



wwPDB EM Validation Summary Report ⓘ

Feb 13, 2024 – 08:52 PM EST

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

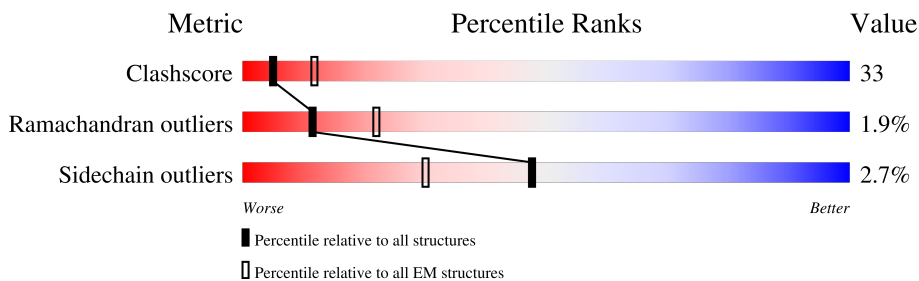
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	4599	 48% 30% 20% 2%
1	C	4599	 48% 30% 20% 2%
1	E	4599	 48% 29% 20% 2%
1	G	4599	 48% 30% 20% 2%
2	B	107	 60% 39% 1%
2	D	107	 62% 37% 1%
2	F	107	 60% 39% 1%
2	H	107	 59% 40% 1%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 111160 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3660	26957	17143	4683	4974	157	1	0
1	C	3660	26957	17143	4683	4974	157	1	0
1	E	3660	26957	17143	4683	4974	157	1	0
1	G	3660	26957	17143	4683	4974	157	1	0

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

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

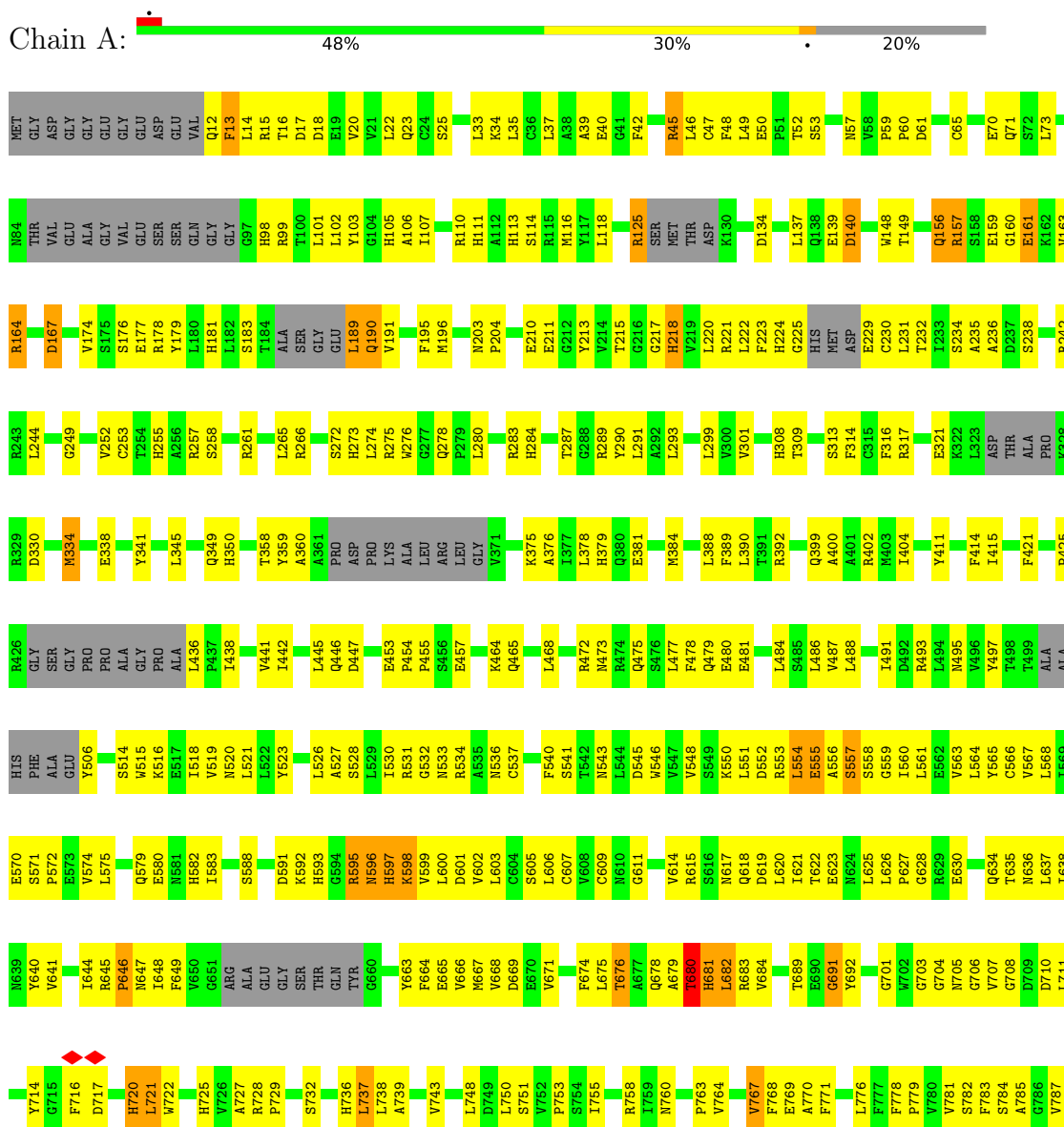
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
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



