



wwPDB EM Validation Summary Report ⓘ

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PDB ID : 5GL1
EMDB ID : EMD-9521
Title : Structure of RyR1 in an open state
Authors : Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-07
Resolution : 5.70 Å (reported)

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

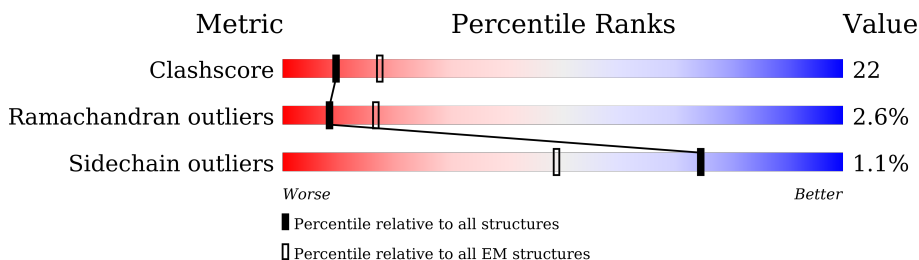
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	5037	
1	C	5037	
1	E	5037	
1	G	5037	
2	B	108	
2	D	108	
2	F	108	
2	H	108	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 110704 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3645	26843	17063	4667	4956	157	0	0
1	C	3645	26843	17063	4667	4956	157	0	0
1	E	3645	26843	17063	4667	4956	157	0	0
1	G	3645	26843	17063	4667	4956	157	0	0

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

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

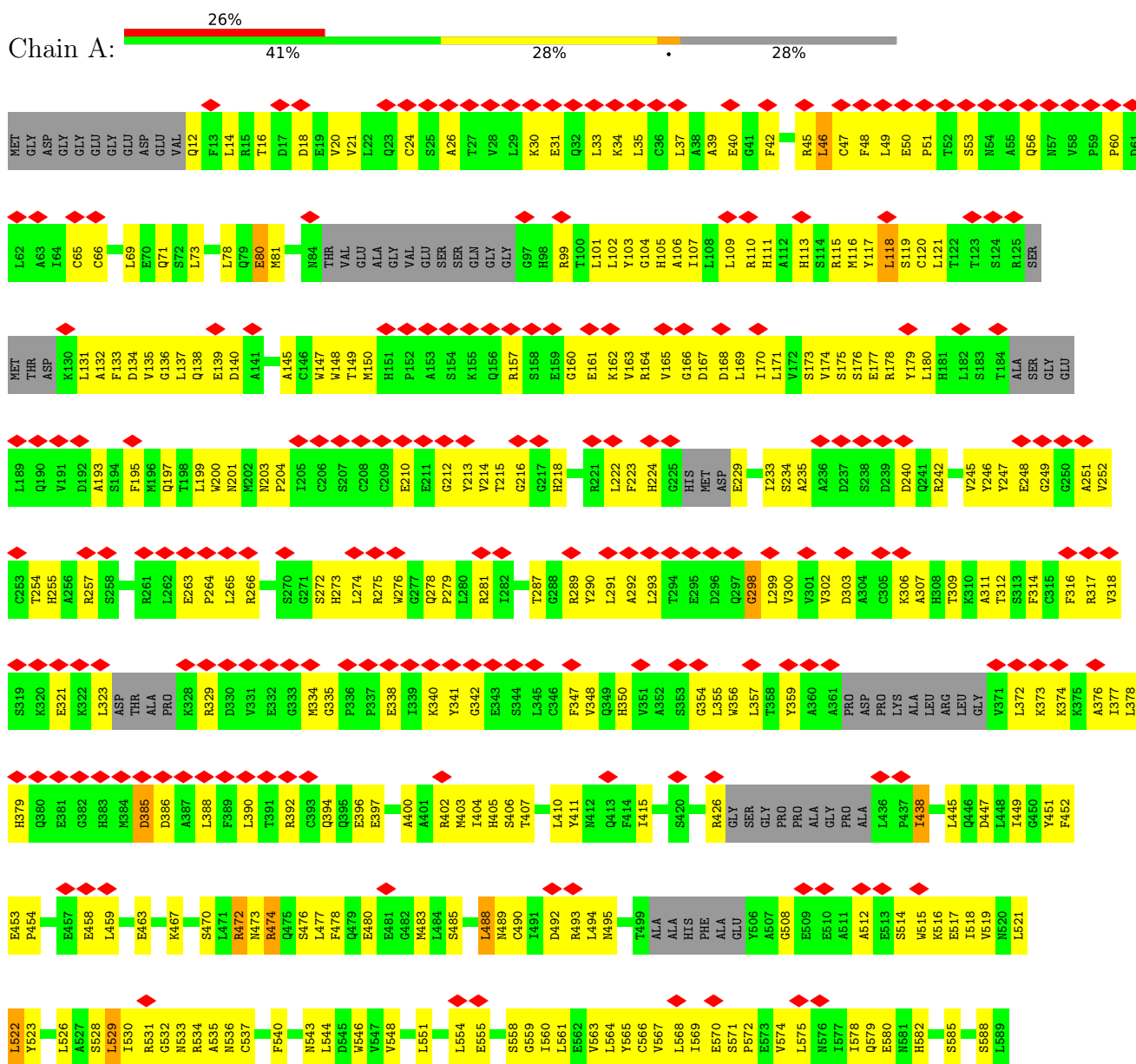
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

