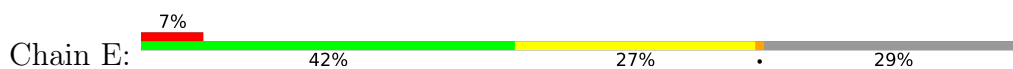


GLU	L2653	A2652	K2724	L2784	M2844	V2904	SER	V3129	ALA	GLY	GLN
GLY	L2653	L2653	Y2725	A2785	M2845	S2905	ALA	V3132	ALA	PRO	LEU
GLU	L2653	L2653	A2726	A2786	M2846	S2906	LYS	R3133	LEU	GLU	LEU
ASP	L2653	L2653	E2727	G2787	E2847	R2907	VAL	R3134	VAL	ASN	LEU
THR	L2653	L2653	H2728	R2788	N2848	PHE	LEU	L3135	PRO	PRO	THR
ALA	L2653	L2653	S2729	W2789	Y2849	LYS	LEU	T3136	LEU	THR	ALA
ILE	L2653	L2653	H2730	I2790	H2850	ASP	LEU	S3137	ILE	ASN	VAL
HIS	L2653	L2653	D2731	E2791	N2851	GLU	ASP	L3138	GLU	VAL	VAL
MET	L2653	L2653	K2732	R2792	I2852	LEU	THR	M3073	THR	ASP	GLU
G2386	L2653	L2653	W2733	T2793	I2853	ASP	PRO	E3074	PHE	CYS	VAL
N2387	L2653	L2653	S2734	R2794	A2854	THR	PRO	M3075	LYS	CYS	PRO
D2464	L2653	L2653	D2735	E2795	K2855	THR	ASP	Q3078	ALA	VAL	ASN
Y2476	L2653	L2653	M2736	G2796	K2856	GLU	GLU	G3079	ASN	PRO	ASN
Y2477	L2653	L2653	K2737	D2797	K2857	LEU	LEU	T3082	ARG	LEU	LEU
F2392	L2653	L2653	L2738	SER	K2858	ARG	ARG	F2983	LYS	SER	GLU
L2399	L2653	L2653	A2739	MET	L2859	PHE	ALA	L2984	HIS	THR	LYS
G2401	L2653	L2653	M2740	ALA	E2860	ALA	ALA	A2987	THR	ILE	LEU
R2402	L2653	L2653	G2741	TYR	L2861	TYR	TYR	C2982	ARG	THR	LEU
P2405	L2653	L2653	W2742	ASN	E2862	PHE	LEU	H2996	ASN	ASN	GLU
E2406	L2653	L2653	I2743	ARG	K2864	LEU	LEU	K3000	GLN	PRO	GLU
H2407	L2653	L2653	Y2744	THR	G2865	LEU	LEU	E3001	ILE	LYS	ILE
L2409	L2653	L2653	G2745	ARG	G2866	LEU	LEU	V3005	VAL	GLY	VAL
A2413	L2653	L2653	E2746	ARG	G2867	ILE	LEU	TRR	THR	VAL	THR
A2417	L2653	L2653	E2747	ARG	N2868	TYR	VAL	SER	THR	ILE	THR
I2418	L2653	L2653	Y2748	THR	H2869	VAL	VAL	LEU	ASP	ILE	THR
R2419	L2653	L2653	S2749	SER	P2870	GLU	GLU	F3009	ASN	ASN	ASN
I2420	L2653	L2653	D2750	GLN	L2871	ALA	ALA	L3012	SER	THR	THR
R2421	L2653	L2653	S2751	VAL	L2872	HIS	VAL	V3016	LEU	LEU	THR
S2422	L2653	L2653	S2752	VAL	V2873	GLN	GLN	I3020	LEU	PRO	THR
I2423	L2653	L2653	K2753	ASP	V2874	TYR	TYR	T3028	VAL	VAL	THR
I2424	L2653	L2653	V2754	ALA	P2874	TYR	ALA	SER	ILE	VAL	THR
R2425	L2653	L2653	Q2755	A2819	D2875	LEU	LEU	ILE	VAL	PRO	THR
S2426	L2653	L2653	P2756	H2820	G2876	LEU	LEU	VAL	ASN	PRO	THR
F2429	L2653	L2653	L2757	G2821	T2877	PHE	PHE	ASP	ASN	VAL	THR
L2430	L2653	L2653	M2758	Y2822	L2878	ASP	ASP	GLY	LYS	GLY	THR
G2431	L2653	L2653	K2759	S2823	T2878	GLY	GLY	GLY	GLY	GLY	THR
D2432	L2653	L2653	F2760	P2824	A2880	SER	SER	GLY	THR	THR	THR
L2433	L2653	L2653	Y2761	R2825	K2881	ARG	ARG	VAL	VAL	VAL	THR
V2436	L2653	L2653	K2762	A2826	E2882	LYS	LYS	CYS	CYS	CYS	THR
I2442	L2653	L2653	L2763	D2828	K2883	GLY	GLY	L3034	LEU	LEU	THR
MET	L2653	L2653	L2764	M2829	A2884	HIS	HIS	H3035	THR	THR	THR
PRO	L2653	L2653	S2765	S2830	K2885	PHE	PHE	I3036	THR	THR	THR
THR	L2653	L2653	E2766	N2831	D2886	PRO	PRO	L3037	THR	THR	THR
ILE	L2653	L2653	E2767	T2832	R2887	TYR	TYR	G3038	THR	THR	THR
ALA	L2653	L2653	K2768	V2833	R2888	GLU	GLU	T3040	THR	THR	THR
LYS	L2653	L2653	E2769	T2834	E2889	GLN	GLN	L3041	THR	THR	THR
ASP	L2653	L2653	K2770	S2835	K2889	ILE	ILE	D3042	THR	THR	THR
GLY	L2653	L2653	F2771	R2836	A2890	LYS	LYS	K3055	THR	THR	THR
ASN	L2653	L2653	L2772	L2837	Q2891	LEU	LEU		THR	THR	THR
VAL	L2653	L2653	E2773	L2838	D2892	LEU	LEU		THR	THR	THR
	L2653	L2653	F2721	H2839	I2893	LEU	LEU		THR	THR	THR
	L2653	L2653	I2722	A2840	K2894	LEU	LEU		THR	THR	THR
	L2653	L2653	N2723	E2841	P2896	LEU	LEU		THR	THR	THR
	L2653	L2653		A2842	L2897	LEU	LEU		THR	THR	THR
	L2653	L2653		E2843	Q2898	LEU	LEU		THR	THR	THR
	L2653	L2653		E2844	I2899	LEU	LEU		THR	THR	THR
	L2653	L2653			M2900	LEU	LEU		THR	THR	THR
	L2653	L2653			G2901	LEU	LEU		THR	THR	THR
	L2653	L2653			A2902	LEU	LEU		THR	THR	THR





