



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 07:23 PM EST

PDB ID : 7MJJ
EMDB ID : EMD-22396
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots
- Frame 37 - State 5 (S5)
Authors : Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.
Deposited on : 2020-07-31
Resolution : 4.50 Å(reported)
Based on initial model : 5TB4

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

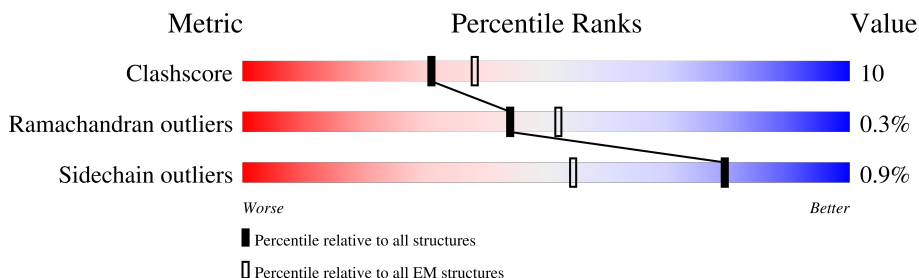
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	107	<div> <div>36%</div> <div>70%</div> <div>30%</div> </div>
1	F	107	<div> <div>52%</div> <div>73%</div> <div>27%</div> </div>
1	H	107	<div> <div>52%</div> <div>72%</div> <div>28%</div> </div>
1	J	107	<div> <div>52%</div> <div>72%</div> <div>28%</div> </div>
2	B	4687	<div> <div>39%</div> <div>70%</div> <div>19%</div> <div>11%</div> </div>
2	E	4687	<div> <div>44%</div> <div>70%</div> <div>18%</div> <div>11%</div> </div>
2	G	4687	<div> <div>49%</div> <div>70%</div> <div>19%</div> <div>11%</div> </div>
2	I	4687	<div> <div>48%</div> <div>70%</div> <div>18%</div> <div>11%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	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 type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	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	G	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of

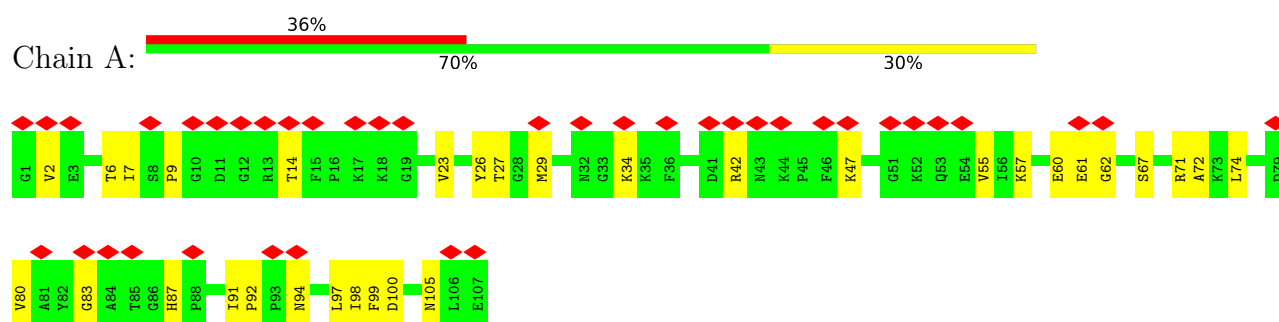
Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0

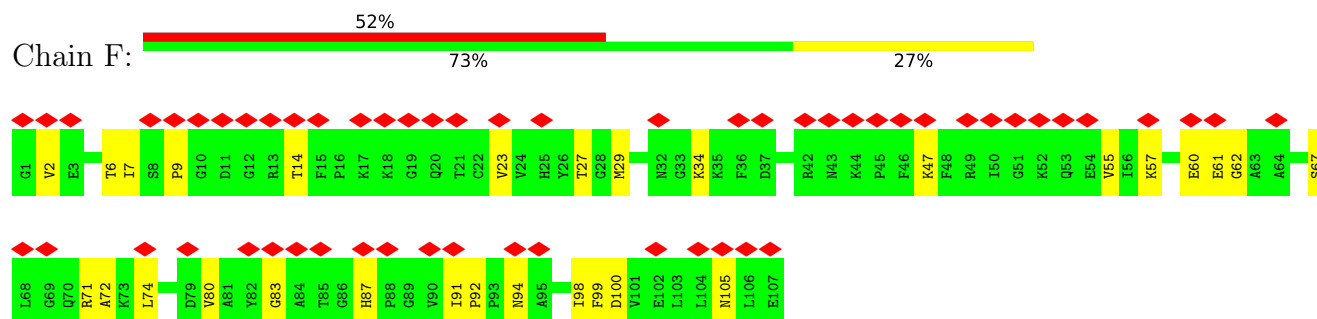
3 Residue-property plots [i](#)

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.

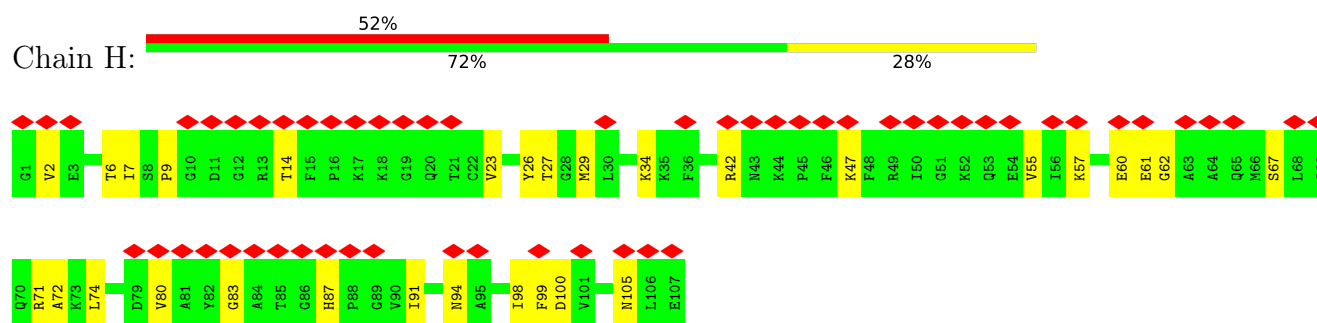
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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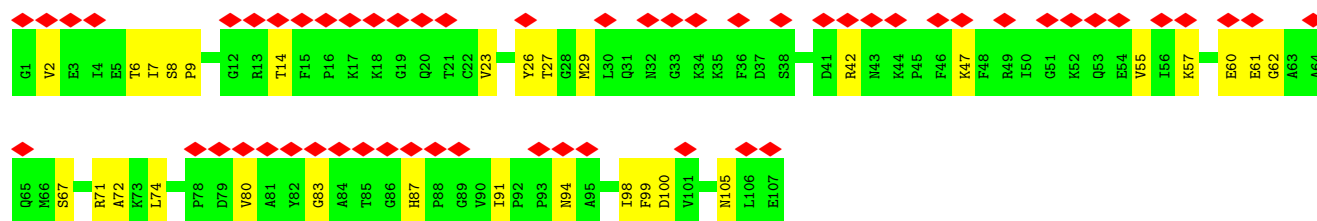


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

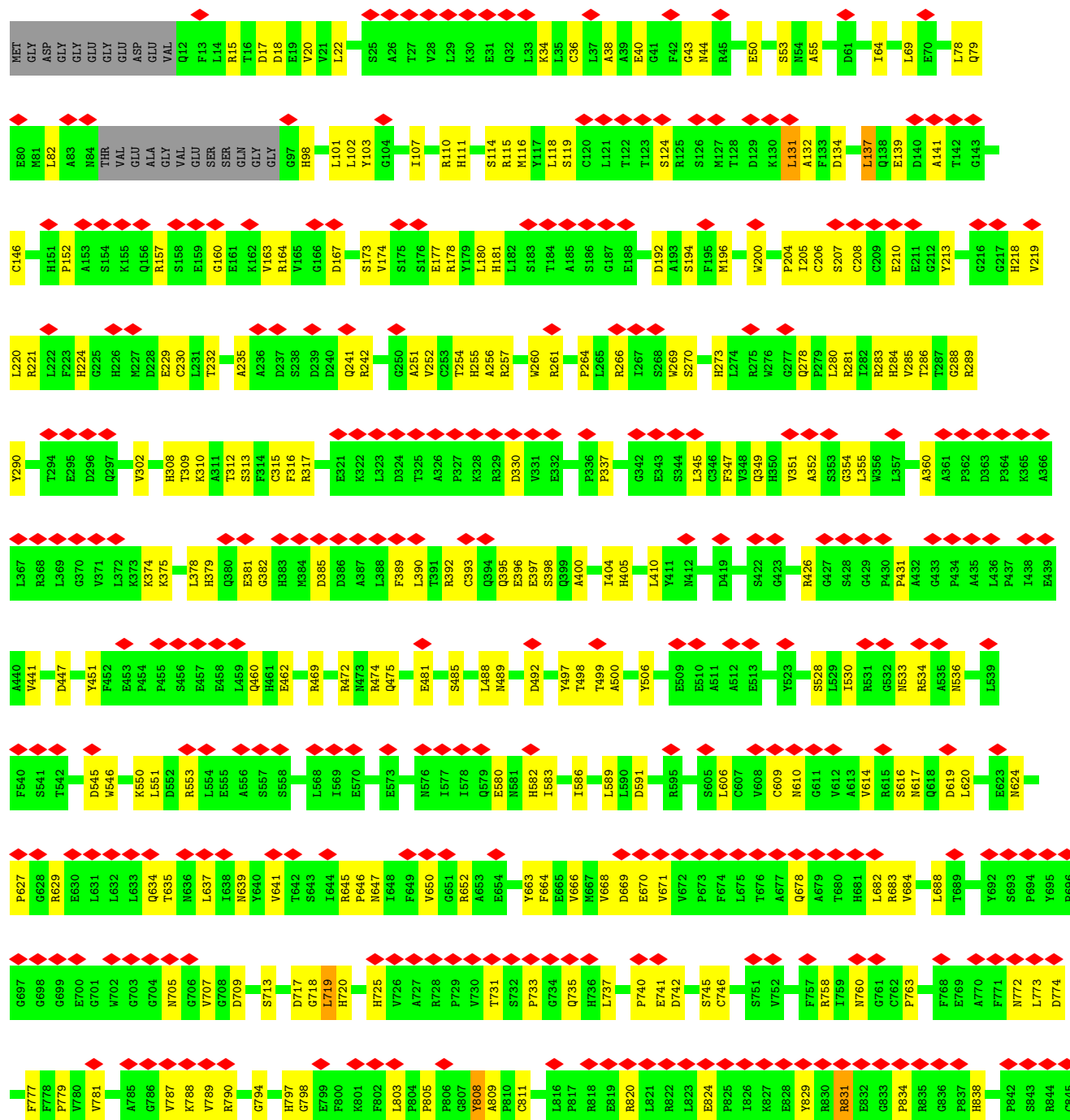
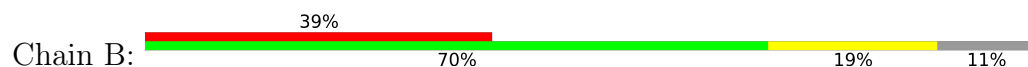