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

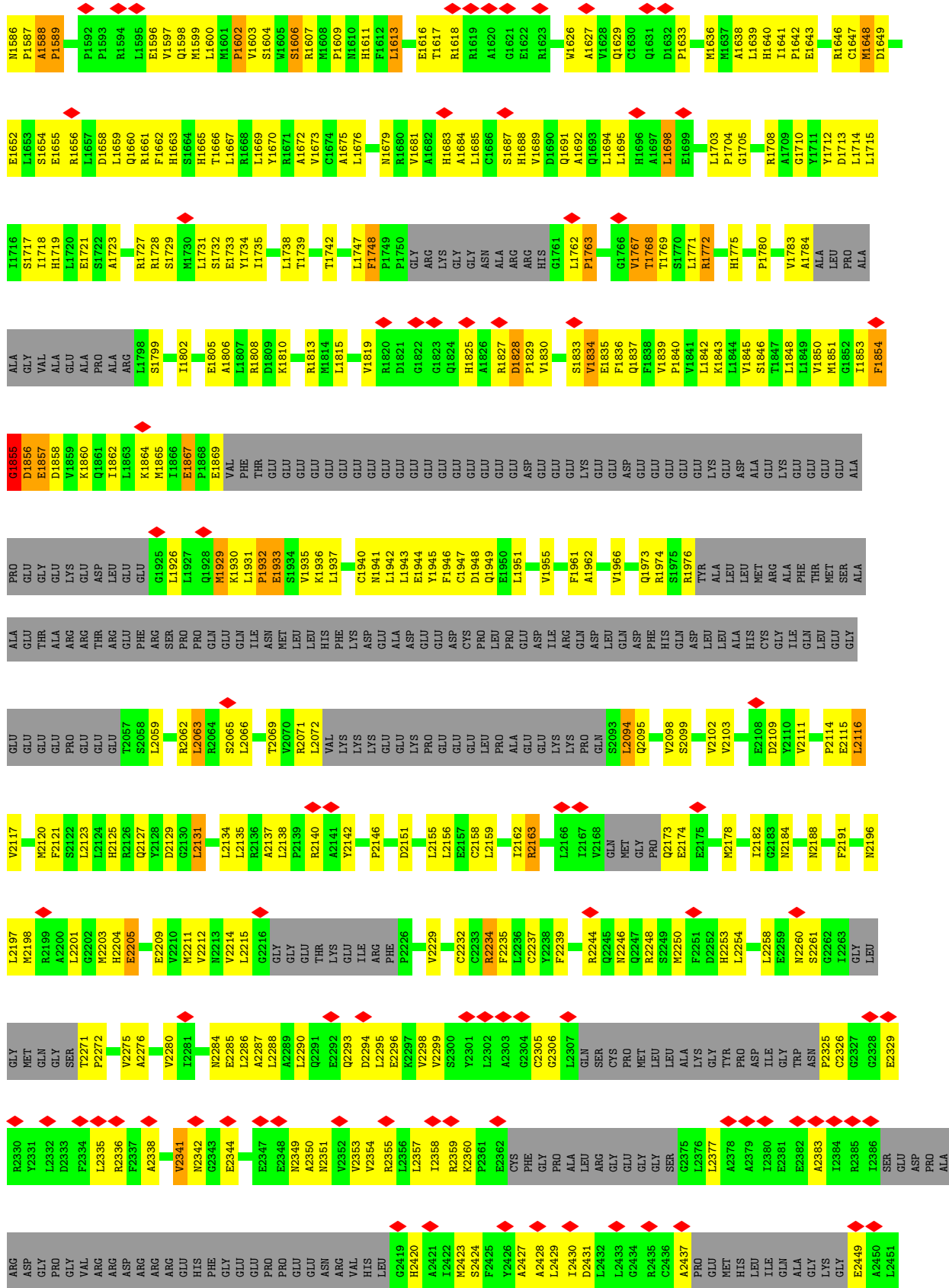
• Molecule 1: Ryanodine receptor 1



L590	D891	K592	H593	G594	R595	N596	H597	K598	V599	V602	L603	L606	C607	M610	G611	V614	M617	Q618	L619	I621	T622	L625	L626	P627	G628	R629	E630	L631	L632	L633	Q634	T635	M636	L637	I638	N639	Y640	V641	T642	S643	I644	R645	N646	I648	F649	V650	G651	ARG	ALA	GLU	GLY								
SER	THR	GLN	TYR	G660	K661	W662	Y663	D669	E670	V671	F674	L675	T676	A677	L682	R683	V684	G685	L688	T689	E690	G691	P696	G697	G698	G699	E700	G701	W702	G703	G704	N705	G706	V707	D710	L711	Y714	G715	F716	D717	H720	H725	V726	A727	R728	T731	S732	P733	G734										
L737	L738	A739	E740	P741	D742	C746	C747	L748	E749	L750	S751	F752	F753	S754	I755	S756	F757	R758	G761	C762	P763	V764	V767	E768	E769	A770	F771	N772	L773	D774	G775	L776	F777	F778	P779	V780	V781	S782	F783	S784	A785	G786	V787	K788	V789	R790	F791	L792	L793	G794	GLY	ARG	HIS	GLY	E799				
F800	K801	F802	L803	P804	P805	G806	G807	H812	E813	A814	V815	L816	P817	R818	E819	R820	L821	R822	L823	E824	P825	I826	K827	E828	Y829	R830	R831	E832	G833	P834	H838	L839	V840	G841	P842	S843	R844	C845	LEU	SER	HIS	THR	ASP	F851	V852	P853	C854	R855	V856	D857	L858	V859	Q860	I861	V862	L863	P864		
P865	H866	L867	E868	R869	I870	P806	R871	E872	H879	E880	A883	L884	T885	R886	I887	E888	Q889	G890	W891	T892	Y893	G894	P895	V896	R897	G898	M899	M900	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	S913	P914	E915	P916	E917	R918	N919	Y920	I921	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	GLU	ASN	LEU	LYS	THR	LYS	THR	LEU	PRO	LYS	THR	Y959	M960	M961	S962	N963	G964	Y965	R966	A968	P969	L970	D971	F910	L972	S973	H974	V975	R976	L977	T978	P979	A980	T983	L984	L988	N991	G992	V1001					
A1002	Q1003	GLY	TRP	SER	TYR	ALA	VAL	ASN	ILE	PRO	ALA	R1016	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	S1033	R1034	M1035	L1036	D1037	S1038	L1039	C1040	Q1041	G964	Y965	V1043	L1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	M1052	I1053	E1054	P1055	PRO	ASP	GLN	GLU	GLY	PRO	PRO	SER	GLN	VAL	GLU	ASN	GLN	SER
ARG	TRP	ASP	R1071	R1072	I1073	I1074	F1075	A1077	K1079	S1080	Y1081	V1083	Q1084	S1085	G1086	R1087	Y1088	F1090	E1091	F1092	E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	V1102	G1103	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	V1123	F1124	G1126	H1127	R1128							
G1129	Q1130	R1131	W1132	H1133	L1134	G1135	S1136	E1137	P1138	F1139	G1140	R1141	P1142	Q1144	S1145	G1146	D1147	V1148	C1151	M1152	T1153	D1154	L1155	T1156	M1157	N1158	F1162	T1163	L1164	H1165	G1166	E1167	V1168	L1169	MET	SER	ASP	SER	GLY	SER	THR	A1178	F1179	R1180	E1181	I1182	G1185	D1186	G1187	F1188	L1189	P1190	V1191	D1261	C1192				
S1193	L1194	G1197	Q1198	V1199	H1200	H1201	M1203	L1204	G1205	Q1206	D1207	S1210	L1211	F1213	F1214	A1215	I1216	E1221	G1222	F1223	E1224	P1225	F1226	A1227	M1230	Q1231	V1234	T1235	T1236	W1237	F1238	S1239	L1240	S1241	L1242	P1243	Q1244	F1245	E1246	P1247	E1251	H1252	P1253	H1254	Y1255	E1256	R1259	M1260	D1261	GLY									
THR	VAL	ASP	THR	PRO	PRO	CYS	LEU	ARG	L1272	R1275	T1276	W1277	G1278	S1279	L1283	V1284	E1285	M1286	L1287	F1288	L1289	R1290	L1291	L1292	L1293	P1294	V1295	Q1296	F1297	HIS	GLN	PHE	ARG	CYS	THR	ALA	GLY	ALA	THR	PRO	LEU	ALA	PRO	VAL	ARG	ALA	PRO	ASN	GLU	GLY	THR	ALA	ARG						
ALA	ALA	GLU	PRO	ASP	PRO	ASP	TYR	GLU	ARG	ARG	ARG	GLY	GLY	GLY	ALA	ALA	GLY	ALA	GLY	LYS	GLU	GLY	THR	ALA	ALA	GLY	THR	THR	ALA	ASN	THR	PHE	THR	GLY	VAL	GLU	ALA	GLN	PRO	VAL	ARG	ALA	ALA	ASN	GLU	GLY	THR	THR	ALA	ALA	ARG								
LYS	LYS	ARG	GLY	PHE	PRO	PHE	LYS	ALA	LYS	ALA	ALA	MET	THR	MET	GLN	PRO	PRO	ALA	THR	PRO	THR	HIS	ASP	VAL	VAL	VAL	PRO	PRO	ALA	ASP	ASN	THR	THR	ILE	ILE	ILE	LEU	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	PRO										

SER	C1447	L1519	E1596	R1661	R1727	ARG	I1862	LEU	THR	GLU	S2192	L2201	SER
C1448	V1520	L1597	V1597	F1662	R1728	ARG	L1863	GLU	ARG	GLU	L2123	G2202	T2271
M1452	ASP	M1598	Q1598	H1663	H1729	THR	K1864	GLU	ARG	GLU	E2125	M2203	P2272
Y1457	LEU	M1601	L1600	H1665	M1730	ARG	M1865	GLU	PHE	GLU	S2058	H2204	M2205
H1458	THR	M1602	M1601	T1666	L1731	ARG	I1866	L1926	SER	PRO	R2126	V2275	E2205
G1459	G1525	V1603	M1601	L1667	S1732	THR	I1867	L1927	PRO	PRO	Q2127	A2276	A2276
M1462	A1531	M1604	V1605	R1668	I1733	THR	P1868	Q1928	PRO	R2062	Y2198	V2280	V2280
M1463	M1532	S1604	M1605	L1669	I1735	THR	I1869	M1929	PRO	L2063	D2129	V2210	I2281
F1465	N1537	M1607	S1606	Y1670	L1738	THR	P1868	K1806	GLN	R2064	R2064	M2211	N2284
L1466	N1537	M1608	M1606	L1671	T1739	THR	I1869	L1931	GLN	S2065	L2066	V2212	E2285
S1467	F1539	M1609	M1607	A1672	T1739	THR	P1868	L1932	GLN	L2066	L2066	V2214	A2287
LYS	P1544	M1610	M1609	A1675	T1742	THR	I1869	E1933	ILE	T2069	L2134	L2215	L2288
VAL	P1544	M1611	M1610	A1675	T1742	THR	I1869	S1934	MET	V2070	L2135	L2216	L2288
ARG	N1546	M1612	M1611	L1676	L1747	THR	M1813	L1935	GLU	R2071	L2136	G2216	L2290
ALA	K1547	L1613	M1611	L1676	F1748	THR	L1815	K1936	GLU	L2072	L2137	GLY	L2290
V1472	K1548	E1616	L1613	L1676	P1749	THR	V1819	L1937	PHE	VAL	P2139	THR	Q2291
G1477	F1549	T1617	L1613	L1676	P1750	THR	R1820	M1941	LYS	LYS	R2140	LYS	Q2291
D1478	P1550	R1618	R1619	L1685	ARG	GLY	D1821	L1942	ASP	LYS	R2141	LYS	Q2293
E1479	V1554	R1618	R1619	L1685	LYS	GLY	G1822	L1943	ASP	LYS	Y2142	ILE	D2294
Q1480	L1555	R1618	R1619	L1685	GLY	GLY	G1822	E1944	ALA	GLU	Y2142	ILE	L2295
G1481	P1556	R1619	R1619	L1685	GLY	GLY	Q1824	Y1945	ASP	LYS	P2146	ARG	E2296
H1482	V1561	R1621	R1621	L1685	ASN	ASN	H1825	F1946	GLU	PRO	D2151	PHE	K2297
H1483	I1562	G1621	G1621	L1685	ALA	ALA	H1825	D1948	GLU	GLU	L2155	V2229	V2298
H1484	Q1563	A1627	A1627	L1685	ARG	ARG	R1827	F1950	ASP	GLU	L2156	G2232	S2300
S1485	F1564	Q1629	Q1629	L1685	ARG	ARG	D1827	L1951	GLU	ALA	E2157	C2232	Y2301
S1486	E1565	C1630	C1630	L1685	HIS	HIS	D1828	L1951	LEU	ALA	C2158	R2234	L2302
L1487	LEU	D1632	D1632	L1685	G1766	GLY	V1955	L1951	LEU	ALA	L2159	F2236	A2303
K1488	LYS	P1633	P1633	L1685	P1763	GLY	V1955	L1951	LEU	ALA	L2162	C2237	G2304
C1489	GLY	M1636	M1636	L1685	P1766	GLY	V1955	L1951	LEU	ALA	R2163	V2238	G2306
S1490	LYS	M1637	M1637	L1685	G1766	GLY	V1955	L1951	LEU	ALA	L2166	V2239	L2307
M1491	GLN	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	I2167	R2244	GLN
CYS	ASN	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	V2168	Q2245	SER
Y1493	ILE	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	GLN	Q2246	PRO
G1497	LEU	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	MET	Q2247	PRO
GLY	ASP	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	GLY	R2248	LEU
ASP	PHE	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	PRO	S2249	LEU
VAL	VAL	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	Q2173	M2250	LEU
SER	SER	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2174	ALA	LEU
PRO	PRO	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	F2251	LYS
GLN	GLN	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	D2252	LYS
GLY	GLY	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	H2253	GLY
ASP	ASP	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	TRP
PHE	PHE	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	PRO
VAL	VAL	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASN
SER	SER	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
PRO	PRO	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ILE
GLY	GLY	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	TRP
GLN	GLN	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASN
ARG	ARG	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
ILE	ILE	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
S1510	S1510	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
H1511	H1511	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
T1512	T1512	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
D1513	D1513	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
L1514	L1514	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
V1515	V1515	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
I1516	I1516	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
L1519	L1519	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
V1520	V1520	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
ASP	ASP	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
LEU	LEU	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
THR	THR	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
G1525	G1525	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
A1531	A1531	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
M1532	M1532	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
N1537	N1537	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
F1465	F1465	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
L1466	L1466	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
S1467	S1467	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
LYS	LYS	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
VAL	VAL	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
ARG	ARG	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
ALA	ALA	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
V1472	V1472	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
G1477	G1477	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
D1478	D1478	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
E1479	E1479	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
Q1480	Q1480	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
G1481	G1481	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
H1482	H1482	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
H1483	H1483	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
H1484	H1484	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
S1485	S1485	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
S1486	S1486	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
L1487	L1487	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
K1488	K1488	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
C1489	C1489	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
S1490	S1490	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
M1491	M1491	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
CYS	CYS	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
Y1493	Y1493	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
G1497	G1497	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
GLY	GLY	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
ASP	ASP	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
PHE	PHE	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
VAL	VAL	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
SER	SER	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
PRO	PRO	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
GLN	GLN	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
GLY	GLY	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
ASP	ASP	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
LEU	LEU	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
LEU	LEU	M1637	M1637	L1685	P1766	GLY	V1955	L1951	LEU	ALA	E2175	L2254	ASP
LEU	LEU	M1637	M1637	L1685									