• Molecule 1: RyR2





LYS	P2656	SER	K2566	GLU	R2304	H2218	G2125	GLN	LYS	D1808	M1722	F1571
L2667	G2559	ASP	V2307	L2219	V2308	L2219	Q2126	ALA	THR	T1813	M1723	K1572
P2668	F2461	THR	F2308	S2220	Y2221	S2221	S2129	GLU	GLY	F1816	E1724	H1575
S2671	C2462	ILE	M2310	L2222	C2462	L2222	V2133	LEU	PHE	F1817	I1726	K1576
A2672	M2319	HIS	N2319	V2298	MET	V2298	ARG	VAL	ARG	F1818	M1729	V1579
P2678	R2323	MET	V2314	GLY	G2366	GLY	GLY	GLU	SER	L1651	I1730	P1580
P2679	E2315	GLY	E2315	LEU	R2367	LEU	MET	SER	LYS	K1652	E1731	L1592
ASP	E2316	ALA	E2316	ALA	R2367	ALA	GLY	ASP	GLY	S1662	I1822	H1593
TYR	M2317	SER	M2317	SER	R2367	SER	LYS	LYS	ASN	V1594	E1732	V1594
MET	A2318	PRO	A2318	PRO	R2367	PRO	VAL	ASP	LYS	L1667	E1733	L1695
GLN	M2319	ALA	M2319	ALA	R2367	ALA	K2141	LYS	HIS	G1668	E1734	R1586
GLY	R2323	MET	R2323	MET	R2367	MET	R2145	PRO	ARG	L1657	S1735	Q1589
LEU	T2326	ARG	T2326	ARG	R2367	ARG	R2145	SER	ASN	L1658	D1741	F1590
THR	R2327	SER	R2327	SER	R2367	SER	G2148	GLY	GLU	R1659	D1741	L1591
GLY	R2328	GLY	R2328	GLY	R2367	GLY	G2148	LEU	LEU	S1662	L1748	H1592
ASP	R2329	ALA	R2329	ALA	R2367	ALA	N2152	ASN	ASN	L1667	L1748	V1594
THR	E2330	ALA	E2330	ALA	R2367	ALA	N2152	PHE	ASN	L1667	L1748	L1695
THR	CYS	ALA	CYS	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	W1596
THR	GLY	ALA	GLY	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	S1597
GLY	PRO	ALA	PRO	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	R1598
GLN	ALA	ALA	GLY	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	R1598
SER	ALA	ALA	GLY	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	P1600
SER	ALA	ALA	GLY	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	W1601
MET	ALA	ALA	GLY	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	Q1602
MET	ALA	ALA	GLY	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	L1603
ASP	L2511	ALA	L2511	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	L1604
SER	L2515	ALA	L2515	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	L1605
SER	A2516	ALA	A2516	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	L1606
GLY	L2517	ALA	L2517	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	V1606
GLY	N2518	ALA	N2518	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	D1607
N2701	R2519	ALA	R2519	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	R1610
F2702	Y2520	ALA	Y2520	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	S1612
N2703	L2521	ALA	L2521	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	E1613
Q2705	L2529	ALA	L2529	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	R1614
P2706	H2541	ALA	H2541	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	W1617
V2707	H2542	ALA	H2542	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	L1618
D2708	A2543	ALA	A2543	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	Q1620
T2709	S2544	ALA	S2544	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	F1627
S2710	L2545	ALA	L2545	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	M1628
N2711	I2546	ALA	I2546	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	S1629
I2712	D2547	ALA	D2547	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	L1630
T2713	L2550	ALA	L2550	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	H1631
I2714	H2551	ALA	H2551	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	I1632
P2715	E2552	ALA	E2552	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	E1635
E2716	V2553	ALA	V2553	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	A1715
K2717	TYR	ALA	TYR	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	A1717
L2718	LEU	ALA	LEU	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	R1718
E2719	LEU	ALA	LEU	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	S1638
Y2720	LEU	ALA	LEU	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	M1720
F2721	LEU	ALA	LEU	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	M1721
I2722	LEU	ALA	LEU	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	I1641
N2723	LEU	ALA	LEU	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	
K2724	LEU	ALA	LEU	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	
Y2725	LEU	ALA	LEU	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	
A2726	LEU	ALA	LEU	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	
E2727	LEU	ALA	LEU	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	
H2728	LEU	ALA	LEU	ALA	R2367	ALA	N2152	ASP	ASN	G1668	L1748	