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

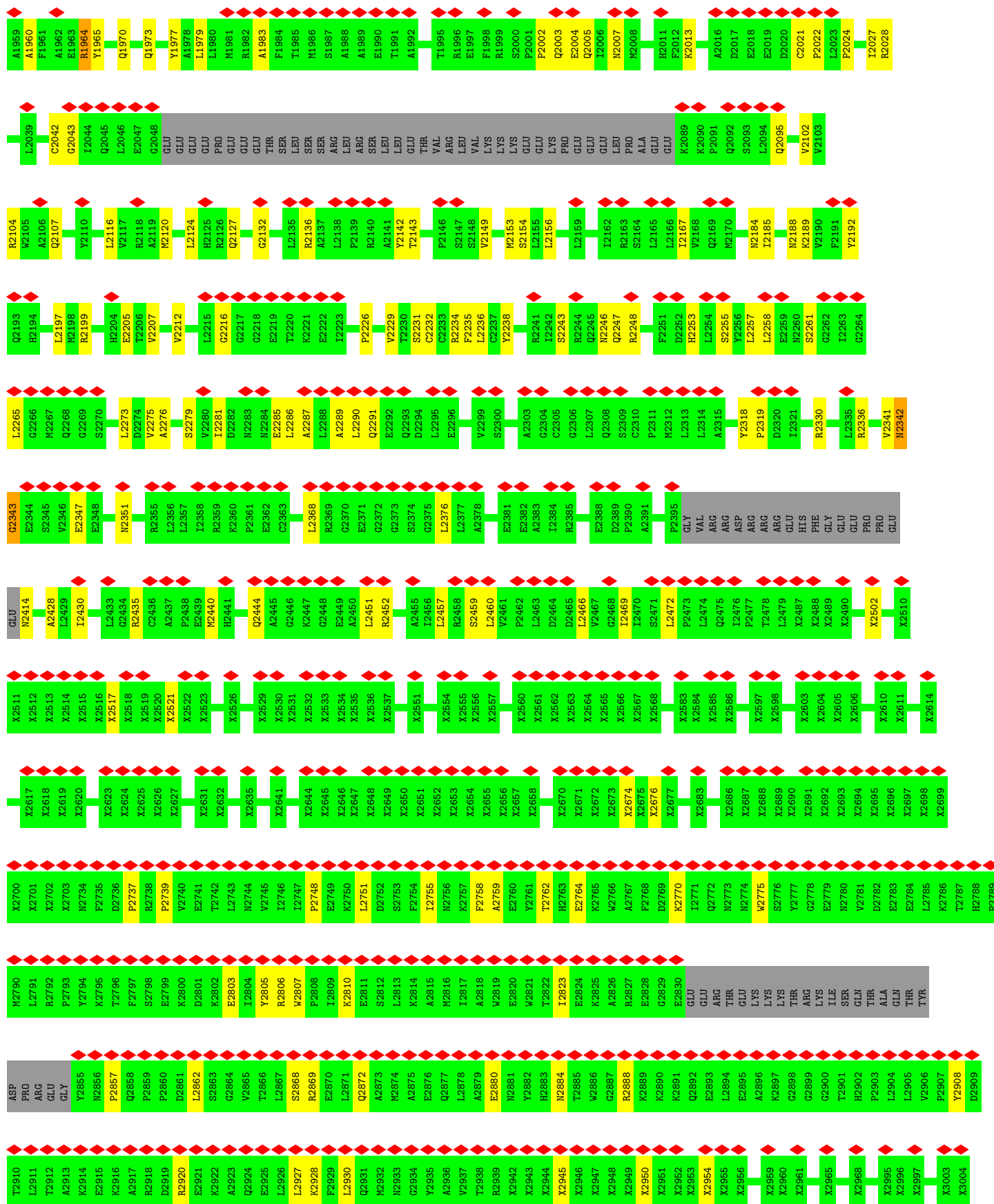


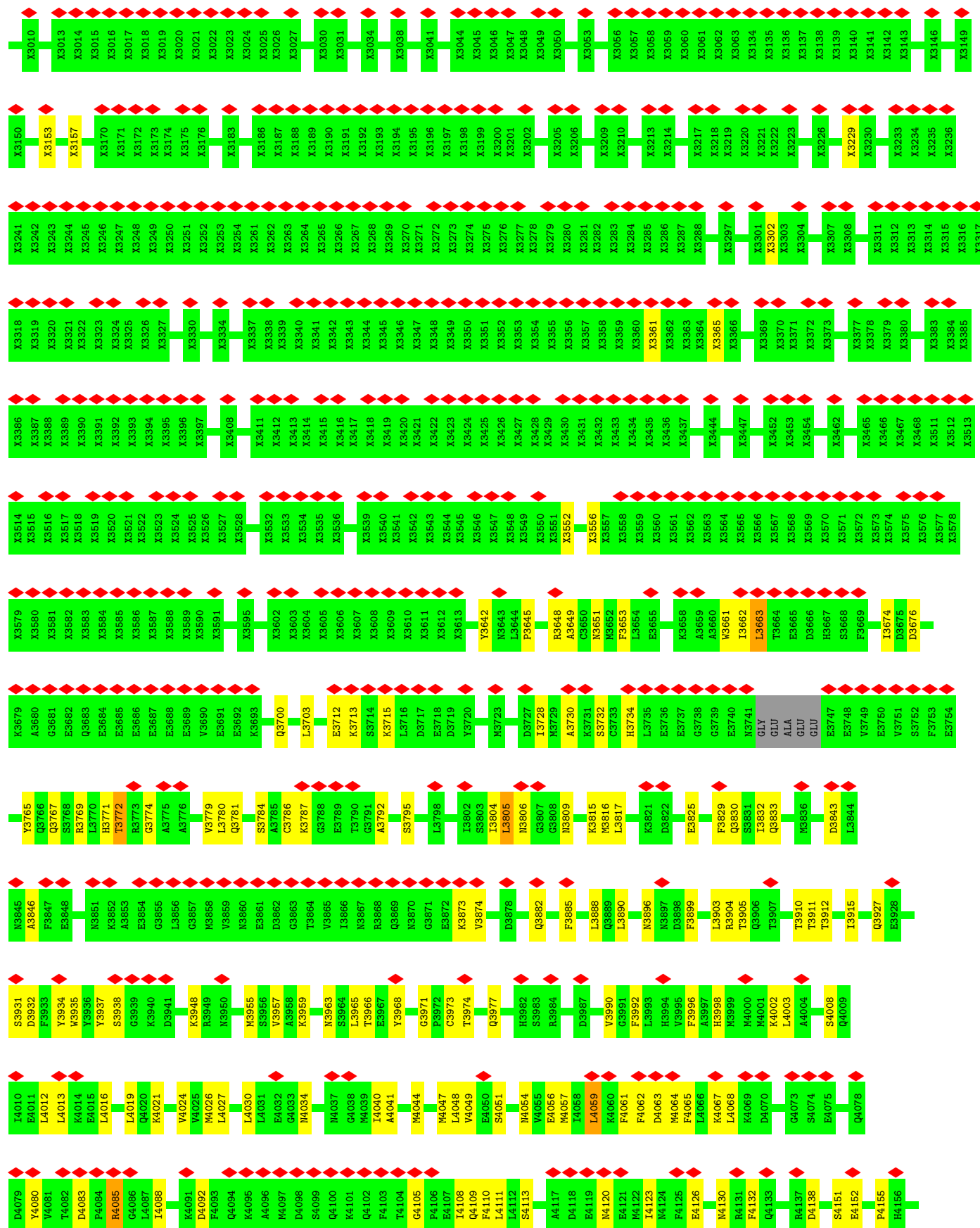


• Molecule 2: ryanodine receptor type 1



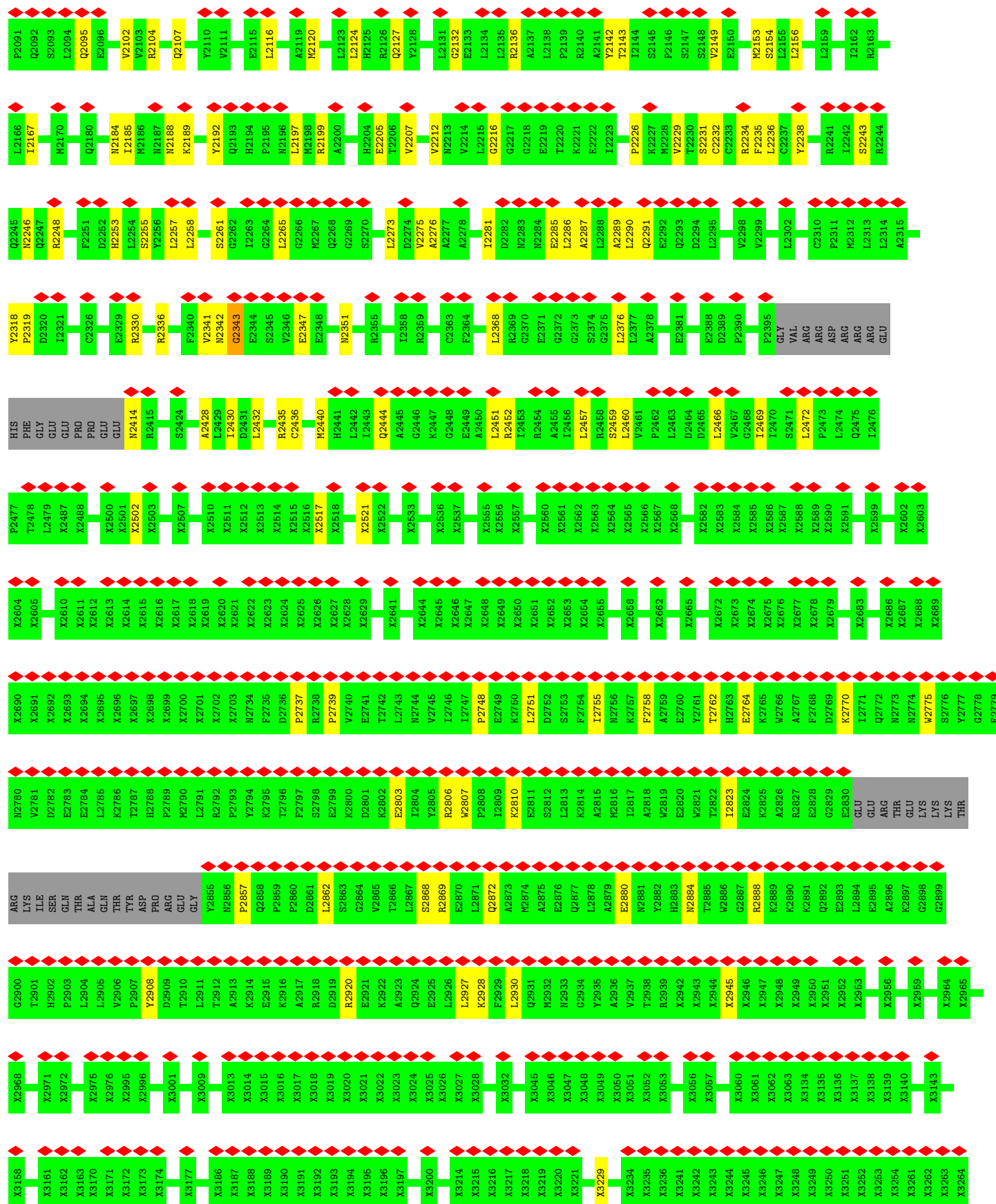




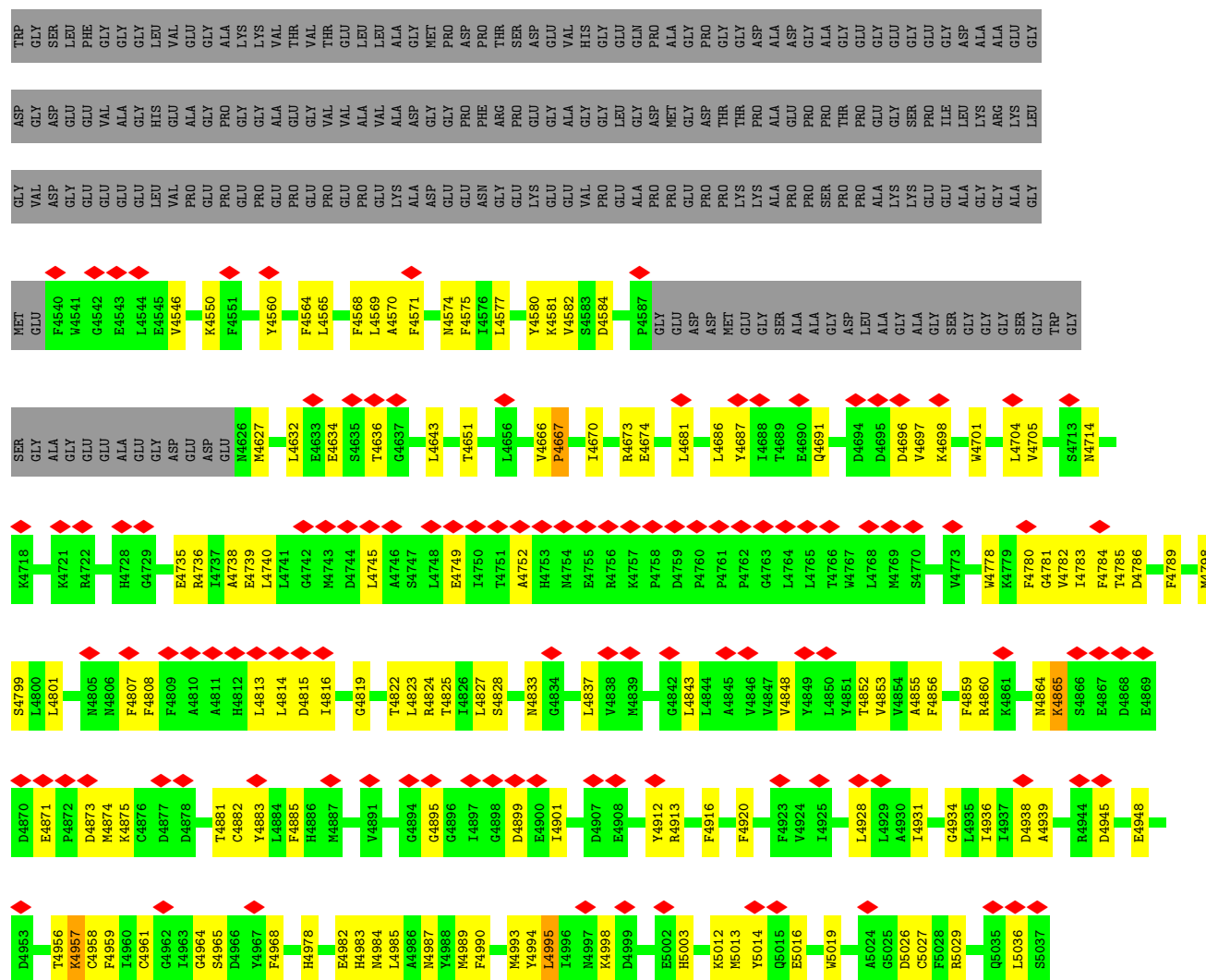




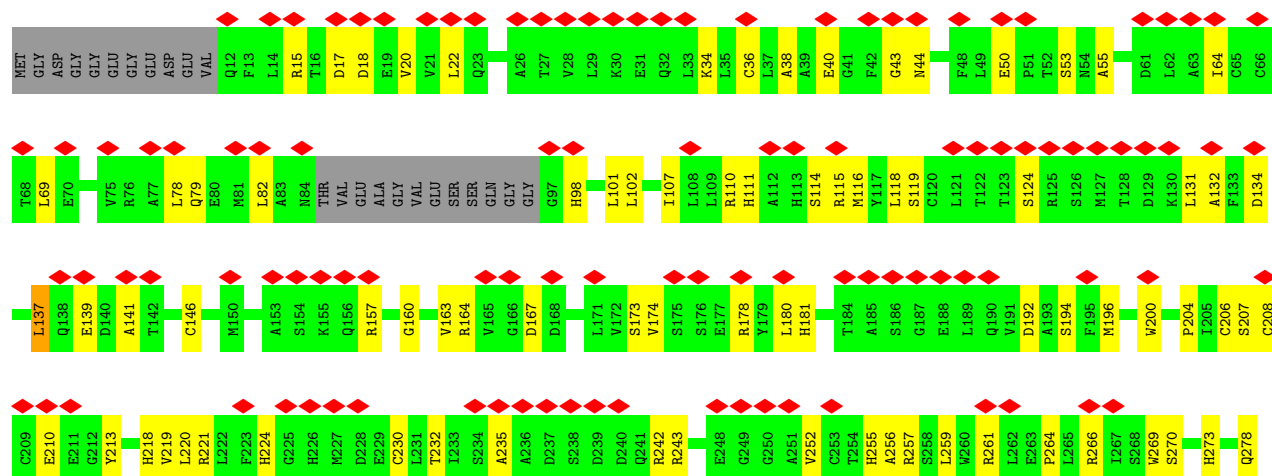
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D2020	V1935	E1873	E1805	R1743	R1671	M1610	X1532	X1445	L1242	E1181	L1039
C2021	K1936	E1874	A1806	I1744	L1676	H1611	X1533	X1446	P1243	I1182	C1040
P2022	L1807	G1U	L1807	I1745	G1677	F1612	X1534	X1447	Q1244	E1183	Q1041
L2023	R1808	G1U	R1808	T1746	N1678	L1613	X1535	X1448	F1245	I1184	A1042
D2024	D1809	G1U	D1809	L1747	N1679	L1614	X1536	X1449	E1246	G1106	V1043
E2025	L1812	G1U	L1812	F1748	V1615	V1615	X1537	X1450	P1247	P1107	R1044
L2026	R1813	G1U	R1813	P1749	G1U	THR	X1538	X1451	V1248	E1108	T1045
L2027	G1816	G1U	G1816	A1682	V1681	ARG	X1539	X1452	P1249	L1109	L1046
R2028	H1863	G1U	H1863	A1684	A1684	ARG	X1540	X1453	P1250	R1110	L1047
C2042	E1817	G1U	E1817	G1751	S1687	ALA	X1541	X1454	E1251	G1048	G1048
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L2046	Q1823	G1U	Q1823	N1756	Q1692	G1625	X1546	X1469	E1256	L1115	I1053
E2047	G1824	G1U	G1824	A1757	Q1693	G1626	X1547	X1470	V1257	G1116	E1054
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GLU	A1826	G1U	A1826	L1762	L1695	V1628	X1549	X1472	R1259	D1118	ASP
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GLU	A1828	G1U	A1828	G1764	A1697	Q1630	X1551	X1474	D1261	H1201	GLU
PRO	D1829	G1U	D1829	V1765	L1698	E1699	X1552	X1487	G1262	L1202	PRO
GLU	V1830	G1U	V1830	G1766	L1699	Q1631	X1561	X1489	T1263	M1203	SER
GLU	L1831	G1U	L1831	A1767	D1700	D1632	X1562	X1493	V1264	L1204	VAL
GLU	P1832	G1U	P1832	T1768	H1702	P1633	X1563	X1497	G1265	G1205	GLU
GLU	E1835	G1U	E1835	L1769	L1703	D1633	X1564	X1498	Q1206	Q1206	ASN
GLU	F1836	G1U	F1836	P1770	P1704	M1636	X1565	X1499	R1141	G1140	GLN
GLU	Q1837	G1U	Q1837	L1771	M1637	M1637	X1566	X1499	P1142	F1139	SER
GLU	F1838	G1U	F1838	R1772	A1638	A1638	X1567	X1499	G1269	G1140	TRP
GLU	V1839	G1U	V1839	P1773	L1639	L1639	X1568	X1500	L1270	W1143	D1070
GLU	P1840	G1U	P1840	H1774	H1640	H1640	X1569	X1501	R1271	Q1144	R1071
GLU	V1841	G1U	V1841	H1775	I1641	I1641	X1570	X1502	L1272	L1211	V1072
GLU	L1842	G1U	L1842	H1776	G1710	G1710	X1571	X1503	L1273	R1212	I1074
GLU	K1843	G1U	K1843	H1777	Y1711	E1643	X1572	X1504	A1273	F1213	F1073
GLU	L1844	G1U	L1844	S1778	Y1712	E1644	X1573	X1505	H1274	F1214	I1075
GLU	V1845	G1U	V1845	P1779	D1713	R1646	X1574	X1506	X1278	A1215	R1076
GLU	L1848	G1U	L1848	P1780	S1717	C1647	X1575	X1507	X1279	I1216	A1077
GLU	V1849	G1U	V1849	C1781	I1718	M1648	X1576	X1508	X1280	C1217	E1078
GLU	M1850	G1U	M1850	G1782	H1719	D1649	X1577	X1509	X1282	G1218	K1079
GLU	G1851	G1U	G1851	V1783	E1721	I1650	X1578	X1510	X1283	L1219	S1080
GLU	I1852	G1U	I1852	A1784	S1722	L1651	X1579	X1511	X1286	L1219	V1081
GLU	F1853	G1U	F1853	A1785	A1723	E1652	X1580	X1512	X1289	E1221	V1082
GLU	G1854	G1U	G1854	L1786	C1724	L1653	X1581	X1513	X1290	G1222	V1083
GLU	D1855	G1U	D1855	P1787	R1725	L1654	X1582	X1514	X1291	F1223	Q1084
GLU	D1856	G1U	D1856	A1788	S1726	E1655	X1583	X1515	X1292	E1224	S1085
GLU	E1857	G1U	E1857	ALA	R1727	R1656	X1584	X1516	X1293	P1225	G1086
GLU	E1858	G1U	E1858	GLY	M1730	D1657	X1585	X1517	X1294	F1226	G1087
GLU	V1859	G1U	V1859	VAL	L1657	L1658	X1586	X1518	X1295	A1227	V1088