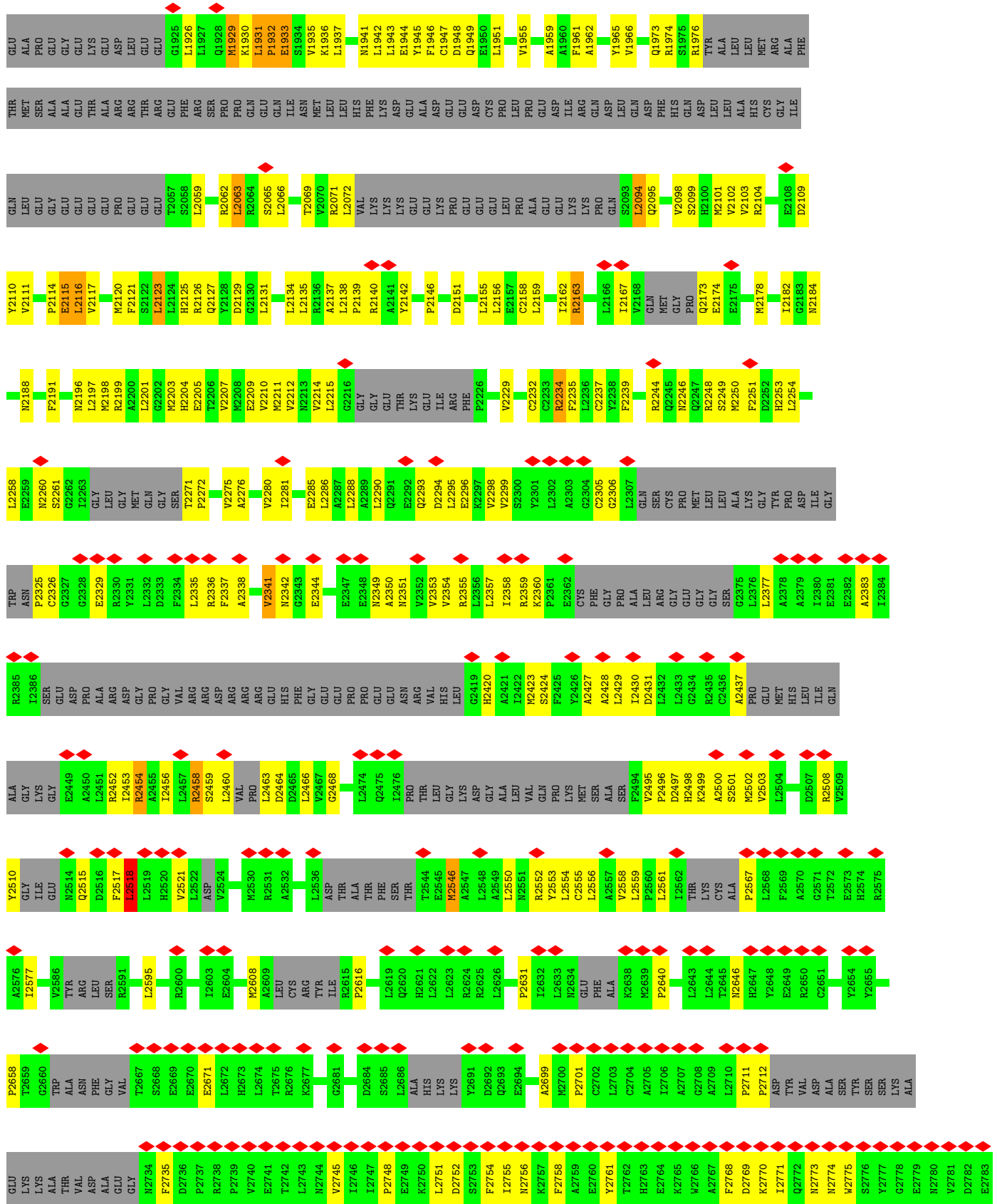
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E799	E799	E799	E927	GLN	N991	GLN	G1126	THR	P1190	GLU	R1259	THR	A1441	D1513	D1513
F900	F900	F900	T928	SER	V1001	SER	R1127	TRP	V1191	ALA	R1260	GLY	G1447	L1514	L1514
F802	F802	F802	L929	ARG	A1002	ARG	G1128	ASP	C1192	ALA	D1261	ALA	G1448	V1515	V1515
P804	P804	P804	L930	TRP	Q1003	TRP	Q1109	TRP	L1194	ALA	G1262	ALA	V1449	I1516	I1516
P805	P805	P805	T931	GLY	GLY	ASP	R1131	ASP	G1195	ALA	H1263	LYS	V1450	L1519	L1519
P806	P806	P806	T932	TRP	GLY	VAL	W1132	THR	F1196	GLU	H1264	GLY	V1451	V1520	V1520
G507	G507	G507	L933	SER	TRP	GLN	L1134	ASP	G1197	GLY	H1265	ALA	V1452	ASP	ASP
HB12	HB12	HB12	L934	TYR	GLY	ASP	G1135	THR	Q1198	GLY	H1266	ALA	V1453	LEU	LEU
E813	E813	E813	A934	SER	ALA	GLN	S1136	PRO	V1199	PRO	H1267	LYS	W1454	THR	THR
L748	L748	L748	L935	ALA	ALA	ASP	R1071	PRO	H1200	ASP	H1268	LYS	Y1455	ALA	ALA
D749	D749	D749	T931	VAL	VAL	GLN	V1072	CYS	H1201	TYR	H1269	ALA	H1456	THR	THR
S751	S751	S751	L932	GLN	VAL	ASP	R1073	LEU	L1202	GLY	H1270	ALA	H1457	GLY	GLY
P817	P817	P817	L933	ASP	GLN	ARG	L1074	LEU	L1203	ALA	H1271	ALA	H1458	GLY	GLY
L750	L750	L750	K873	ASP	ASP	ILE	L1075	LEU	L1204	ARG	H1272	ALA	H1459	GLY	GLY
S752	S752	S752	R879	PRO	PRO	PRO	F1075	LEU	G1205	ALA	H1273	ALA	H1460	LEU	LEU
P753	P753	P753	E880	ALA	ALA	ALA	F1076	LEU	Q1206	ARG	H1274	ALA	H1461	GLY	GLY
S754	S754	S754	E881	ALA	R1016	VAL	Q1084	LEU	D1207	ARG	H1275	ALA	H1462	ARG	ARG
S755	S755	S755	E882	ALA	Y1024	VAL	S1085	LEU	S1210	ARG	H1276	ALA	H1463	ARG	ARG
S756	S756	S756	L821	ALA	R1025	GLN	G1086	LEU	L1211	ARG	H1277	ALA	H1464	ARG	ARG
R757	R757	R757	L822	ALA	L1026	GLN	R1087	LEU	R1212	ARG	H1278	ALA	H1465	ARG	ARG
R758	R758	R758	R886	ALA	L1027	GLN	W1088	LEU	F1214	ARG	H1279	ALA	H1466	ARG	ARG
G761	G761	G761	I887	ALA	D1028	GLY	F1089	LEU	F1215	ARG	H1280	ALA	H1467	ARG	ARG
C762	C762	C762	E888	ALA	E1029	GLY	C1151	LEU	A1215	ARG	H1281	ALA	H1468	ARG	ARG
P825	P825	P825	E889	ALA	F1090	GLY	M1152	LEU	E1285	ARG	H1282	ALA	H1469	ARG	ARG
K827	K827	K827	G889	ALA	A1030	GLY	I1153	LEU	C1217	ARG	H1283	ALA	H1470	ARG	ARG
V764	V764	V764	G890	ALA	T1031	GLY	D1154	LEU	E1286	ARG	H1284	ALA	H1471	ARG	ARG
V767	V767	V767	G891	ALA	K1032	GLY	L1155	LEU	F1288	ARG	H1285	ALA	H1472	ARG	ARG
F768	F768	F768	W891	ALA	LYS	GLY	T1156	LEU	L1289	ARG	H1286	ALA	H1473	ARG	ARG
E769	E769	E769	T892	ALA	THR	GLY	E1157	LEU	R1290	ARG	H1287	ALA	H1474	ARG	ARG
A770	A770	A770	G894	ALA	THR	GLY	L1158	LEU	L1291	ARG	H1288	ALA	H1475	ARG	ARG
F771	F771	F771	P895	ALA	LYS	GLY	T1096	LEU	S1292	ARG	H1289	ALA	H1476	ARG	ARG
N772	N772	N772	P896	ALA	LYS	GLY	V1095	LEU	L1293	ARG	H1290	ALA	H1477	ARG	ARG
L773	L773	L773	V896	ALA	THR	GLY	T1097	LEU	F1223	ARG	H1291	ALA	H1478	ARG	ARG
D774	D774	D774	R897	ALA	THR	GLY	G1098	LEU	F1224	ARG	H1292	ALA	H1479	ARG	ARG
G775	G775	G775	D898	ALA	LYS	GLY	E1099	LEU	P1225	ARG	H1293	ALA	H1480	ARG	ARG
L776	L776	L776	N900	ALA	LYS	GLY	M1100	LEU	F1226	ARG	H1294	ALA	H1481	ARG	ARG
F777	F777	F777	G841	ALA	LYS	GLY	R1101	LEU	A1227	ARG	H1295	ALA	H1482	ARG	ARG
F778	F778	F778	P842	ALA	LYS	GLY	V1102	LEU	Q1296	ARG	H1296	ALA	H1483	ARG	ARG
V780	V780	V780	S843	ALA	THR	GLY	G1103	LEU	F1297	ARG	H1297	ALA	H1484	ARG	ARG
S782	S782	S782	R844	ALA	THR	GLY	W1104	LEU	HIS	ARG	H1298	ALA	H1485	ARG	ARG
F783	F783	F783	C845	ALA	THR	GLY	E1107	LEU	GLN	ARG	H1299	ALA	H1486	ARG	ARG
S784	S784	S784	R845	ALA	THR	GLY	P1107	LEU	GLN	ARG	H1300	ALA	H1487	ARG	ARG
G786	G786	G786	R845	ALA	THR	GLY	ASP	LEU	PHE	ARG	H1301	ALA	H1488	ARG	ARG
V787	V787	V787	R844	ALA	THR	GLY	ASP	LEU	THR	ARG	H1302	ALA	H1489	ARG	ARG
K788	K788	K788	R844	ALA	THR	GLY	ASP	LEU	THR	ARG	H1303	ALA	H1490	ARG	ARG
V789	V789	V789	C845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1304	ALA	H1491	ARG	ARG
R790	R790	R790	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1305	ALA	H1492	ARG	ARG
F791	F791	F791	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1306	ALA	H1493	ARG	ARG
L792	L792	L792	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1307	ALA	H1494	ARG	ARG
L793	L793	L793	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1308	ALA	H1495	ARG	ARG
L794	L794	L794	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1309	ALA	H1496	ARG	ARG
G794	G794	G794	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1310	ALA	H1497	ARG	ARG
V859	V859	V859	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1311	ALA	H1498	ARG	ARG
Q860	Q860	Q860	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1312	ALA	H1499	ARG	ARG
I861	I861	I861	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1313	ALA	H1500	ARG	ARG
V862	V862	V862	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1314	ALA	H1501	ARG	ARG
L863	L863	L863	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1315	ALA	H1502	ARG	ARG
P864	P864	P864	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1316	ALA	H1503	ARG	ARG
P865	P865	P865	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1317	ALA	H1504	ARG	ARG
H866	H866	H866	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1318	ALA	H1505	ARG	ARG
L867	L867	L867	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1319	ALA	H1506	ARG	ARG
P805	P805	P805	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1320	ALA	H1507	ARG	ARG
E868	E868	E868	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1321	ALA	H1508	ARG	ARG
R869	R869	R869	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1322	ALA	H1509	ARG	ARG
I870	I870	I870	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1323	ALA	H1510	ARG	ARG
R871	R871	R871	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1324	ALA	H1511	ARG	ARG
E872	E872	E872	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1325	ALA	H1512	ARG	ARG
K873	K873	K873	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1326	ALA	H1513	ARG	ARG
H879	H879	H879	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1327	ALA	H1514	ARG	ARG
E880	E880	E880	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1328	ALA	H1515	ARG	ARG
A883	A883	A883	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1329	ALA	H1516	ARG	ARG
L884	L884	L884	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1330	ALA	H1517	ARG	ARG
T885	T885	T885	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1331	ALA	H1518	ARG	ARG
R886	R886	R886	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1332	ALA	H1519	ARG	ARG
I887	I887	I887	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1333	ALA	H1520	ARG	ARG
E888	E888	E888	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1334	ALA	H1521	ARG	ARG
Q889	Q889	Q889	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1335	ALA	H1522	ARG	ARG
G890	G890	G890	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1336	ALA	H1523	ARG	ARG
W891	W891	W891	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1337	ALA	H1524	ARG	ARG
T892	T892	T892	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1338	ALA	H1525	ARG	ARG
G894	G894	G894	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1339	ALA	H1526	ARG	ARG
P895	P895	P895	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1340	ALA	H1527	ARG	ARG
V896	V896	V896	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1341	ALA	H1528	ARG	ARG
R897	R897	R897	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1342	ALA	H1529	ARG	ARG
D898	D898	D898	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1343	ALA	H1530	ARG	ARG
N899	N899	N899	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1344	ALA	H1531	ARG	ARG
G900	G900	G900	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1345	ALA	H1532	ARG	ARG
K901	K901	K901	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1346	ALA	H1533	ARG	ARG
R902	R902	R902	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1347	ALA	H1534	ARG	ARG
L903	L903	L903	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1348	ALA	H1535	ARG	ARG
H904	H904	H904	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1349	ALA	H1536	ARG	ARG
P905	P905	P905	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1350	ALA	H1537	ARG	ARG
C906	C906	C906	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1351	ALA	H1538	ARG	ARG
S908	S908	S908	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1352	ALA	H1539	ARG	ARG
N909	N909	N909	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1353	ALA	H1540	ARG	ARG
F910	F910	F910	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1354	ALA	H1541	ARG	ARG
H911	H911	H911	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1355	ALA	H1542	ARG	ARG
S912	S912	S912	R845	ALA	THR	GLY	ASP	LEU	THR	ARG	H1356	ALA	H1543	ARG	ARG
L913	L91														



