



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 02:26 PM EDT

PDB ID : 5TB3
EMDB ID : EMD-8394
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-11
Resolution : 4.70 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

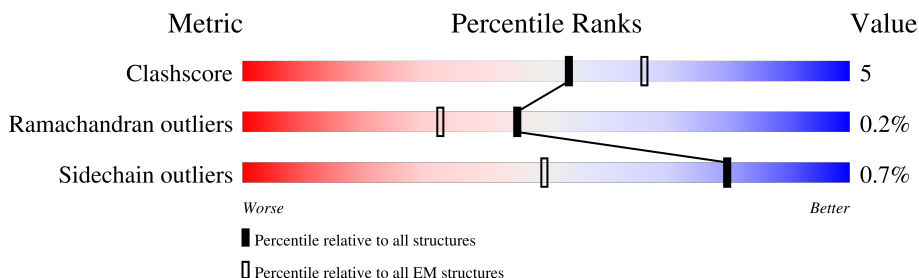
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	108	<div> <div>80%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	F	108	<div> <div>80%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	H	108	<div> <div>80%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	J	108	<div> <div>80%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
2	B	4416	<div> <div>66%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
2	E	4416	<div> <div>67%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
2	G	4416	<div> <div>66%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
2	I	4416	<div> <div>67%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121312 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	E	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	I	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	G	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		

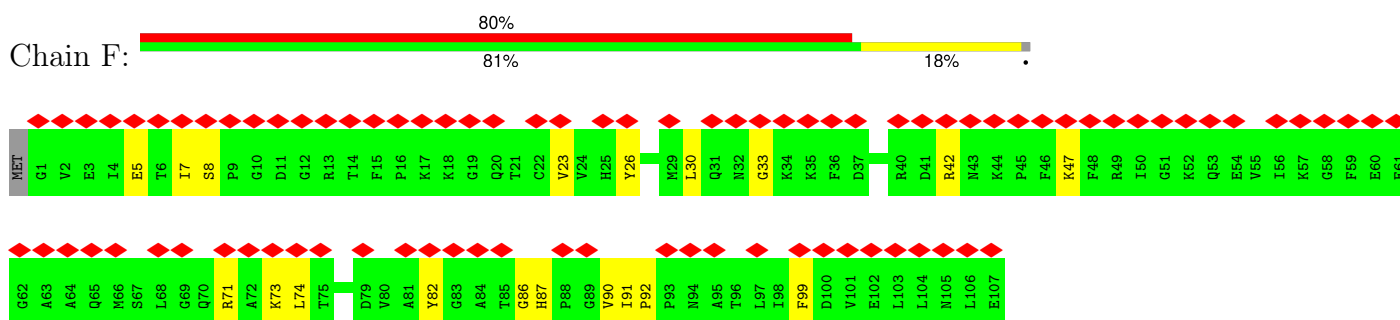
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

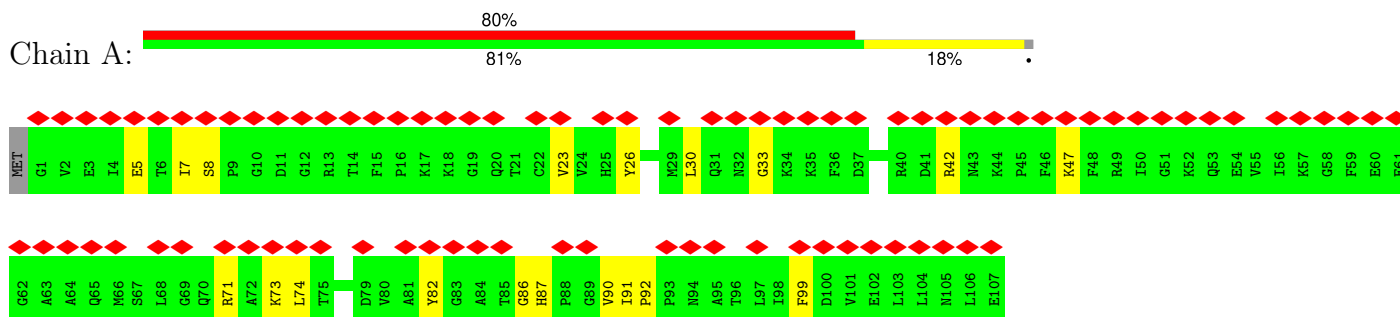
3 Residue-property plots [i](#)

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.

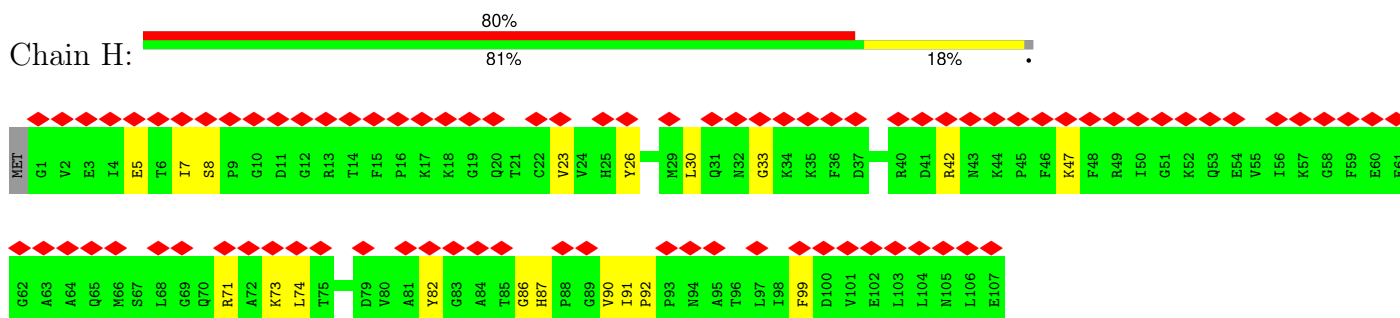
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



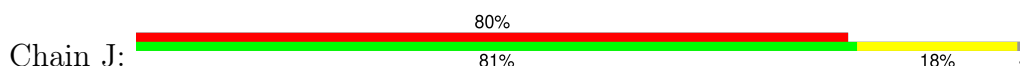
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