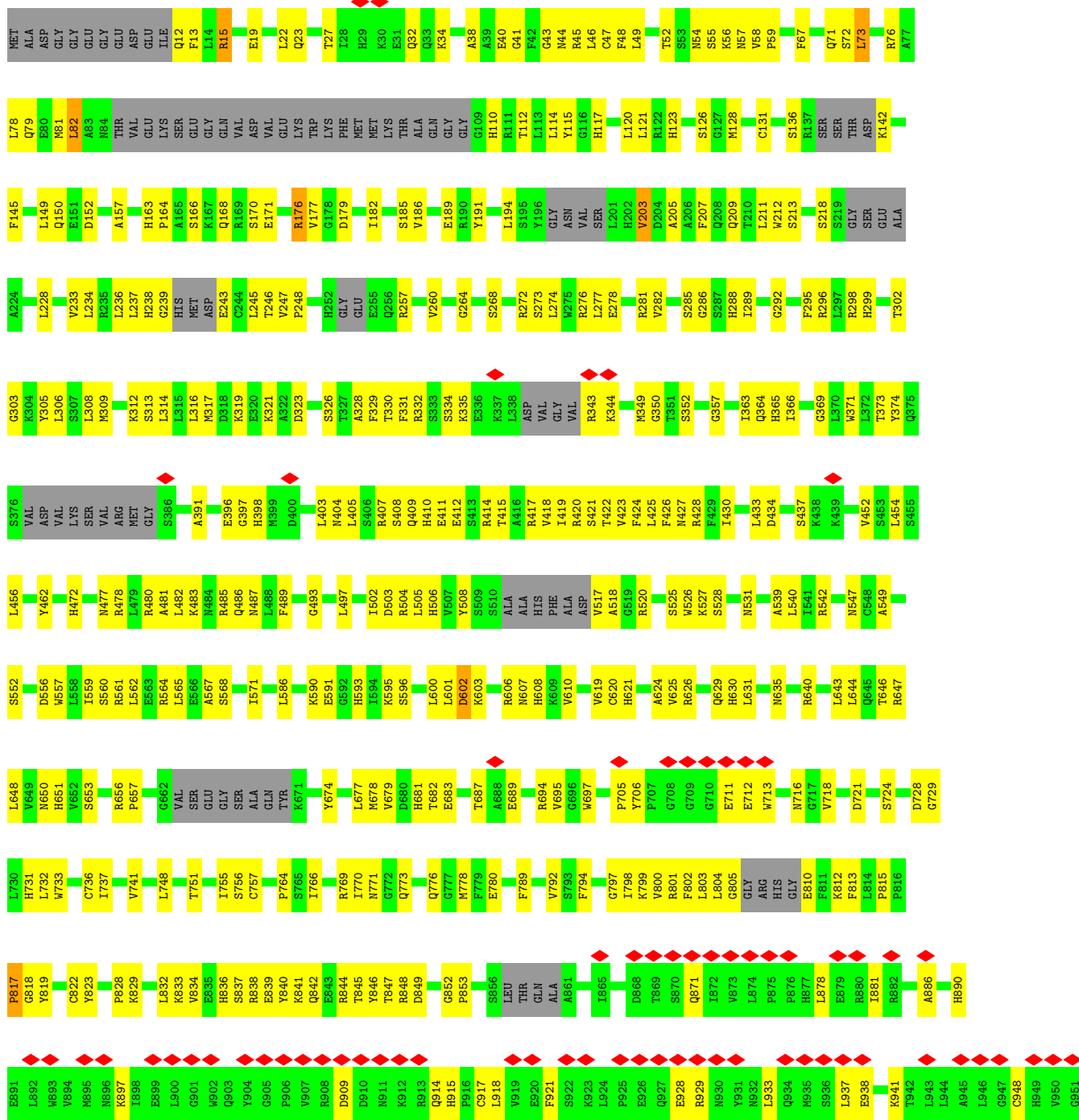






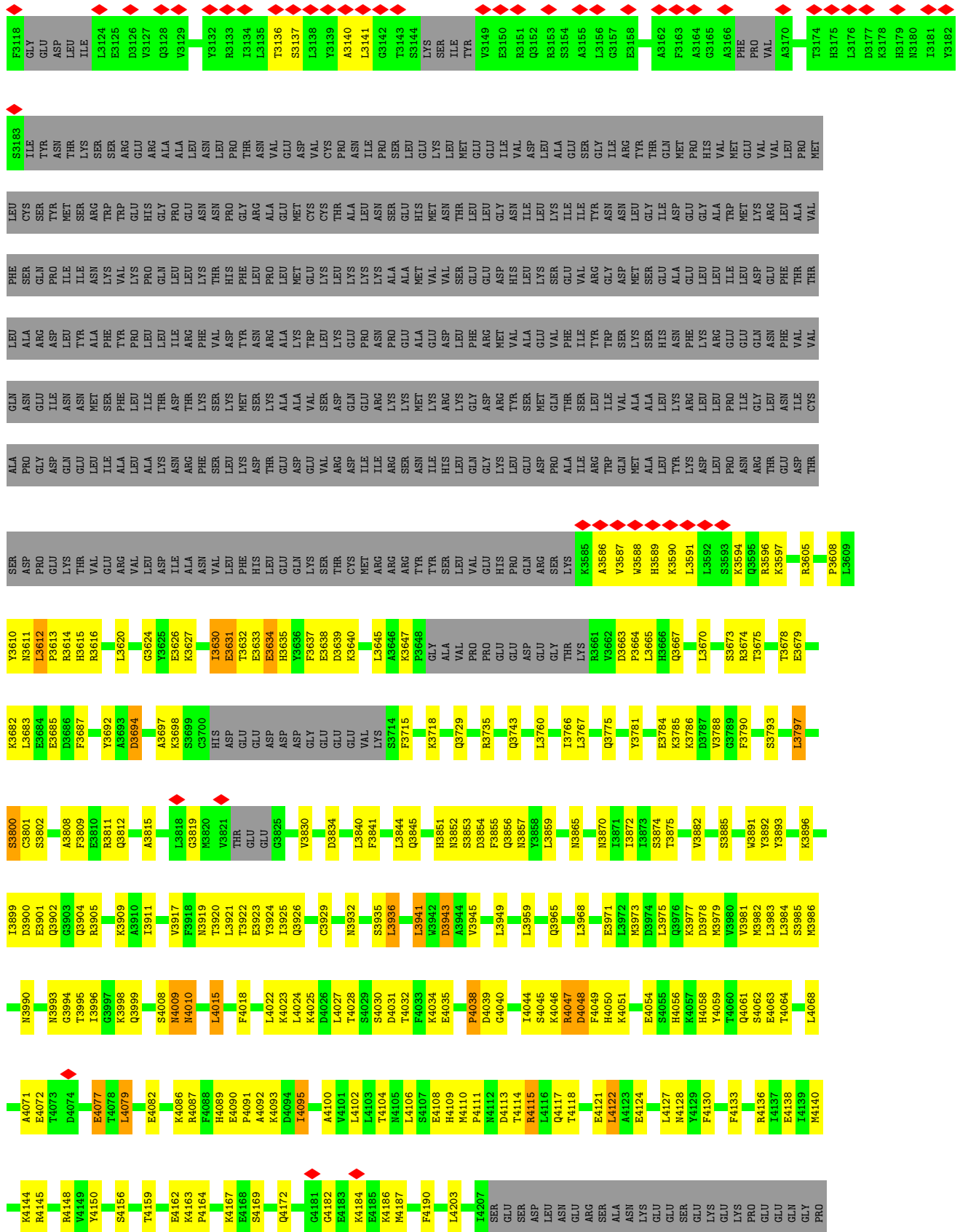


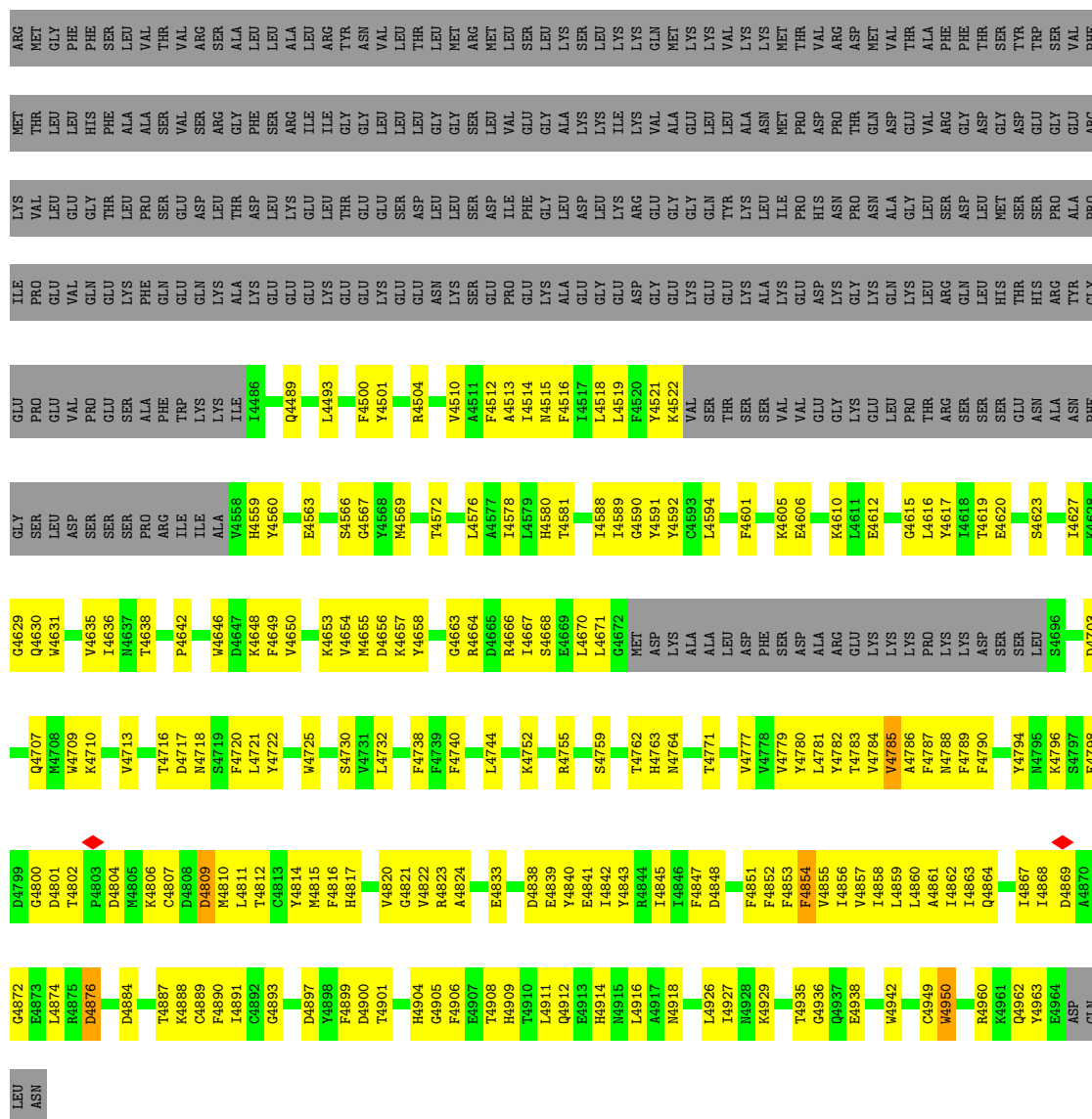
• Molecule 1: RyR2



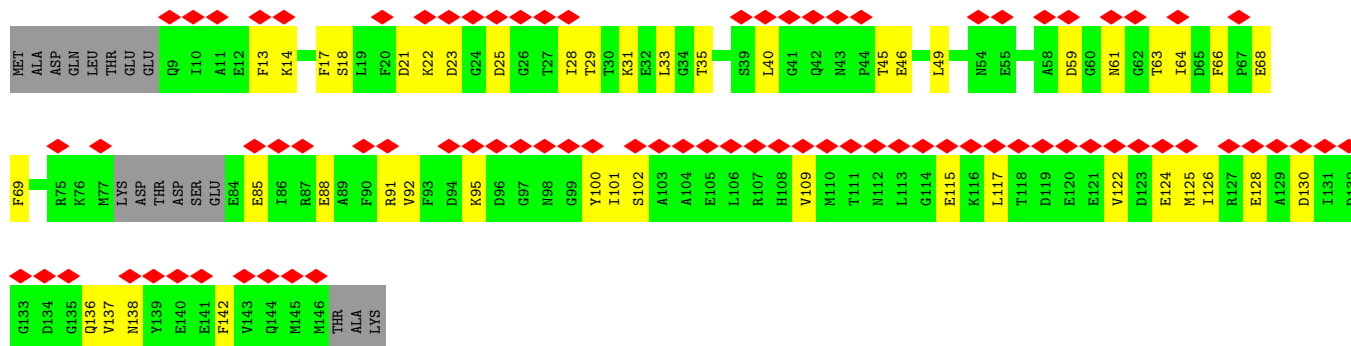




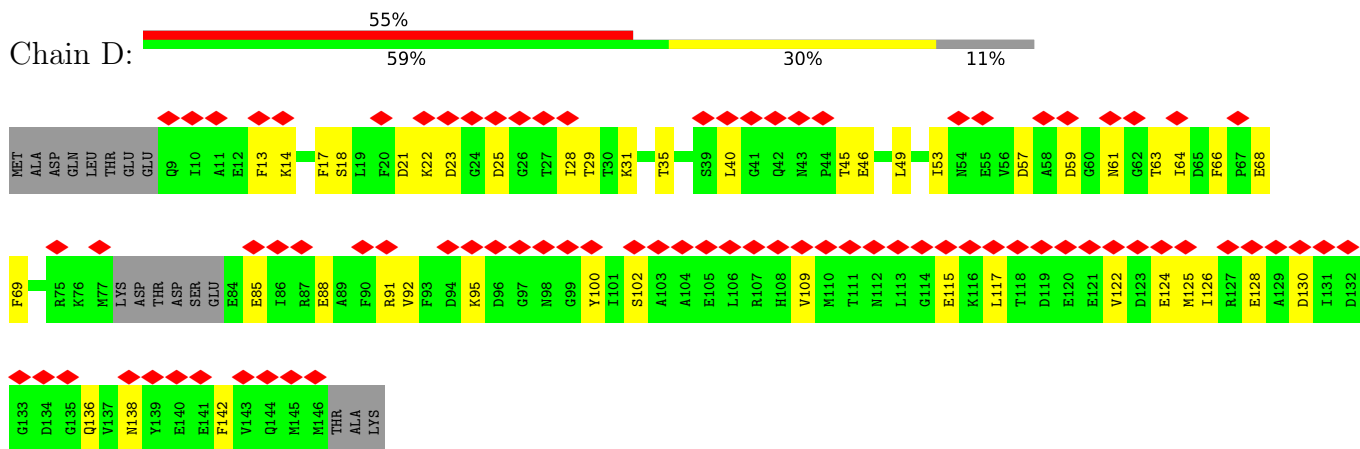




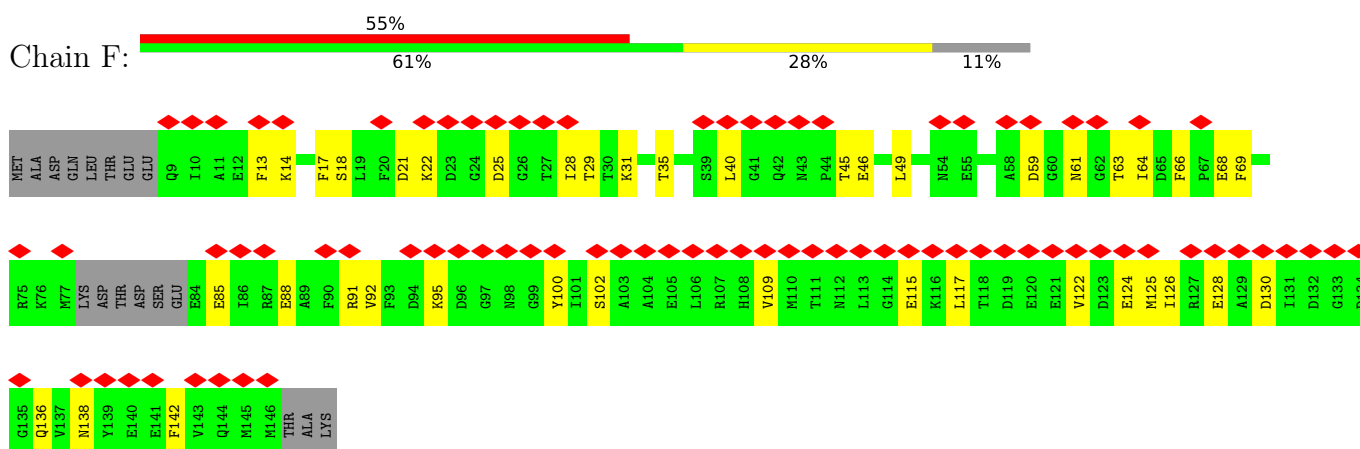
● Molecule 2: Calmodulin-1



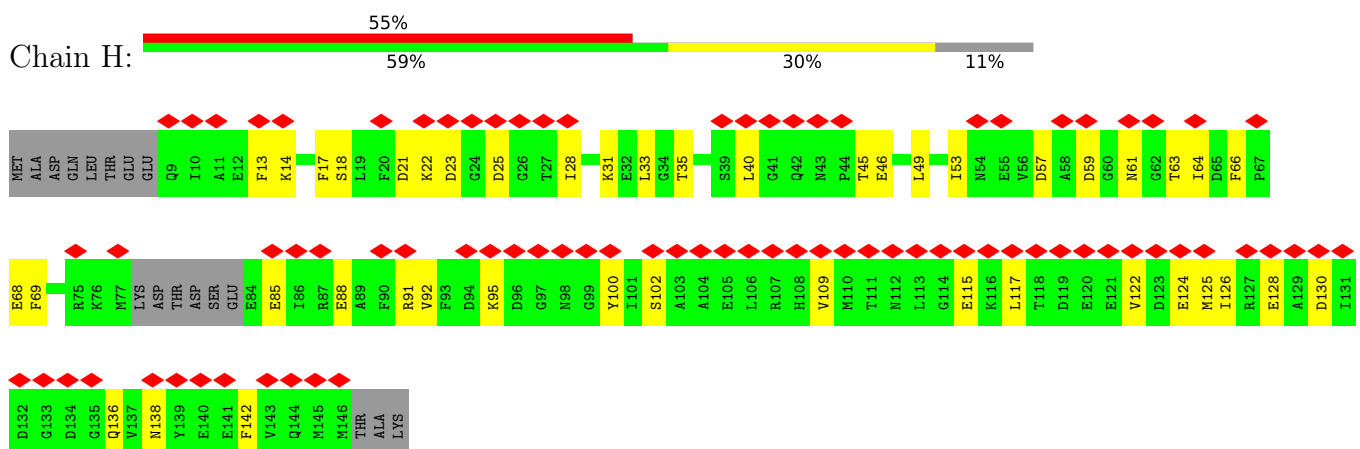
● Molecule 2: Calmodulin-1



• Molecule 2: Calmodulin-1



• Molecule 2: Calmodulin-1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	22876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size ( $\text{\AA}$ )	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.091, 1.091, 1.091	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.56	2/27223 (0.0%)	0.69	7/36827 (0.0%)
1	C	0.56	2/27223 (0.0%)	0.69	8/36827 (0.0%)
1	E	0.56	2/27223 (0.0%)	0.69	8/36827 (0.0%)
1	G	0.56	2/27223 (0.0%)	0.69	7/36827 (0.0%)
2	B	0.33	0/1053	0.52	0/1411
2	D	0.33	0/1053	0.52	0/1411
2	F	0.33	0/1053	0.52	0/1411
2	H	0.33	0/1053	0.52	0/1411
All	All	0.56	8/113104 (0.0%)	0.69	30/152952 (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	33
1	C	0	33
1	E	0	33
1	G	0	33
All	All	0	132

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4950	TRP	CB-CG	-5.59	1.40	1.50
1	C	4950	TRP	CB-CG	-5.59	1.40	1.50
1	E	4950	TRP	CB-CG	-5.59	1.40	1.50
1	G	4950	TRP	CB-CG	-5.59	1.40	1.50
1	A	4942	TRP	CB-CG	-5.18	1.41	1.50

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4519	LEU	CB-CA-C	-9.78	91.61	110.20
1	A	3797	LEU	CA-CB-CG	-6.82	99.61	115.30
1	C	3797	LEU	CA-CB-CG	-6.82	99.61	115.30
1	E	3797	LEU	CA-CB-CG	-6.82	99.61	115.30
1	G	3797	LEU	CA-CB-CG	-6.82	99.61	115.30

There are no chirality outliers.

5 of 132 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	729	GLY	Peptide
1	A	817	PRO	Peptide
1	A	818	GLY	Peptide
1	A	819	TYR	Peptide
1	A	829	LYS	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	26722	0	25168	1034	0
1	C	26722	0	25168	1062	0
1	E	26722	0	25168	1051	0
1	G	26722	0	25168	1057	0
2	B	1042	0	979	31	0
2	D	1042	0	979	31	0
2	F	1042	0	979	31	0
2	H	1042	0	979	33	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