R2452	R2453	R2454	R2455	R2456	R2457	R2458	S2459	L2460	VAL	PRO	L2463	L2464	D2465	D2466	L2467	G2468	L2474	Q2475	L2476	PRO	THR	LEU	GLY	LYS	ASP	GLY	ALA	VAL	GLN	PRO	L2563	L2564	C2565	L2566	SER	ALA	SER	F2494	V2495	F2496	H2498	K2499	A2500	S2501	M2502	V2503	L2504	D2507	R2508	V2509	Y2510	GLY	ILE	GLU	W2514	Q2515	D2516				
F2517	L2518	L2519	H2520	V2521	L2522	ASP	V2524	M2530	R2531	A2532	L2536	ASP	THR	ALA	ALA	THR	PHE	PHE	SER	THR	T2544	E2545	M2546	A2547	L2548	A2549	L2550	N2551	R2552	Y2553	L2554	C2555	L2556	V2558	L2559	P2567	L2568	F2569	G2571	T2572	H2574	R2575	A2576	L2577	V2586	TYR	ARG	LEU													
SER	R2591	L2595	R2600	L2603	E2604	M2608	A2609	LEU	CYS	ARG	TYR	ILE	R2615	P2616	L2619	Q2620	H2621	L2622	L2623	R2624	R2625	L2626	P2631	L2632	L2633	M2634	PHE	ALA	ALA	R2638	M2639	P2640	L2643	L2644	T2645	M2646	H2647	Y2648	E2649	R2650	C2651	Y2654	SER	THR	TYR	SER	THR	THR	P2658	T2659	G2660	TRP	ALA	ASN	PHE						
GLY	VAL	T2667	S2668	E2669	E2670	E2671	L2672	H2673	L2674	T2675	R2676	K2677	L2678	G2681	D2684	S2685	L2686	ALA	HIS	LYS	LYS	Y2691	D2692	Q2693	E2694	A2699	M2700	P2701	C2702	L2703	C2704	A2705	I2706	A2707	G2708	A2709	L2710	P2711	P2712	ASP	TYR	VAL	ASP	ALA	SER	THR	THR	SER	SER	LYS	LYS	ALA	GLU	LYS	LYS	ALA	THR	VAL			
ASP	ALA	GLU	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	D2782	E2783	L2785	K2786	H2788	P2789						
W2790	L2791	R2792	P2793	K2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	E2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	L2822	T2823	E2824	K2825	A2826	R2827	E2828	K2829	E2830	GLU	GLU	ARG	THR	GLY	LYS	LYS	THR	ARG	LYS	ILE	LEU	ARG	TRP	GLN	THR	THR	ALA	GLN	THR	Y2849
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T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	A2922	K2923	Q2924	E2925	L2926	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	G2940	LEU	LEU	ASP	MET	GLU	LEU	LEU	ASP	HIS	CYS	LYS	Y3016	F3017	L3018	S3019	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029							
SER	GLN	GLU	PHE	ILE	ALA	HIS	LEU	VAL	VAL	SER	SER	GLY	ARG	VAL	GLU	LYS	SER	PRO	HIS	GLN	GLU	ILE	PHE	ALA	LYS	ILE	LEU	PRO	LEU	ILE	ASN	GLN	TYR	THR	THR	ASN	HIS	CYS	LYS	Y3016	F3017	L3018	S3019	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029								
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LEU	GLY	PRO	ASN	VAL	GLU	MET	CYS	PRO	ASP	ILE	PRO	VAL	LEU	ARG	LEU	MET	ALA	ASP	ILE	THR	LYS	ALA	GLU	GLY	ALA	ARG	TYR	THR	GLU	MET	ILE	VAL	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	A3215	C3216	S3217	VAL	TYR	THR	THR	THR	SER	SER	PRO	ARG	GLU	ARG	ALA	ILE						
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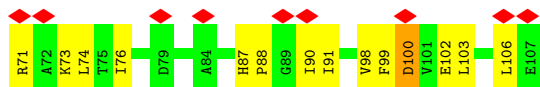
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C3839	S3840	V3841	L3842	D3843	L3844	R3849	F3852	ALA	GLU	GLY	LEU	GLY	GLY	VAL	ASN	ASP	GLY	THR	VAL	ILE	ASN	ARG	GLN	ASN	GLY	GLU	VAL	D3877	D3878	F3879	F3880	T3881	Q3882	D3883	L3884	F3885	R3886	L3887	Q3888	Q3889	L3890	L3891	C3892	E3893	F3899	Q3900	N3901	Y3902	T3905	Q3906	T3907																		
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LYS	SER	LYS	LYS	ALA	VAL	TRP	HIS	LYS	LEU	SER	LYS	GLN	ARG	ARG	ALA	VAL	VAL	VAL	ALA	CYS	PHE	VAL	MET	THR	PRO	GLY	N3651	L3654	E3655	K3658	A3659	K3660	K3661	I3662	E3665	K3668	A3669	H3667	D3666	H3667	S3668	F3669	E3670	I3674	D3675	D3676	L3677	A3680	GLY	GLU	GLN																		
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C3839	S3840	V3841	L3842	D3843	L3844	R3849	F3852	ALA	GLU	GLY	LEU	GLY	GLY	VAL	ASN	ASP	GLY	THR	VAL	ILE	ASN	ARG	GLN	ASN	GLY	GLU	VAL	D3877	D3878	F3879	F3880	T3881	Q3882	D3883	L3884	F3885	R3886	L3887	Q3888	Q3889	L3890	L3891	C3892	E3893	F3899	Q3900	N3901	Y3902	T3905	Q3906	T3907																		
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ILE	ALA	HIS	LEU	GLU	ALA	VAL	VAL	SER	SER	GLY	ARG	VAL	GLU	LYS	PRO	HIS	GLU	GLN	GLU	ILE	LYS	PHE	PHE	ALA	ALA	ILE	LYS	LEU	PRO	ILE	ILE	ASN	GLN	TVR	PHE	THR	ASN	HIS	CYS	Y3016	F3017	L3018	S3019	T3020	P3021	A3022	K3023	V3024	L3025	G3026	G3027	G3028	H3030	A3031	S3032	R3033							
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E3097	S3098	A3099	S3100	T3103	E3104	K3105	M3106	V3107	E3108	M3109	L3110	R3111	L3112	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	LYS	GLY	VAL	GLN	ASN	GLN	LEU	THR	T3132	T3133	L3137	F3138	V3139	L3140	H3146	I3147	Q3151	F3152	GLY	ASP	ASP	VAL	ILE	L3158	D3159	D3160	V3161	Q3162	S3164	C3165											
Y3166	R3167	T3168	L3169	C3170	S3171	I3172	Y3173	S3174	L3175	G3176	T3177	T3178	LYS	ASN	THR	TVR	V3183	E3184	K3185	L3186	R3187	P3188	A3195	R3196	L3197	A3198	A3199	A3200	MET	PRO	VAL	T3273	F3205	L3206	E3207	P3208	Q3209	L3210	A3215	C3216	S3217	VAL	TVR	THR	THR	GLN	LYS	SER	PRO	ARG	G3288	P3289	E3290	ALA	PRO	PRO							
ASN	SER	VAL	GLU	GLU	MET	CYS	PRO	ASP	ILE	PRO	VAL	LEU	ASP	ARG	LEU	ALA	ALA	ASP	ILE	GLY	GLY	LEU	LEU	ALA	TYR	THR	GLU	MET	HIS	PRO	VAL	ILE	GLU	ILE	T3273	L3274	P3275	M3276	L3277	C3278	S3279	Y3280	L3281	P3282	R3283	W3284	W3285	E3286	K3287	G3288	P3289	E3290	ALA	PRO	PRO								
P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	G3304	T3305	A3306	V3307	T3308	S3309	D3310	H3311	L3312	M3313	SER	LEU	LEU	G3317	M3318	I3319	L3320	V3324	N3325	M3326	L3327	G3328	I3329	D3330	E3331	A3332	T3333	W3334	M3335	L3338	A3339	VAL	PHE	ALA	ALA	Y3406	A3407	L3408	Y3409	P3410	L3411	L3412	L3413	R3414	Y3415	V3416	D3417	N3418	N3419	R3420	S3356			
H3357	F3358	I3359	P3360	T3361	I3362	G3363	ARG	LEU	ARC	K3367	R3368	A3369	V3373	A3374	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3387	E3388	E3389	G3390	E3391	V3394	R3395	D3396	E3397	PHE	ALA	SER	SER	VAL	LEU	C3402	R3403	D3404	L3405	Y3406	A3407	L3408	Y3409	P3410	L3411	L3412	L3413	R3414	Y3415	V3416	D3417	N3418	N3419	R3420					
A3421	H3422	H3423	L3424	THR	GLU	P3427	N3428	A3429	N3430	A3431	E3432	E3433	L3434	F3435	ARG	M3437	S3446	K3447	S3448	H3449	N3450	E3455	G3456	N3457	H3458	F3469	L3470	THR	ALA	ASP	SER	LYS	C3402	R3403	D3404	L3405	Y3406	A3407	L3408	Y3409	P3410	L3411	L3412	L3413	R3414	Y3415	V3416	D3417	N3418	N3419	R3420												
A3478	A3479	K3480	A3481	G3482	D3483	A3484	Q3485	S3486	G3487	G3488	D3490	GLU	ARG	H3478	A3479	K3480	A3481	G3482	D3483	A3484	Q3485	S3486	G3487	G3488	D3490	GLU	ARG																																				