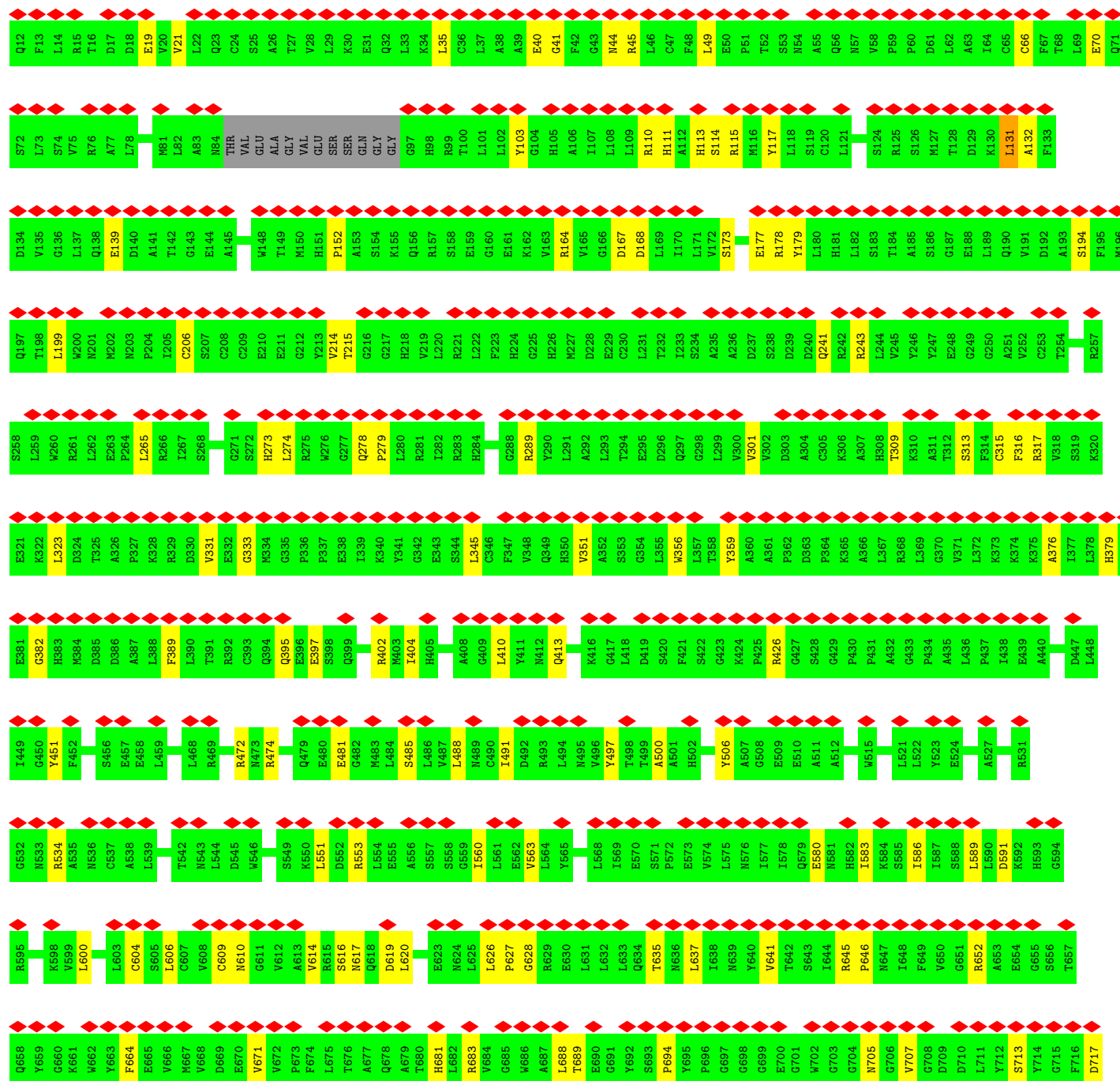


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



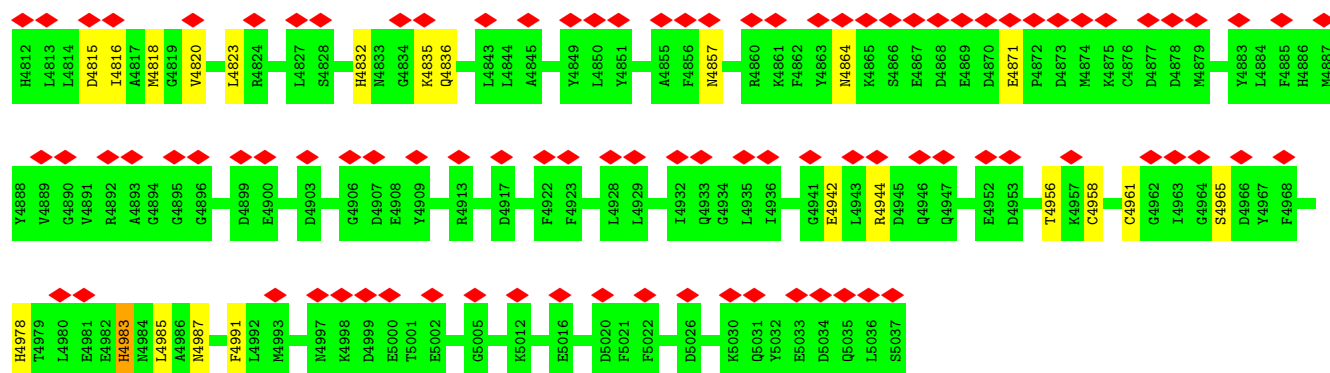


A1638	L1639	H1640	E1643	E1644	N1645	L1646	C1647	M1648	D1649	E1652	L1653	S1654	E1655	L1657	D1658	L1659	Q1660	R1661	H1665	T1666	L1667	R1668	R1671	A1672	A1675	L1676	M1679	R1680	V1681	A1682	H1683	A1684	L1685	H1688	V1689	D1690	Q1691	H1696	A1697	L1698	E1699	D1700	A1701	H1702	L1707	R1708	A1709	G1710	Y1711										
S1576	A1577	A1578	M1579	F1580	L1581	S1582	R1584	K1585	M1586	P1587	A1588	P1589	Q1590	C1591	P1592	P1593	R1594	L1595	E1596	V1597	Q1598	M1599	L1600	M1601	P1602	V1603	S1606	R1607	M1608	H1611	F1612	L1613	Q1614	V1615	GLU	THR	ARG	ALA	GLY	E1622	R1623	L1624	G1625	W1626	A1627	V1628	Q1629	C1630	Q1631	D1632	P1633	L1634	A1709	G1710	Y1711				
X1497	X1504	X1505	X1506	X1510	X1511	X1512	X1513	X1514	X1515	X1516	X1517	X1518	X1519	X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1534	X1537	X1538	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1561	X1562	X1563	X1564	M1573	P1574	L1575					
X1288	X1289	X1290	X1291	X1292	X1293	X1294	X1295	X1430	X1431	X1434	X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1455	X1456	X1457	X1458	X1459	X1460	X1464	X1473	X1474	X1475	X1476	X1477	X1478	X1479	X1480	X1481	X1482	X1483	X1484	X1485	X1486	X1487	X1488	X1489	X1492								
G1218	L1219	Q1220	E1221	G1222	F1223	E1224	A1227	I1228	Q1231	R1232	T1235	T1236	F1238	S1239	G1240	S1241	F1245	E1246	E1251	H1254	Y1255	E1256	V1257	A1258	R1259	M1260	D1261	G1262	T1263	V1264	D1265	T1266	P1267	P1268	C1269	L1270	R1271	L1272	A1273	H1274	R1275	X1276	X1277	X1278	S1279	L1280	X1281	X1282	X1285	X1286	X1287								
E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	G1116	A1117	D1118	E1119	L1120	A1121	G1122	V1123	F1124	N1125	G1126	H1127	R1128	C1129	Q1130	R1131	W1132	H1133	L1134	G1135	S1136	F1139	G1140	R1141	P1142	W1143	Q1144	S1145	G1146	D1147	V1148	Y1149	G1150	C1151	M1152	I1153		
T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRO	PRO	GLN	GLU	PRO	PRO	GLN	VAL	ASN	GLN	GLN	GLN	ARG	TRP	D1070	R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	Q1084	S1085	G1086	Y1089	F1090	E1091	F1092			
M961	S962	N963	G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	D999	Q1003	G1004	W1005	S1006	Y1007	S1008	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	D1028	E1029	A1030				
G841	P842	S843	R844	C845	L846	S847	H848	T849	D850	F851	V852	P853	C854	P855	V856	D857	THR	VAL	GLN	I861	V862	L863	P864	P865	H866	L867	E868	R869	I870	R871	R872	K873	L874	A875	E876	N877	I878	H879	E880	L881	W882	A883	L884	T885	R886	I887	E888	Q889	N890	W891	T892	Y893	G894	P895	V896	R897	D898	N899	M900
K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	M924	G925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	M941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	M960
V781	S782	F783	S784	A785	G786	V787	K788	V789	R790	F791	L792	G794	G795	R796	H797	G798	E799	F800	K801	F802	L803	P804	P805	P806	G807	Y808	A809	P810	C811	H812	E813	A814	V815	L816	P817	R818	E819	R820	L821	R822	L823	E824	P825	I826	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	V840	
G718	L719	H720	L721	G724	H725	V726	A727	R728	P729	V730	T731	S732	P733	Q734	Q735	H736	L737	L738	A739	P740	E741	S745	G746	C747	L748	D749	L750	S751	V752	P753	S754	I755	S756	F757	R758	I759	N760	G761	C762	P763	V764	Q765	G766	V767	F768	E769	A770	F771	N772	L773	D774	G775	L776	F777	F778	P779	V780		

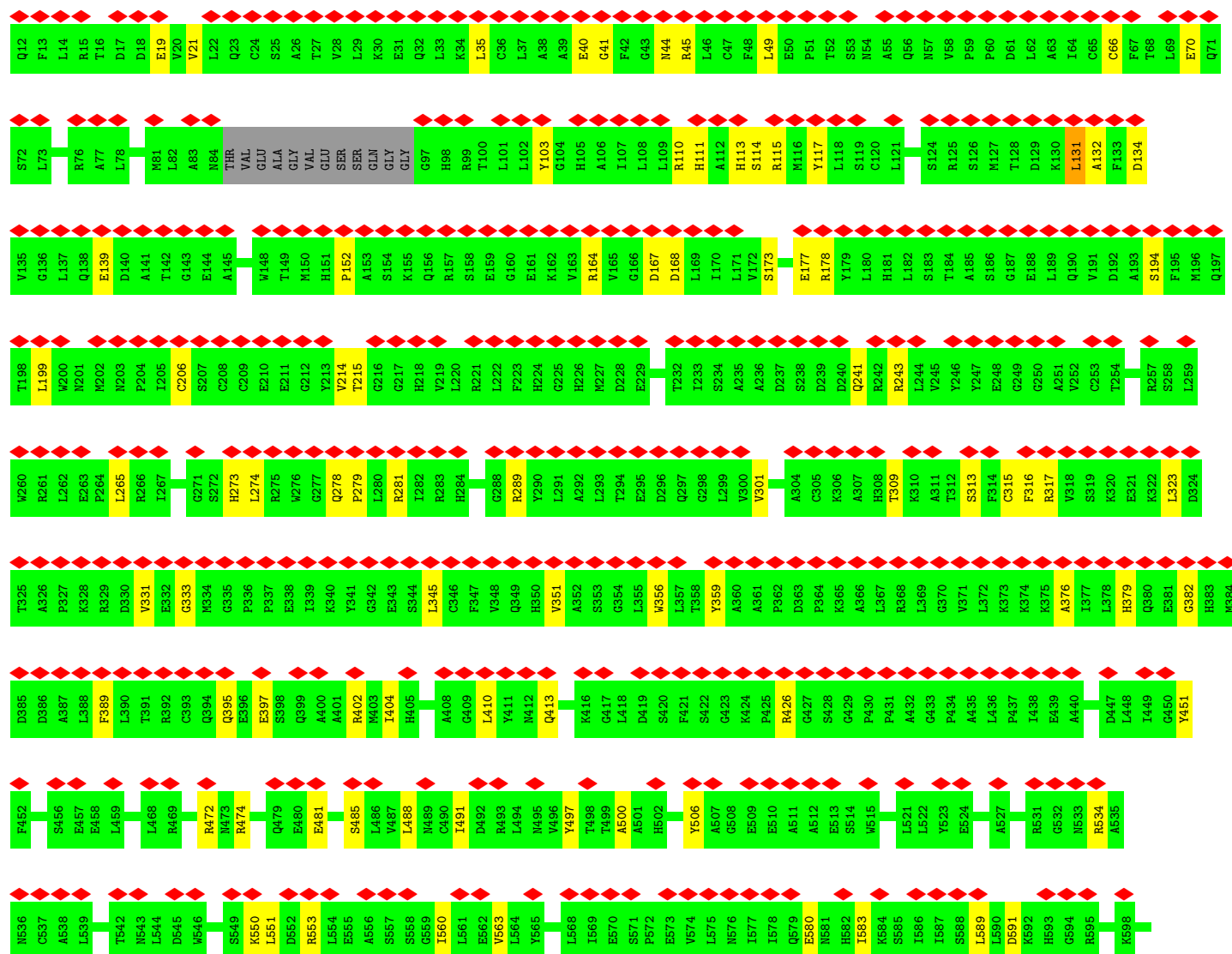
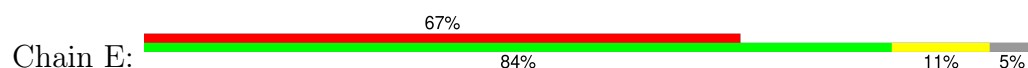
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D2464	D2465	L2466	V2467	Q2468	L2469	L2470	S2471	L2472	P2473	L2474	L2475	L2476	P2477	T2478	L2479	L2487	X2488	X2489	X2490	X2493	X2494	X2495	X2496	X2497	X2498	X2499	X2500	X2501	X2502	X2506	X2509	X2510	X2511	X2512	X2513	X2514	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2526	X2527	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535		
R2336	F2337	F2340	V2341	N2342	E2344	S2345	V2346	E2347	E2348	N2349	A2350	R2355	L2356	L2357	I2358	R2359	K2360	P2361	E2362	C2363	F2364	G2365	P2366	A2367	L2368	R2369	G2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378	I2379	E2380	E2381	E2382	A2383	I2384	R2385	L2386	S2387	D2388	L2389	P2390	A2391	R2392	L2393	G2394	P2395	GLY	VAL	ARG		
ASP	ARG	ARG	ARG	HIS	PHE	GLY	GLU	GLU	PRO	PRO	GLU	N2414	N2415	V2416	H2417	L2418	G2419	H2420	L2421	L2422	N2423	S2424	F2425	Y2426	A2427	I2430	D2431	L2432	L2433	G2434	R2435	A2436	A2437	F2438	N2439	M2440	H2441	L2442	G2446	K2447	G2448	L2451	R2452	I2453	R2454	A2455	L2456	L2457	R2458	S2459	L2460	V2461	P2462	L2463			
D2464	D2465	L2466	V2467	Q2468	L2469	L2470	S2471	L2472	P2473	L2474	L2475	L2476	P2477	T2478	L2479	L2487	X2488	X2489	X2490	X2493	X2494	X2495	X2496	X2497	X2498	X2499	X2500	X2501	X2502	X2506	X2509	X2510	X2511	X2512	X2513	X2514	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2526	X2527	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535		
H1775	H1776	F1777	F1778	F1782	V1783	A1784	L1785	L1786	P1787	A1788	ALA	GLY	V1791	A1792	E1793	A1794	P1795	A1796	R1797	L1798	S1799	I1802	A1806	L1807	R1808	R1813	M1814	L1815	G1816	D1821	G1822	G1823	Q1824	H1825	A1826	G1754	G1755	M1756	A1757	R1758	R1759	H1760	G1761	L1762	P1763	G1764	V1765	G1766	L1842	K1843	L1844	L1848					
G1852	I1853	F1854	G1855	D1856	E1857	D1858	V1859	K1864	M1865	I1866	E1867	P1868	E1869	V1870	F1871	T1872	E1873	E1874	GLU	GLU	GLU	R1797	N1941	L1942	L1943	E1944	Y1945	F1946	Q1949	E1950	R1954	V1955	E1956	S1957	L1958	A2016	A1959	A1960	F1961	A1962	E1963	R1964	Y1965	V1966	D1967	K1968	L1969	Q1970	A1971	N1972	Q1973	R1974	S1975	R1976	Y1977	A1978	L1980
H1775	H1776	F1777	S1778	F1782	V1783	A1784	L1785	L1786	P1787	A1788	ALA	GLY	V1791	A1792	E1793	A1794	P1795	A1796	R1797	L1798	S1799	I1802	A1806	L1807	R1808	R1813	M1814	L1815	G1816	D1821	G1822	G1823	Q1824	H1825	A1826	G1754	G1755	M1756	A1757	R1758	R1759	H1760	G1761	L1762	P1763	G1764	V1765	G1766	L1842	K1843	L1844	L1848					
G1852	I1853	F1854	G1855	D1856	E1857	D1858	V1859	K1864	M1865	I1866	E1867	P1868	E1869	V1870	F1871	T1872	E1873	E1874	GLU	GLU	GLU	R1797	N1941	L1942	L1943	E1944	Y1945	F1946	Q1949	E1950	R1954	V1955	E1956	S1957	L1958	A2016	A1959	A1960	F1961	A1962	E1963	R1964	Y1965	V1966	D1967	K1968	L1969	Q1970	A1971	N1972	Q1973	R1974	S1975	R1976	Y1977	A1978	L1980
H1775	H1776	F1777	S1778	F1782	V1783	A1784	L1785	L1786	P1787	A1788	ALA	GLY	V1791	A1792	E1793	A1794	P1795	A1796	R1797	L1798	S1799	I1802	A1806	L1807	R1808	R1813	M1814	L1815	G1816	D1821	G1822	G1823	Q1824	H1825	A1826	G1754	G1755	M1756	A1757	R1758	R1759	H1760	G1761	L1762	P1763	G1764	V1765	G1766	L1842	K1843	L1844	L1848					
G1852	I1853	F1854	G1855	D1856	E1857	D1858	V1859	K1864	M1865	I1866	E1867	P1868	E1869	V1870	F1871	T1872	E1873	E1874	GLU	GLU	GLU	R1797	N1941	L1942	L1943	E1944	Y1945	F1946	Q1949	E1950	R1954	V1955	E1956	S1957	L1958	A2016	A1959	A1960	F1961	A1962	E1963	R1964	Y1965	V1966	D1967	K1968	L1969	Q1970	A1971	N1972	Q1973	R1974	S1975	R1976	Y1977	A1978	L1980
H1775	H1776	F1777	S1778	F1782	V1783	A1784	L1785	L1786	P1787	A1788	ALA	GLY	V1791	A1792	E1793	A1794	P1795	A1796	R1797	L1798	S1799	I1802	A1806	L1807	R1808	R1813	M1814	L1815	G1816	D1821	G1822	G1823	Q1824	H1825	A1826	G1754	G1755	M1756	A1757	R1758	R1759	H1760	G1761	L1762	P1763	G1764	V1765	G1766	L1842	K1843	L1844	L1848					
G1852	I1853	F1854	G1855	D1856	E1857	D1858	V1859	K1864	M1865	I1866	E1867	P1868	E1869	V1870	F1871	T1872	E1873	E1874	GLU	GLU	GLU	R1797	N1941	L1942	L1943	E1944	Y1945	F1946	Q1949	E1950	R1954	V1955	E1956	S1957	L1958	A2016	A1959	A1960	F1961	A1962	E1963	R1964	Y1965	V1966	D1967	K1968	L1969	Q1970	A1971	N1972	Q1973	R1974	S1975	R1976	Y1977	A1978	L1980
H1775	H1776	F1777	S1778	F1782	V1783	A1784	L1785	L1786	P1787	A1788	ALA	GLY	V1791	A1792	E1793	A1794	P1795	A1796	R1797	L1798	S1799	I1802	A1806	L1807	R1808	R1813	M1814	L1815	G1816	D1821	G1822	G1823	Q1824	H1825	A1826	G1754	G1755	M1756	A1757	R1758	R1759	H1760	G1761	L1762	P1763	G1764	V1765	G1766	L1842	K1843	L1844	L1848					
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X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423		X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441		X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455		X3457	X3458	X3459	X3460	X3461	X3462	X3463	X3464	X3465																																																																						
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A2815	M2816	L2817	A2818	R2819	Y2820	M2821	T2822	X2823	Y2824	M2825	A2826	R2827	X2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TTR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	R2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874																																																																						
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G4742	V4686	ALA	X4322	Y4173	Q4102	G4038	L3884	S3803	A3726	L3654	X3568
M4743	P4667	ALA	X4325	F4174	F4103	M4039	F3885	S3805	M3729	E3655	X3569
D4744	L4668	ASP	R4175	R4175	T4104	M4039	R3886	L3804	X3730	X3570	X3571
L4745	V4669	LEU	P4176	P4176	G4105	A4041	Q3889	N3806	K3731	X3572	X3573
A4746	R4673	ALA	G4179	G4179	P4106	D4046	L3890	N3809	A3730	X3574	X3575
S4747	E4674	ALA	R4180	R4180	E4107	M4047	L3891	A3660	S3732	X3576	X3577
L4748	K4675	GLY	X4334	X4334	I4108	E4050	C3892	W3661	L3735	X3578	X3579
E4749	R4679	SER	X4340	M4184	F4109	E4051	E3893	L3816	L3736	X3580	X3581
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L4751	L4681	GLY	X4342	A4186	L4111	E4054	D3898	K3821	E3738	X3584	X3585
A4752	E4682	SER	X4343	R4188	L4112	M4054	F3899	D3822	G3739	X3586	X3587
M4753	G4683	GLY	X4344	R4189	S4113	E4056	Q3900	E3825	E3740	X3588	X3589
H4754	F4683	TRP	X4345	I4190	S4115	M4057	N3901	E3825	E3741	X3590	X3591
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P4758	Y4687	GLY	E4543	E4196	E4119	F4061	Q3906	E3834	GLU	X3598	X3599
I4758	I4688	GLU	E4544	I4197	M4120	F4062	T3910	L3842	E3747	X3600	X3601
T4759	T4689	ALA	E4545	S4198	E4121	D4063	T3911	D3843	E3748	X3602	X3603
P4760	E4690	GLY	E4546	E4199	M4122	M4064	T3912	E3846	V3749	X3604	X3605
K4761	Q4691	GLY	V4546	T4200	I4123	F4065	T3913	E3846	E3750	X3606	X3607
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L4765	D4695	GLU	L4552	M4205	E4128	K4069	D3932	E3846	E3754	X3614	X3615
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L4768	Y4699	GLU	S4556	Q4209	M4130	H3999	Q3927	E3846	E3757	X3620	X3621
M4769	F4631	GLU	R4557	V4210	R4131	M4000	E3928	E3846	E3758	X3622	X3623
S4770	L4632	GLU	E4633	E4211	F4132	K4002	E3928	E3846	E3759	X3624	X3625
D4771	E4633	GLU	E4634	E4212	Q4133	L4003	E3928	E3846	E3760	X3626	X3627
R4772	E4634	GLU	S4635	E4213	E4134	A4004	E3928	E3846	E3761	X3628	X3629
L4773	T4636	GLU	L4667	E4214	E4135	Q4005	E3928	E3846	E3762	X3630	X3631
K4774	C4637	GLU	F4568	E4215	E4136	D4006	E3928	E3846	E3763	X3632	X3633
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G4781	P4641	GLU	E4571	E4218	T4139	D4008	E3928	E3846	E3766	X3638	X3639
V4782	E4644	GLU	A4572	E4219	F4141	S4008	E3928	E3846	E3767	X3640	X3641
L4783	C4645	GLU	I4573	E4220	E4142	E4009	E3928	E3846	E3768	X3642	X3643
F4784	E4645	GLU	E4574	E4221	E4143	E4010	E3928	E3846	E3769	X3644	X3645
T4785	E4646	GLU	E4575	E4222	E4144	E4011	E3928	E3846	E3770	X3646	X3647
D4786	L4648	GLU	E4576	E4223	E4145	E4012	E3928	E3846	E3771	X3648	X3649
F4789	L4649	GLU	E4577	E4224	E4146	E4013	E3928	E3846	E3772	X3650	X3651
L4790	H4650	GLU	E4582	E4225	E4147	E4014	E3928	E3846	E3773	X3652	X3653
Y4791	F4655	GLU	E4583	E4226	E4148	E4015	E3928	E3846	E3774	X3654	X3655
W4794	L4656	GLU	E4584	E4227	E4149	E4016	E3928	E3846	E3775	X3656	X3657
L4800	L4657	GLU	E4585	E4228	E4150	E4017	E3928	E3846	E3776	X3658	X3659
G4801	C4657	GLU	E4586	E4229	E4151	E4018	E3928	E3846	E3777	X3660	X3661
A4802	L4658	GLU	E4587	E4230	E4152	E4019	E3928	E3846	E3778	X3662	X3663
M4805	L4659	GLU	E4588	E4231	E4153	E4020	E3928	E3846	E3779	X3664	X3665
N4806	L4660	GLU	E4589	E4232	E4154	E4021	E3928	E3846	E3780	X3666	X3667
F4807	L4661	GLU	E4590	E4233	E4155	E4022	E3928	E3846	E3781	X3668	X3669
F4808	L4662	GLU	E4591	E4234	E4156	E4023	E3928	E3846	E3782	X3670	X3671
P4809	L4663	GLU	E4592	E4235	E4157	E4024	E3928	E3846	E3783	X3672	X3673
A4810	L4664	GLU	E4593	E4236	E4158	E4025	E3928	E3846	E3784	X3674	X3675
A4811	L4665	GLU	E4594	E4237	E4159	E4026	E3928	E3846	E3785	X3676	X3677