• Molecule 1: Ryanodine receptor 1

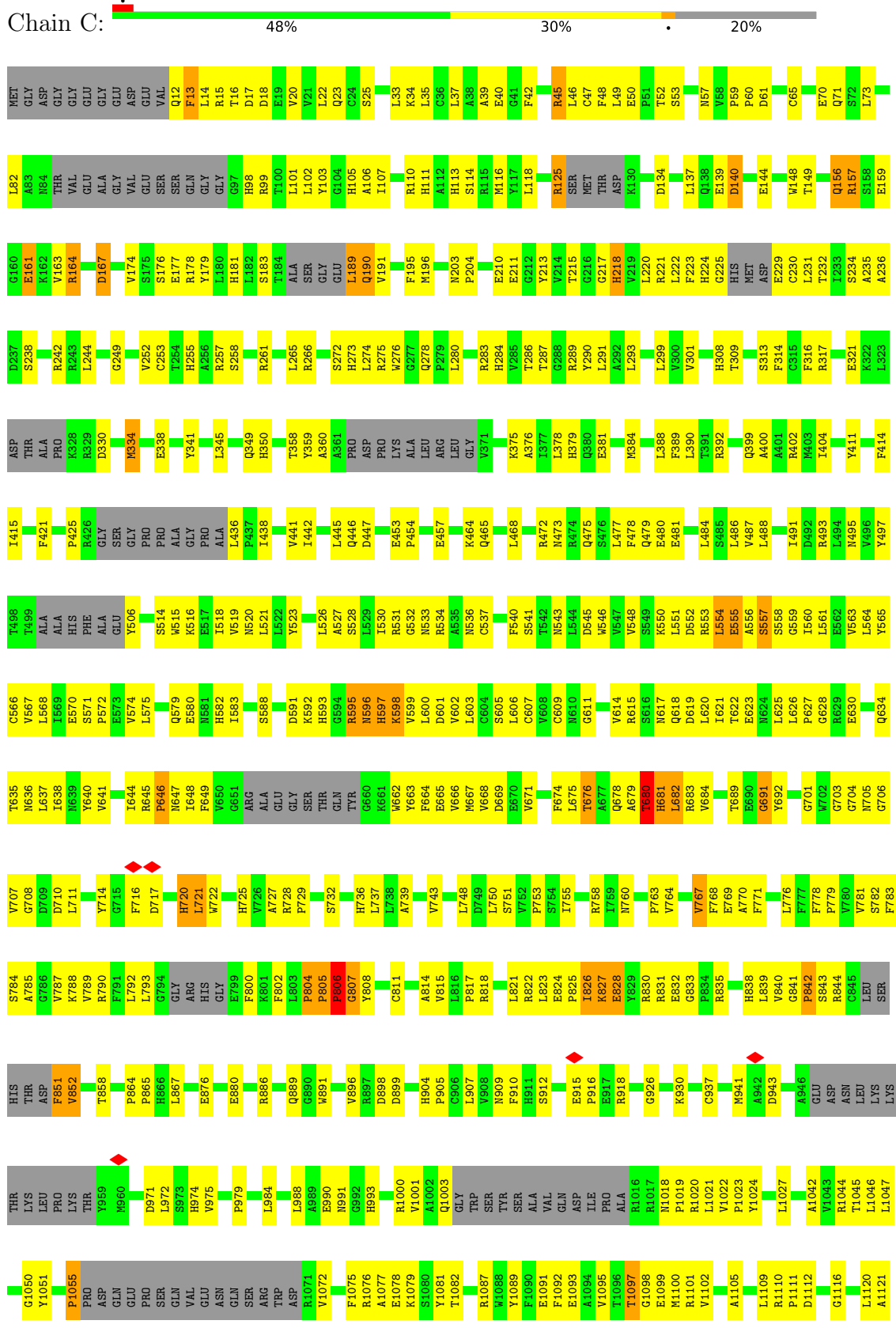
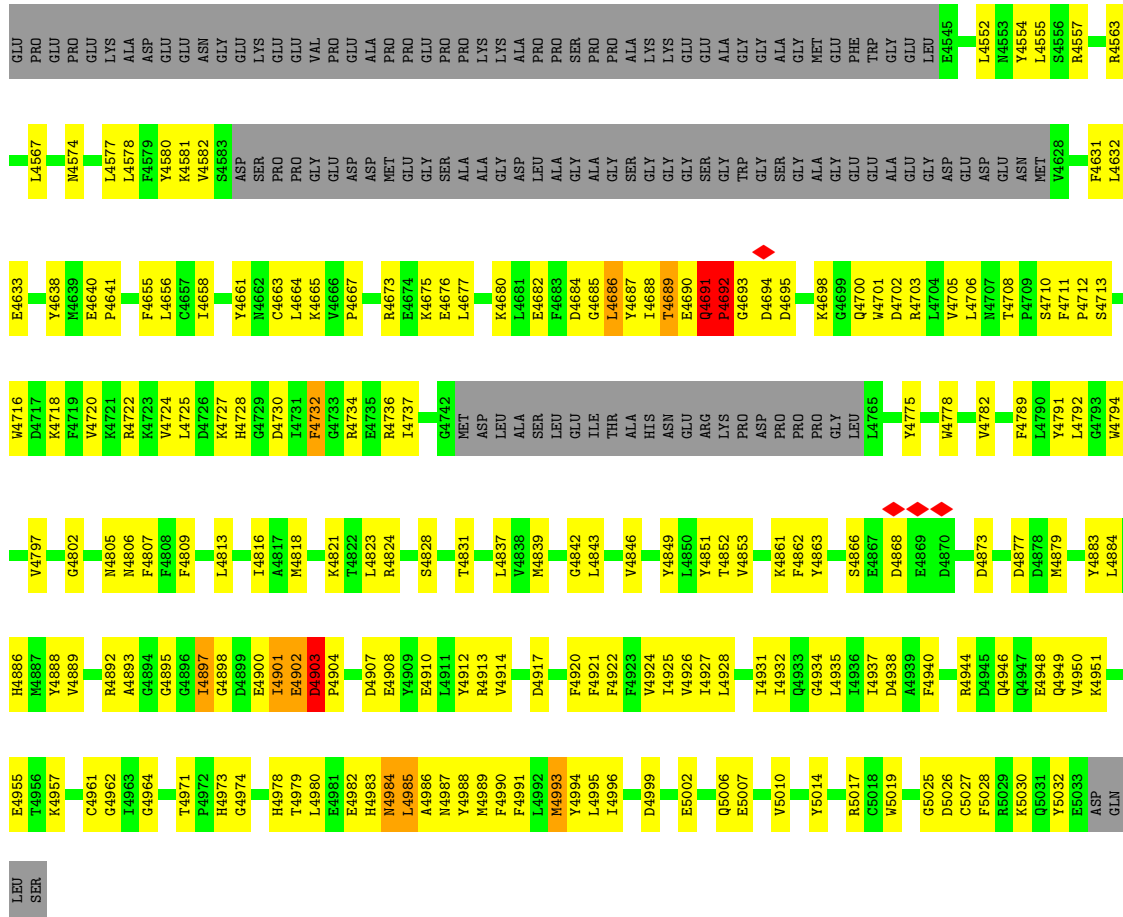