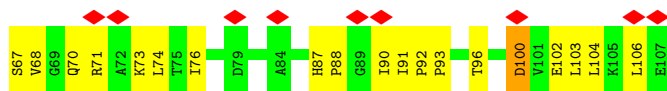
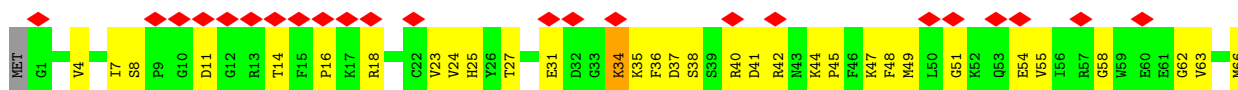




- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.243	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.21	41/27312 (0.2%)	1.12	151/37004 (0.4%)
1	C	1.20	39/27312 (0.1%)	1.12	154/37004 (0.4%)
1	E	1.21	35/27312 (0.1%)	1.12	158/37004 (0.4%)
1	G	1.21	38/27312 (0.1%)	1.11	145/37004 (0.4%)
2	B	0.91	1/851 (0.1%)	0.93	2/1146 (0.2%)
2	D	0.91	1/851 (0.1%)	0.92	2/1146 (0.2%)
2	F	0.91	1/851 (0.1%)	0.92	2/1146 (0.2%)
2	H	0.93	1/851 (0.1%)	0.90	0/1146
All	All	1.20	157/112652 (0.1%)	1.11	614/152600 (0.4%)

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	36
1	C	0	35
1	E	0	36
1	G	0	34
All	All	0	141

The worst 5 of 157 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	80	GLU	CG-CD	11.12	1.68	1.51
1	G	3661	TRP	CB-CG	10.06	1.68	1.50
1	A	3661	TRP	CB-CG	9.81	1.68	1.50
1	G	1976	ARG	NE-CZ	9.78	1.45	1.33
1	A	741	GLU	CG-CD	9.74	1.66	1.51

The worst 5 of 614 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	G	80	GLU	OE1-CD-OE2	-10.92	110.20	123.30
1	A	1212	ARG	NE-CZ-NH1	10.39	125.49	120.30
1	G	4796	MET	CG-SD-CE	10.33	116.73	100.20
1	G	1976	ARG	CD-NE-CZ	10.23	137.93	123.60
1	C	1212	ARG	NE-CZ-NH1	10.17	125.39	120.30

There are no chirality outliers.

5 of 141 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	GLU	Mainchain,Peptide
1	A	329	ARG	Mainchain,Peptide
1	A	734	GLY	Peptide
1	A	841	GLY	Mainchain,Peptide
1	A	894	GLY	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	26843	0	24428	1190	0
1	C	26843	0	24428	1200	0
1	E	26843	0	24428	1194	0
1	G	26843	0	24427	1209	0
2	B	832	0	831	58	0
2	D	832	0	831	54	0
2	F	832	0	831	58	0
2	H	832	0	831	58	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	110704	0	101035	4733	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 22.

The worst 5 of 4733 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4880:MET:HA	1:G:4578:LEU:HD11	1.26	1.17
1:A:4578:LEU:HD11	1:C:4880:MET:HA	1.18	1.17
1:E:4578:LEU:HD11	1:G:4880:MET:HA	1.25	1.16
1:C:4578:LEU:HD11	1:E:4880:MET:HA	1.17	1.10
1:A:4822:THR:HG22	1:C:4839:MET:SD	1.93	1.08

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	3483/5037 (69%)	3132 (90%)	258 (7%)	93 (3%)	5	31
1	C	3483/5037 (69%)	3133 (90%)	254 (7%)	96 (3%)	5	30
1	E	3483/5037 (69%)	3134 (90%)	255 (7%)	94 (3%)	5	31
1	G	3483/5037 (69%)	3137 (90%)	252 (7%)	94 (3%)	5	31
2	B	105/108 (97%)	95 (90%)	9 (9%)	1 (1%)	15	54
2	D	105/108 (97%)	95 (90%)	9 (9%)	1 (1%)	15	54
2	F	105/108 (97%)	96 (91%)	8 (8%)	1 (1%)	15	54
2	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
All	All	14352/20580 (70%)	12919 (90%)	1053 (7%)	380 (3%)	8	31

5 of 380 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	806	PRO
1	A	900	ASN
1	A	914	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	916	PRO
1	A	971	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2502/4276 (58%)	2472 (99%)	30 (1%)	71 83
1	C	2504/4276 (59%)	2476 (99%)	28 (1%)	73 84
1	E	2501/4276 (58%)	2472 (99%)	29 (1%)	71 83
1	G	2501/4276 (58%)	2474 (99%)	27 (1%)	73 84
2	B	89/90 (99%)	88 (99%)	1 (1%)	73 84
2	D	89/90 (99%)	88 (99%)	1 (1%)	73 84
2	F	89/90 (99%)	88 (99%)	1 (1%)	73 84
2	H	89/90 (99%)	88 (99%)	1 (1%)	73 84
All	All	10364/17464 (59%)	10246 (99%)	118 (1%)	74 84

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4207	MET
1	G	2555	CYS
1	E	1211	LEU
1	G	2518	LEU
1	G	978	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 155 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	4947	GLN
1	G	3809	ASN
1	G	224	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	1130	GLN
1	G	4728	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

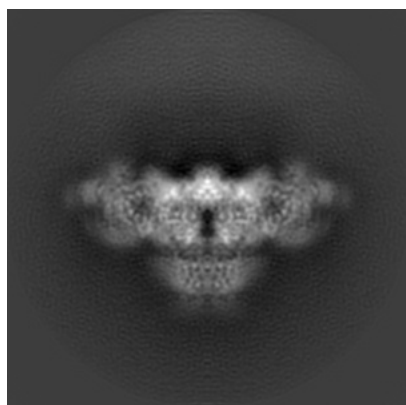
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9521. These allow visual inspection of the internal detail of the map and identification of artifacts.