• Molecule 2: Ryanodine receptor 1

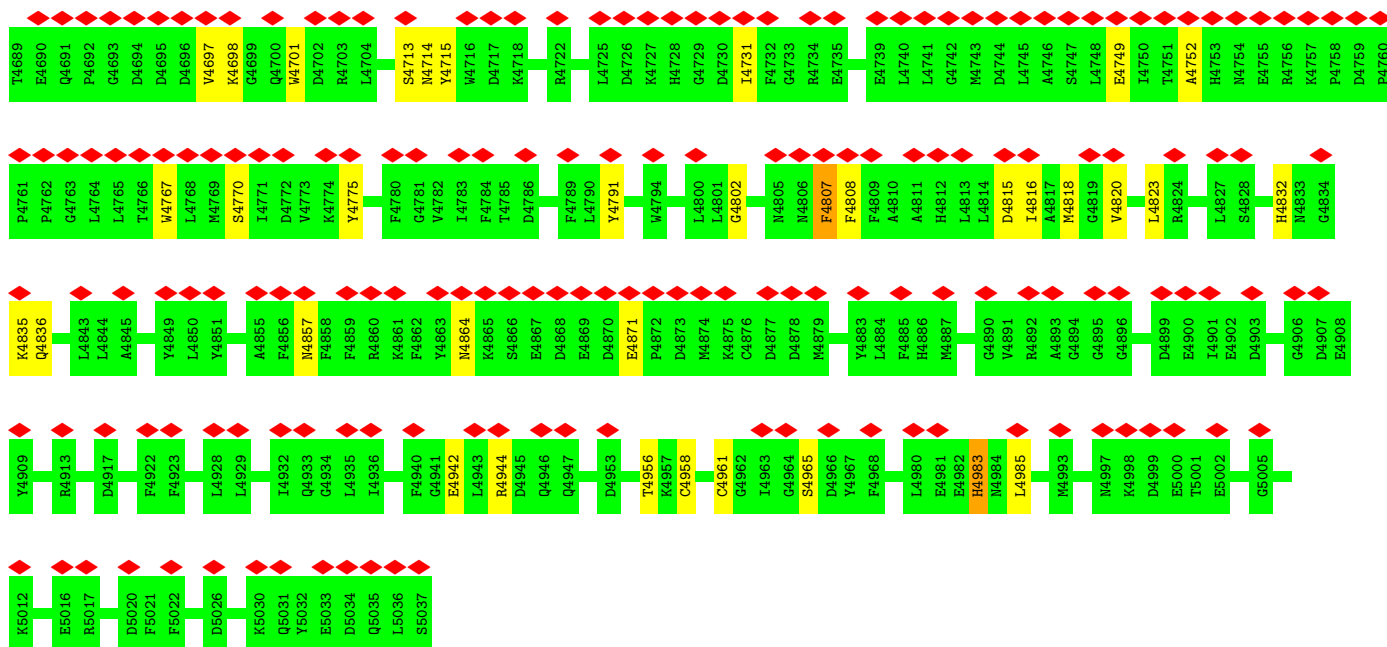


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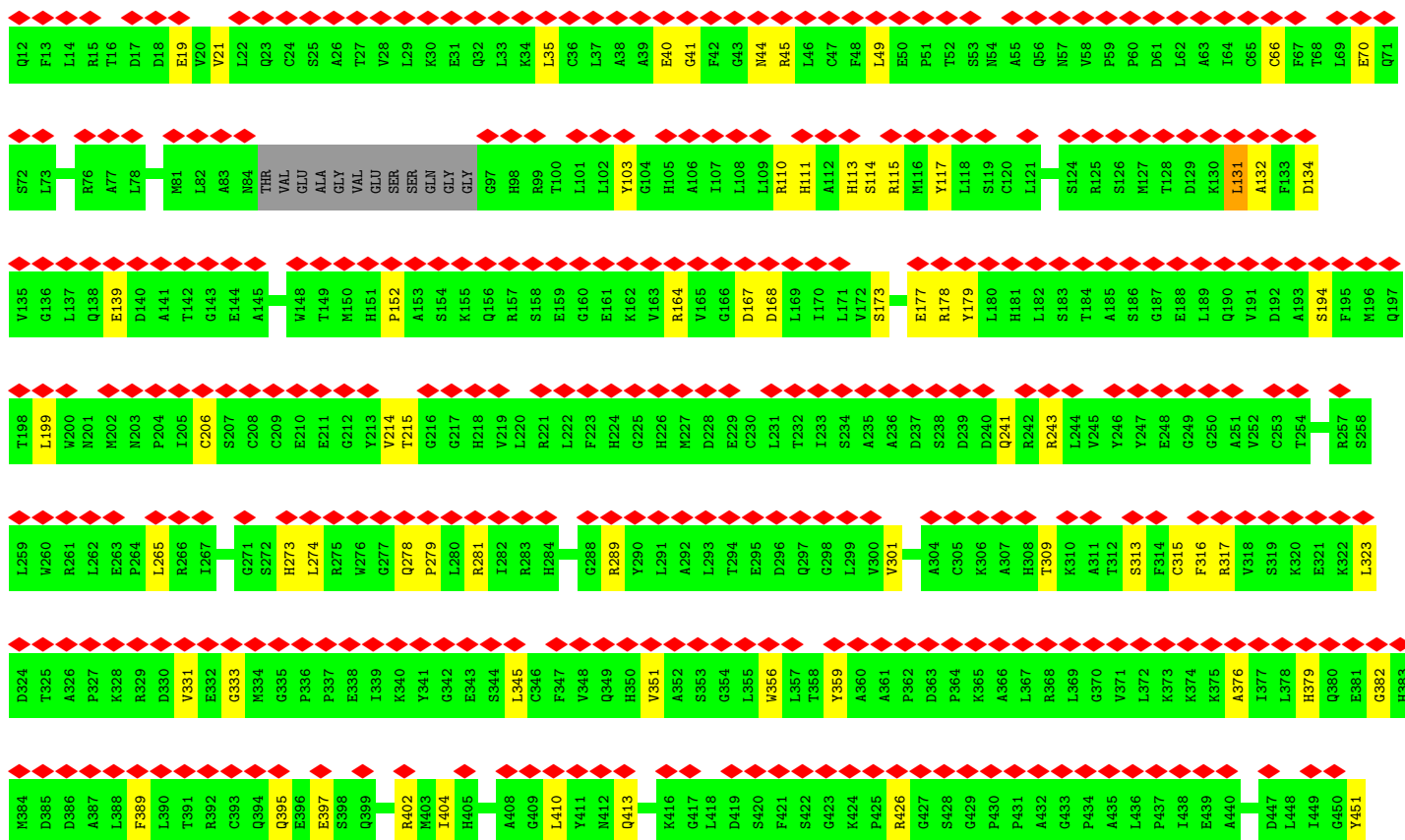
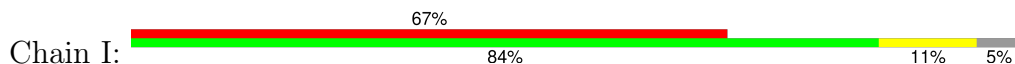