GLU	K1860	G1U	K1860	ALA	D1658	L1659	X1587	X1519	X1296	I1228	V1089
GLU	Q1861	G1U	Q1861	E1793	Q1660	Q1660	X1588	X1520	X1297	D1172	F1090
GLU	M1865	G1U	M1865	A1794	H1663	H1663	X1589	X1521	X1298	M1230	E1091
GLU	I1866	G1U	I1866	P1795	Y1734	E1596	X1590	X1522	X1299	Q1231	F1092
GLU	E1867	G1U	E1867	A1796	I1735	Q1597	X1591	X1523	X1300	R1232	E1093
GLU	F1868	G1U	F1868	P1797	V1736	L1598	X1592	X1524	X1301	P1233	A1094
GLU	E1869	G1U	E1869	L1738	H1665	H1665	X1593	X1525	X1302	V1234	V1095
GLU	V1870	G1U	V1870	L1739	T1666	T1666	X1594	X1526	X1303	T1235	T1096
GLU	F1871	G1U	F1871	T1739	L1667	L1667	X1595	X1527	X1304	T1236	T1097
GLU	K2089	G1U	K2089	P1800	R1668	R1668	X1596	X1528	X1305	W1237	
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	E2018	G1U	E2018	F1803			X1599	X1531	X1308	K1240	







• Molecule 2: ryanodine receptor type 1



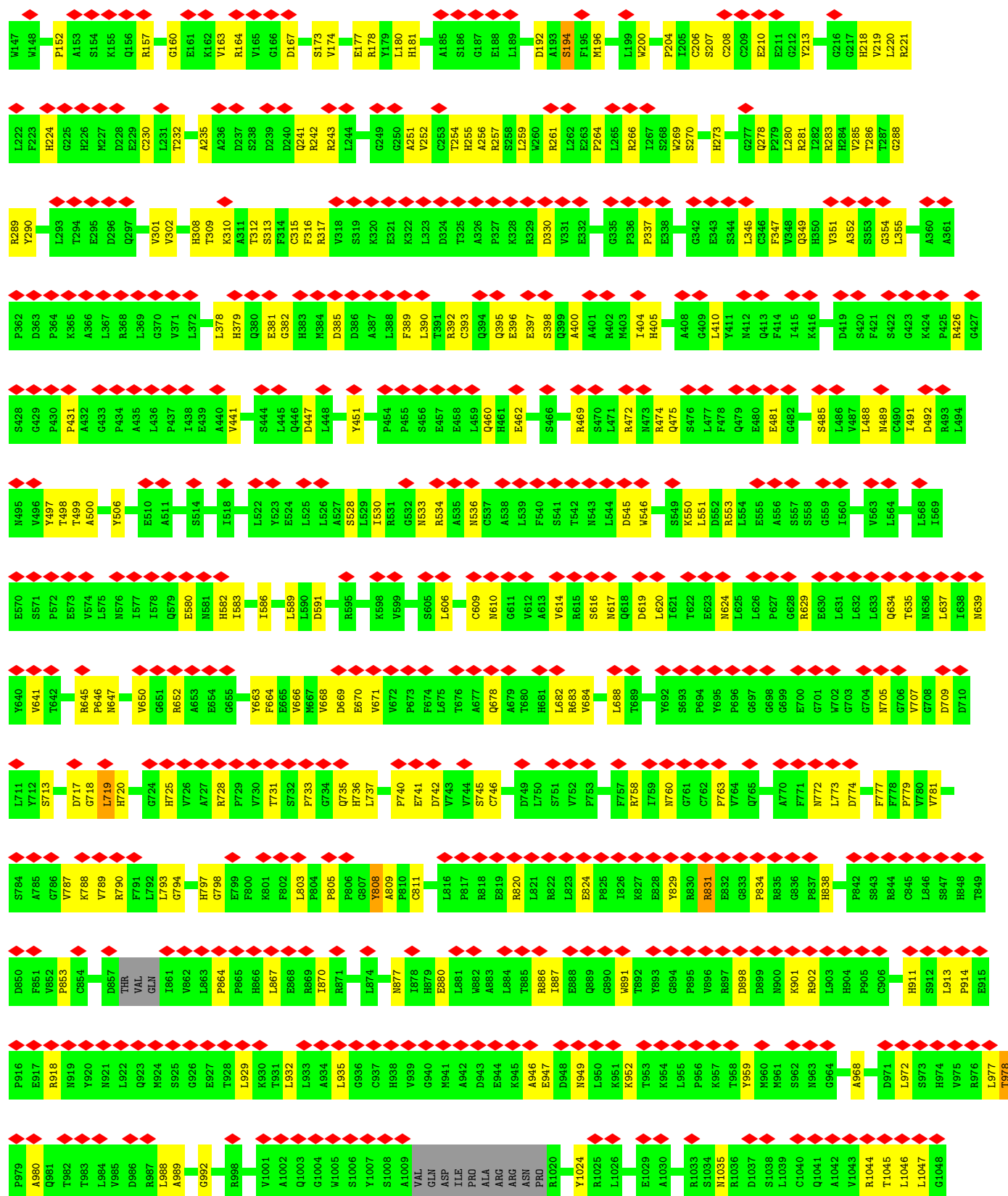
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V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	Y1122	V1123	F1124	N1125		F1139	G1140	R1141		Q1144	S1145	G1146	D1147	V1149		M1152	I1153	D1154	L1155	T1156	E1157	N1158		I1161	F1162	L1163	L1164	N1165		V1168		G1174	S1175	E1176		F1179	R1180	E1181	I1182			
F347	V348	Q349	H350	F351	A352	S353	G354	L355		Y359	A360	A361	P362	D363	P364	K365	A366	L367	R368	L369	G370	V371	L372	K373	K374	K375		L378	H379	Q380	E381	G382		A511	S514	W515	K516	V519	L522	Y523		L526	A527	S528	L529	I530	R531	G532	N533	R534	A535	N536		C537	A538	L539	F540	S541	T542		
Y411	N412	Q413	F414	I415	K416	G417	L418	D419	S420	F421	S422	G423	K424	P425	R426	G427	S428	G429	P430	A431	A432	G433	P434	A435	L436	P437	I438		V441	I442	L443	S444	L445	Q446	D447	L448	I449	G450	F452	E453	P454	P455	S456	E457	E458	L459	Q460	H461	E462	E463		S466	K467	A468	R469		R472	N473			
R474	Q475	S476	L477	F478	Q479	E480	E481	G482	M483	L484	S485	L486	L487	L488	N489	C490	I491	D492	R493	L494	N495	Y496	Y497	T498	T499	A500		F503	Y506		A511	S514	W515	K516	V519	L522	Y523		L526	A527	S528	L529	I530	R531	G532	N533	R534	A535	N536		C537	A538	L539	F540	S541	T542					
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L688		Y692	S693	P694	Y695	P696		W772	L773	D774		F777	F778	F779	W780	W781		S784	A785	G786	W787	K788	W789	R790		L793	G794		H797	G798	E799	F800	R801	F802	L803	P804	P805	P806	G807	Y808	A809	P810	C811		L816	P817	R818	E819	R820	L821	R822	L823	E824	P825	I826	K827	E828	Y829	R830		
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D898	D899	N900	K901	R902	L903	H904	P905		H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	M924	S925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	M941	A942	D943	E944	K945	A946	E947	D948	N949		K952	T953	K954	L955	P956	K957	T958	Y959	M960	N961	S962		
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L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	L1051	N1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	VAL	ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	L1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	T1082	V1083	Q1084	S1085	G1086	R1087	W1088	Y1089	F1090	E1091	F1092	E1093	A1094	V1095	T1096		R1101				
V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	Y1122	V1123	F1124	N1125		F1139	G1140	R1141		Q1144	S1145	G1146	D1147	V1149		M1152	I1153	D1154	L1155	T1156	E1157	N1158		I1161	F1162	L1163	L1164	N1165		V1168		G1174	S1175	E1176		F1179	R1180	E1181	I1182			