Table with 15 columns of residue identifiers and labels. The labels are color-coded: green for good, yellow for warnings, and red for errors. A red diamond symbol is present above the residue 'R1623'.

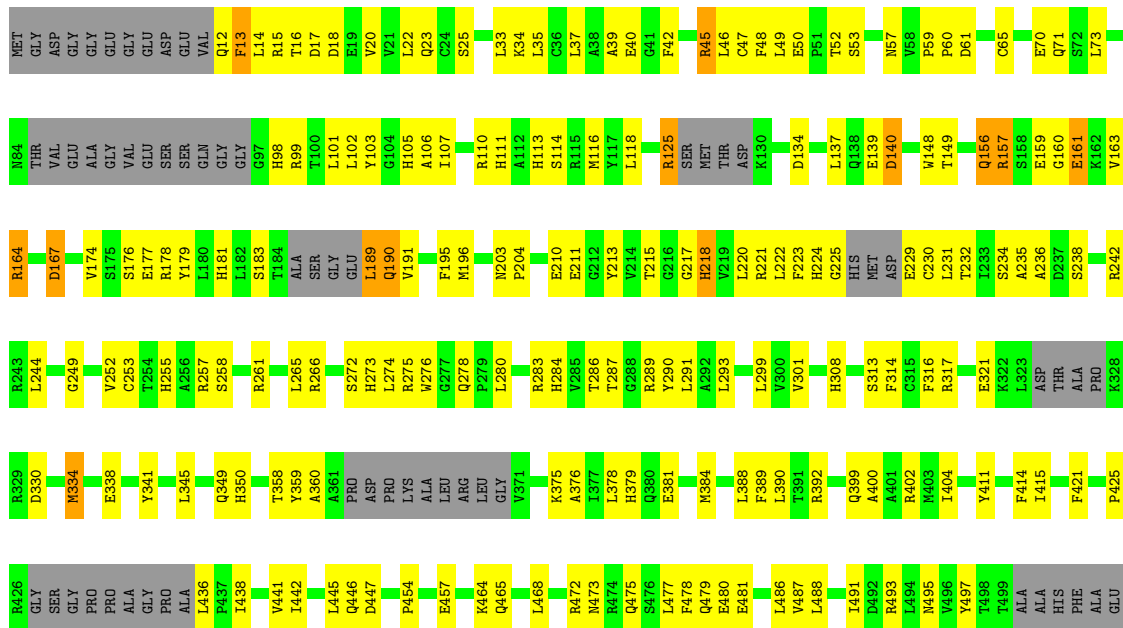
V4049	S3983	R3904	T3838	Q2892	Q2893	Q2894	T2823	A2759	P2529	L2419	L2356	T2271
E4050	R3984	T3905	C3839	E2893	E2894	E2895	E2824	E2760	A2529	G2419	L2357	L2357
S4051	L3985	Q3906	S3840	L2894	L2894	E2895	K2825	T2762	A2533	M2423	R2358	R2358
F4141	A3988	Q3908	V3841	E2896	E2896	E2897	A2826	H2763	L2537	D2431	K2360	A2277
M4142	A3989	M3909	D3843	A2897	A2897	K2827	R2827	E2764	ASP	D2431	A2278	A2278
M4145	V3990	M3909	L3844	K2896	K2896	G2828	G2828	E2765	THR	G2434	S2279	S2279
L4146	G3991	I3915	R3849	G2898	G2898	G2899	E2830	F2768	ALA	R2435	V2280	V2280
L4147	F3992	I3916	K3852	G2899	G2899	G2900	E2830	D2769	THR	R2436	L2281	L2281
M4148	L3993	T3919	L3852	T2901	T2901	T2901	E2830	D2769	THR	R2436	N2283	N2283
M4149	L3994	T3919	L3852	G2902	G2902	H2902	E2830	D2769	THR	R2436	N2284	N2284
L4150	F3996	V3920	A3852	L2903	L2903	H2903	E2830	D2769	THR	R2436	E2286	E2286
V4154	A3997	L3924	ALA	L2904	L2904	H2904	E2830	D2769	THR	R2436	E2286	E2286
F4155	H3998	R3925	GLU	L2904	L2904	H2904	E2830	D2769	THR	R2436	E2286	E2286
H4156	H3998	R3925	GLU	L2904	L2904	H2904	E2830	D2769	THR	R2436	E2286	E2286
D4157	M3999	L3926	GLU	L2904	L2904	H2904	E2830	D2769	THR	R2436	E2286	E2286
P4158	M4000	Q3927	GLU	L2904	L2904	H2904	E2830	D2769	THR	R2436	E2286	E2286
M4159	M4001	Q3928	VAL	L2905	L2905	H2905	E2830	D2769	THR	R2436	E2286	E2286
L4160	K4002	S3929	GLU	V2906	V2906	H2906	E2830	D2769	THR	R2436	E2286	E2286
R4161	L4003	I3930	GLU	P2907	P2907	H2907	E2830	D2769	THR	R2436	E2286	E2286
L4164	A4004	ASP	ASP	D2908	D2908	H2908	E2830	D2769	THR	R2436	E2286	E2286
L4164	Q4005	GLY	GLY	T2910	T2910	H2910	E2830	D2769	THR	R2436	E2286	E2286
L4164	Q4006	THR	THR	L2911	L2911	H2911	E2830	D2769	THR	R2436	E2286	E2286
G4072	S4007	Y3934	VAL	T2912	T2912	H2912	E2830	D2769	THR	R2436	E2286	E2286
G4073	S4008	Y3935	VAL	T2913	T2913	H2913	E2830	D2769	THR	R2436	E2286	E2286
S4074	Q4009	Y3937	ASN	K2914	K2914	H2914	E2830	D2769	THR	R2436	E2286	E2286
F4077	L4010	S3938	ARG	E2915	E2915	H2915	E2830	D2769	THR	R2436	E2286	E2286
F4077	E4011	G3939	GLN	R2918	R2918	H2918	E2830	D2769	THR	R2436	E2286	E2286
D4083	L4012	K3940	ASN	R2919	R2919	H2919	E2830	D2769	THR	R2436	E2286	E2286
P4084	L4013	K3941	GLY	E2921	E2921	H2921	E2830	D2769	THR	R2436	E2286	E2286
R4085	L4013	V3942	GLU	Q2924	Q2924	H2924	E2830	D2769	THR	R2436	E2286	E2286
R4085	L4013	V3942	GLU	Q2924	Q2924	H2924	E2830	D2769	THR	R2436	E2286	E2286
G4086	L4017	F3951	VAL	R2924	R2924	H2924	E2830	D2769	THR	R2436	E2286	E2286
G4086	L4017	F3951	VAL	R2924	R2924	H2924	E2830	D2769	THR	R2436	E2286	E2286
L4178	L4018	M3793	LYS	R2924	R2924	H2924	E2830	D2769	THR	R2436	E2286	E2286
G4179	L4018	M3793	LYS	R2924	R2924	H2924	E2830	D2769	THR	R2436	E2286	E2286
R4180	L4087	S3796	GLY	R2924	R2924	H2924	E2830	D2769	THR	R2436	E2286	E2286
L4181	L4088	S3797	GLY	R2924	R2924	H2924	E2830	D2769	THR	R2436	E2286	E2286
E4182	L4088	S3797	GLY	R2924	R2924	H2924	E2830	D2769	THR	R2436	E2286	E2286
S4187	F4093	A3954	ALA	Q2924	Q2924	H2924	E2830	D2769	THR	R2436	E2286	E2286
R4188	Q4100	F3880	LYS	L2927	L2927	H2927	E2830	D2769	THR	R2436	E2286	E2286
R4189	Q4102	F3881	LYS	K2928	K2928	H2928	E2830	D2769	THR	R2436	E2286	E2286
R4192	L4028	Q3882	GLY	F2929	F2929	H2929	E2830	D2769	THR	R2436	E2286	E2286
I4193	S4029	D3883	GLY	L2930	L2930	H2930	E2830	D2769	THR	R2436	E2286	E2286
Y4194	L4030	F3885	ASP	M2932	M2932	H2932	E2830	D2769	THR	R2436	E2286	E2286
F4195	L4031	R3886	ARG	N2933	N2933	H2933	E2830	D2769	THR	R2436	E2286	E2286
E4196	E4032	F3887	ARG	M2933	M2933	H2933	E2830	D2769	THR	R2436	E2286	E2286
I4197	M4035	L3888	GLY	N2933	N2933	H2933	E2830	D2769	THR	R2436	E2286	E2286
P4208	V4036	Q3889	GLY	Y2935	Y2935	H2935	E2830	D2769	THR	R2436	E2286	E2286
L4111	L4111	I3969	GLY	A2936	A2936	H2936	E2830	D2769	THR	R2436	E2286	E2286
L4112	L4112	I3969	GLY	T2937	T2937	H2937	E2830	D2769	THR	R2436	E2286	E2286
S4113	M4037	Q3970	ASN	T2938	T2938	H2938	E2830	D2769	THR	R2436	E2286	E2286
M4120	G4038	C3871	ASN	R2939	R2939	H2939	E2830	D2769	THR	R2436	E2286	E2286
F4214	M4039	P3972	HIS	H3647	H3647	H3648	E2830	D2769	THR	R2436	E2286	E2286
F4217	I4040	C3973	LEU	R3648	R3648	H3649	E2830	D2769	THR	R2436	E2286	E2286
L4218	A4041	T3974	LEU	A3649	A3649	H3650	E2830	D2769	THR	R2436	E2286	E2286
R4042	D3898	G3975	GLU	N3651	N3651	H3651	E2830	D2769	THR	R2436	E2286	E2286
D4220	Q4043	N3976	GLY	Y3657	Y3657	H3657	E2830	D2769	THR	R2436	E2286	E2286
V4221	M4044	Q3977	GLY	I3662	I3662	H3662	E2830	D2769	THR	R2436	E2286	E2286
V4222	PHE	Q3977	GLY	H3667	H3667	H3668	E2830	D2769	THR	R2436	E2286	E2286
M4223	GLU	Y3902	GLY	F3669	F3669	H3669	E2830	D2769	THR	R2436	E2286	E2286
E4224	P4135	L3903	ASN	E3670	E3670	H3670	E2830	D2769	THR	R2436	E2286	E2286