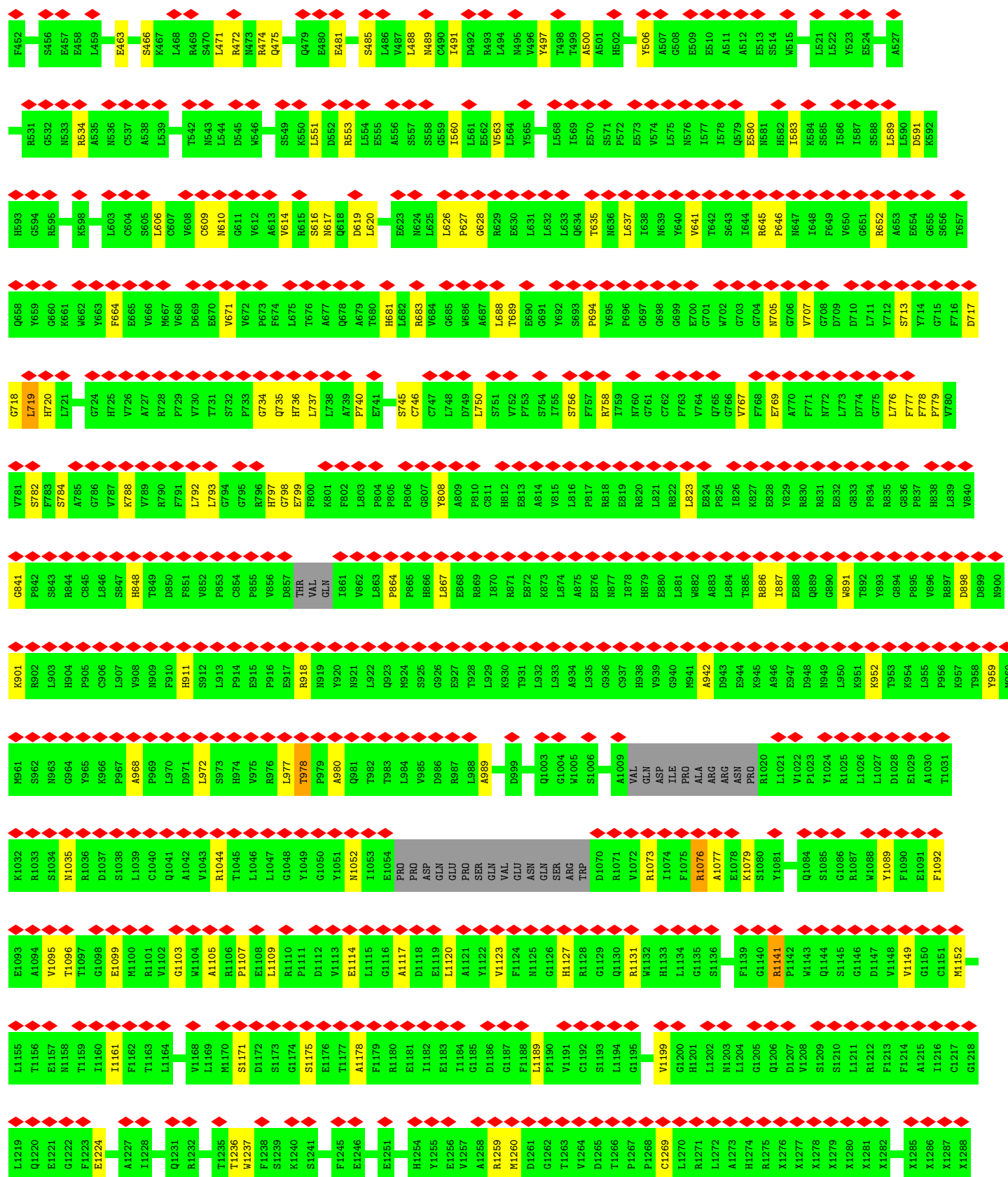
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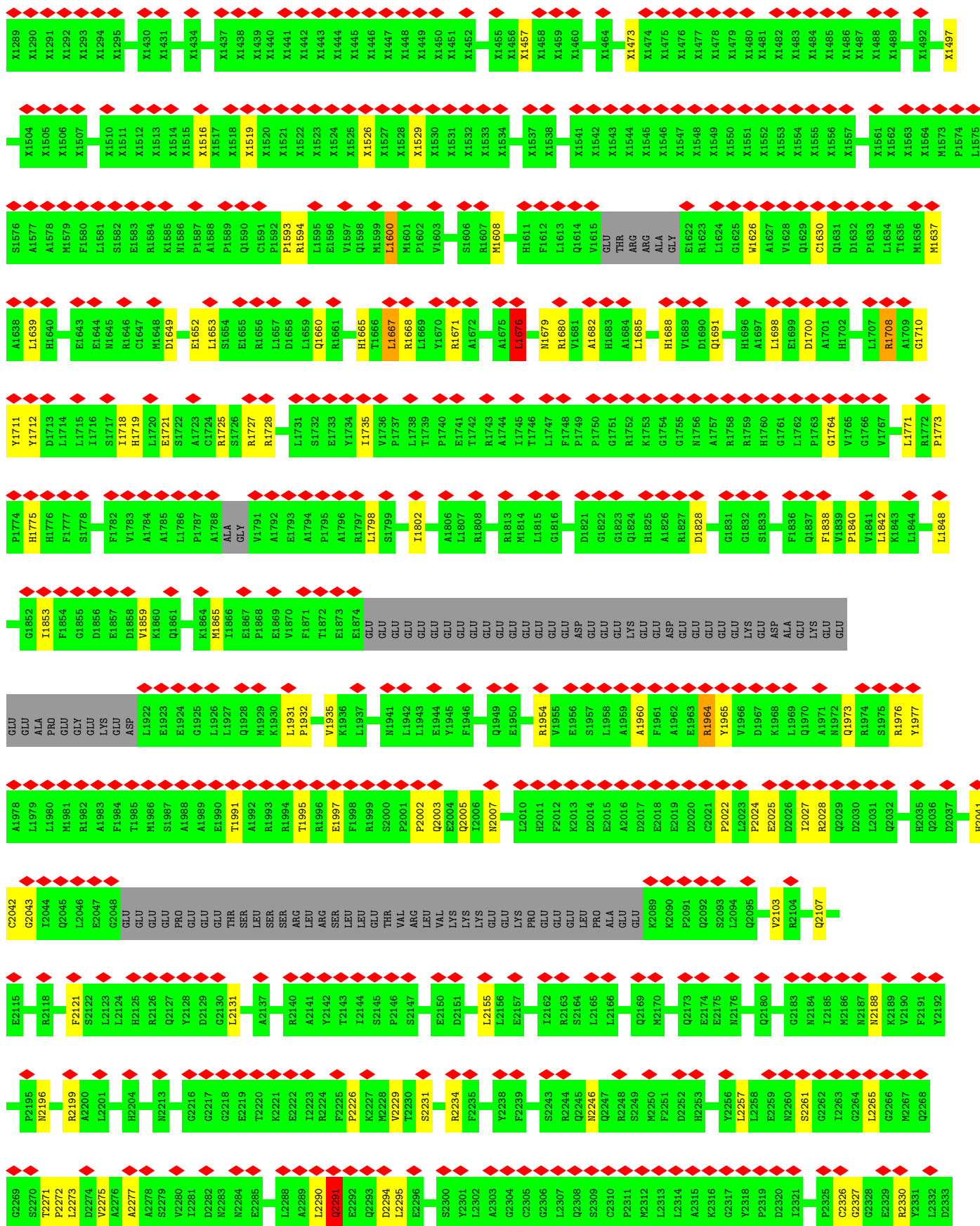




• Molecule 2: Ryanodine receptor 1







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X2602	X2603	X2604	X2605	X2606	X2607	X2608	X2609	X2610	X2611	X2612	X2613	X2614	X2615	X2616	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2641	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2656	X2657	X2660	X2661	X2662	X2663	X2664											
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L2460	V2461	P2462	L2463	D2464	D2465	L2466	V2467	G2468	L2469	I2470	S2471	L2472	P2473	L2474	Q2475	L2476	P2477	L2478	L2479	X2487	X2488	X2489	X2490	X2493	X2494	X2495	X2496	X2497	X2498	X2499	X2500	X2501	X2502	X2506	X2511	X2512	X2513	X2514	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2526	X2527	X2528	X2529	X2530	X2531	X2532	X2533													
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P4176	R4180	M4184	G4185	A4186	S4187	R4188	R4189	I4190	E4191	R4192	E4196	I4197	S4198	E4199	T4200	N4201	R4202	A4203	Q4204	V4205	E4206	M4207	P4208	Q4209	V4210	K4211	E4212	R4215	F4219	M4223	E4224	G4225	G4226	E4227	A4228	E4229	L4233	E4239	Q4250	I4251	S4252	E4253	X4320	X4321	X4322	X4323	X4324	X4325	X4330										
G4105	P4106	E4107	I4108	Q4109	F4110	L4111	L4112	S4113	C4114	S4115	E4116	A4117	D4118	E4119	N4120	E4121	M4122	I4123	M4124	F4125	E4126	E4127	M4128	N4129	A4130	R4131	F4132	Q4133	E4134	R4137	D4138	I4139	Q4140	F4141	N4142	L4147	E4152	H4153	H4156	R4159	L4160	R4161	L4164	E4165	L4166	A4167	E4168	S4169	E4172	Y4173	F4174	R4175	T4104						
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S3732	C3733	H3734	L3735	E3736	E3737	G3738	X3739	E3740	X3741	GLY	ALA	ALA	GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	M3758	X3759	K3760	Q3761	R3762	L3763	L3764	Y3765	Q3766	Q3767	S3768	R3769	L3770	H3771	T3772	R3773	G3774	A3775	X3776	E3777	M3778	X3779	L3780	K3787	S3795	X3799	S3803	I3804	L3805	M3806					
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E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	P1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	Y1122	V1123	F1124	N1125	G1126	H1127	R1128	S1006	D1070	A1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	Q1084	S1085	G1086	Y1089	F1090	E1091	F1092	M1152					
T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	T1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	SER	TRP	D1070	R1071	V1072	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030
M961	S962	N963	G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	D999	G999	Q1003	G1004	W1005	Y1007	S1008	A1009	VAL	GLN	ASP	ASP	PRO	ALA	ARG	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030				
K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	N924	S925	Q926	E927	T928	L929	K930	T931	L932	L933	A934	L935	Q936	C937	H938	V939	G940	M941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	Y959	N960			
G841	P842	S843	R844	C845	L846	S847	H848	T849	D850	F851	W852	P853	C854	P855	W856	D857	THR	VAL	GLN	I861	W862	L863	P864	P865	H866	L867	E868	R869	L870	R871	E872	K873	L874	A875	E876	R877	R878	H879	E880	L881	W882	A883	L884	T885	R886	L887	E888	Q889	G890	W891	T892	Y893	G894	P895	W896	R897	D898	D899	Y959	N960	
V780	V781	S782	F783	S784	A785	G786	V787	K788	V789	R790	F791	L792	L793	G794	G795	R796	H797	G798	E799	F800	K801	F802	L803	P804	P805	P806	G807	Y808	A809	H812	E813	A814	W815	L816	P817	R818	E819	R820	L821	R822	L823	E824	P825	L826	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	Y840			
D717	G718	L719	H720	L721	G724	H725	V726	A727	R728	F729	W730	T731	S732	F733	G734	Q735	H736	L737	L738	A739	P740	E741	S745	C746	G747	L748	L749	L750	S751	V752	F753	Y754	I755	S756	F757	Y758	P759	N760	G761	G762	C763	V764	G765	G766	V767	F768	E769	A770	F771	W772	L773	D774	G775	L776	F777	F778	P779				
T657	Q658	Y659	K598	V599	L600	L603	C604	S605	L606	C607	V608	C609	N610	G611	V612	A613	R615	S616	Q617	Q618	D619	L620	E623	N624	L625	L626	P627	E628	R629	E630	L631	L632	L633	Q634	T635	N636	L637	T638	N639	Y640	V641	T642	S643	T644	R645	P646	N647	T648	F649	V650	G651	R652	A653	E654	G655	S656					
G594	R595	K598	V599	L600	L603	C604	S605	L606	C607	V608	C609	N610	G611	V612	A613	R615	S616	Q617	Q618	D619	L620	E623	N624	L625	L626	P627	E628	R629	E630	L631	L632	L633	Q634	T635	N636	L637	T638	N639	Y640	V641	T642	S643	T644	R645	P646	N647	T648	F649	V650	G651	R652	A653	E654	G655	S656						
R531	G532	N533	R534	A535	N536	C537	A538	L539	T542	N543	L544	D545	W546	S549	K550	L551	D552	R553	L554	E555	A556	S557	S558	G559	I560	L561	E562	V563	L564	Y565	L568	I569	E570	S571	P572	E573	V574	L575	N576	I577	I578	Q579	E580	N581	H582	I583	K584	S585	I586	I587	S588	L589	L590	D591	K592	H593					
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X3020	X2942	E2880	E2820	E2760	X2670	X2607	X2540	L2466	GLU	V2341	V2275	L2201
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X3028	X2950	R2888	E2828	F2768	X2678	X2615	X2553	Q2475	GLU	N2349	N2283	T2220
X3029	X2951	G2889	G2829	D2769	X2679	X2616	X2554	L2476	GLU	A2350	N2284	E2221
X3030	X2952	K2890	E2830	K2770	X2680	X2617	X2555	Q2477	GLU	G2355	E2285	T2222
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X3035	X2957	E2895	LYS	W2775	X2685	X2622	X2561	X2494	GLU	K2360	E2292	K2227
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X3039	X2961	G2899	LYS	E2779	X2689	X2626	X2565	X2498	GLU	G2364	S2231	G2231
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X3042	X2964	H2902	ALA	D2782	X2692	X2629	X2568	X2502	GLU	L2368	V2238	V2238
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X3046	X2968	V2906	ASP	K2786	X2696	X2633	X2572	X2513	GLU	G2372	H2250	H2250
X3047	X2969	P2907	ARG	T2787	X2697	X2634	X2575	X2514	GLU	S2373	F2251	F2251
X3048	X2970	Y2908	GLU	H2788	X2698	X2635	X2576	X2517	GLU	G2374	D2252	D2252
X3049	X2971	D2909	GLY	P2789	X2699	X2636	X2577	X2518	GLU	L2375	H2253	H2253
X3050	X2972	T2910	Y2855	M2790	X2700	X2637	X2578	X2519	GLU	G2376	V2256	V2256
X3051	X2973	L2911	N2856	M2791	X2701	X2638	X2579	X2520	GLU	L2377	L2257	L2257
X3052	X2974	T2912	P2857	R2792	X2702	X2639	X2580	X2521	GLU	L2378	L2258	L2258
X3053	X2975	A2913	Q2858	P2793	X2703	X2640	X2581	X2522	GLU	G2379	E2259	E2259
X3054	X2976	K2914	P2859	Y2794	N2734	X2641	X2582	X2523	GLU	E2380	R2260	R2260
X3055	X2977	E2915	D2860	K2795	F2735	X2642	X2583	X2524	GLU	E2381	S2261	S2261
X3056	X2978	A2916	L2861	T2796	D2736	X2643	X2584	X2525	GLU	E2382	G2262	G2262
X3057	X2979	G2917	L2862	T2797	P2737	X2644	X2585	X2526	GLU	A2383	I2263	I2263
X3058	X2980	R2918	S2863	S2798	R2738	X2645	X2586	X2527	GLU	G2448	G2264	G2264
X3059	X2981	D2919	G2864	E2799	P2739	X2646	X2587	X2528	GLU	E2449	L2265	L2265
X3060	X2982	N2920	V2865	W2740	X2740	X2647	X2588	X2529	GLU	A2450	E2329	E2329
X3061	X3001	E2921	L2867	E2741	X2651	X2648	X2589	X2530	GLU	L2451	R2330	R2330
X3062	X3002	T2922	T2868	T2742	X2652	X2649	X2590	X2531	GLU	G2452	G2267	G2267
X3063	X3003	A2923	S2868	T2743	X2653	X2650	X2591	X2532	GLU	I2453	Q2268	Q2268
X3064	X3004	Q2924	E2870	L2744	X2654	X2651	X2592	X2533	GLU	R2454	P2325	P2325
X3065	X3005	E2925	L2871	W2745	X2655	X2652	X2593	X2534	GLU	A2455	C2326	C2326
X3066	X3006	L2926	Q2872	L2746	X2656	X2653	X2594	X2535	GLU	G2456	G2327	G2327
X3067	X3007	L2927	X2873	W2807	X2657	X2654	X2595	X2536	GLU	L2457	E2328	E2328
X3068	X3008	G2928	A2873	P2748	X2660	X2655	X2596	X2537	GLU	R2458	E2329	E2329
X3069	X3009	F2929	M2874	E2749	X2661	X2656	X2597	X2538	GLU	S2459	R2330	R2330
X3070	X3010	A2875	K2875	K2750	X2662	X2657	X2598	X2539	GLU	L2460	Y2331	Y2331
X3071	X3011	Q2931	E2811	L2751	X2663	X2658	X2599	X2540	GLU	V2461	Q2269	Q2269
X3072	X3012	N2932	S2812	D2752	X2664	X2659	X2600	X2541	GLU	P2462	Q2270	Q2270
X3073	X3013	N2933	L2813	S2753	X2665	X2660	X2601	X2542	GLU	L2463	S2271	S2271
X3074	X3014	G2934	K2814	F2754	X2666	X2661	X2602	X2543	GLU	A2464	R2273	R2273
X3075	X3015	Y2935	A2815	I2755	X2667	X2662	X2603	X2544	GLU	ASP	L2274	L2274
X3076	X3016	T2936	N2816	W2756	X2668	X2663	X2604	X2545	GLU	ARG	D2275	D2275
X3077	X3017	V2937	L2817	K2757	X2669	X2664	X2605	X2546	GLU	ARG	F2337	F2337
X3078	X3018	T2938	A2818	F2758	X2670	X2665	X2606	X2547	GLU	ARG	F2340	F2340
X3079	X3019	R2939	N2819	A2759	X2671	X2666	X2607	X2548	GLU	ARG		