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F1612	L1613	Q1614	V1615	GLU	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	W1625	W1626	A1627	V1628	Q1629	C1630	Q1631	D1632	P1633	L1634	T1635	M1636	M1637	A1638	L1639	H1640	E1643	M1644	N1645	R1646	C1647	M1648	D1649	L1650	L1651	E1652	L1653	E1654	E1655	R1656	L1657	D1658	L1659	Q1660	R1661	F1662	H1663	S1664	H1665	T1666	L1667	R1668	L1669	Y1670	R1671	
L1676	G1677	M1678	N1679	R1680	V1681	A1682	H1683	A1684	S1687	D1690	Q1691	A1692	Q1693	L1694	L1695	H1696	A1697	L1698	E1699	D1700	A1701	H1702	M1636	L1703	P1704	G1705	P1706	L1707	R1708	A1709	G1710	Y1711	Y1712	D1713	S1717	I1718	H1719	L1720	E1721	S1722	A1723	C1724	R1725	S1726	R1727	F1728	S1729	M1730	L1731	S1732	E1733	Y1734	L1735	V1736	P1737	L1738	T1739	
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L1804	E1805	A1806	L1807	R1808	A1811	L1812	R1813	M1814	L1815	G1816	E1817	A1818	V1819	R1820	D1821	G1822	G1823	Q1824	H1825	A1826	R1827	D1828	P1829	V1830	E1835	F1836	Q1837	F1838	V1839	P1840	V1841	L1842	K1843	L1844	L1848	L1849	V1850	M1851	G1852	I1853	F1854	G1855	D1856	E1857	D1858	M1859	T1862	L1863	K1864	M1865	I1866	V1870	F1871	T1872				
E1873	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP	GLU	GLU	GLU	GLU	ASP	GLU	GLU	GLU	GLU	LYS	ASP	ALA	GLU	LYS	P1839	P1840	V1841	L1842	K1843	L1844	L1848	L1849	V1850	M1851	G1852	I1853	F1854	G1855	D1856	E1857	D1858	M1859	T1862	L1863	K1864	M1865	I1866	V1870	F1871	T1872			
V1935	K1936	L1937	C1940	H1941	E1944	Y1945	D1948	Q1949	E1950	L1951	Q1952	H1953	R1954	V1955	L1958	A1959	A1960	R1964	Y1965	Q1970	Q1973	Y1977	A1978	L1979	L1980	M1981	R1982	A1983	F1984	T1985	M1986	S1987	A1988	A1989	E1990	T1991	A1992	T1995	R1996	E1997	F1998	P2002	Q2003	E2004	Q2005	I2006	N2007	M2008										
L2009	L2010	H2011	F2012	K2013	A2016	D2017	E2018	E2019	D2020	C2021	P2022	L2023	P2024	E2025	D2026	I2027	R2028	C2042	G2043	L2044	Q2045	L2046	E2047	G2048	GLU	GLU	GLU	GLU	PRO	GLU	GLU	GLU	THR	SER	LEU	SER	SER	ARG	LEU	SER	ARG	SER	LEU	GLU	THR	VAL	ARG	LEU	VAL	LYS	LYS	GLU	GLU	LYS	PRO	GLU		
GLU	GLU	PRO	ALA	GLU	K2089	K2090	P2091	Q2092	S2093	L2094	Q2095	E2096	V2102	V2103	R2104	W2105	A2106	Q2107	E2108	D2109	Y2110	V2111	E2115	L2116	V2117	R2118	A2119	M2120	F2121	S2122	GLU	GLU	L2124	R2125	R2126	Q2127	L2131	G2132	E2133	L2134	L2135	R2136	A2137	L2138	P2139	R2140	A2141	Y2142	T2143	I2144	S2145	P2146	S2147	V2148	V2149			
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L2433	G2434	R2435	C2436	A2437	M2440	H2441	L2442	I2443	Q2444	A2445	G2446	K2447	G2448	E2449	A2450	L2451	R2452	L2453	R2454	A2455	I2456	L2457	R2458	S2459	V2461	L2463	D2464	D2465	L2466	V2467	G2468	I2469	I2470	S2471	L2472	P2473	L2474	Q2475	I2476	P2477	T2478	L2479	X2487	X2488	X2499	X2500	X2501	X2502	X2503	X2506	X2507	X2508	X2509	X2510							
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E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	G2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	N2874	E2875	E2876	Q2877	L2878	A2879	E2880	N2881	T2882	H2883	N2884	T2885	T2886	G2887	R2888	K2889			
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X3050	X3051	X3052	X3053	X3056	X3057	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3141	X3142	X3143	X3158	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3177	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3198	X3199	X3200	X3201	X3202	X3203	X3204	X3205	X3206	X3207	X3208	X3209	X3291	X3292	X3295	X3296	X3297	X3298	X3299	X3300	X3301

H4245	K4095	K3953	E3872	I3802	E3740	D3675	X3573	X3439	X3369	X3302
A4248	A4096	A3954	K3873	S3803	E3741	D3676	X3574	X3458	X3370	X3303
A4249	M4097	M3955	V3874	I3804	GLU		X3575	X3459	X3371	
	D4098	S3956	M3875	N3805	ALA		X3576	X3464	X3372	X3309
	A4099	V3957	A3876	N3806	GLU		X3577	X3465	X3373	X3310
S4252	S4099	A3958	D3877	G3807	GLU		X3578	X3466	X3374	X3311
E4253	Q4100	K3959	D3878	G3808			X3579	X3467	X3375	X3312
PRO	K4101		E3879	N3809	E3747		X3580	X3468	X3376	X3313
GLU	Q4102	F3962	F3880		E3748		X3581	X3469	X3377	X3314
GLY	F4103	N3963	T3881	Q3813	E3749		X3582	X3470	X3378	X3315
GLU	F4104	S3964		K3814	V3750		X3583	X3471	X3379	X3316
PRO	G4105	L3965	Q3882	K3815	V3751		X3584	X3472	X3380	X3317
ASP	P4106	E3967		M3816	S3752		X3585	X3473	X3381	X3318
ASP	E4107	Y3968	F3885	L3817	F3753		X3586	X3474	X3382	X3319
GLU	I4108	I3969	R3886	D3818	F3754		X3587	X3475	X3383	X3320
ASP	Q4109	Q3970	F3887	Y3819	E3755		X3588	X3476	X3384	X3321
GLU	F4110	G3971	L3888	L3820	K3756		X3589	X3477		
GLY	I4181	C3972	Q3889				X3590	X3478	X3387	X3324
E4182	L4112	T3974	L3900	E3825	E3759		X3591	X3479	X3388	X3325
GLY	S4113		E3993	F3829	K3760		X3592	X3480	X3389	
ALA		Q3977	N3896	Q3830	Q3761		X3593	X3481	X3390	X3328
ALA	A4116	L3980		S3831	R3762		X3594	X3482	X3391	
ALA	A4117	A3981	F3999	I3832	L3763		X3595	X3483	X3392	
GLY	D4118			Q3833	L3764		X3596	X3484	X3393	X3331
ALA	E4119		L3903	M3836	Y3765		X3597	X3485	X3394	X3332
GLU	N4120	R3984	T3905		Q3766		X3598	X3486	X3395	X3333
GLU	E4121	D3987			S3768		X3599	X3487	X3396	X3334
GLY	M4122		G3908	S3840	R3769		X3600	X3488	X3397	X3335
ALA	I4123		N3909	V3841	L3770		X3601	X3489	X3398	X3336
ALA	N4124	V3990	S3910	L3842	H3771		X3602	X3490	X3399	
GLY	F4125	G3991	T3911	D3843	R3772		X3603	X3491		X3409
GLU	E4126	F3992	T3912	L3844	G3774		X3604	X3492	X3410	X3411
ALA		F3996	I3913	N3845	A3775		X3605	X3493	X3412	X3413
ALA	N4130	A3997	N3914	A3846	R3776		X3606	X3494	X3414	X3414
ALA	R4131	H3998	S3915	F3847	A3777		X3607	X3495	X3415	X3415
ALA	E4132		Q3927	R3848	E3777		X3608	X3496	X3416	X3416
THR	F4133			Q3850	N3778		X3609	X3497	X3417	X3417
VAL	E4134	M4001	S3931	K3851	V3779		X3610	X3498	X3418	X3418
ALA	P4135	K4002	D3932	E3853	L3780		X3611	X3499	X3419	X3419
ALA	A4136	L4003	Y3934	E3854	Q3781		X3612	X3500	X3420	X3420
GLY	A4137	A4004	W3935	G3855	L3782		X3613	X3501	X3421	X3421
ALA	R4138	S4008	Y3937	L3856	S3784		X3614	X3502		
ALA	D4139	Q4009	S3938	G3857	C3785		X3615	X3503	X3422	X3422
ALA	F4141	I4010	G3939	M3858	C3786		X3616	X3504	X3423	X3423
ALA	V4142	E4011	K3940	V3859	K3787		X3617	X3505	X3424	X3424
ALA	V4143	L4012	D3941	E3860	G3788		X3618	X3506	X3425	X3425
ALA	A4144	L4013	V3942	E3861	E3789		X3619	X3507	X3426	X3426
ALA		K4014	T3943	D3862	T3790		X3620	X3508	X3427	X3427
LEU	L4147	L4015	E3944	G3863	G3791		X3621	X3509	X3428	X3428
ALA	S4151	L4016	E3945	T3864	A3792		X3622	X3510	X3429	X3429
ARG	E4152	L4017		V3865			X3623	X3511	X3430	X3430
GLY		L4018	K3948	I3866	S3796		X3624	X3512	X3431	X3431
		L4019		N3867	T3797		X3625	X3513	X3432	X3432
		Q4020	F3961	R3868	L3798		X3626	X3514	X3433	X3433
		K4021	S3952	Q3869	K3799		X3627	X3515	X3434	X3434
				N3870	L3800		X3628	X3516	X3435	X3435
				G3871	G3801		X3629	X3517	X3436	X3436
							X3630	X3518	X3437	X3437
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							X3750			