4	A	1	0	0	0	0
4	B	4	0	0	0	0
4	C	1	0	0	0	0
4	D	4	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	F	4	0	0	0	0
4	G	1	0	0	0	0
4	H	4	0	0	0	0
All	All	111080	0	104588	4092	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 4092 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:4811:LEU:CD2	1:G:4519:LEU:HD13	1.75	1.15
1:A:4860:LEU:HD13	1:C:4863:ILE:HD12	1.29	1.11
1:A:4863:ILE:HD12	1:G:4860:LEU:HD13	1.29	1.11
1:E:4860:LEU:HD13	1:G:4863:ILE:HD12	1.29	1.10
1:C:4860:LEU:HD13	1:E:4863:ILE:HD12	1.29	1.09

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	3387/4968 (68%)	2919 (86%)	459 (14%)	9 (0%)	41	76
1	C	3387/4968 (68%)	2917 (86%)	460 (14%)	10 (0%)	41	76
1	E	3387/4968 (68%)	2921 (86%)	457 (14%)	9 (0%)	41	76
1	G	3387/4968 (68%)	2920 (86%)	458 (14%)	9 (0%)	41	76
2	B	128/149 (86%)	120 (94%)	8 (6%)	0	100	100
2	D	128/149 (86%)	120 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	128/149 (86%)	120 (94%)	8 (6%)	0	100	100
2	H	128/149 (86%)	120 (94%)	8 (6%)	0	100	100
All	All	14060/20468 (69%)	12157 (86%)	1866 (13%)	37 (0%)	44	76

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	4521	TYR
1	A	853	PRO
1	A	1580	PRO
1	A	2309	CYS
1	C	853	PRO

### 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	2675/4355 (61%)	2627 (98%)	48 (2%)	59	77
1	C	2675/4355 (61%)	2627 (98%)	48 (2%)	59	77
1	E	2676/4355 (61%)	2626 (98%)	50 (2%)	57	75
1	G	2675/4355 (61%)	2626 (98%)	49 (2%)	59	77
2	B	112/127 (88%)	112 (100%)	0	100	100
2	D	112/127 (88%)	112 (100%)	0	100	100
2	F	112/127 (88%)	112 (100%)	0	100	100
2	H	112/127 (88%)	112 (100%)	0	100	100
All	All	11149/17928 (62%)	10954 (98%)	195 (2%)	62	78

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1601	ASN
1	E	4809	ASP

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	2198	CYS
1	E	3943	ASP
1	G	81	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 202 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1265	HIS
1	E	3993	ASN
1	G	4643	ASN
1	E	1602	GLN
1	E	2442	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 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.