H4983	N4984	L4985	M4993	M4997	M4998	M4999	E5000	T5001	E5002	G5005	K5012	E5016	R5017	D5020	F5021	F5022	D5026	K5030	Q5031	Y5032	E5033	D5034	Q5035	L5036	S5037																															
G4896	D4899	E4900	I4901	E4902	D4903	G4906	D4907	E4908	Y4909	R4913	D4917	F4922	F4923	L4928	L4929	I4932	Q4933	G4934	L4935	I4936	F4940	G4941	E4942	L4943	R4944	D4945	Q4946	Q4947	D4953	T4956	K4957	C4958	C4961	G4962	I4963	G4964	S4965	D4966	Y4967	F4968	E4976	T4977	D4978	T4979	L4980	E4981	E4982									
L4823	R4824	L4827	S4828	M4832	M4833	G4834	K4835	Q4836	L4843	L4844	A4845	Y4849	L4850	Y4851	A4855	F4856	M4857	F4858	F4859	R4860	K4861	F4862	Y4863	M4864	K4865	S4866	E4867	D4868	E4869	D4870	E4871	F4872	D4873	M4874	K4875	C4876	D4877	D4878	M4879	Y4883	L4884	F4885	H4886	M4887	Y4888	V4889	G4890	V4891	R4892	A4893	G4894	G4895				
T4751	A4752	H4753	M4754	E4755	M4756	K4757	P4758	D4759	P4760	P4761	P4762	G4763	L4764	L4765	T4766	M4767	M4769	S4770	I4771	D4772	V4773	K4774	Y4775	F4780	G4781	V4782	L4783	F4784	T4785	D4786	F4789	L4790	Y4791	M4794	L4800	L4801	C4802	M4805	M4806	F4807	F4808	F4809	A4810	A4811	H4812	L4813	L4814	D4815	I4816	A4817	M4818	G4819	V4820			
R4679	K4680	L4681	E4682	F4683	D4684	G4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	G4693	D4694	D4695	D4696	V4697	K4698	G4699	Q4700	M4701	D4702	E4634	S4635	T4636	G4637	Y4638	P4641	M4644	C4645	L4648	L4649	H4650	F4655	L4656	C4657	I4658	T4659	Q4660	Y4661	M4662	V4666	P4667	L4668	V4669	R4673	E4674	K4675							
GLY	GLY	GLY	SER	GLY	TRP	GLY	SER	GLY	ALA	GLY	GLY	GLU	GLU	ALA	GLY	GLY	ASP	ASP	GLU	ASP	GLU	M4626	Y4629	Y4630	F4631	L4632	E4633	E4634	S4635	T4636	G4637	Y4638	P4641	M4644	C4645	L4648	L4649	H4650	F4655	L4656	C4657	I4658	T4659	Q4660	Y4661	M4662	V4666	P4667	L4668	V4669	R4673	E4674	K4675			
X4341	X4342	X4343	X4344	X4345	F4340	M4341	G4342	E4343	E4344	L4345	E4346	V4347	R4348	F4351	L4352	M4353	Y4354	L4355	S4356	R4357	L4362	L4367	P4368	F4371	A4372	I4373	M4374	P4375	I4376	L4377	V4382	S4383	D4384	S4385	P4386	P4387	GLY	GLU	ASP	ASP	ASP	ASP	ASP	ASP	GLY	SER	ALA	ALA	GLY	ASP	LEU	ALA	GLY	ALA	GLY	SER
S4187	R4188	R4189	I4190	E4191	R4192	E4196	I4197	S4198	E4199	T4200	N4201	R4202	A4203	Q4204	W4205	E4206	M4207	Y4208	Q4209	V4210	K4211	E4212	R4215	F4219	N4223	E4224	G4225	G4226	E4227	E4228	E4229	L4233	S4236	E4239	Q4250	I4251	S4252	E4253	ASP	ASP	ASP	ASP	GLY	SER	ALA	ALA	GLY	ASP	LEU	ALA	GLY	ALA	GLY	SER	X4340	
L4112	S4113	C4114	S4115	E4116	A4117	D4118	E4119	M4120	E4121	M4122	I4123	M4124	F4125	E4126	F4127	F4128	A4129	M4130	M4131	F4132	Q4133	E4134	R4137	D4138	G4140	F4141	M4142	L4147	E4152	H4153	H4156	R4159	L4160	R4161	L4164	E4165	L4166	A4167	E4168	S4169	E4172	Y4173	F4174	R4175	P4176	R4180	M4184	C4185	A4186							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	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 ($e^-/\text{\AA}^2$)	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	0.060	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	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	0.32	0/834	0.53	0/1123
1	F	0.32	0/834	0.53	0/1123
1	H	0.32	0/834	0.53	0/1123
1	J	0.32	0/834	0.53	0/1123
2	B	0.30	0/25438	0.54	8/34548 (0.0%)
2	E	0.30	0/25438	0.54	8/34548 (0.0%)
2	G	0.30	0/25438	0.54	8/34548 (0.0%)
2	I	0.30	0/25438	0.54	8/34548 (0.0%)
All	All	0.30	0/105088	0.54	32/142684 (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	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	56

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	131	LEU	CA-CB-CG	7.74	133.11	115.30
2	B	131	LEU	CA-CB-CG	7.73	133.09	115.30
2	I	131	LEU	CA-CB-CG	7.73	133.08	115.30
2	G	131	LEU	CA-CB-CG	7.73	133.08	115.30
2	E	1600	LEU	CA-CB-CG	7.38	132.27	115.30

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	11	0
1	F	818	0	824	11	0
1	H	818	0	824	11	0
1	J	818	0	824	11	0
2	B	29509	0	24752	277	0
2	E	29509	0	24753	269	0
2	G	29509	0	24753	269	0
2	I	29509	0	24753	276	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	121312	0	102307	1111	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 5.

The worst 5 of 1111 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.10	0.70
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.10	0.70
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.10	0.69
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.10	0.67
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.61	0.65

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	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	44	78
2	E	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	44	78
2	G	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	44	78
2	I	3237/4416 (73%)	2890 (89%)	341 (10%)	6 (0%)	44	78
All	All	13368/18096 (74%)	11931 (89%)	1413 (11%)	24 (0%)	45	78

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2475 (99%)	18 (1%)	81	87
2	E	2493/3022 (82%)	2475 (99%)	18 (1%)	81	87
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	81	87
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	81	87
All	All	10324/12444 (83%)	10252 (99%)	72 (1%)	80	87

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	719	LEU
2	G	4983	HIS
2	G	1076	ARG
2	G	3787	LYS
2	E	1141	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	3960	GLN
2	G	1775	HIS
2	I	479	GLN
2	G	1719	HIS
2	G	3950	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	14
2	G	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.38
1	E	4345:UNK	C	4540:PHE	N	73.38
1	I	4345:UNK	C	4540:PHE	N	73.38
1	G	4345:UNK	C	4540:PHE	N	73.38

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	48.21

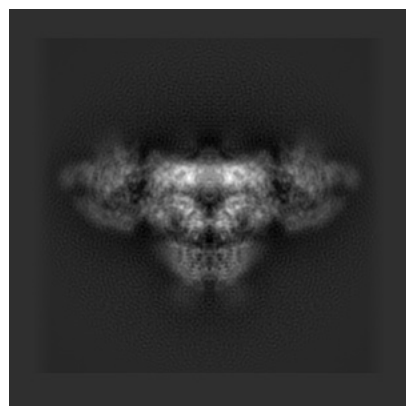
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8394. These allow visual inspection of the internal detail of the map and identification of artifacts.