ALA	THR	PRO	ALA	ARG	LEU	PRO	ARG	LEU	LEU	PRO	HIS	ASP	VAL	VAL	PRO	ALA	ASP	ASN	ARG	ASP	PRO	THR	THR	Y1432	Y1433	Y1434	Y1435	Y1436	Y1437	Y1438	Y1439	Y1440	Y1441	GLY	GLN	PRO	PRO	SER	C1447	V1448	V1449	V1450	G1451	G1452	G1453	K1547	T1454	P1455	H1462	D1463	M1464	N1465	F1466	L1467	L1468																																																								
S1469	LYS	VAL	ARG	ALA	V1472	T1473	V1474	T1475	M1476	G1477	D1478	E1479	Q1480	G1481	N1482	V1483	S1486	X1493	D1510	I1511	V1515	L1516	G1517	C1518	L1519	V1520	ASP	LEU	ALA	THR	G1525	L1526	F1527	T1528	F1529	T1530	T1538	Q1541	V1542	E1543	P1544	M1545	T1546	K1547	L1548	F1549	P1550	A1551	V1552	M1553	V1554	L1555	P1556	L1562																																																									
M1560	V1561	Q1562	F1564	E1565	LEU	GLY	GLN	ALA	ASN	ASN	E1577	A1578	M1579	F1580	L1581	E1582	E1583	R1584	K1585	V1586	F1587	H1588	A1589	P1589	R1594	L1595	V1597	Q1598	M1599	L1600	M1601	P1602	R1607	M1608	P1609	M1610	F1611	F1612	L1613	Q1614	V1615	E1616	T1617	G1621	E1622	R1623	M1626	L1703	P1704																																																														
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G1706	P1706	R1707	R1708	Y1712	D1713	L1714	L1715	I1716	L1720	E1721	S1726	R1727	R1728	S1729	M1730	L1731	S1732	E1733	Y1734	I1735	V1736	P1737	L1738	T1739	T1742	R1743	P1750	G1751	L1752	G1753	V1754	G1755	G1756	ASN	ALA	ARG	H1761	L1762	P1763	G1764	V1765	G1766	V1767	T1768	T1769	S1770	L1771	R1772	H1775	H1776	F1777																																																												
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LYS	GLU	GLU	GLU	GLU	ALA	PRO	GLU	GLY	GLU	GLY	VAL	ASP	LEU	GLU	GLU	G1925	P1932	L1937	C1940	L1943	E1944	Y1945	Y1946	C1947	D1948	Q1952	V1955	E1956	S1957	L1958	F1961	A1962	E1963	R1964	Y1965	V1966	L1969	N1972	M1975	S1975	L2063	L2066	T2069	V2070	R2071	L2072	VAL																																																																
LYS	LYS	LYS	GLU	GLU	LYS	PRO	GLU	GLU	PRO	GLU	ALA	ASP	LEU	GLU	GLU	G1925	P1932	L1937	C1940	L1943	E1944	Y1945	Y1946	C1947	D1948	Q1952	V1955	E1956	S1957	L1958	F1961	A1962	E1963	R1964	Y1965	V1966	L1969	N1972	M1975	S1975	L2063	L2066	T2069	V2070	R2071	L2072	VAL																																																																
L2094	Q2095	E2096	L2097	V2098	S2099	H2100	R2104	N2188	K2189	V2190	F2191	Y2192	P2195	N2196	L2197	M2198	A2200	L2201	Q2202	M2203	H2204	E2205	T2206	M2208	E2209	V2210	M2211	R2212	M2213	Y2214	T2215	G2216	GLY	GLY	P2214	P2215	P2216	E2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	L2261	L2262	L2263	L2264	L2265	L2266	L2267	L2268	L2269	L2270	L2271	L2272	L2273	L2274	L2275	L2276	L2277	L2278	L2279	L2280	L2281	D2282	M2283	N2284	E2285	L2286	V2289	S2300	Y2301	L2307
V2149	E2150	D2151	T2152	L2155	L2156	L2159	T2162	R2163	S2164	L2165	L2166	I2167	V2168	GLN	MET	GLY	PRO	Q2245	M2246	Q2247	R2248	S2249	Y2256	L2257	L2258	E2259	M2260	L2263	Y2268	L2269	L2270	L2271	V2275	A2276	A2277	A2278	S2279	V2280	L2281	D2282	M2283	N2284	E2285	L2286	V2289	S2300	Y2301	L2307																																																															
THR	LYS	GLU	ILE	ARG	PHE	P2226	K2227	T2230	R2234	C2237	Y2238	F2239	C2240	R2241	L2242	Q2245	M2246	Q2247	R2248	S2249	Y2256	L2257	L2258	E2259	M2260	L2263	Y2268	L2269	L2270	L2271	V2275	A2276	A2277	A2278	S2279	V2280	L2281	D2282	M2283	N2284	E2285	L2286	V2289	S2300	Y2301	L2307																																																																	
GLN	SER	CYS	PRO	MET	LEU	LEU	ALA	GLY	TYR	PRO	ASP	ILE	TRP	ASN	P2325	C2326	E2329	R2330	Y2331	F2337	A2338	V2339	F2340	V2341	N2342	G2343	V2346	N2349	A2350	N2351	V2354	R2355	L2356	L2357	I2358	R2359	K2360	P2361	CYS	PHE	GLY	PRO	ALA	LEU	ARG	GLY	GLU	ILE	GLN	GLY	ALA	GLY	GLY	SER	THR	THR	THR	PHE	SER	THR	T2544	A2547	L2550	M2551	R2552	Y2553																																													
L2376	L2377	L2380	A2383	L2384	R2385	L2386	L2456	L2457	R2458	X2465	X2466	X2467	P2496	D2497	R2498	K2499	A2500	S2501	M2502	V2503	L2504	F2505	Y2510	GLY	ILE	GLY	GLU	PRO	P2517	V2521	L2522	ASP	V2525	P2529	A2533	L2537	ASP	THR	ALA	THR	PHE	SER	THR	T2544	A2547	L2550	M2551	R2552	Y2553																																																														