Y1049	G1050	Y1051	I1052	E1054	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	SER	ARG	TRP	D1070	R1071	Y1072	R1073	R1076	A1077	E1078	K1079	S1080	Y1081	T1082	V1083	Q1084	S1085	G1086	R1087	Y1088	Y1089	F1090	E1091	F1092	E1093	A1094	V1095	T1096	R1101	V1102	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	Y1122	V1123	L1134	G1135	S1136	F1139	G1140	R1141	Q1144	S1145	G1146	V1149	M1152	L1153	D1154	L1155	T1156	E1157	N1158	T1161	F1162	T1163	L1164	N1165	V1168	L1169	M1170	S1173	G1174	S1175	E1176	R1180	E1181	I1182	I1183	I1184	G1185	D1186	L1189	P1190	V1191	C1192																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
S1193	L1194	E1195	P1196	G1197	Q1198	V1199	G1200	H1201	L1202	M1203	G1205	Q1206	D1207	V1208	S1209	S1210	L1211	R1212	F1213	F1214	A1215	G1218	L1219	Q1220	E1221	G1222	F1223	E1224	P1225	F1226	I1228	M1229	M1230	Q1231	R1232	P1233	V1234	T1235	K1240	S1241	L1242	P1243	Q1244	F1245	E1246	P1247	V1248	P1249	P1250	E1251	H1252	P1253	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	X1279	X1280	X1281	X1282	X1285	X1289	X1290	X1291	X1292	X1293	X1294	X1295	X1296	X1297	X1298	X1299	X1300	X1301	X1302	X1303	X1304	X1305	X1306	X1307	X1308	X1309	X1310	X1311	X1312	X1313	X1314	X1315	X1316	X1317	X1318	X1319	X1320	X1321	X1322	X1323	X1324	X1325	X1326	X1327	X1328	X1329	X1330	X1331	X1332	X1333	X1334	X1335	X1336	X1337	X1338	X1339	X1340	X1341	X1342	X1343	X1344	X1345	X1346	X1347	X1348	X1349	X1350	X1351	X1352	X1353	X1354	X1355	X1356	X1357	X1358	X1359	X1360	X1361	X1362	X1363	X1364	X1365	X1366	X1367	X1368	X1369	X1370	X1371	X1372	X1373	X1374	X1375	X1376	X1377	X1378	X1379	X1380	X1381	X1382	X1383	X1384	X1385	X1386	X1387	X1388	X1389	X1390	X1391	X1392	X1393	X1394	X1395	X1396	X1397	X1398	X1399	X1400	X1401	X1402	X1403	X1404	X1405	X1406	X1407	X1408	X1409	X1410	X1411	X1412	X1413	X1414	X1415	X1416	X1417	X1418	X1419	X1420	X1421	X1422	X1423	X1424	X1425	X1426	X1427	X1428	X1429	X1430	X1431	X1432	X1433	X1434	X1435	X1436	X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1453	X1454	X1455	X1456	X1457	X1458	X1459	X1460	X1461	X1462	X1463	X1464	X1465	X1466	X1467	X1468	X1469	X1470	X1471	X1472	X1473	X1474	X1475	X1476	X1477	X1478	X1479	X1480	X1481	X1482	X1483	X1484	X1485	X1486	X1487	X1488	X1489	X1490	X1491	X1492	X1493	X1494	X1495	X1496	X1497	X1498	X1499	X1500	X1501	X1502	X1503	X1504	X1505	X1506	X1507	X1508	X1509	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	X1535	X1536	X1537	X1538	X1539	X1540	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1558	X1559	X1560	X1561	X1562	X1563	X1564	X1565	X1566	X1567	X1568	X1569	X1570	X1571	X1572	X1573	X1574	X1575	X1576	X1577	X1578	X1579	X1580	X1581	X1582	X1583	X1584	X1585	X1586	X1587	X1588	X1589	X1590	X1591	X1592	X1593	X1594	X1595	X1596	X1597	X1598	X1599	X1600	X1601	X1602	X1603	X1604	X1605	X1606	X1607	X1608	X1609	X1610	X1611	X1612	X1613	X1614	X1615	X1616	X1617	X1618	X1619	X1620	X1621	X1622	X1623	X1624	X1625	X1626	X1627	X1628	X1629	X1630	X1631	X1632	X1633	X1634	X1635	X1636	X1637	X1638	X1639	X1640	X1641	X1642	X1643	X1644	X1645	X1646	X1647	X1648	X1649	X1650	X1651	X1652	X1653	X1654	X1655	X1656	X1657	X1658	X1659	X1660	X1661	X1662	X1663	X1664	X1665	X1666	X1667	X1668	X1669	X1670	X1671	X1672	X1673	X1674	X1675	X1676	X1677	X1678	X1679	X1680	X1681	X1682	X1683	X1684	X1685	X1686	X1687	X1688	X1689	X1690	X1691	X1692	X1693	X1694	X1695	X1696	X1697	X1698	X1699	X1700	X1701	X1702	X1703	X1704	X1705	X1706	X1707	X1708	X1709	X1710	X1711	X1712	X1713	X1714	X1715	X1716	X1717	X1718	X1719	X1720	X1721	X1722	X1723	X1724	X1725	X1726	X1727	X1728	X1729	X1730	X1731	X1732	X1733	X1734	X1735	X1736	X1737	X1738	X1739	X1740	X1741	X1742	X1743	X1744	X1745	X1746	X1747	X1748	X1749	X1750	X1751	X1752	X1753	X1754	X1755	X1756	X1757	X1758	X1759	X1760	X1761	X1762	X1763	X1764	X1765	X1766	X1767	X1768	X1769	X1770	X1771	X1772	X1773	X1774	X1775	X1776	X1777	X1778	X1779	X1780	X1781	X1782	X1783	X1784	X1785	X1786	X1787	X1788	X1789	X1790	X1791	X1792	X1793	X1794	X1795	X1796	X1797	X1798	X1799	X1800	X1801	X1802	X1803	X1804	X1805	X1806	X1807	X1808	X1809	X1810	X1811	X1812	X1813	X1814	X1815	X1816	X1817	X1818	X1819	X1820	X1821	X1822	X1823	X1824	X1825	X1826	X1827	X1828	X1829	X1830	X1831	X1832	X1833	X1834	X1835	X1836	X1837	X1838	X1839	X1840	X1841	X1842	X1843	X1844	X1845	X1846	X1847	X1848	X1849	X1850	X1851	X1852	X1853	X1854	X1855	X1856	X1857	X1858	X1859	X1860	X1861	X1862	X1863	X1864	X1865	X1866	X1867	X1868	X1869	X1870	X1871	X1872	X1873	X1874	X1875	X1876	X1877	X1878	X1879	X1880	X1881	X1882	X1883	X1884	X1885	X1886	X1887	X1888	X1889	X1890	X1891	X1892	X1893	X1894	X1895	X1896	X1897	X1898	X1899	X1900	X1901	X1902	X1903	X1904	X1905	X1906	X1907	X1908	X1909	X1910	X1911	X1912	X1913	X1914	X1915	X1916	X1917	X1918	X1919	X1920	X1921	X1922	X1923	X1924	X1925	X1926	X1927	X1928	X1929	X1930	X1931	X1932	X1933	X1934	X1935	X1936	X1937	X1938	X1939	X1940	X1941	X1942	X1943	X1944	X1945	X1946	X1947	X1948	X1949	X1950	X1951	X1952	X1953	X1954	X1955	X1956	X1957	X1958	X1959	X1960	X1961	X1962	X1963	X1964	X1965	X1966	X1967	X1968	X1969	X1970	X1971	X1972	X1973	X1974	X1975	X1976	X1977	X1978	X1979	X1980	X1981	X1982	X1983	X1984	X1985	X1986	X1987	X1988	X1989	X1990	X1991	X1992	X1993	X1994	X1995	X1996	X1997	X1998	X1999	X2000	X2001	X2002	X2003	X2004	X2005	X2006	X2007	X2008	X2009	X2010	X2011	X2012	X2013	X2014	X2015	X2016	X2017	X2018	X2019	X2020	X2021	X2022	X2023	X2024	X2025	X2026	X2027	X2028	X2029	X2030	X2031	X2032	X2033	X2034	X2035	X2036	X2037	X2038	X2039	X2040	X2041	X2042	X2043	X2044	X2045	X2046	X2047	X2048	X2049	X2050	X2051	X2052	X2053	X2054	X2055	X2056	X2057	X2058	X2059	X2060	X2061	X2062	X2063	X2064	X2065	X2066	X2067	X2068	X2069	X2070	X2071	X2072	X2073	X2074	X2075	X2076	X2077	X2078	X2079	X2080	X2081	X2082	X2083	X2084	X2085	X2086	X2087	X2088	X2089	X2090	X2091	X2092	X2093	X2094	X2095	X2096	X2097	X2098	X2099	X2100	X2101	X2102	X2103	X2104	X2105	X2106	X2107	X2108	X2109	X2110	X2111	X2112	X2113	X2114	X2115	X2116	X2117	X2118	X2119	X2120	X2121	X2122	X2123	X2124	X2125	X2126	X2127	X2128	X2129	X2130	X2131	X2132	X2133	X2134	X2135	X2136	X2137	X2138	X2139	X2140	X2141	X2142	X2143	X2144	X2145	X2146	X2147	X2148	X2149	X2150	X2151	X2152	X2153	X2154	X2155	X2156	X2157	X2158	X2159	X2160	X2161	X2162	X2163	X2164	X2165	X2166	X2167	X2168	X2169	X2170	X2171	X2172	X2173	X2174	X2175	X2176	X2177	X2178	X2179	X2180	X2181	X2182	X2183	X2184	X2185	X2186	X2187	X2188	X2189	X2190	X2191	X2192	X2193	X2194	X2195	X2196	X2197	X2198	X2199	X2200	X2201	X2202	X2203	X2204	X2205	X2206	X2207	X2208	X2209	X2210	X2211	X2212	X2213	X2214	X2215	X2216	X2217	X2218	X2219	X2220	X2221	X2222	X2223	X2224	X2225	X2226	X2227	X2228	X2229	X2230	X2231	X2232	X2233	X2234	X2235	X2236	X2237	X2238	X2239	X2240	X2241	X2242	X2243	X2244	X2245	X2246	X2247	X2248	X2249	X2250	X2251	X2252	X2253	X2254	X2255	X2256	X2257	X2258	X2259	X2260	X2261	X2262	X2263	X2264	X2265	X2266	X2267	X2268	X2269	X2270	X2271	X2272	X2273	X2274	X2275	X2276	X2277	X2278	X2279	X2280	X2281	X2282	X2283	X2284	X2285	X2286	X2287	X2288	X2289	X2290	X2291	X2292	X2293	X2294	X2295	X2296	X2297	X2298	X2299	X2300	X2301	X2302	X2303	X2304	X2305	X2306	X2307	X2308	X2309	X2310	X2311	X2312	X2313	X2314	X2315	X2316	X2317	X2318	X2319	X2320	X2321	X2322	X2323	X2324	X2325	X2326	X2327	X2328	X2329	X2330	X2331	X2332	X2333	X2334	X2335	X2336	X2337	X2338	X2339	X2340	X2341	X2342	X2343	X2344	X2345	X2346	X2347	X2348	X2349	X2350	X2351	X2352	X2353	X2354	X2355	X2356	X2357	X2358	X2359	X2360	X2361	X2362	X2363	X2364	X2365	X2366	X2367	X2368	X2369	X2370	X2371	X2372	X2373	X2374	X2375	X2376	X2377	X2378	X2379	X2380	X2381	X2382	X2383	X2384	X2385	X2386	X2387	X2388	X2389	X2390	X2391	X2392	X2393	X2394	X2395	X2396	X2397	X2398	X2399	X2400	X2401	X2402	X2403	X2404	X2405	X2406	X2407	X2408	X2409	X2410	X2411	X2412	X2413	X2414	X2415	X2416	X2417	X2418	X2419	X2420	X2421	X2422	X2423	X2424	X2425	X2426	X2427	X2428	X2429	X2430	X2431	X2432	X2433	X2434	X2435	X2436	X2437	X2438	X2439	X2440	X2441	X2442	X2443	X2444	X2445	X2446	X2447	X2448	X2449	X2450	X2451	X2452	X2453	X2454	X2455	X2456	X2457	X2458	X2459	X2460	X2461	X2462