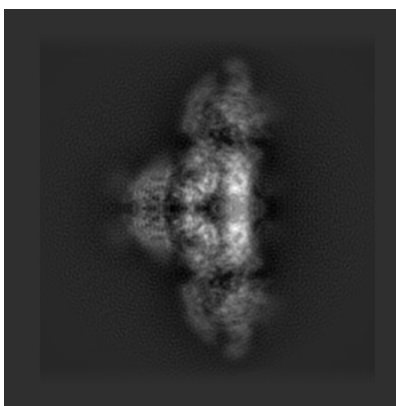
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

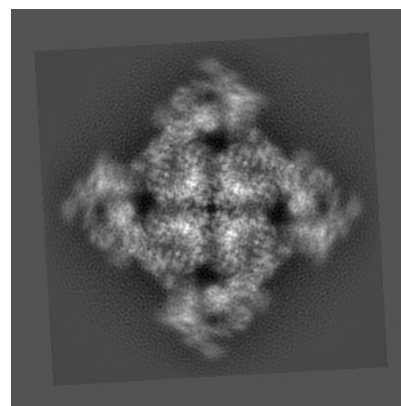
6.1.1 Primary map



X

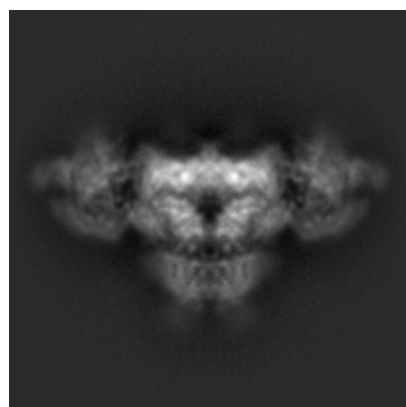


Y

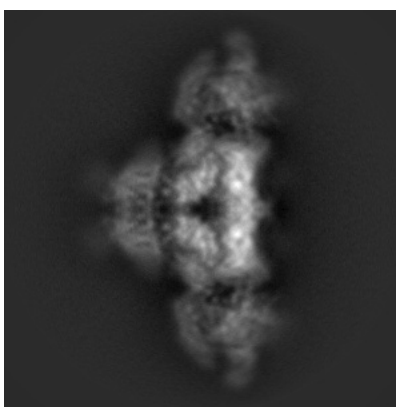


Z

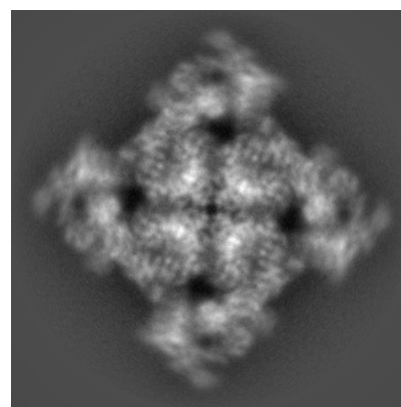
6.1.2 Raw map



X



Y

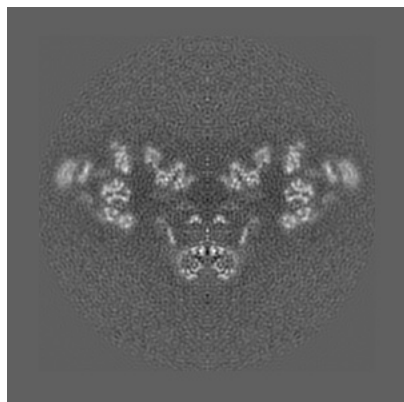


Z

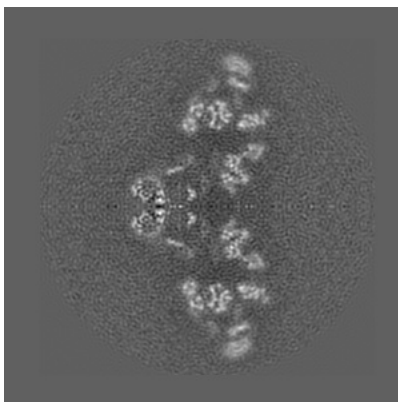
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

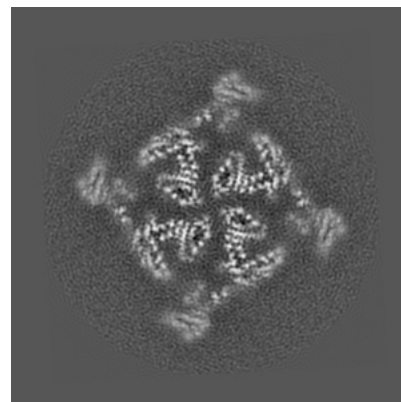
6.2.1 Primary map



X Index: 200

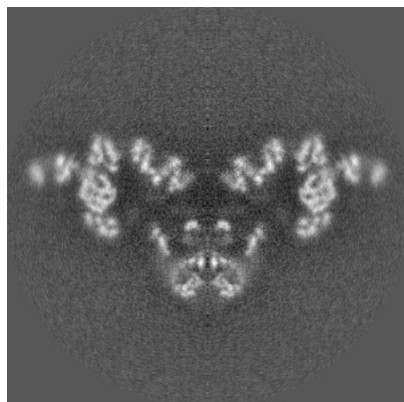


Y Index: 200

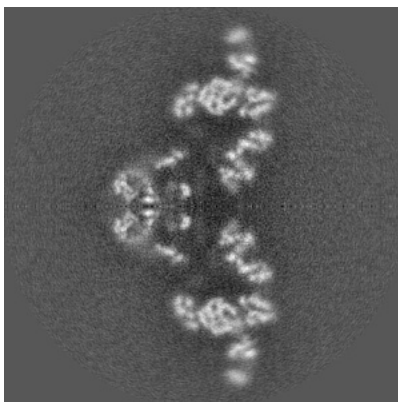


Z Index: 200

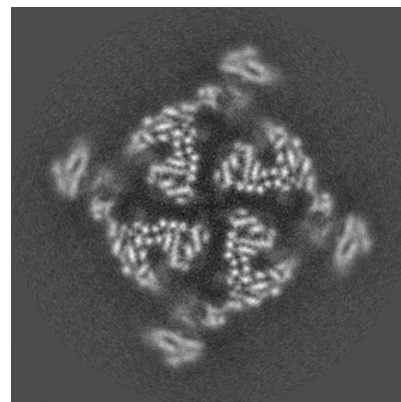
6.2.2 Raw map



X Index: 168



Y Index: 168

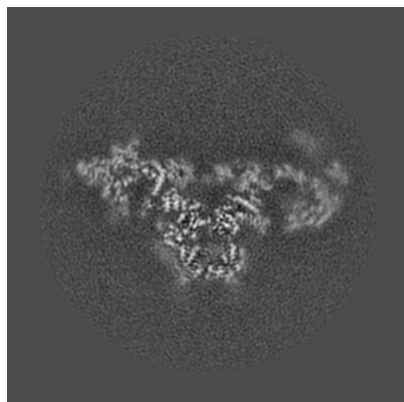


Z Index: 168

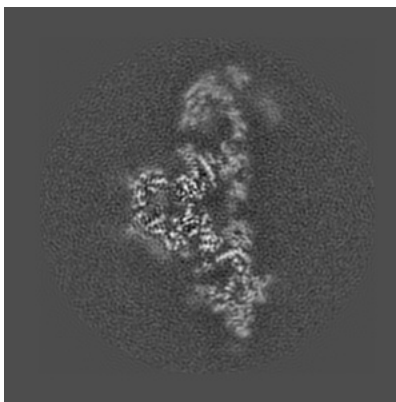
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

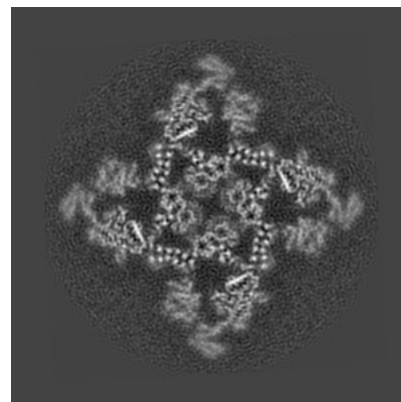
6.3.1 Primary map



X Index: 217

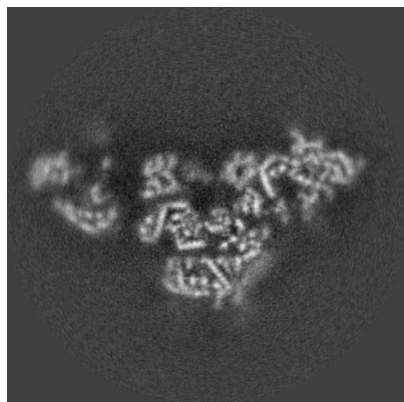


Y Index: 183

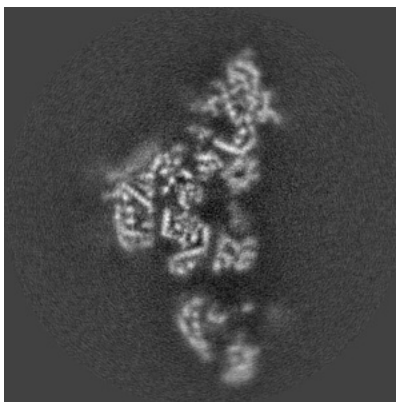


Z Index: 227

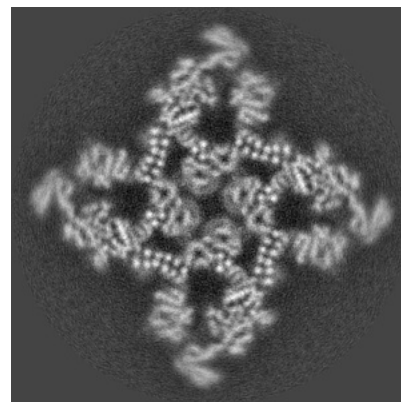
6.3.2 Raw map



X Index: 154



Y Index: 182

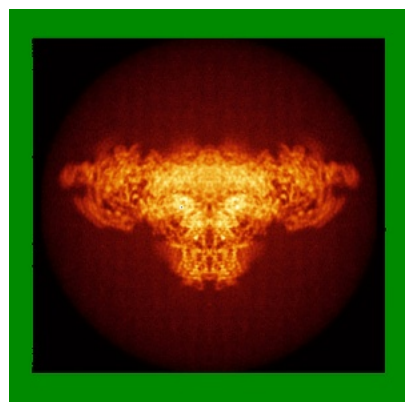


Z Index: 193

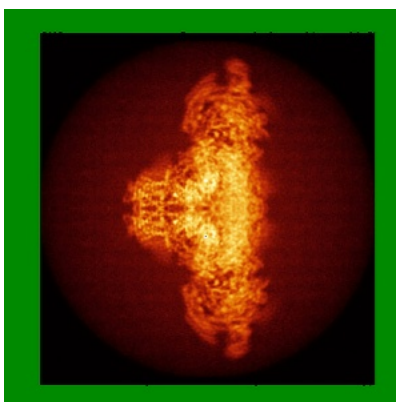
The images above show the largest variance slices of the map in three orthogonal directions.

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

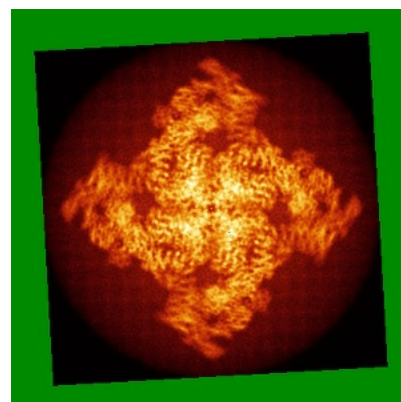
6.4.1 Primary map



X



Y

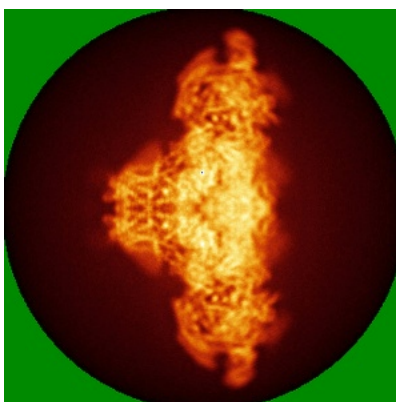


Z

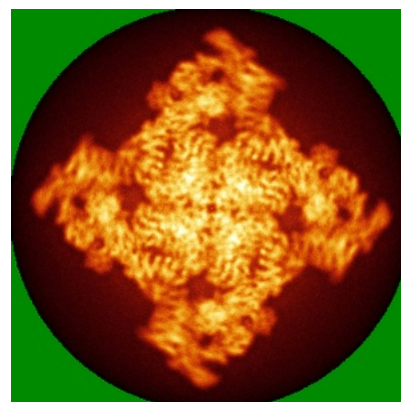
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

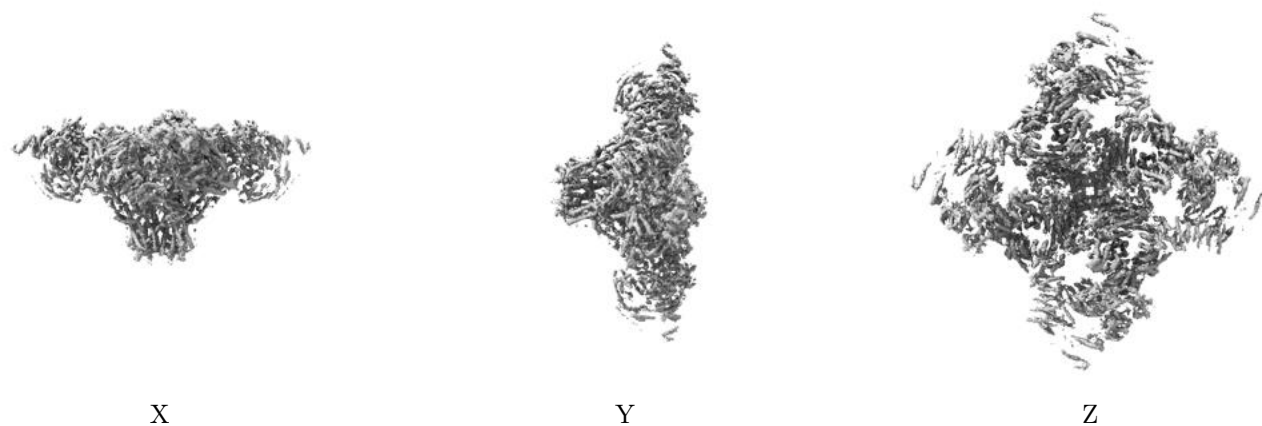
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