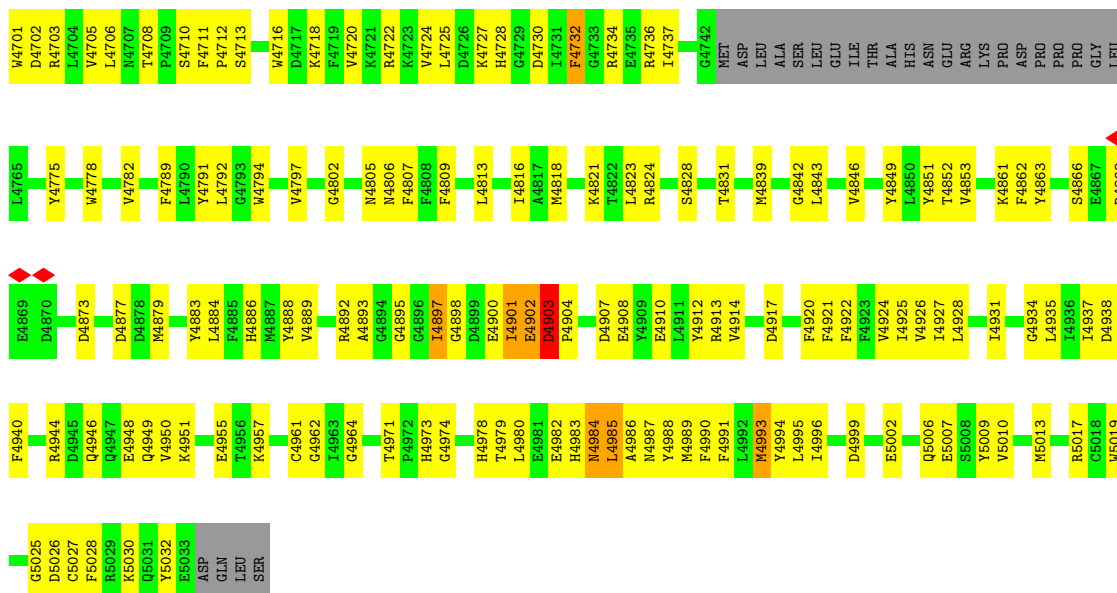
Table with 22 columns (residue ID, chain, atom name, occupancy, B-factor, etc.) displaying validation data for residues L2554 through P4159. The table is organized into 12 horizontal bands, each representing a different chain (GLN, THR, ALA, THR, D2849, D2850, P2851, R2852, E2853, E2854, Y2855, Y2856, P2857, Q2858, P2859, P2860, D2861, E2862, S2863, Y2864, Y2865, T2866, R2867, S2868, E2869, E2870, Q2871, E2872, E2873, L2874, Y2875, Q2876, Q2877, E2878, E2879, E2880, N2881, Y2882, K2883, K2884, Q2885, Q2886, Q2887, E2888, E2889, E2890, E2891, E2892, E2893, L2894, E2895, E2896, E2897, E2898, E2899, E2900, H2901, H2902, P2903, L2904, L2905, L2906, P2907, D2908, T2909, L2910, T2911, T2912).