V4081	L4013	V3942	E3872	I3802	E3737	M3673	X3571	X3462	X3379	X3311	X3230	X3135
T4082	K4014	K3948	K3873	S3803	G3738	M3674	X3572	X3463	X3380	X3312	X3233	X3136
D4083	E4015	K3949	V3874	L3805	G3739	D3675	X3573	X3464	X3383	X3313	X3234	X3137
F4084	L4016	R3949	D3877	N3806	E3740	D3676	X3574	X3465	X3384	X3314	X3235	X3138
B4085	D4018	N3950	D3878	G3807	M3741	A3680	X3575	X3466	X3385	X3315	X3236	X3139
I4088	L4019	F3951	GLY	G3808	ALA	E3681	X3576	X3467	X3386	X3316	X3241	X3140
	Q4020	A3954	GLU	N3809	GLU	E3682	X3577	X3468	X3387	X3317	X3242	X3141
K4091	K4021	M3955	GLU	K3815	E3747	E3683	X3578	X3469	X3388	X3318	X3243	X3142
D4092	V4024	V3957	F3885	M3816	E3748	E3684	X3579	X3470	X3389	X3319	X3244	X3143
Q4094	L4027	A3958	F3886	L3820	E3749	E3685	X3580	X3471	X3390	X3320	X3245	X3146
K4095	L4028	K3959	L3888	K3821	V3749	E3686	X3581	X3472	X3391	X3321	X3246	
A4096	S4029	F3962	Q3889	L3822	E3750	E3687	X3582	X3473	X3392	X3322	X3247	X3162
D4098	L4030	N3963	L3890	K3824	V3751	E3688	X3583	X3474	X3393	X3323	X3248	X3163
M4034		S3964	S3752	E3825	E3752	E3689	X3584	X3475	X3394	X3324	X3249	X3170
N4037		L3965	F3753	E3826	E3753	E3690	X3585	X3476	X3395	X3325	X3250	X3171
I4040		T3966	E3754	E3827	E3754	E3691	X3586	X3477	X3396	X3326	X3251	X3172
A4041		E3967	E3755	F3829	E3755	E3692	X3587	X3478	X3397	X3327	X3252	X3173
Q4043		Y3968	K3756	Q3830	X3756	K3694	X3588	X3479	X3398	X3328	X3253	X3174
M4044		Y3969	E3759	S3831	E3759	P3695	X3589	X3480	X3399	X3329	X3254	X3183
V4045		Q3970	K3760	Q3832	K3760		X3590	X3481	X3400	X3330	X3255	X3184
D4046		Q3971	L3763	Q3833	L3763		X3591	X3482	X3401	X3331	X3256	X3185
M4047		P3972	L3764	M3836	L3764		X3602	X3483	X3402	X3332	X3257	X3186
L4048		C3973	Y3765	Q3837	L3765		X3603	X3484	X3403	X3333	X3258	X3187
V4049		T3974	Y3766	T3838	Y3766		X3604	X3485	X3404	X3334	X3259	X3188
E4107		Q3977	Q3767	C3839	Q3767		X3605	X3486	X3405	X3335	X3260	X3189
D4108		Q3978	Q3768	L3842	Q3768		X3606	X3487	X3406	X3336	X3261	X3190
Q4109		A3981	R3769	D3843	R3769		X3607	X3488	X3407	X3337	X3262	X3191
F4110		S3982	L3770	L3844	L3770		X3608	X3489	X3408	X3338	X3263	X3192
L4111		H3984	H3771	L3845	H3771		X3609	X3490	X3409	X3339	X3264	X3193
L4112		A3846	T3772	A3846	T3772		X3610	X3491	X3410	X3340	X3265	X3194
S4113		F3847	R3773	F3847	R3773		X3611	X3492	X3411	X3341	X3266	X3195
A4117		E3848	G3774	E3848	G3774		X3612	X3493	X3412	X3342	X3267	X3196
D4118		E3849	A3775	E3849	A3775		X3613	X3494	X3413	X3343	X3268	X3197
F4119		Q3987	A3776	Q3849	A3776		X3614	X3495	X3414	X3344	X3269	X3198
N4120		V3990	V3779	Q3850	V3779		X3615	X3496	X3415	X3345	X3270	X3199
F4121		G3991	L3780	N3851	L3780		X3616	X3497	X3416	X3346	X3271	X3200
I4122		F3992	Q3781	K3852	Q3781		X3617	X3498	X3417	X3347	X3272	X3201
L4123		L3993	L3782	A3853	L3782		X3618	X3499	X3418	X3348	X3273	X3202
F4125		H3994	M3783	E3854	M3783		X3619	X3500	X3419	X3349	X3274	X3205
E4126		V3995	L3784	G3855	L3784		X3620	X3501	X3420	X3350	X3275	X3206
N4130		F3996	A3785	L3856	A3785		X3621	X3502	X3421	X3351	X3276	X3209
R4131		A3997	S3786	G3857	S3786		X3622	X3503	X3422	X3352	X3277	X3210
F4132		H3998	K3787	M3858	K3787		X3623	X3504	X3423	X3353	X3278	X3214
Q4133		M3999	C3788	V3859	C3788		X3624	X3505	X3424	X3354	X3279	X3217
L4136		M4001	G3788	N3860	G3788		X3625	X3506	X3425	X3355	X3280	X3218
R4137		K4002	E3789	E3861	E3789		X3626	X3507	X3426	X3356	X3281	X3219
D4138		L4003	T3790	D3862	T3790		X3627	X3508	X3427	X3357	X3282	X3220
F4139		A4004	Q3791	G3863	Q3791		X3628	X3509	X3428	X3358	X3283	X3221
Q4140		Q4005	A3792	T3864	A3792		X3629	X3510	X3429	X3359	X3284	X3222
G4073		S4008	L3798	V3865	L3798		X3630	X3511	X3430	X3360	X3285	X3223
S4074		Q4009	K3799	I3866	K3799		X3631	X3512	X3431	X3361	X3286	X3226
E4075		I4010	E3799	N3867	E3799		X3632	X3513	X3432	X3362	X3287	X3229
A4076		E4011	S3795	T3867	S3795		X3633	X3514	X3433	X3363	X3288	
D4079		L4012	L3798	Q3868	L3798		X3634	X3515	X3434	X3364	X3289	X3301
Y4080			K3799	N3870	K3799		X3635	X3516	X3435	X3365	X3290	X3302
				G3871			X3636	X3517	X3436	X3366	X3291	X3307
							X3637	X3518	X3437	X3367	X3292	X3308
							X3638	X3519	X3438	X3368	X3293	X3309
							X3639	X3520	X3439	X3369	X3294	X3310
							X3640	X3521	X3440	X3370	X3295	
							X3641	X3522	X3441	X3371	X3296	
							X3642	X3523	X3442	X3372	X3297	
							X3643	X3524	X3443	X3373	X3298	
							X3644	X3525	X3444	X3374	X3299	
							X3645	X3526	X3445	X3375	X3300	
							X3646	X3527	X3446	X3376	X3301	
							X3647	X3528	X3447	X3377	X3302	
							X3648	X3529	X3448	X3378	X3303	
							X3649	X3530	X3449	X3379	X3304	
							X3650	X3531	X3450	X3380	X3305	
							X3651	X3532	X3451	X3381	X3306	
							X3652	X3533	X3452	X3382	X3307	
							X3653	X3534	X3453	X3383	X3308	
							X3654	X3535	X3454	X3384	X3309	
							X3655	X3536	X3455	X3385	X3310	
							X3656	X3537	X3456	X3386	X3311	
							X3657	X3538	X3457	X3387	X3312	
							X3658	X3539	X3458	X3388	X3313	
							X3659	X3540	X3459	X3389	X3314	
							X3660	X3541	X3460	X3390	X3315	
							X3661	X3542	X3461	X3391	X3316	
							X3662	X3543	X3462	X3392	X3317	
							X3663	X3544	X3463	X3393	X3318	
							X3664	X3545	X3464	X3394	X3319	
							X3665	X3546	X3465	X3395	X3320	
							X3666	X3547	X3466	X3396	X3321	
							X3667	X3548	X3467	X3397	X3322	
							X3668	X3549	X3468	X3398	X3323	
							X3669	X3550	X3469	X3399	X3324	
							X3670	X3551	X3470	X3400	X3325	
							X3671	X3552	X3471	X3401	X3326	
							X3672	X3553	X3472	X3402	X3327	
							X3673	X3554	X3473	X3403	X3328	
							X3674	X3555	X3474	X3404	X3329	
							X3675	X3556	X3475	X3405	X3330	
							X3676	X3557	X3476	X3406	X3331	
							X3677	X3558	X3477	X3407	X3332	
							X3678	X3559	X3478	X3408	X3333	
							X3679	X3560	X3479	X3409	X3334	
							X3680	X3561	X3480	X3410	X3335	
							X3681	X3562	X3481	X3411	X3336	
							X3682	X3563	X3482	X3412	X3337	
							X3683	X3564	X3483	X3413	X3338	
							X3684	X3565	X3484	X3414	X3339	
							X3685	X3566	X3485	X3415	X3340	
							X3686	X3567	X3486	X3416	X3341	
							X3687	X3568	X3487	X3417	X3342	
							X3688	X3569	X3488	X3418	X3343	
							X3689	X3570	X3489	X3419	X3344	
							X3690	X3571	X3490	X3420	X3345	
							X3691	X3572	X3491	X3421	X3346	
							X3692	X3573	X3492	X3422	X3347	
							X3693	X3574	X3493	X3423	X3348	
							X3694	X3575	X3494	X3424	X3349	
							X3695	X3576	X3495	X3425	X3350	
							X3696	X3577	X3496	X3426	X3351	
							X3697	X3578	X3497	X3427	X3352	
							X3698	X3579	X3498	X3428	X3353	
							X3699	X3580	X3499	X3429	X3354	
							X3700	X3581	X3500	X3430	X3355	
							X3701	X3582	X3501	X3431	X3356	
							X3702	X3583	X3502	X3432	X3357	
							X3703	X3584	X3503	X3433	X3358	
							X3704	X3585	X3504	X3434	X3359	
							X3705	X3586	X3505	X3435	X3360	
							X3706	X3587	X3506	X3436	X3361	
							X3707	X3588	X3507	X3437	X3362	
							X3708	X3589	X3508	X3438	X3363	
							X3709	X				



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	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	0.466	Depositor
Minimum map value	-0.266	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.16	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, 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	0.37	0/834	0.61	0/1123
1	F	0.37	0/834	0.61	0/1123
1	H	0.37	0/834	0.61	0/1123
1	J	0.37	0/834	0.61	0/1123
2	B	0.40	0/25428	0.61	5/34534 (0.0%)
2	E	0.40	0/25428	0.61	5/34534 (0.0%)
2	G	0.40	0/25428	0.61	5/34534 (0.0%)
2	I	0.40	0/25428	0.61	5/34534 (0.0%)
All	All	0.40	0/105048	0.61	20/142628 (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
2	B	0	19
2	E	0	19
2	G	0	19
2	I	0	20
All	All	0	77

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4985	LEU	CA-CB-CG	6.40	130.01	115.30
2	B	4985	LEU	CA-CB-CG	6.39	130.00	115.30
2	I	719	LEU	CA-CB-CG	6.39	130.00	115.30
2	B	719	LEU	CA-CB-CG	6.38	129.99	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	719	LEU	CA-CB-CG	6.38	129.97	115.30

There are no chirality outliers.

5 of 77 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	137	LEU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	808	TYR	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	21	0
1	F	818	0	824	19	0
1	H	818	0	824	19	0
1	J	818	0	824	20	0
2	B	29369	0	24716	533	0
2	E	29369	0	24712	519	0
2	G	29369	0	24713	531	0
2	I	29369	0	24713	522	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
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102150	2154	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 10.

The worst 5 of 2154 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:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.65	0.79
2:B:853:PRO:HB3	2:B:1024:TYR:H	1.51	0.76
2:B:379:HIS:HD2	2:B:382:GLY:H	1.35	0.75
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.51	0.75
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.51	0.75

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	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
1	F	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
1	H	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
1	J	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4687 (69%)	2859 (88%)	367 (11%)	9 (0%)	41	76
2	E	3235/4687 (69%)	2860 (88%)	367 (11%)	8 (0%)	47	81
2	G	3235/4687 (69%)	2859 (88%)	367 (11%)	9 (0%)	41	76
2	I	3235/4687 (69%)	2860 (88%)	366 (11%)	9 (0%)	41	76
All	All	13360/19176 (70%)	11818 (88%)	1507 (11%)	35 (0%)	44	76

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3772	THR
2	B	4667	PRO
2	E	3772	THR
2	E	4667	PRO

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Mol	Chain	Res	Type
2	G	3772	THR

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	88/88 (100%)	88 (100%)	0	100	100
1	F	88/88 (100%)	88 (100%)	0	100	100
1	H	88/88 (100%)	88 (100%)	0	100	100
1	J	88/88 (100%)	88 (100%)	0	100	100
2	B	2493/3209 (78%)	2469 (99%)	24 (1%)	76	86
2	E	2493/3209 (78%)	2469 (99%)	24 (1%)	76	86
2	G	2493/3209 (78%)	2469 (99%)	24 (1%)	76	86
2	I	2493/3209 (78%)	2469 (99%)	24 (1%)	76	86
All	All	10324/13188 (78%)	10228 (99%)	96 (1%)	79	87

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	3663	LEU
2	G	4995	LEU
2	G	3805	LEU
2	G	4180	ARG
2	I	688	LEU

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

Mol	Chain	Res	Type
2	G	3978	GLN
2	I	1598	GLN
2	G	4120	ASN
2	I	218	HIS

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Mol	Chain	Res	Type
2	I	2005	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 8 ligands modelled in this entry, 8 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	G	12
2	I	12

Continued on next page...

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Mol	Chain	Number of breaks
2	B	12
2	E	12

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	3613:UNK	C	3639:THR	N	44.11
1	I	3613:UNK	C	3639:THR	N	44.00
1	B	3613:UNK	C	3639:THR	N	43.94
1	E	3613:UNK	C	3639:THR	N	43.92
1	B	3163:UNK	C	3170:UNK	N	16.36

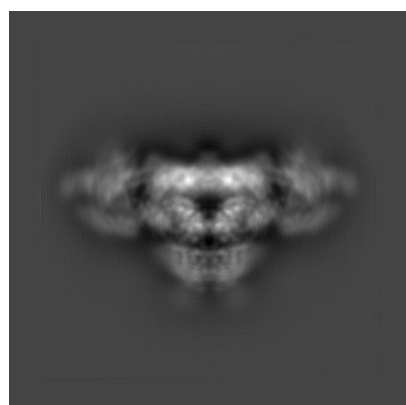
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22396. These allow visual inspection of the internal detail of the map and identification of artifacts.