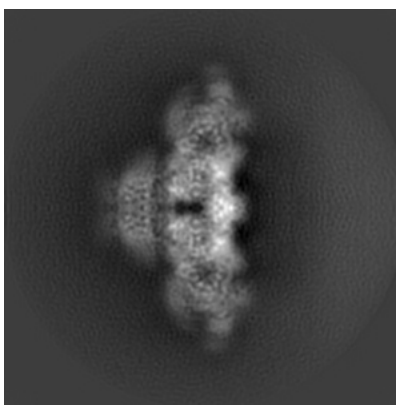
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

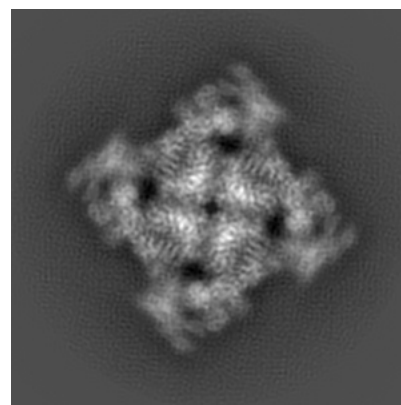
6.1.1 Primary map



X



Y

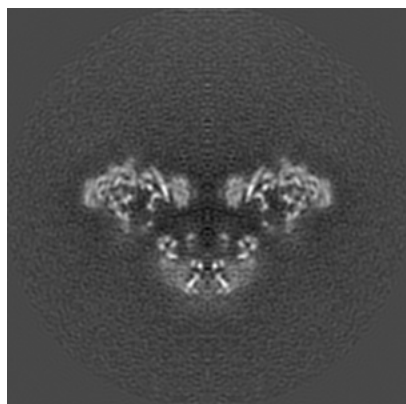


Z

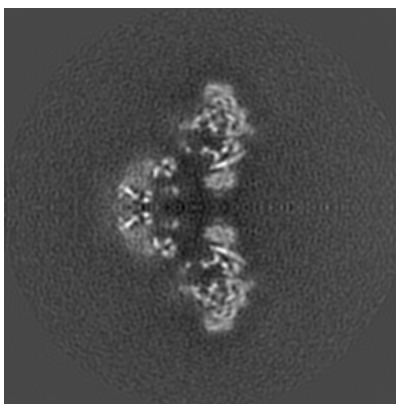
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

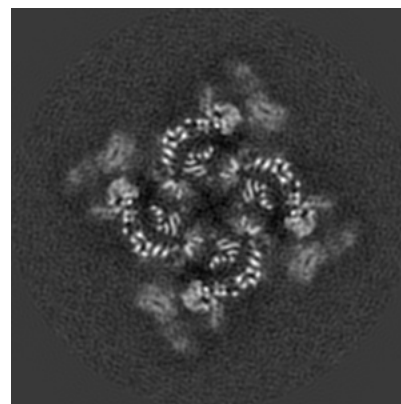
6.2.1 Primary map



X Index: 180



Y Index: 180

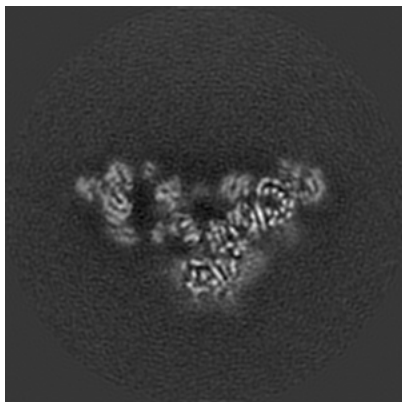


Z Index: 180

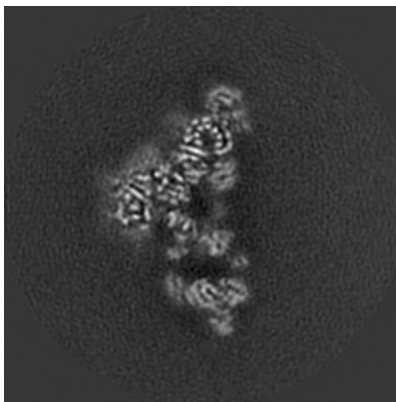
The images above show central slices of the map in three orthogonal directions.

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

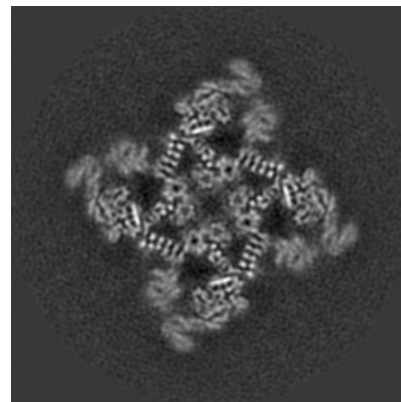
6.3.1 Primary map



X Index: 169



Y Index: 191

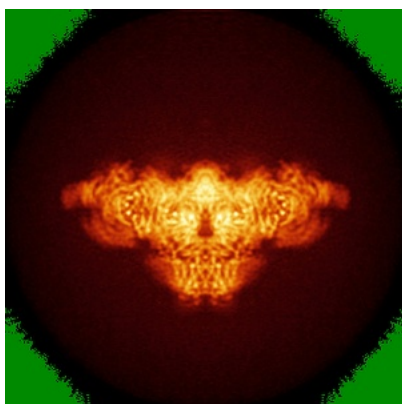


Z Index: 190

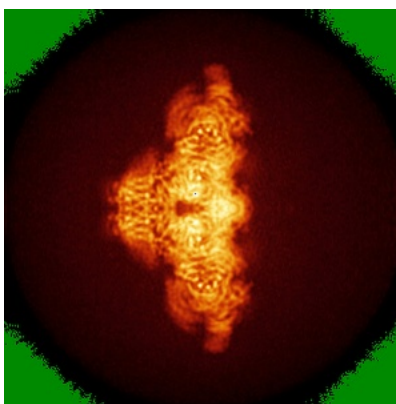
The images above show the largest variance slices of the map in three orthogonal directions.