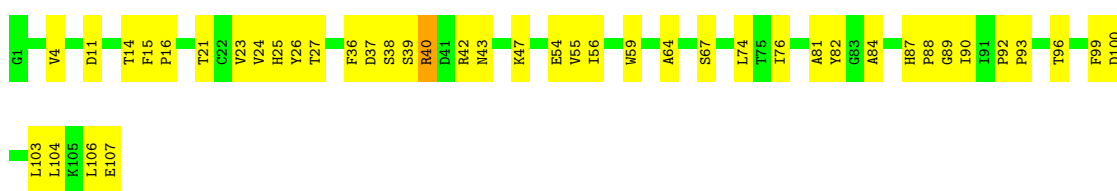
• Molecule 1: Ryanodine receptor 1



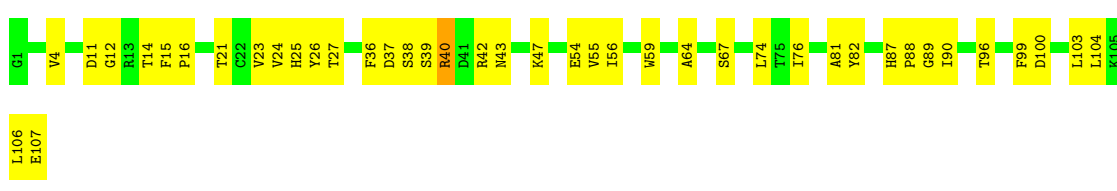
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L1585	M1561	L1467	S1210	L1134	S1279	G1219	F1158	I1162	I1097	L1028	E881	L793	D717	R645	L575	S514
P1556	M1562	L1469	L1211	G1135	Q1280	L1212	E1159	I1163	G1098	R1017	R886	L794	H720	P646	Q579	M515
M1563	L1562	S1469	R1212	S1136	V1283	R1213	D1154	D1154	E1099	A1077	R887	GLY	H721	E580	E580	K516
F1564	L1562	L1470	R1213	E1137	L1283	F1213	L1155	L1155	F1092	E1078	E876	HIS	L722	F649	M581	E517
E1565	L1564	ALA	F1214	F1139	E1285	F1214	T1156	T1156	A1094	K1079	E880	GLY	W722	V650	I518	I518
LEU	V1472	ARG	G1218	G1140	M1286	G1218	E1157	E1157	S1080	S1081	E880	E799	H725	G651	V519	N520
ARG	T1473	PRO	E1221	W1143	F1288	E1221	W1143	W1143	T1082	T1082	R886	F800	W726	ALA	N520	N520
LEU	V1474	LEU	G1222	D1147	S1291	G1222	D1147	D1147	R1076	R1076	R886	F801	A727	ALA	L521	L521
PRO	T1475	PRO	F1223	V1148	L1293	F1223	V1148	V1148	A1077	A1077	R889	F802	R728	GLU	L522	L522
HIS	M1476	HIS	E1224	C1151	L1293	E1224	C1151	C1151	E1078	E1078	G889	F803	P729	GLY	Y523	Y523
ASP	G1477	ASP	P1225	M1152	P1294	P1225	M1152	M1152	K1079	K1079	G890	P804	P729	THR	L526	L526
ASP	D1478	VAL	Q1226	D1153	F1296	F1226	D1153	D1153	S1080	S1080	G891	P805	S732	GLN	A527	A527
VAL	Q1479	VAL	F1227	L1154	Q1297	F1227	L1154	L1154	R1076	R1076	V896	P806	H736	TYR	R595	R595
ALA	G1481	ALA	A1227	L1155	L1297	A1227	L1155	L1155	E1078	E1078	G897	Y808	L737	TYR	L530	L530
ASN	M1482	ASN	M1230	T1156	HIS	M1230	T1156	T1156	K1079	K1079	V899	Y809	L738	GLN	I531	I531
ASP	V1483	ASP	Q1231	E1157	GLN	Q1231	E1157	E1157	S1080	S1080	V899	Y809	A739	GLN	G532	G532
ASP	S1486	ASP	R1232	N1158	HIS	R1232	N1158	N1158	T1082	T1082	V899	Y809	V743	TYR	L536	L536
PRO	X1493	PRO	T1235	I1161	PHE	T1235	I1161	I1161	R1087	R1087	V899	Y809	V743	TYR	L536	L536
GLU	D1510	GLU	T1236	V1168	ARG	T1236	V1168	V1168	Y1089	Y1089	V899	Y809	V743	TYR	L536	L536
ILE	L1511	ILE	W1237	W1169	CYS	W1237	W1169	W1169	F1090	F1090	V899	Y809	V743	TYR	L536	L536
LEU	V1515	LEU	F1238	MET	THR	F1238	MET	MET	E1091	E1091	V899	Y809	V743	TYR	L536	L536
ASN	K1585	ASN	K1240	SER	ALA	K1240	SER	SER	F1092	F1092	V899	Y809	V743	TYR	L536	L536
THR	G1517	THR	F1245	GLY	THR	F1245	GLY	GLY	A1094	A1094	V899	Y809	V743	TYR	L536	L536
THR	C1518	THR	F1246	SER	LEU	F1246	SER	SER	E1094	E1094	V899	Y809	V743	TYR	L536	L536
LEU	L1519	LEU	V1248	GLY	ALA	V1248	GLY	GLY	A1096	A1096	V899	Y809	V743	TYR	L536	L536
ASP	V1520	ASP	P1249	THR	PRO	P1249	THR	THR	I1096	I1096	V899	Y809	V743	TYR	L536	L536
LEU	S1436	LEU	G1250	THR	GLY	G1250	THR	THR	G1098	G1098	V899	Y809	V743	TYR	L536	L536
ALA	W1437	ALA	E1251	THR	GLY	E1251	THR	THR	E1099	E1099	V899	Y809	V743	TYR	L536	L536
THR	W1437	THR	H1252	F1179	GLN	H1252	F1179	F1179	M1100	M1100	V899	Y809	V743	TYR	L536	L536
G1525	L1526	G1525	P1253	R1180	PRO	P1253	R1180	R1180	R1101	R1101	V899	Y809	V743	TYR	L536	L536
L1527	M1528	L1527	H1254	E1181	PRO	H1254	E1181	E1181	V1102	V1102	V899	Y809	V743	TYR	L536	L536