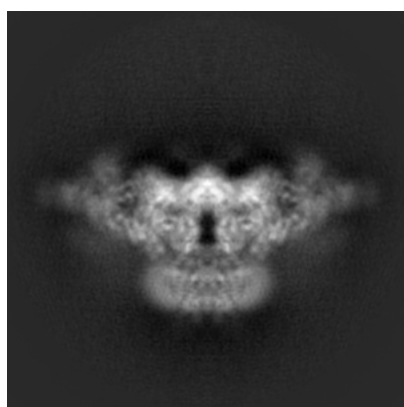
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9889. These allow visual inspection of the internal detail of the map and identification of artifacts.

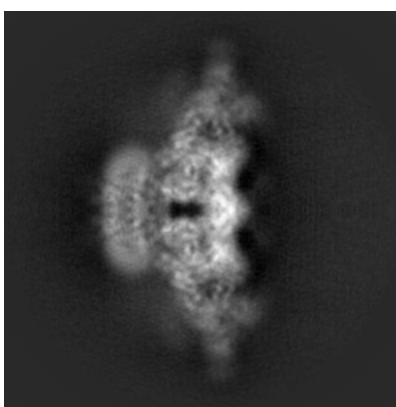
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

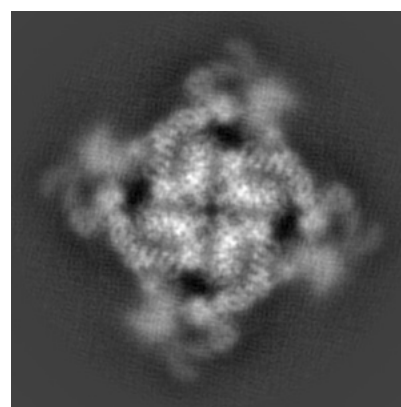
#### 6.1.1 Primary map



X



Y

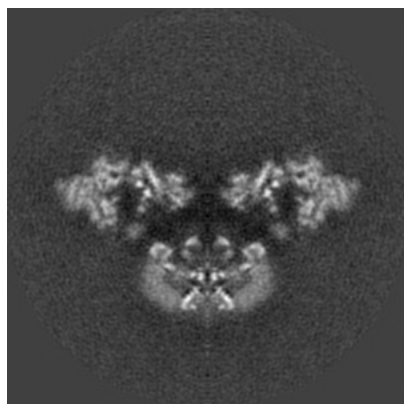


Z

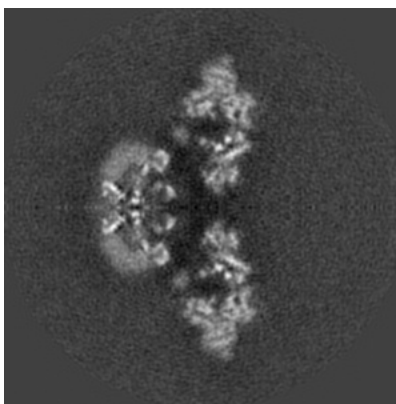
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

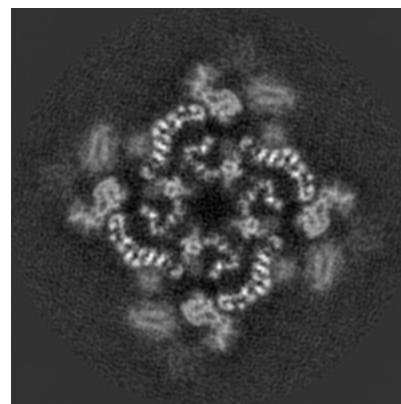
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



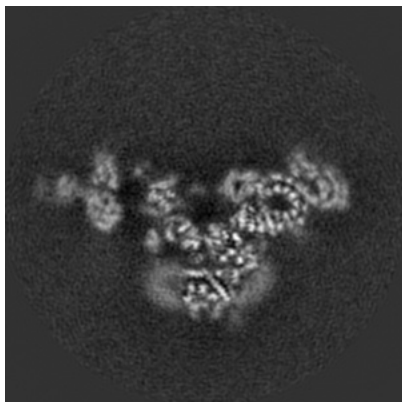
Z Index: 200



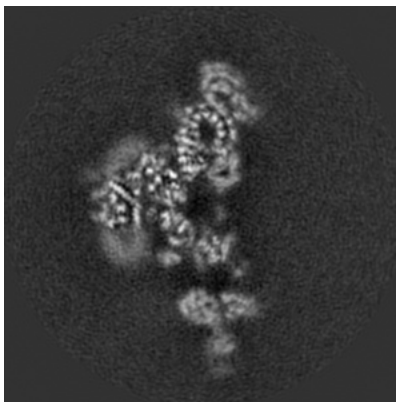
The images above show central slices of the map in three orthogonal directions.

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

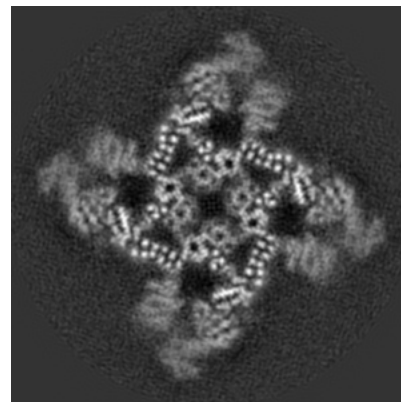
### 6.3.1 Primary map



X Index: 187



Y Index: 213

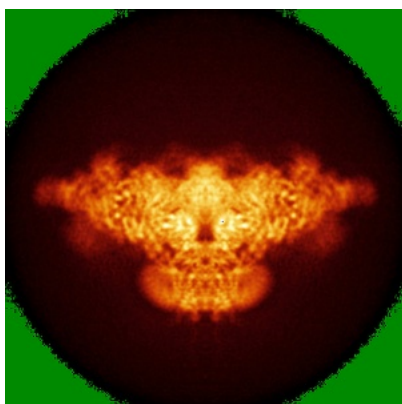


Z Index: 211

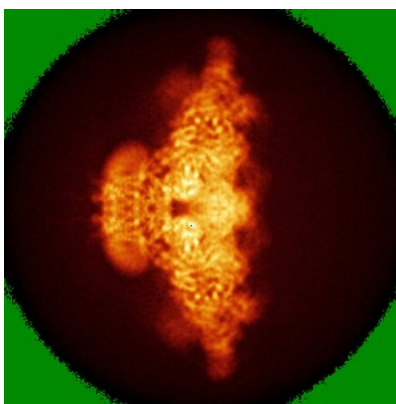
The images above show the largest variance slices of the map in three orthogonal directions.

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

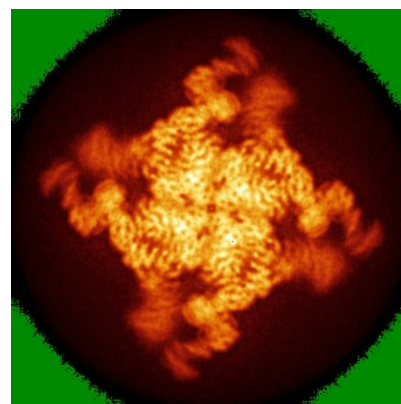
### 6.4.1 Primary map



X



Y

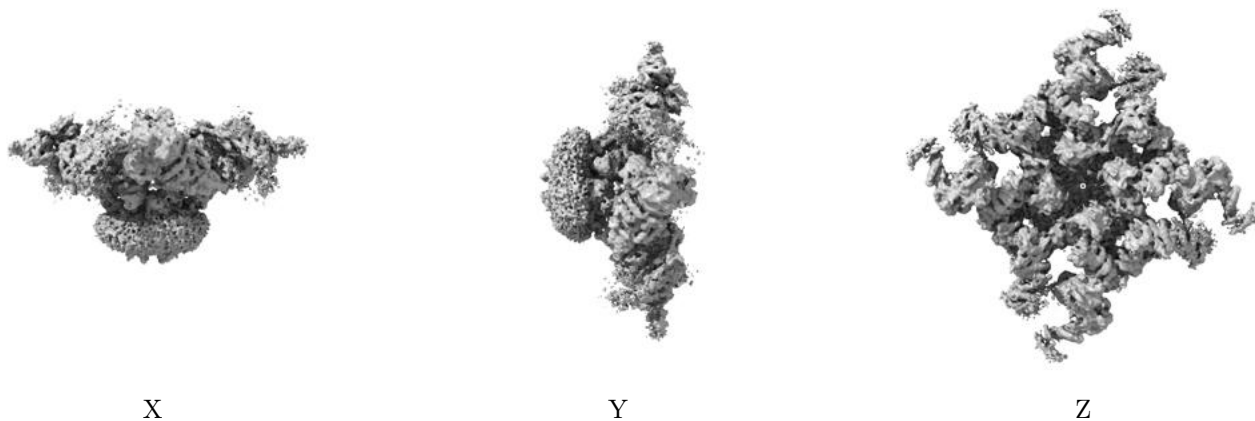


Z

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 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