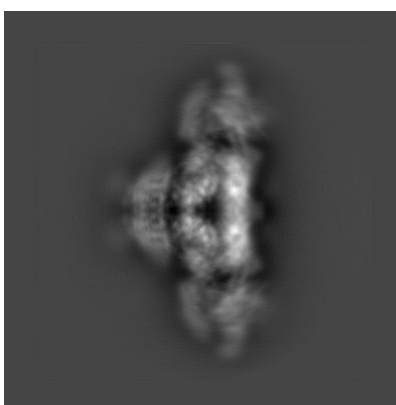
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

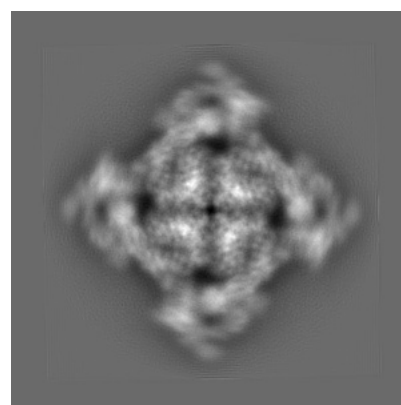
6.1.1 Primary map



X



Y

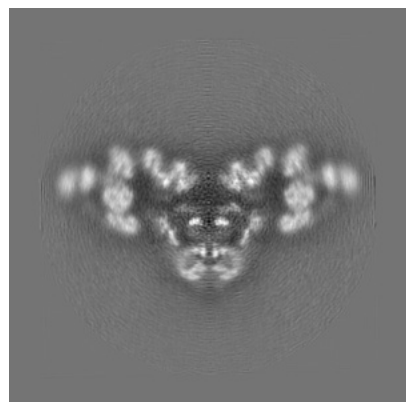


Z

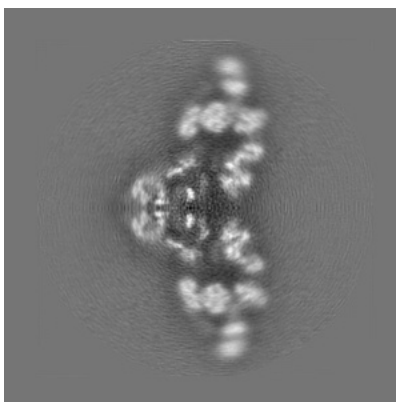
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

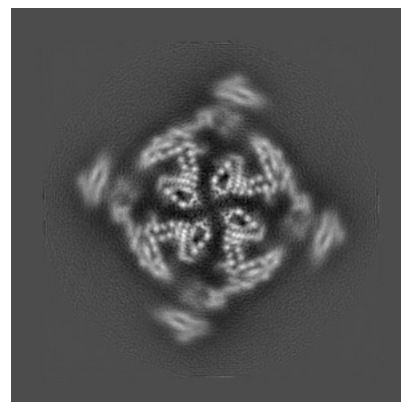
6.2.1 Primary map



X Index: 200



Y Index: 200

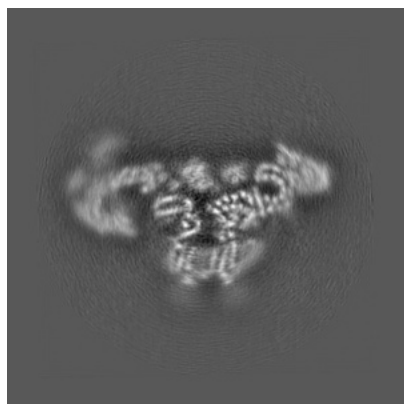


Z Index: 200

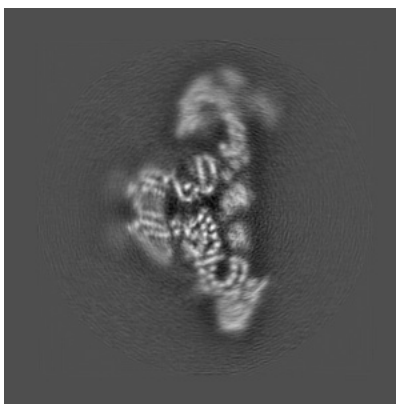
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

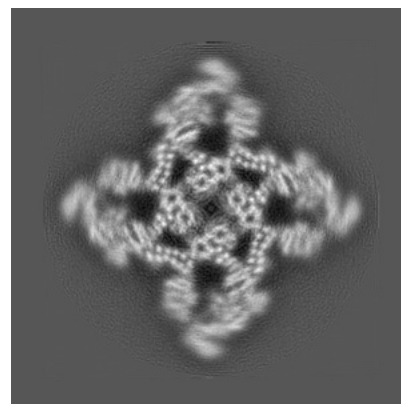
6.3.1 Primary map



X Index: 177



Y Index: 177



Z Index: 227

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

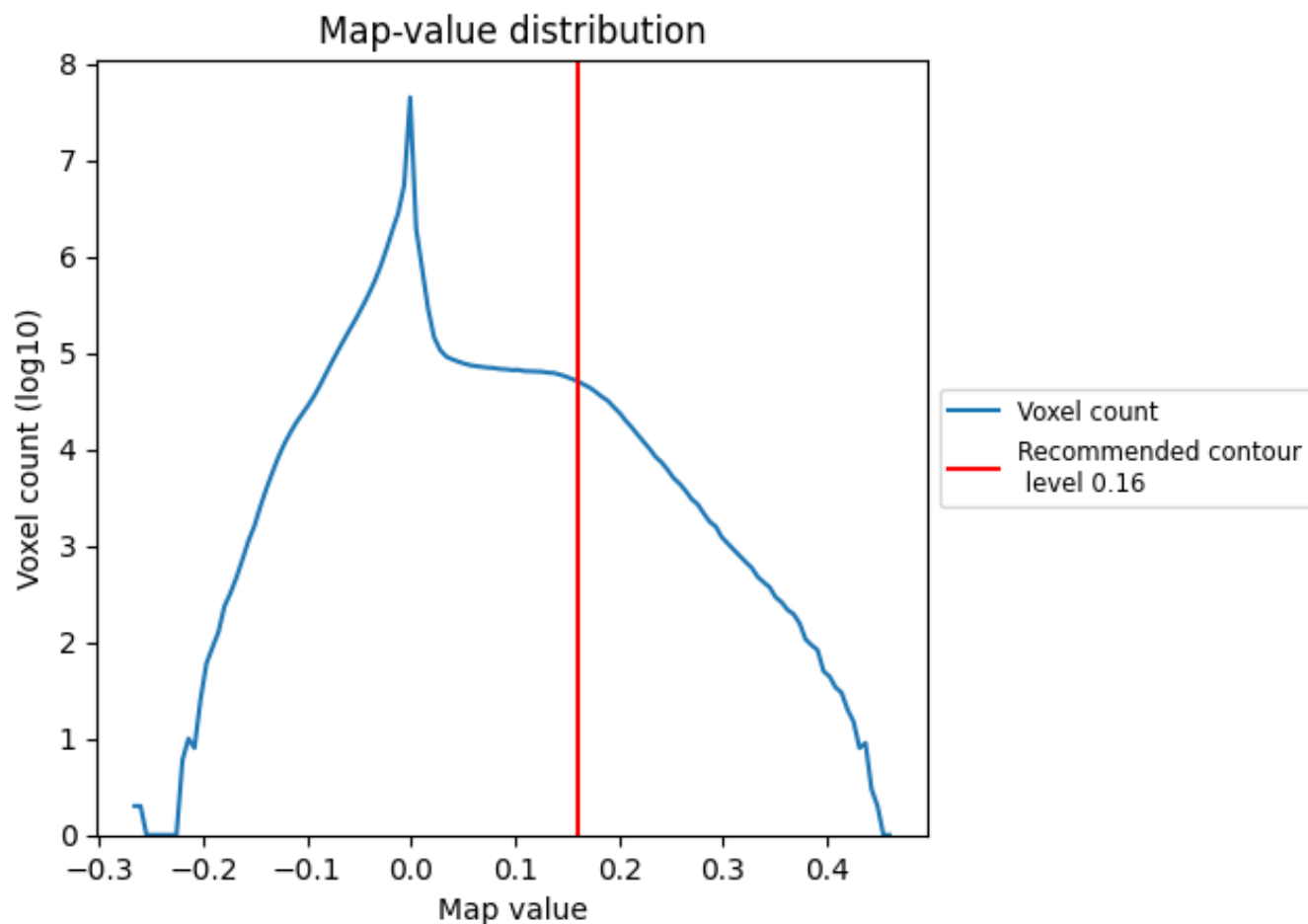
6.5 Mask visualisation

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

7 Map analysis [i](#)

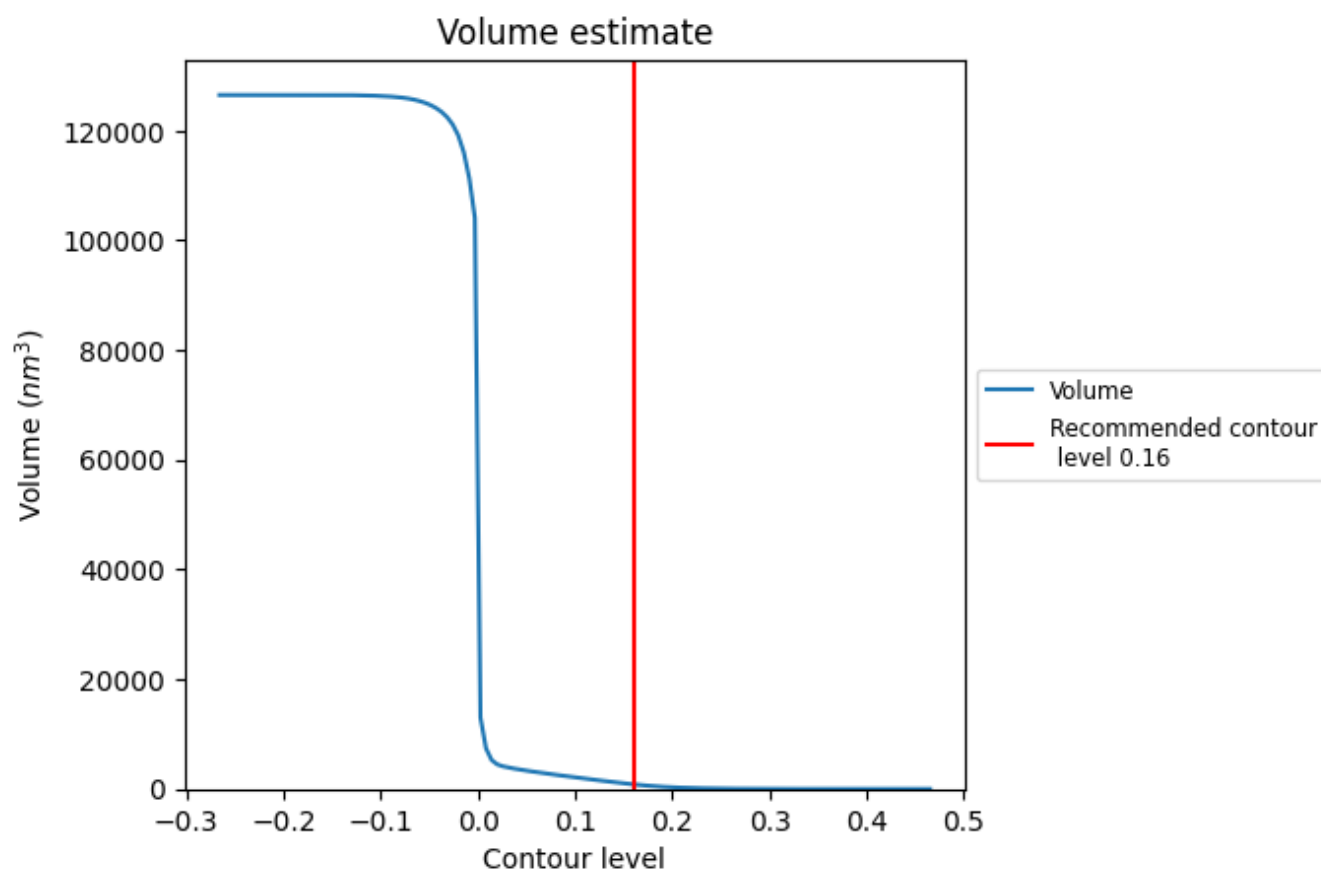
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