T1528	F1440	T1528	Y1255	I1182	ALA	Y1255	I1182	I1182	A1105	A1105	V899	Y809	V743	TYR	L536	L536
F1529	A1441	F1529	E1256	E1183	GLU	E1256	E1183	E1183	L1109	L1109	V899	Y809	V743	TYR	L536	L536
GLY	A1441	GLY	V1257	I1184	GLU	V1257	I1184	I1184	L1110	L1110	V899	Y809	V743	TYR	L536	L536
GLN	T1442	GLN	D1261	F1188	ALA	D1261	F1188	F1188	P1111	P1111	V899	Y809	V743	TYR	L536	L536
PRO	Y1433	PRO	GLY	L1189	ARG	GLY	L1189	L1189	G1116	G1116	V899	Y809	V743	TYR	L536	L536
PRO	Y1434	PRO	THR	P1190	ALA	Y1434	P1190	P1190	G1116	G1116	V899	Y809	V743	TYR	L536	L536
ASP	Y1434	ASP	VAL	F1191	ALA	Y1434	F1191	F1191	G1116	G1116	V899	Y809	V743	TYR	L536	L536
LEU	S1436	LEU	ARG	C1192	GLU	S1436	C1192	C1192	L1120	L1120	V899	Y809	V743	TYR	L536	L536
ALA	W1437	ALA	THR	S1193	PRO	W1437	S1193	S1193	L1121	L1121	V899	Y809	V743	TYR	L536	L536
THR	W1437	THR	THR	L1194	ASP	W1437	L1194	L1194	L1122	L1122	V899	Y809	V743	TYR	L536	L536
G1525	L1526	G1525	PRO	G1195	PRO	G1525	G1195	G1195	L1123	L1123	V899	Y809	V743	TYR	L536	L536
L1527	M1528	L1527	PRO	P1196	PRO	L1527	P1196	P1196	L1124	L1124	V899	Y809	V743	TYR	L536	L536
T1528	F1440	T1528	CYS	G1197	LEU	F1440	G1197	G1197	L1125	L1125	V899	Y809	V743	TYR	L536	L536
F1529	A1441	F1529	ARG	Q1198	LEU	F1529	Q1198	Q1198	L1126	L1126	V899	Y809	V743	TYR	L536	L536
GLY	A1441	GLY	THR	V1199	ARG	GLY	V1199	V1199	L1127	L1127	V899	Y809	V743	TYR	L536	L536
GLN	T1442	GLN	LEU	G1200	ALA	T1442	G1200	G1200	L1128	L1128	V899	Y809	V743	TYR	L536	L536
GLU	Y1433	GLU	ALA	H1201	ARG	Y1433	H1201	H1201	L1129	L1129	V899	Y809	V743	TYR	L536	L536
PRO	Y1434	PRO	ARG	G1205	ALA	Y1434	G1205	G1205	L1130	L1130	V899	Y809	V743	TYR	L536	L536
PRO	Y1434	PRO	ASN	R1111	ARG	Y1434	R1111	R1111	L1131	L1131	V899	Y809	V743	TYR	L536	L536
SER	C1447	SER	VAL	F1188	VAL	C1447	F1188	F1188	W1132	W1132	V899	Y809	V743	TYR	L536	L536
V1541	L1448	V1541	ARG	P1190	ALA	V1541	P1190	P1190	G1116	G1116	V899	Y809	V743	TYR	L536	L536
E1543	W1449	E1543	GLY	F1191	ALA	W1449	F1191	F1191	G1116	G1116	V899	Y809	V743	TYR	L536	L536
P1544	W1449	P1544	PHE	C1192	GLU	P1544	C1192	C1192	L1120	L1120	V899	Y809	V743	TYR	L536	L536
F1545	G1451	F1545	LEU	S1193	PRO	F1545	S1193	S1193	L1121	L1121	V899	Y809	V743	TYR	L536	L536
T1546	G1451	T1546	PRO	L1194	PRO	T1546	L1194	L1194	L1122	L1122	V899	Y809	V743	TYR	L536	L536
K1547	W1452	K1547	CYS	G1195	PRO	K1547	G1195	G1195	L1123	L1123	V899	Y809	V743	TYR	L536	L536
L1548	V1453	L1548	THR	P1196	LEU	L1548	P1196	P1196	L1124	L1124	V899	Y809	V743	TYR	L536	L536
F1549	T1454	F1549	ARG	Q1198	LEU	F1549	Q1198	Q1198	L1125	L1125	V899	Y809	V743	TYR	L536	L536
P1550	P1455	P1550	LEU	V1199	ARG	P1550	V1199	V1199	L1126	L1126	V899	Y809	V743	TYR	L536	L536
A1551	H1462	A1551	ALA	G1200	ARG	A1551	H1462	H1462	L1127	L1127	V899	Y809	V743	TYR	L536	L536
L1552	E1463	L1552	ALA	H1201	ARG	L1552	H1201	H1201	L1128	L1128	V899	Y809	V743	TYR	L536	L536
F1553	M1464	F1553	MET	G1205	ALA	F1553	G1205	G1205	L1129	L1129	V899	Y809	V743	TYR	L536	L536
			MET	R1111	ARG		R1111	R1111	L1130	L1130	V899	Y809	V743	TYR	L536	L536
				W1277	ALA		W1277	W1277	W1132	W1132	V899	Y809	V743	TYR	L536	L536