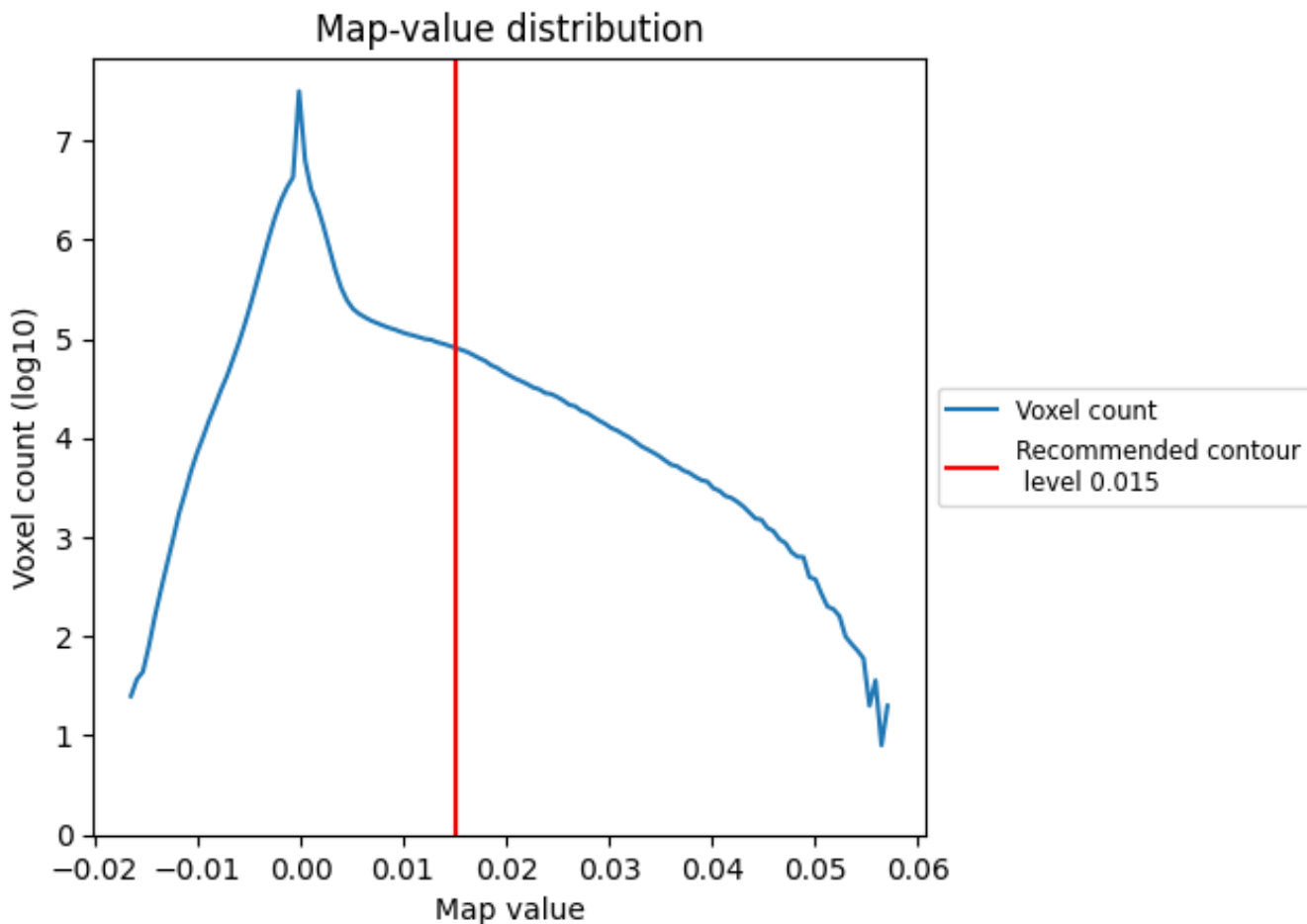
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

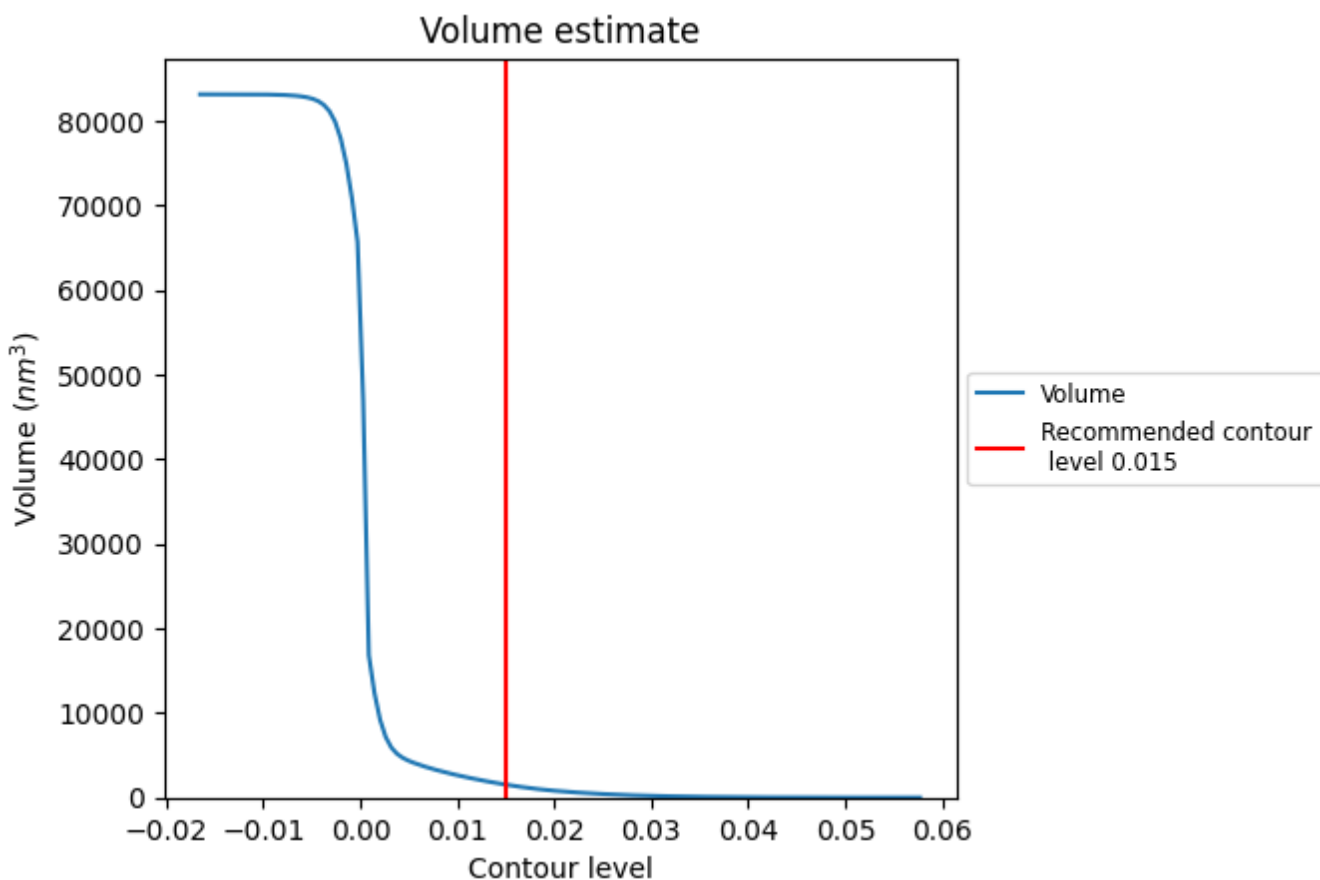
This section contains the results of statistical analysis of the map.