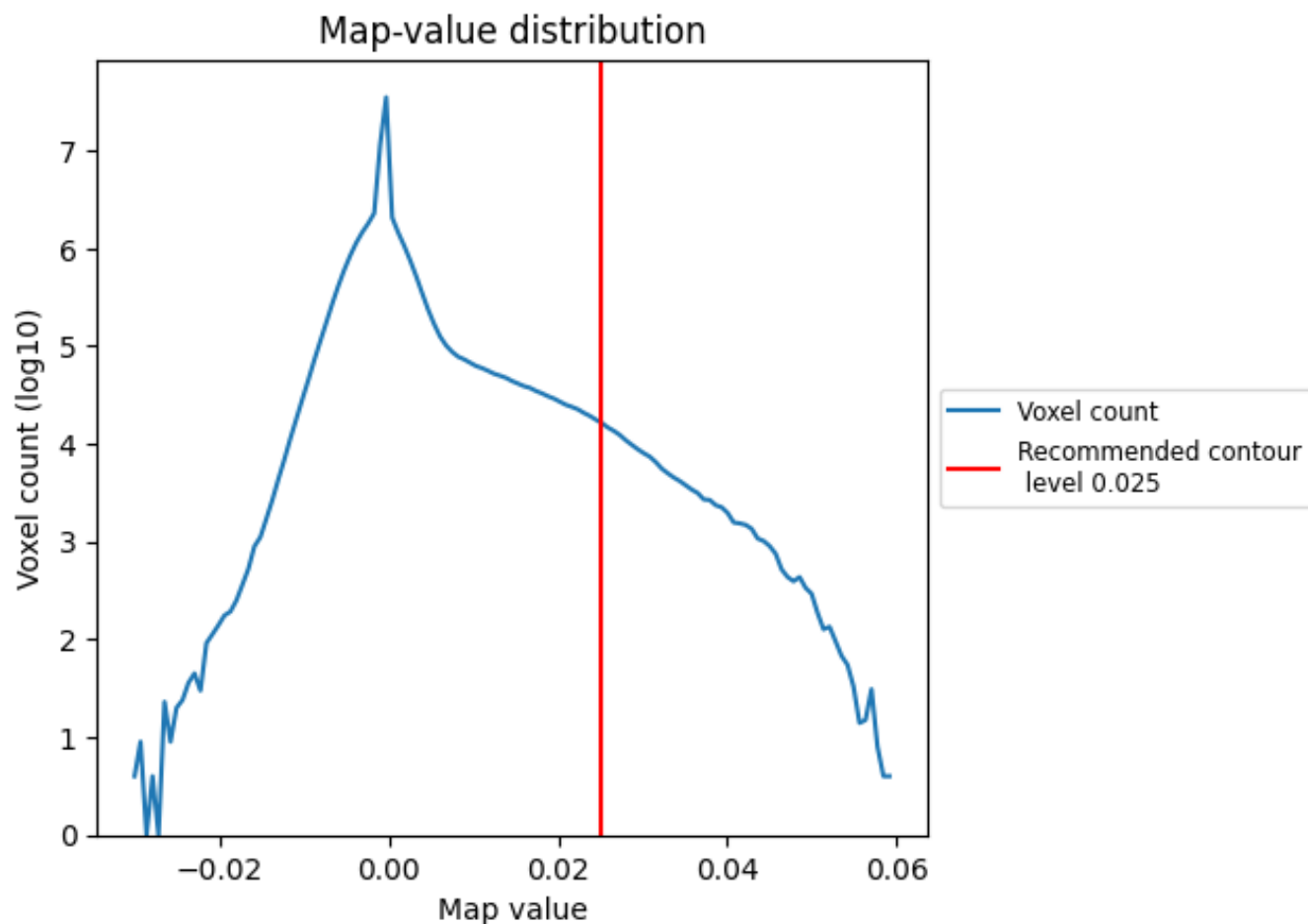
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

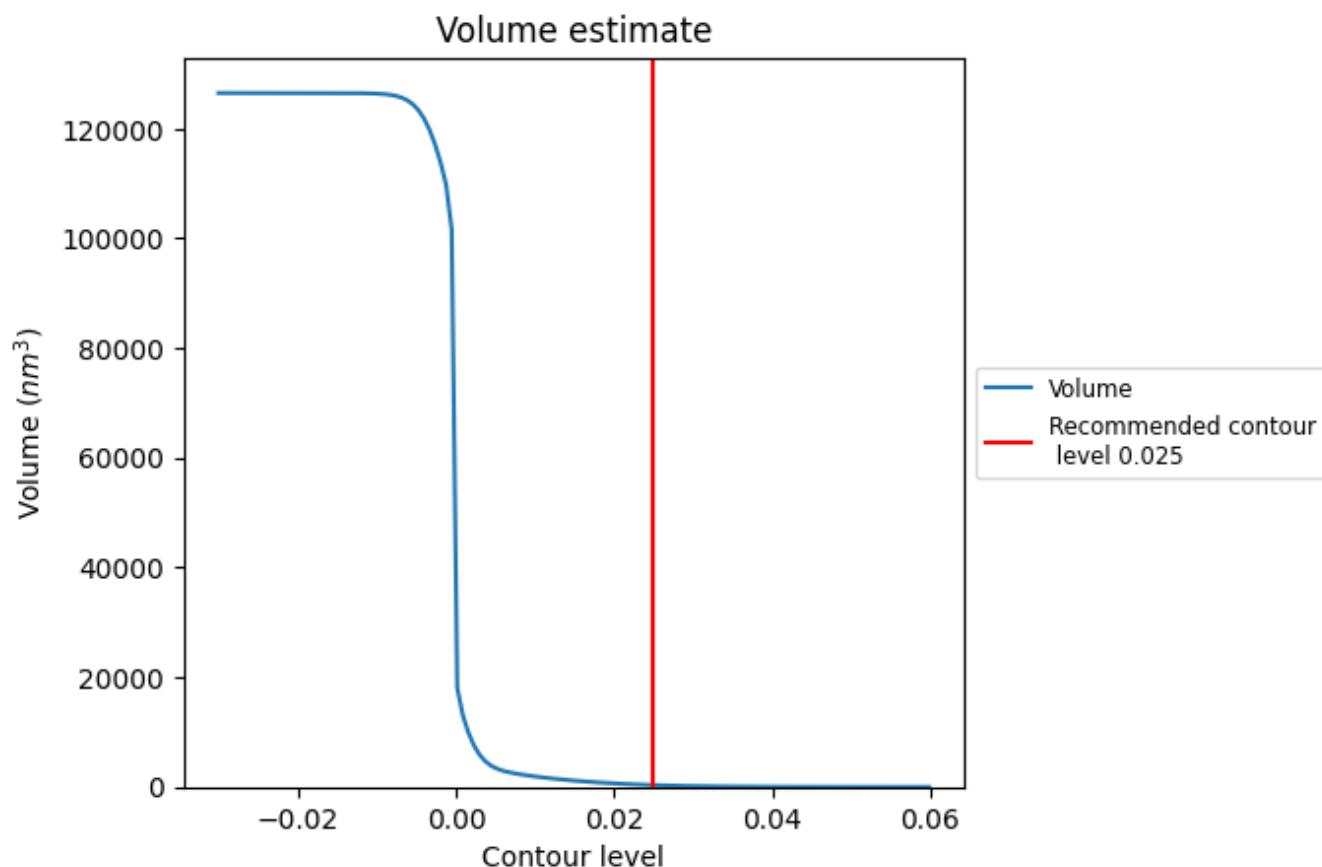
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

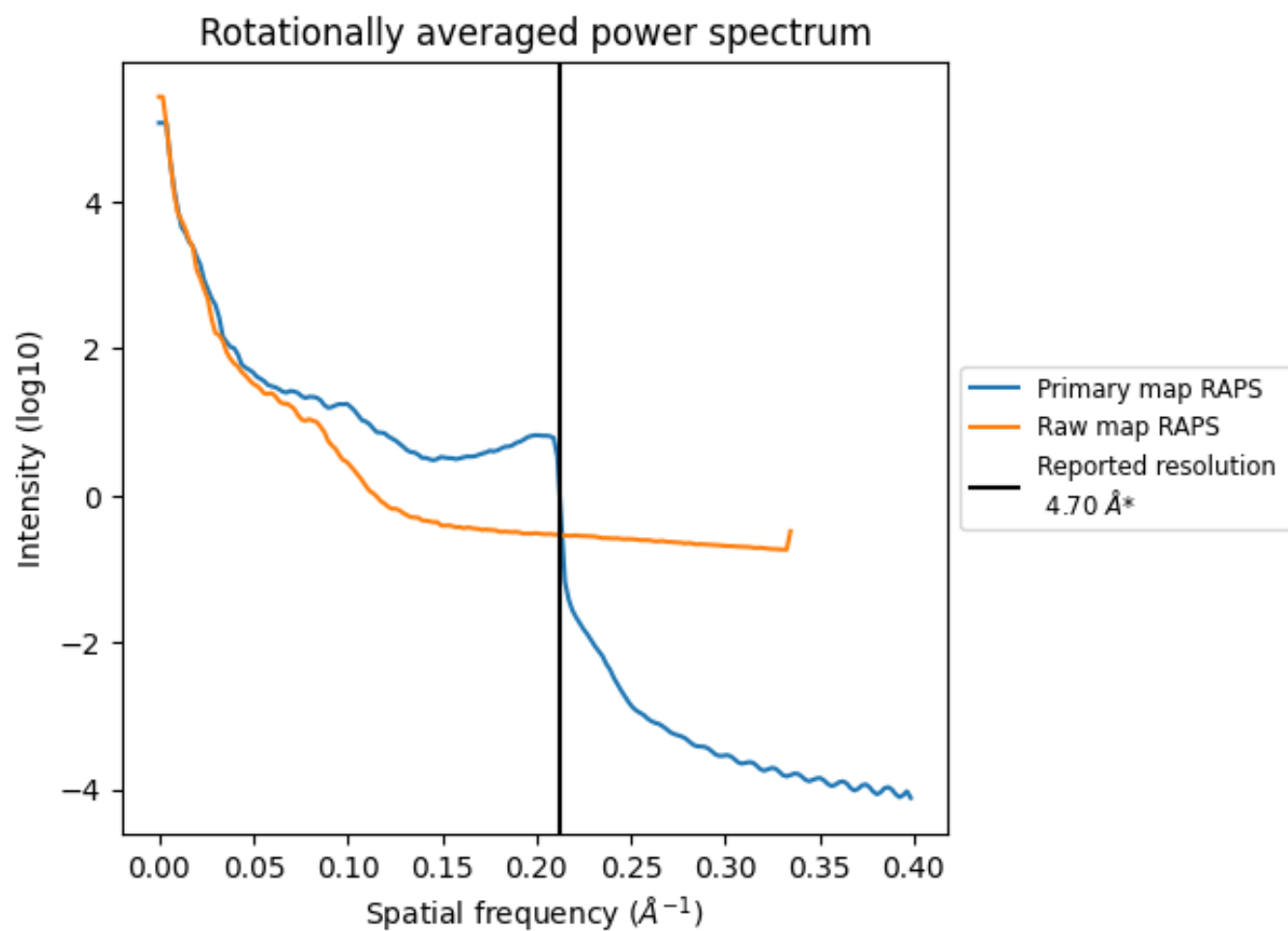
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 330 nm³; this corresponds to an approximate mass of 299 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 ⓘ