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

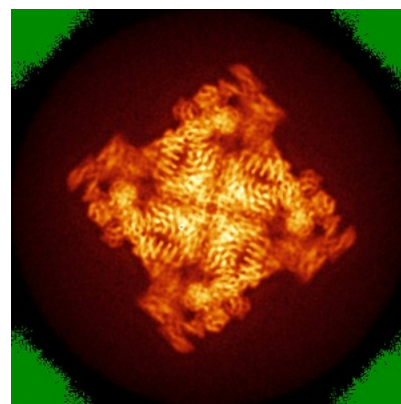
6.4.1 Primary map



X



Y

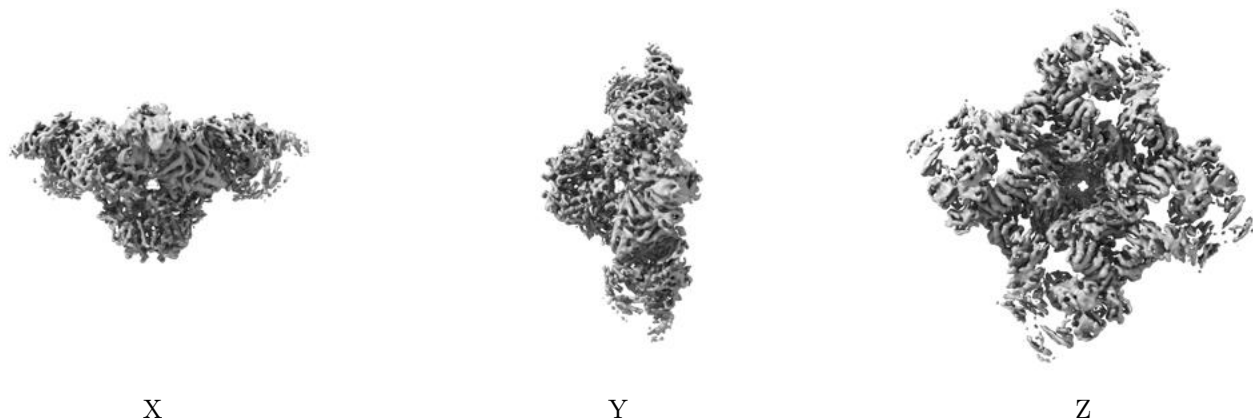


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

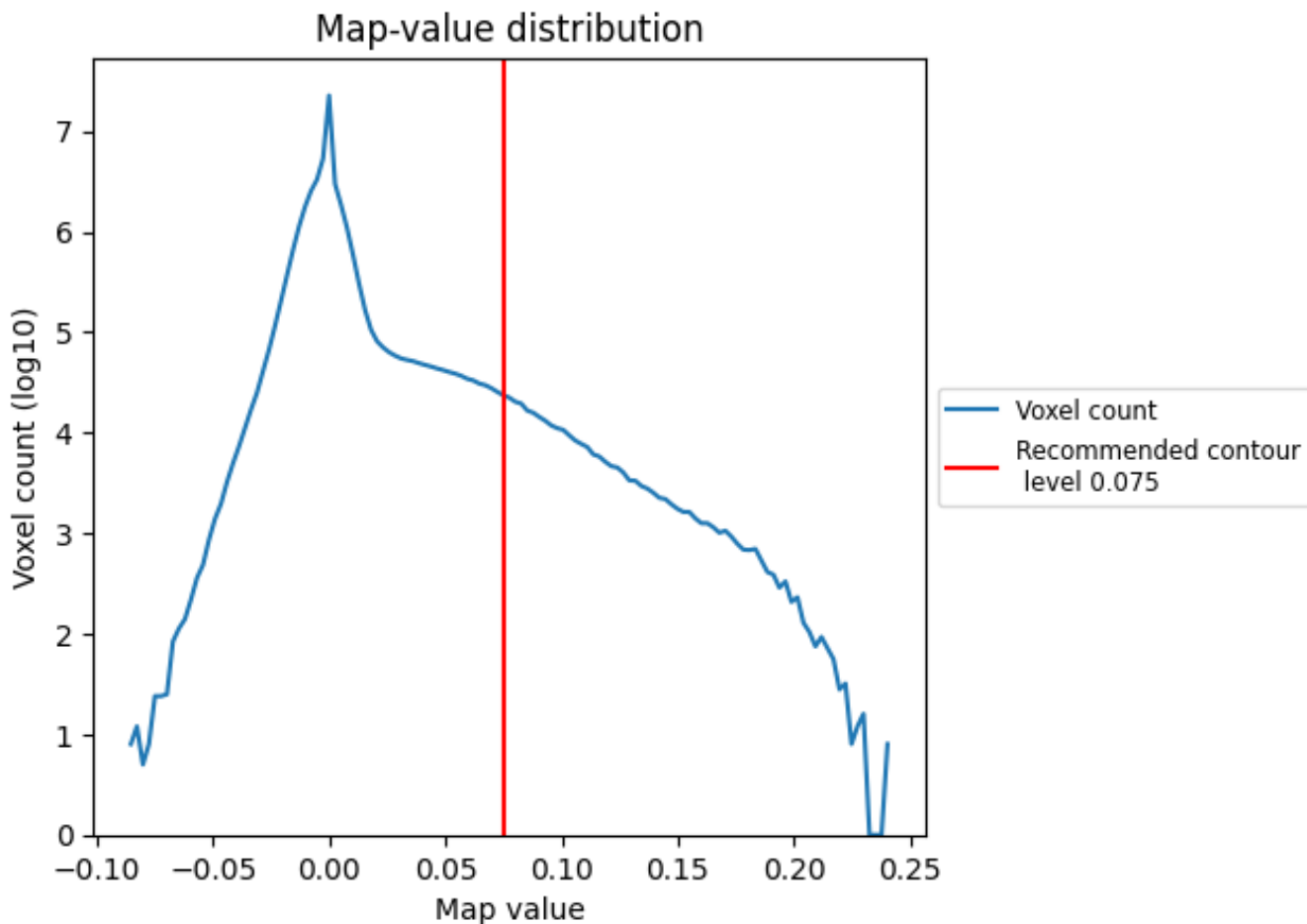
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

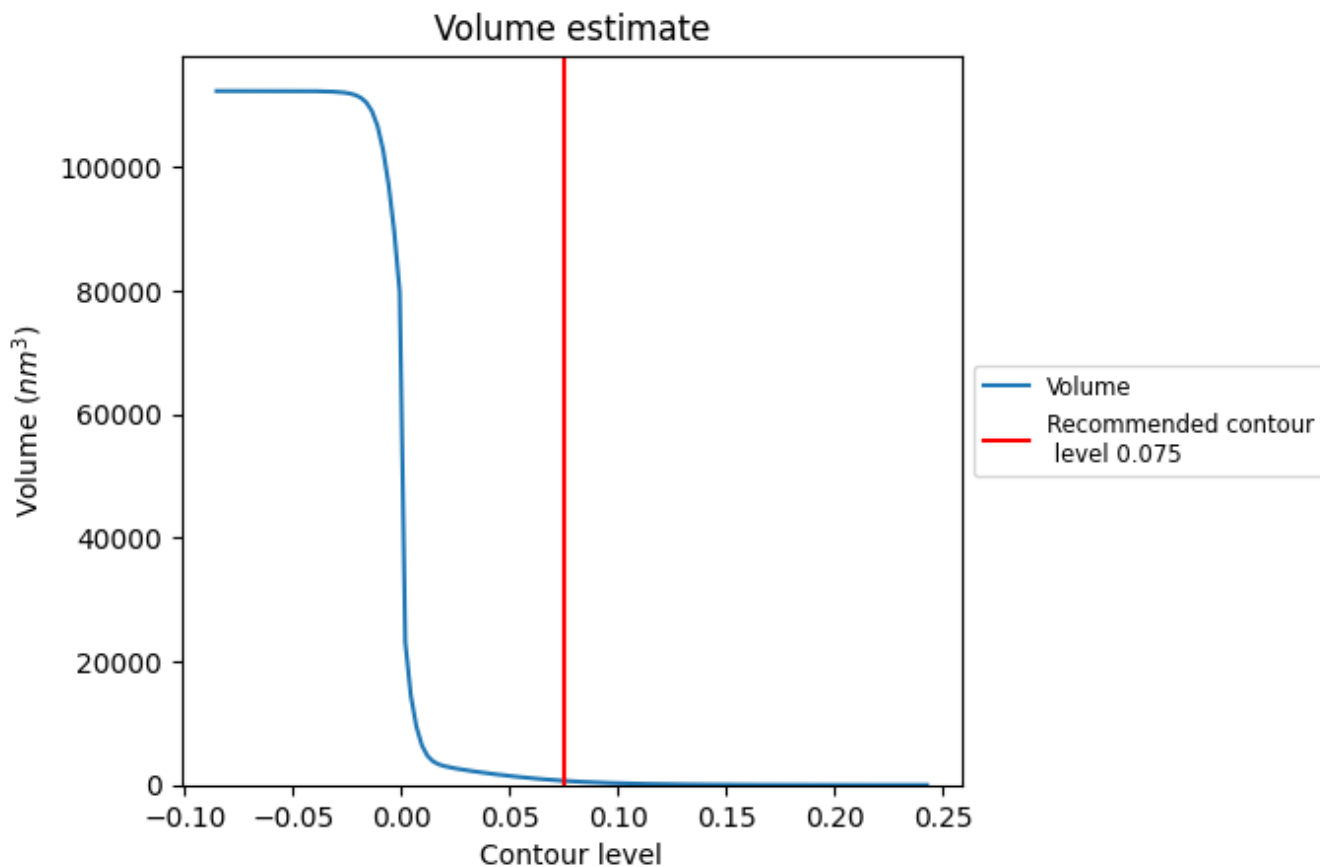
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

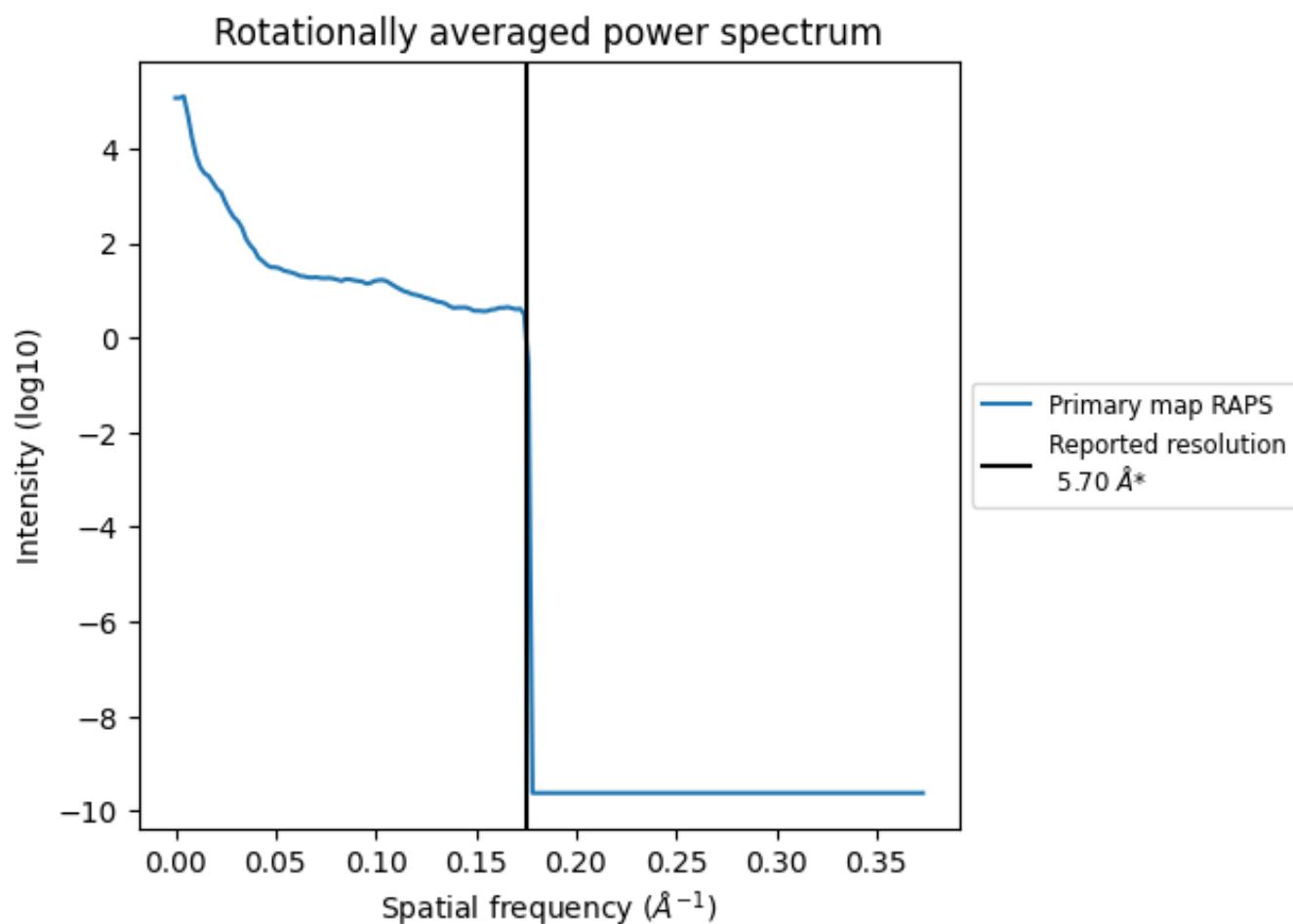
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 679 nm^3 ; this corresponds to an approximate mass of 613 kDa.