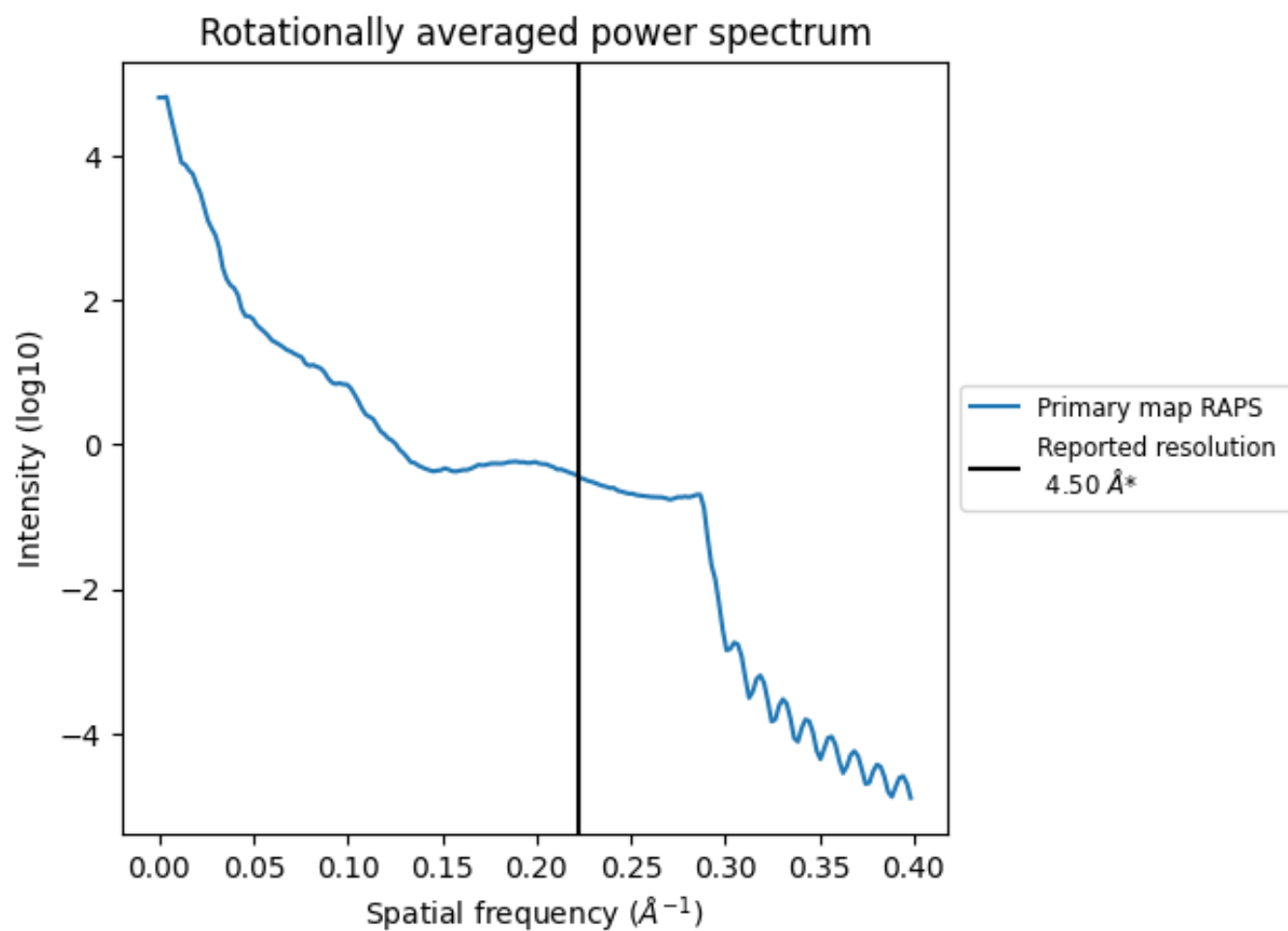
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 846 nm³; this corresponds to an approximate mass of 764 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 0.222 Å⁻¹

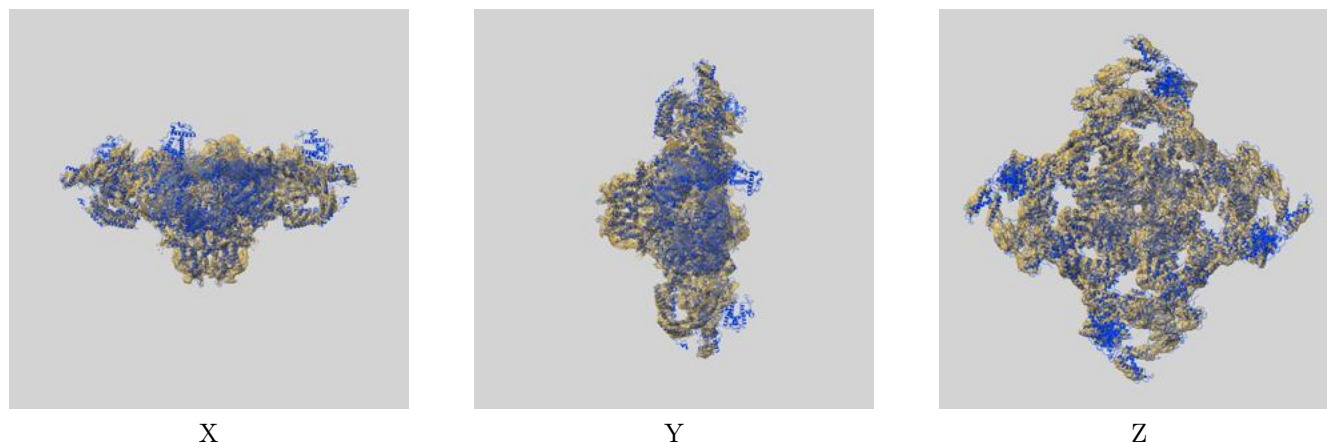
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

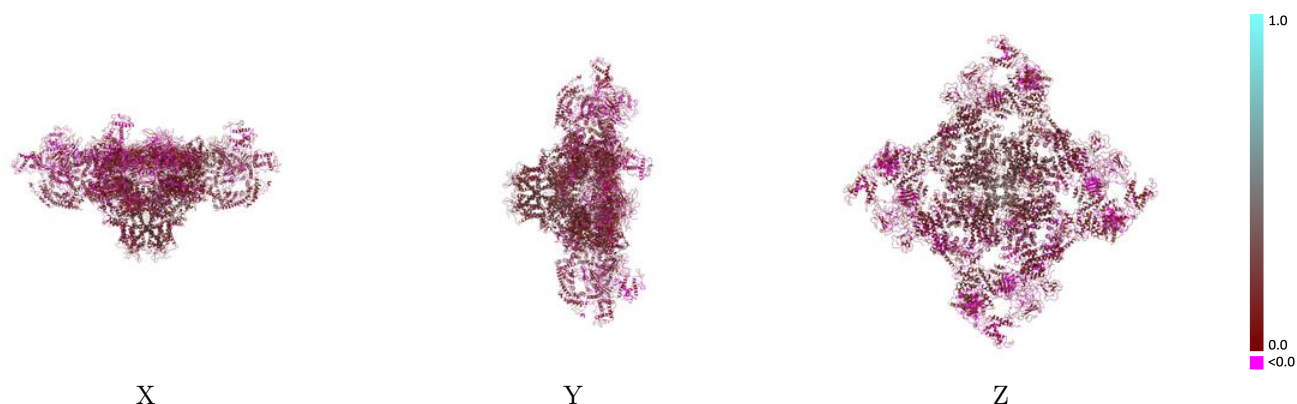
This section contains information regarding the fit between EMDB map EMD-22396 and PDB model 7JMJ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



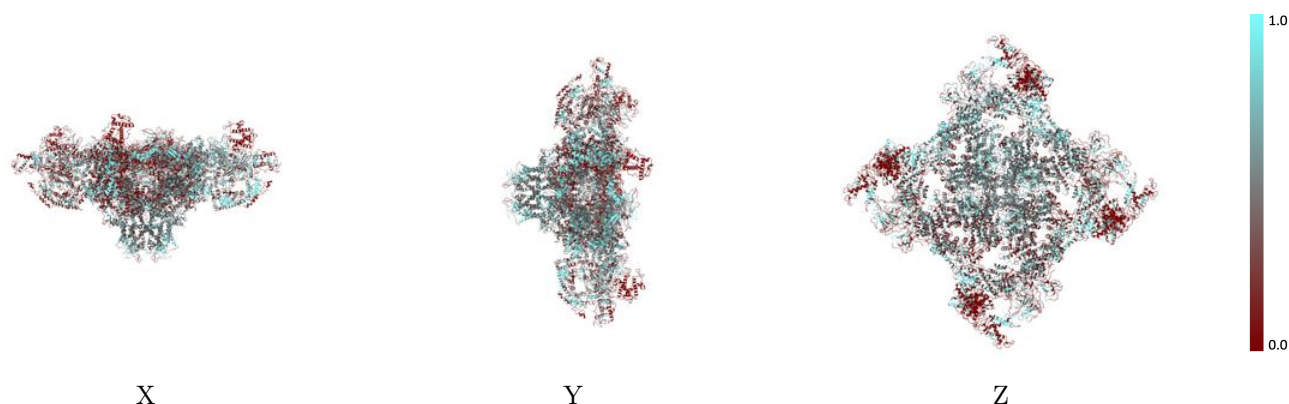
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



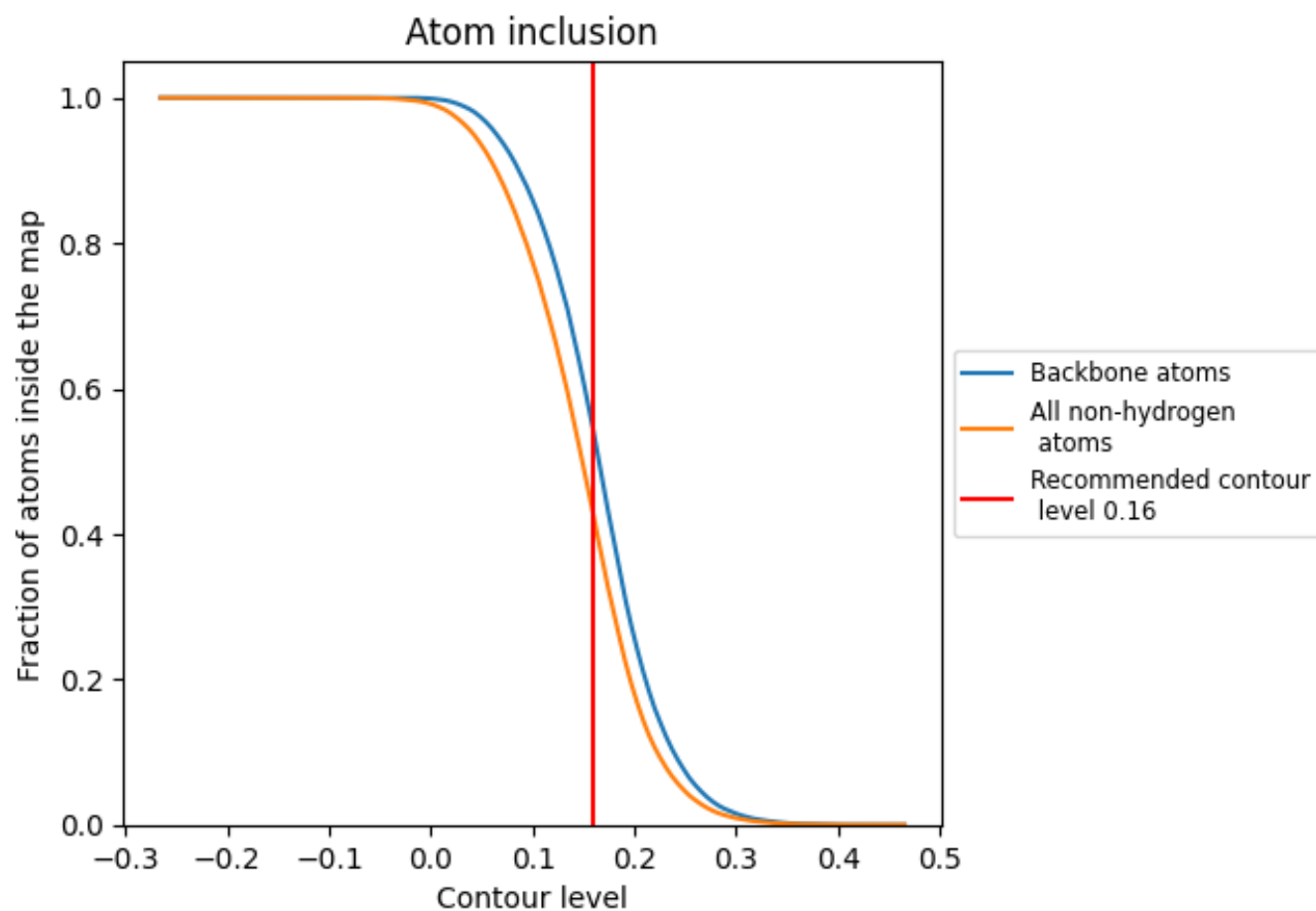
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 42% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.4247	<div><div></div></div> 0.1330
A	<div><div></div></div> 0.4529	<div><div></div></div> 0.1410
B	<div><div></div></div> 0.4630	<div><div></div></div> 0.1670
E	<div><div></div></div> 0.4324	<div><div></div></div> 0.1360
F	<div><div></div></div> 0.4256	<div><div></div></div> 0.1110
G	<div><div></div></div> 0.3976	<div><div></div></div> 0.1060
H	<div><div></div></div> 0.3921	<div><div></div></div> 0.1210
I	<div><div></div></div> 0.4065	<div><div></div></div> 0.1230
J	<div><div></div></div> 0.4020	<div><div></div></div> 0.1150

1.0

0.0

<0.0