### 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.

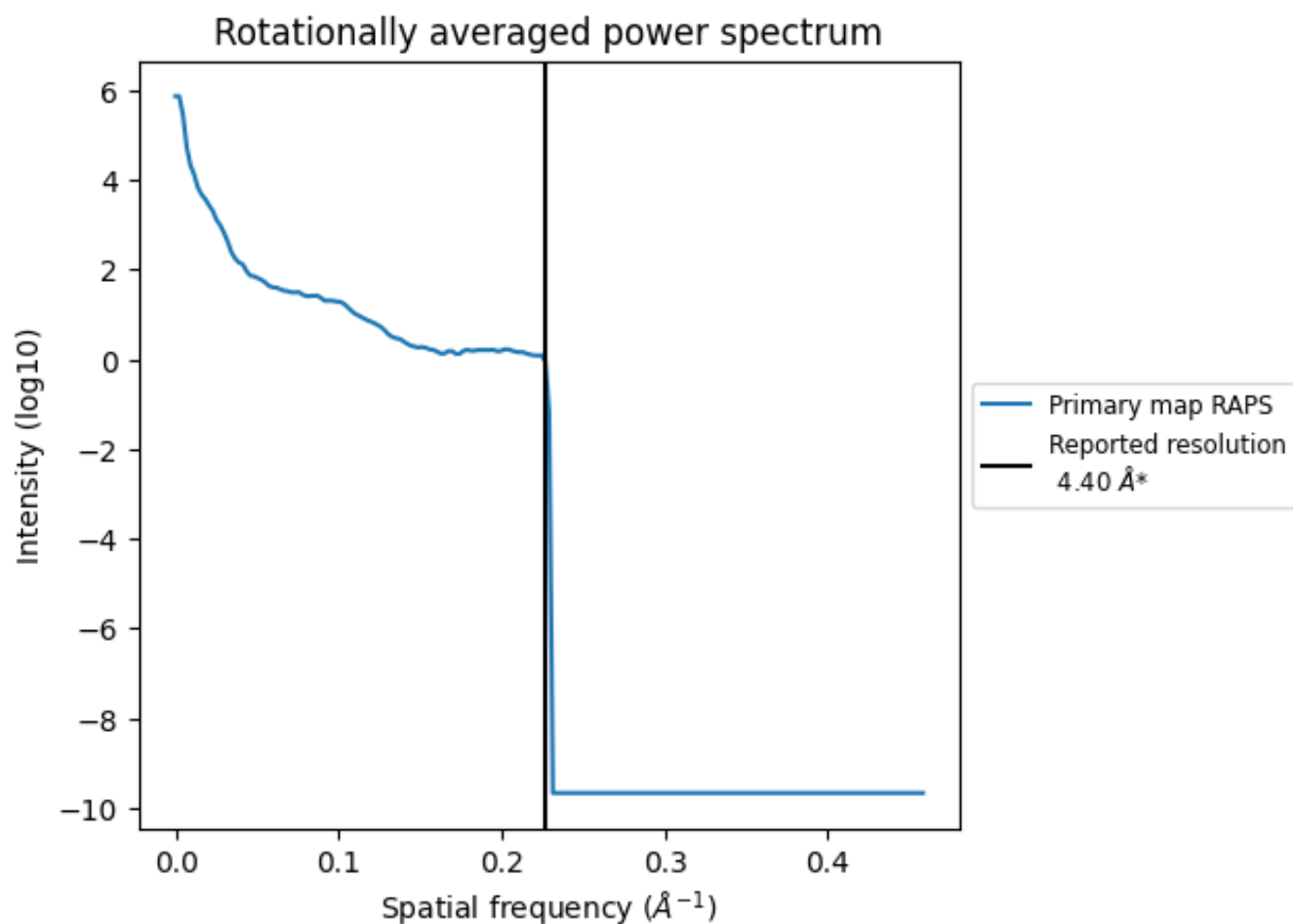
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1535 nm<sup>3</sup>; this corresponds to an approximate mass of 1386 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i

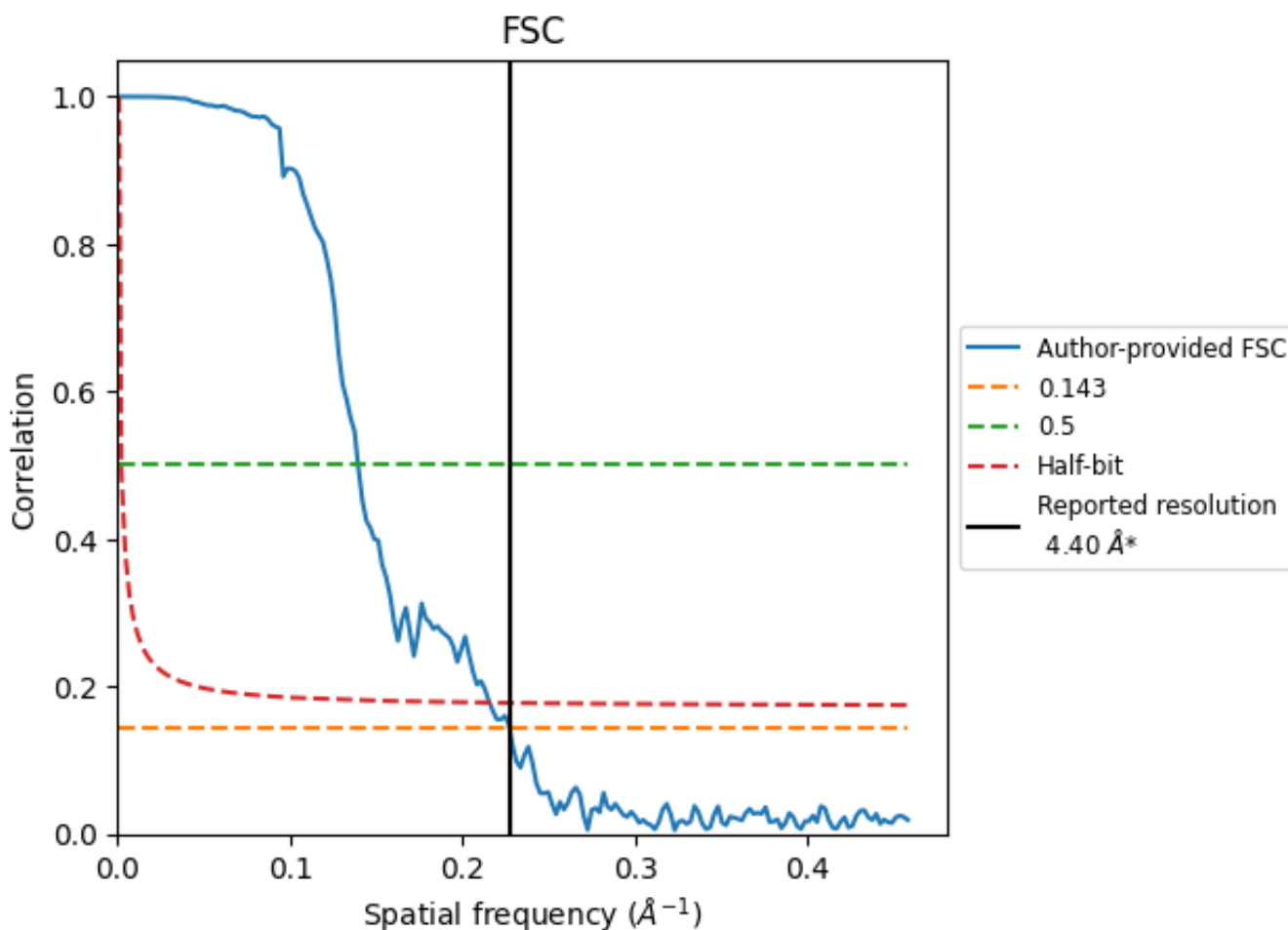


\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

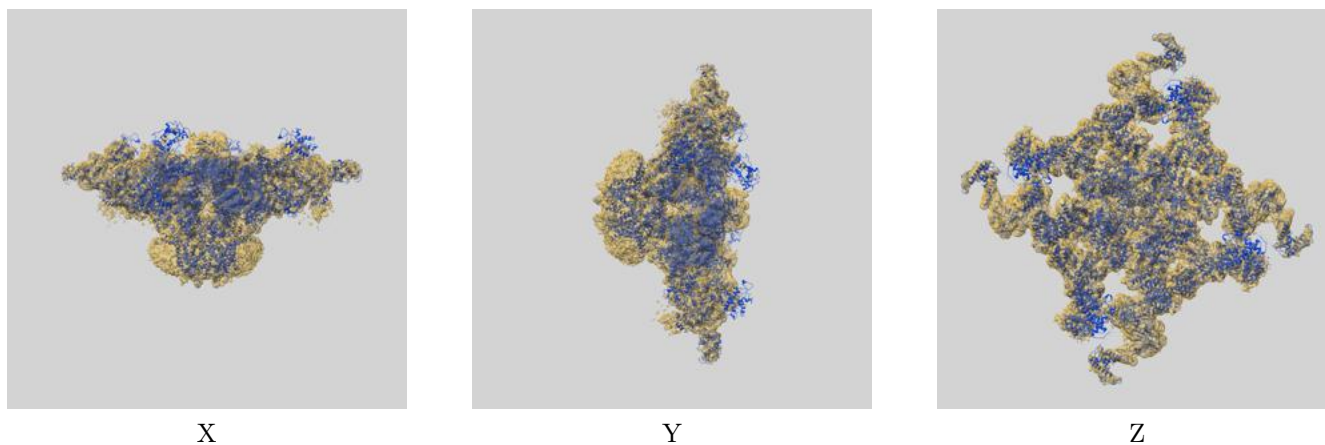
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.40	7.17	4.64
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

This section contains information regarding the fit between EMDB map EMD-9889 and PDB model 6JV2. Per-residue inclusion information can be found in section 3 on page 5.