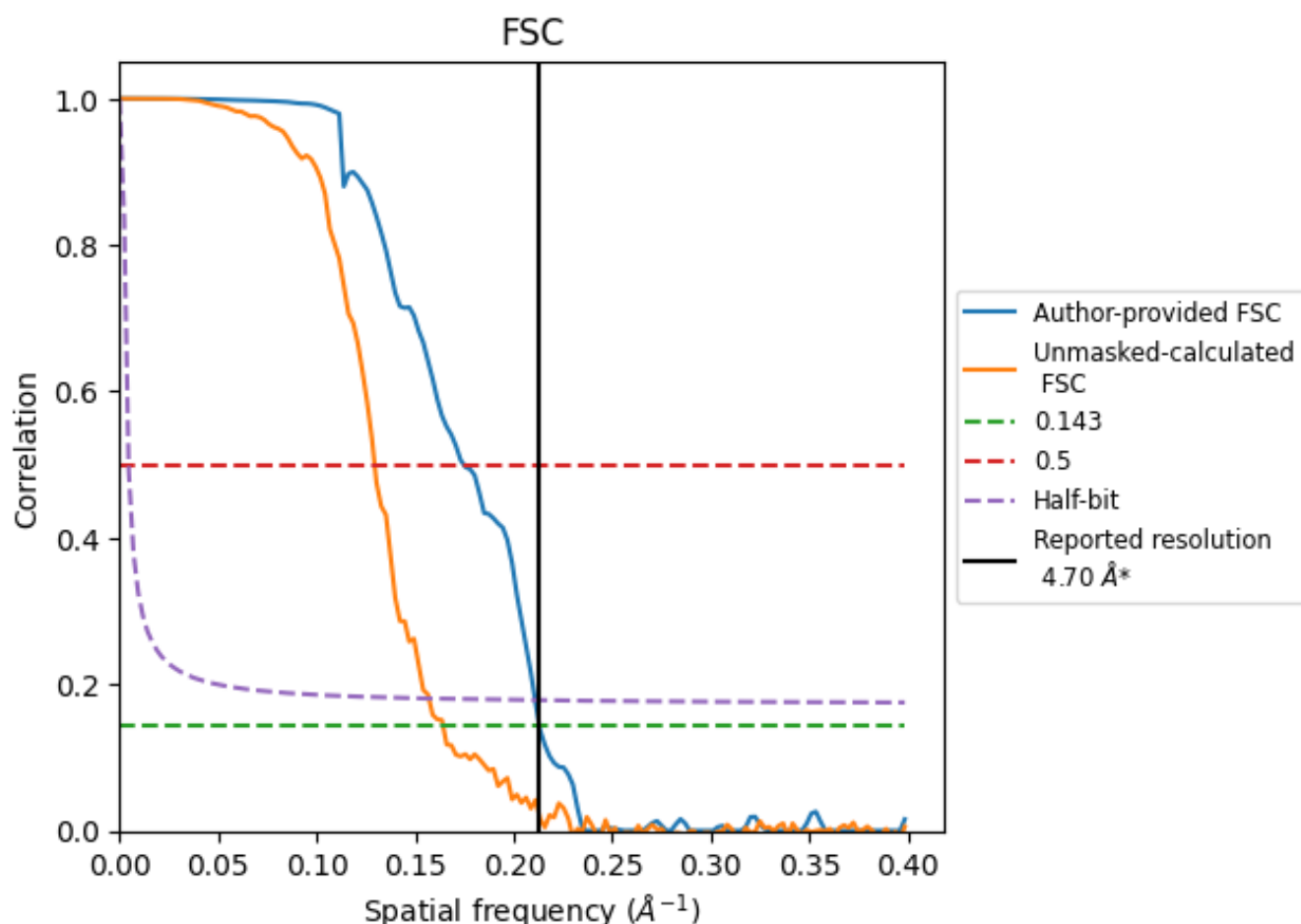


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.213 \AA^{-1}

8.2 Resolution estimates [i](#)

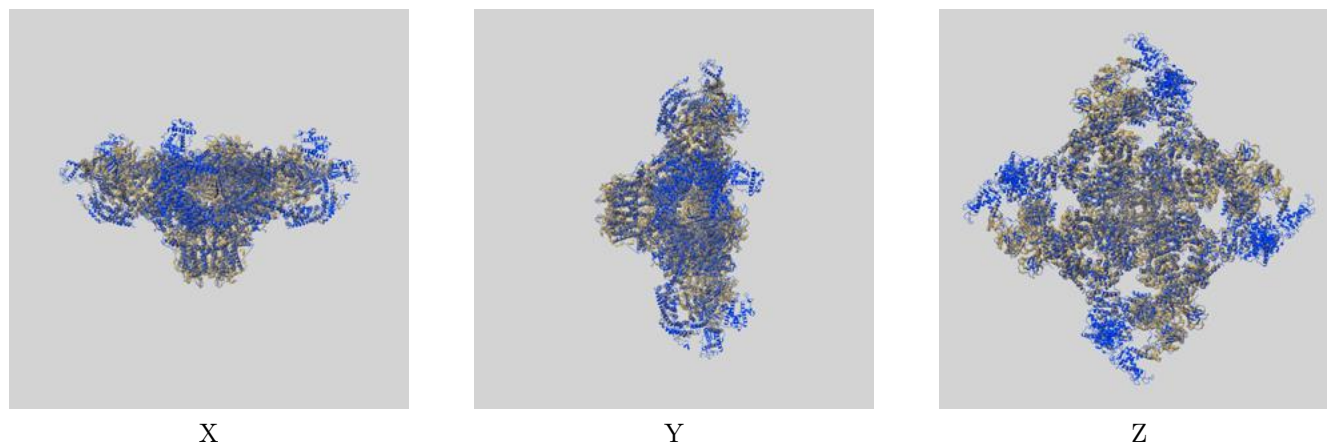
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.69	5.73	4.74
Unmasked-calculated*	6.09	7.73	6.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.09 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

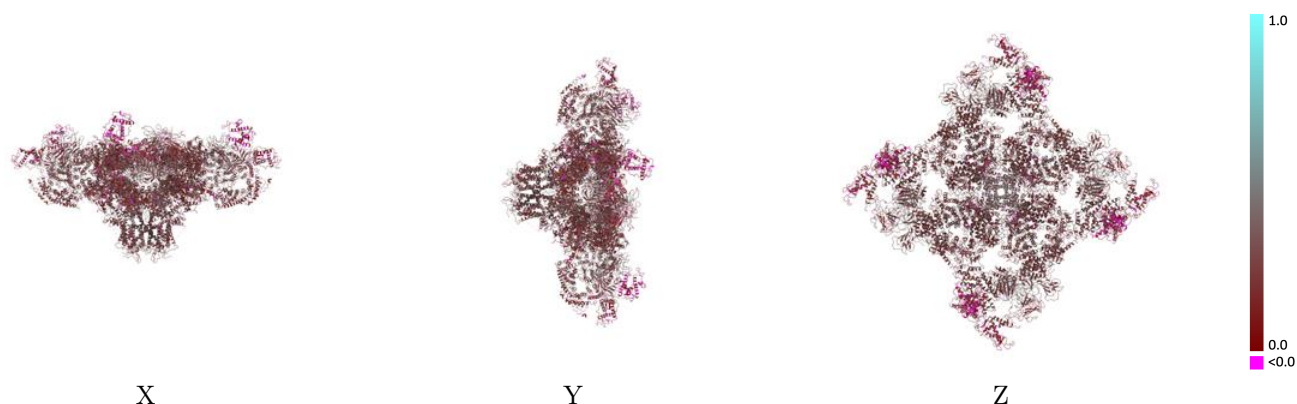
This section contains information regarding the fit between EMDB map EMD-8394 and PDB model 5TB3. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



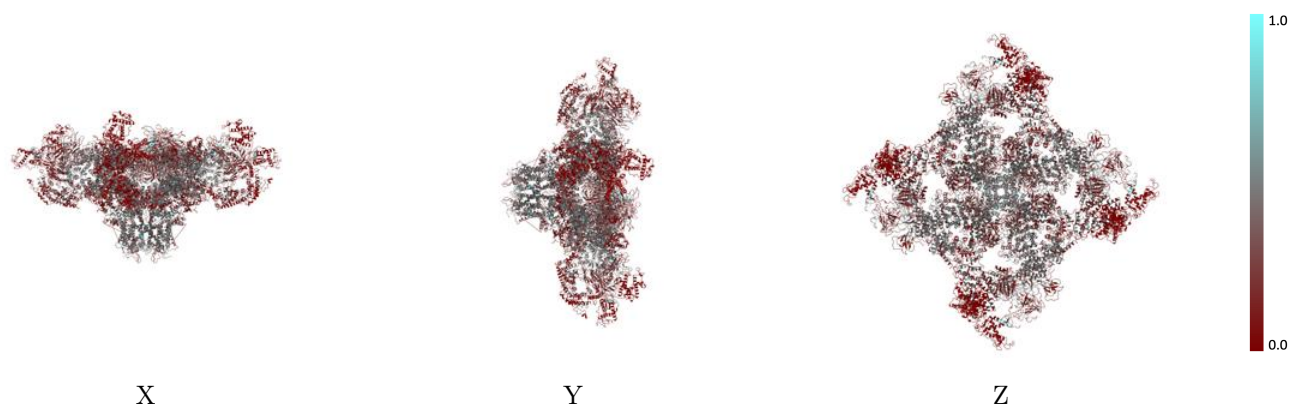
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



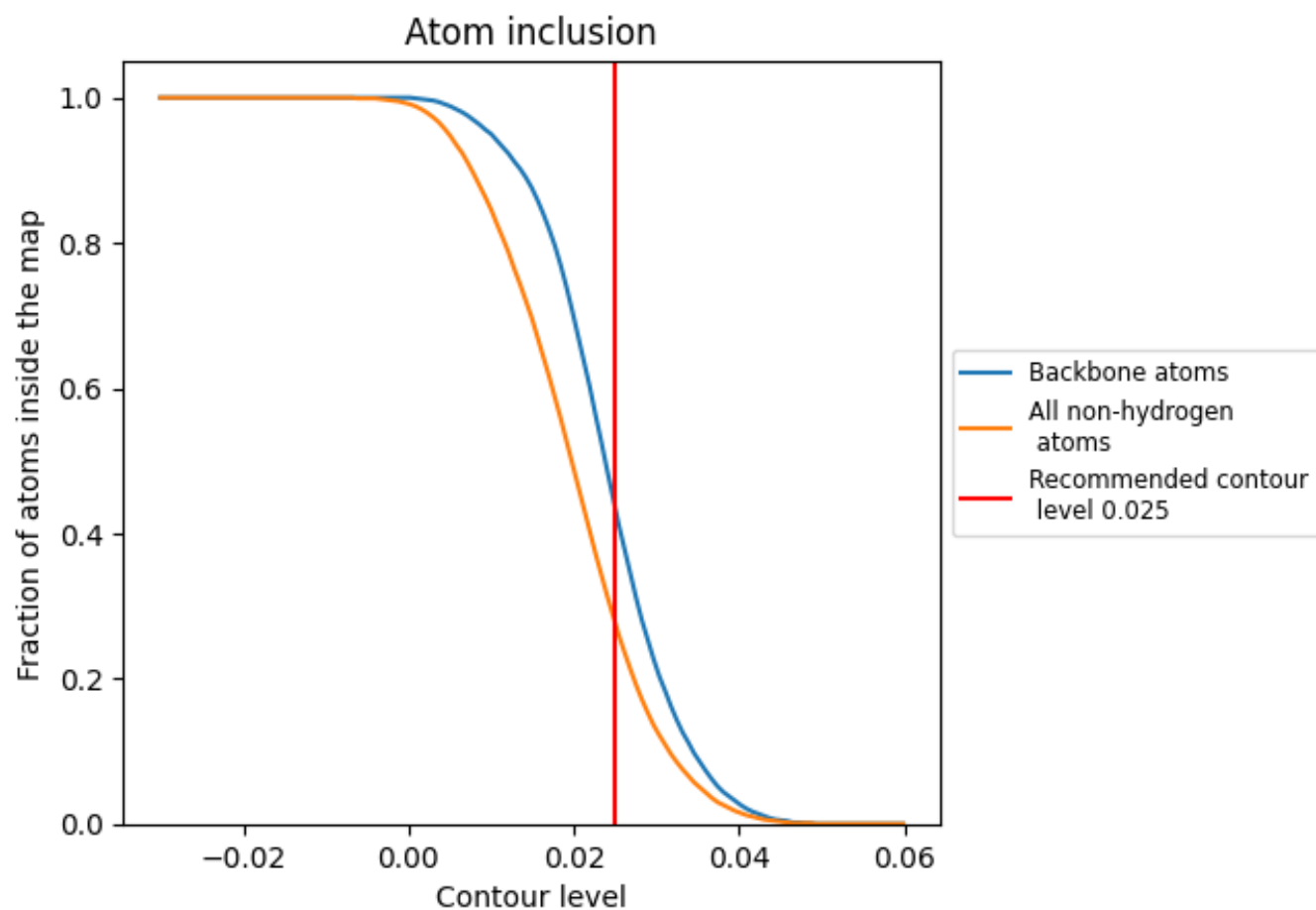
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 28% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.2760</div>	<div><div></div>0.2630</div>
A	<div><div></div>0.2390</div>	<div><div></div>0.2880</div>
B	<div><div></div>0.2780</div>	<div><div></div>0.2620</div>
E	<div><div></div>0.2770</div>	<div><div></div>0.2620</div>
F	<div><div></div>0.2380</div>	<div><div></div>0.2900</div>
G	<div><div></div>0.2770</div>	<div><div></div>0.2620</div>
H	<div><div></div>0.2390</div>	<div><div></div>0.2920</div>
I	<div><div></div>0.2770</div>	<div><div></div>0.2620</div>
J	<div><div></div>0.2390</div>	<div><div></div>0.2900</div>

1.0

0.0

<0.0