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

7.3 Rotationally averaged power spectrum [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.175 Å⁻¹

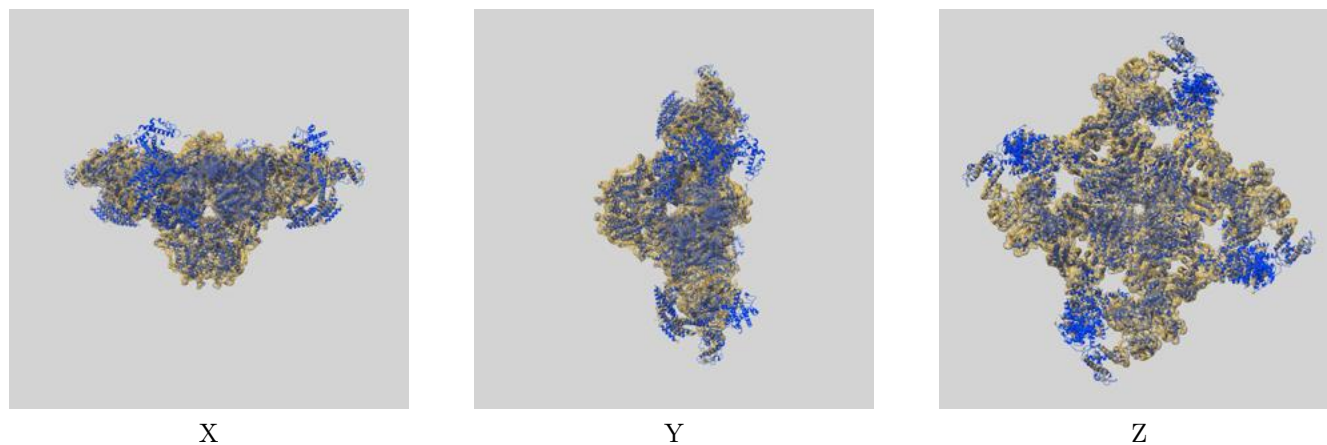
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

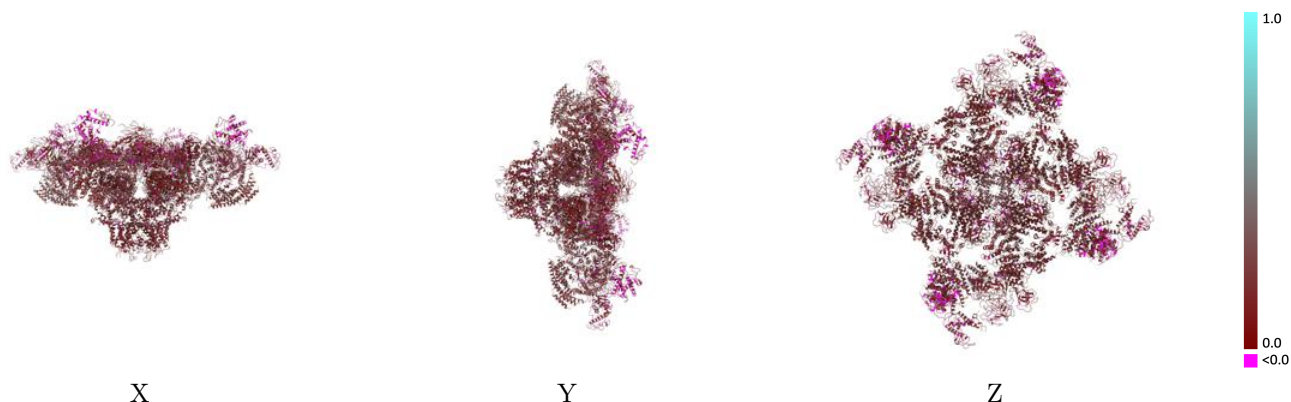
This section contains information regarding the fit between EMDB map EMD-9521 and PDB model 5GL1. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



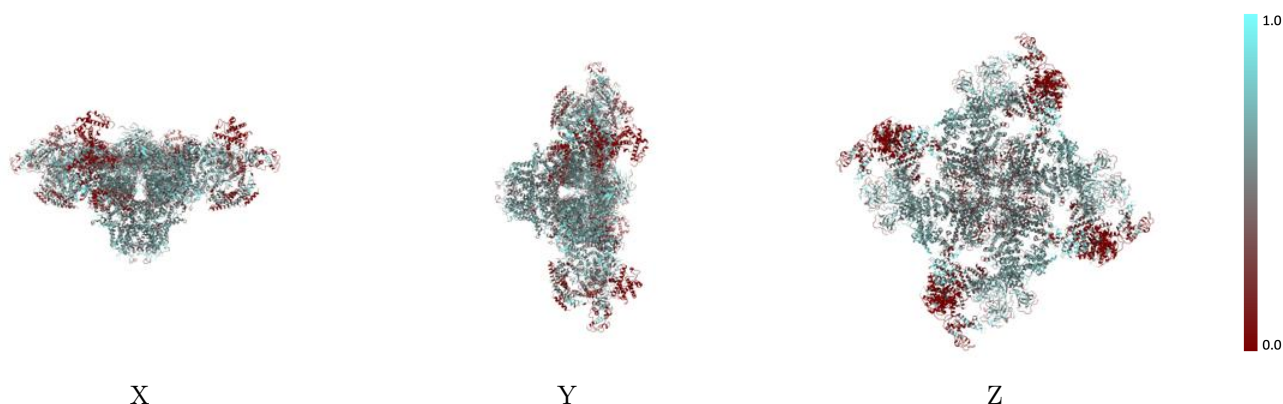
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



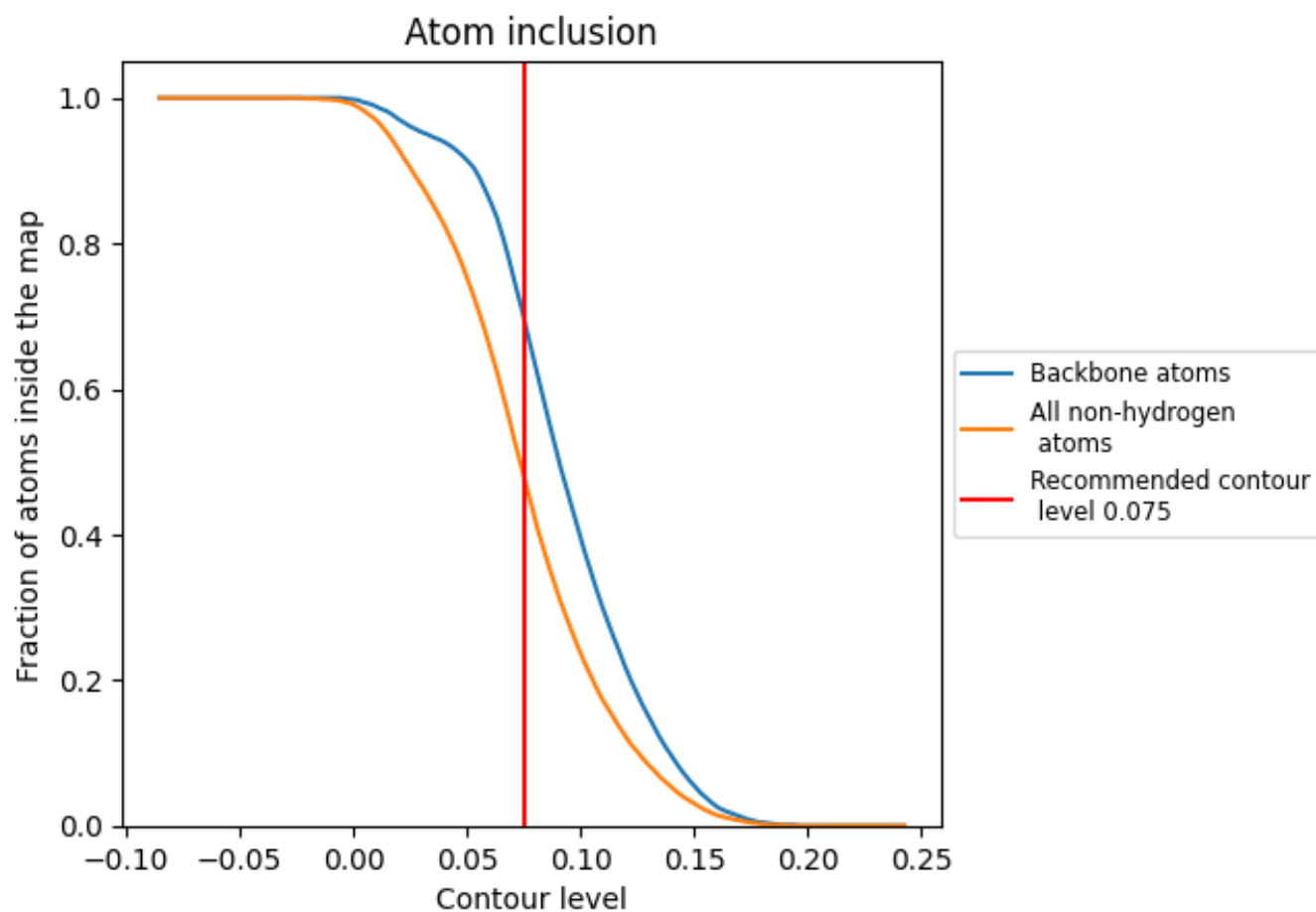
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4830	0.2010
A	0.4820	0.2020
B	0.4990	0.2060
C	0.4820	0.2010
D	0.4990	0.2080
E	0.4820	0.2010
F	0.5000	0.2050
G	0.4820	0.2010
H	0.4970	0.2040