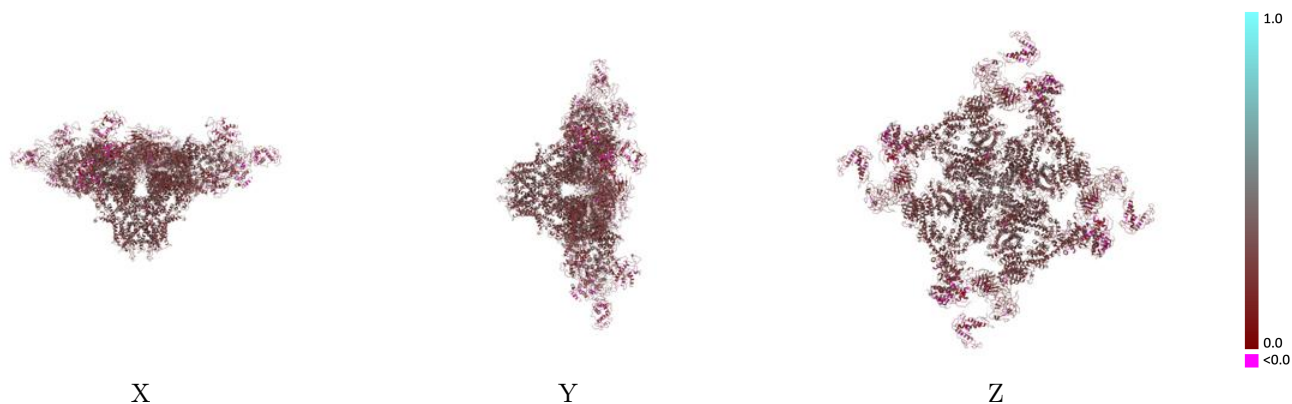
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

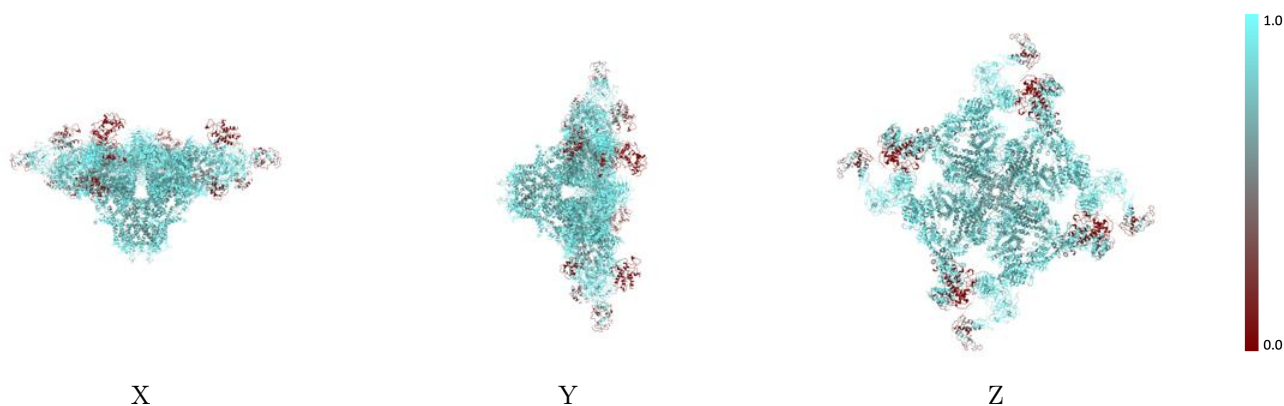


## 9.2 Q-score mapped to coordinate model [i](#)



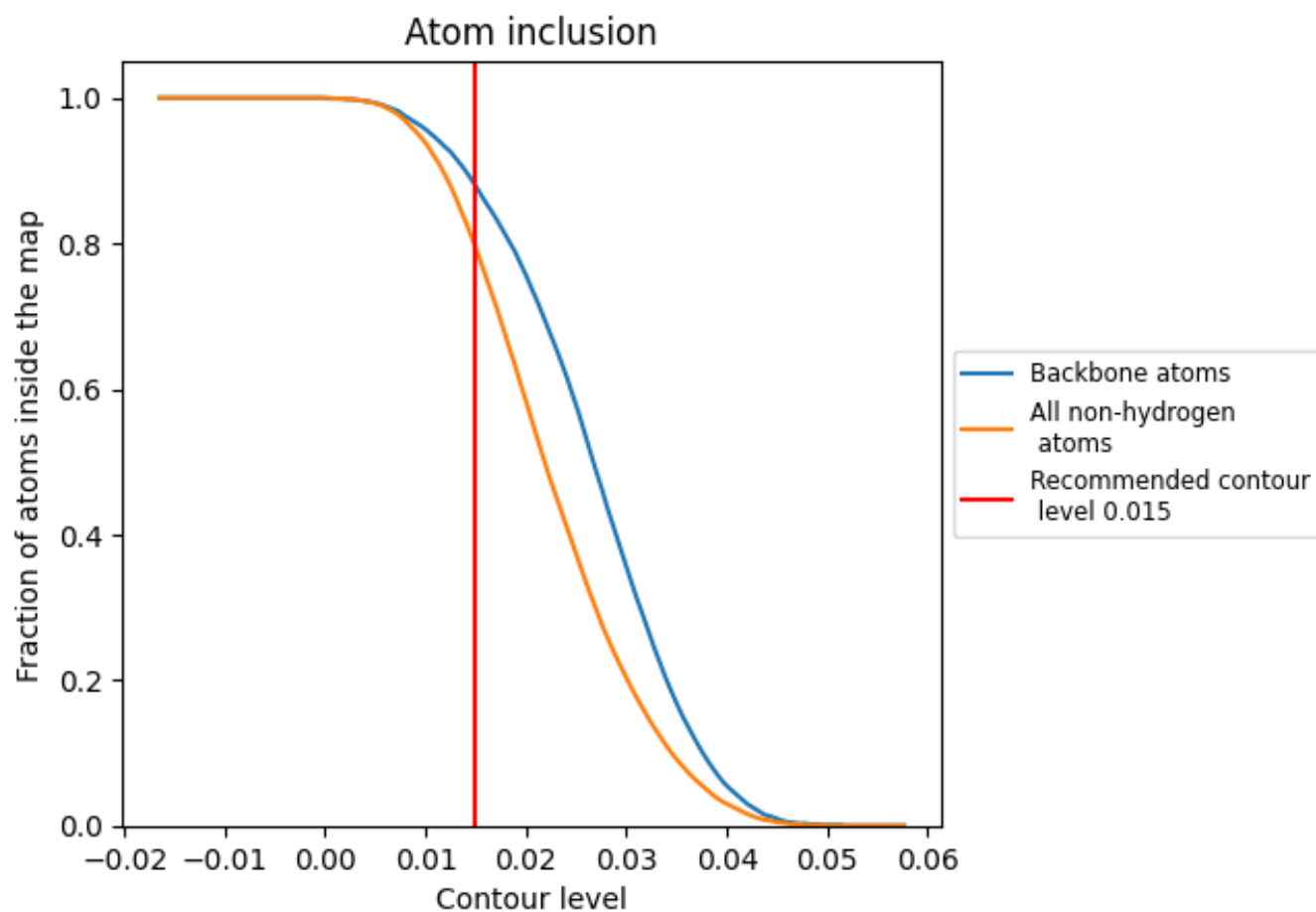
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 79% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7940	 0.2670
A	 0.8120	 0.2680
B	 0.3300	 0.2230
C	 0.8130	 0.2690
D	 0.3290	 0.2250
E	 0.8130	 0.2680
F	 0.3300	 0.2220
G	 0.8120	 0.2680
H	 0.3290	 0.2210