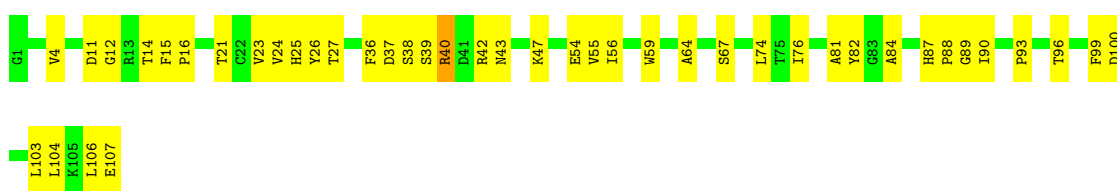
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



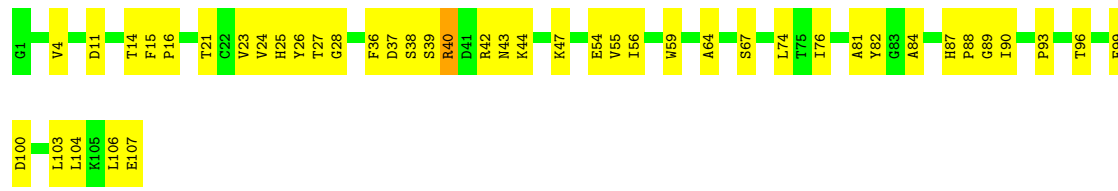
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• 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, C4	Depositor
Number of particles used	65872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Contrast transfer function parameters were estimated using CTFFIND3	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	5600	Depositor
Magnification	104748	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.336	Depositor
Minimum map value	-0.183	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.04	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	0.33	2/24616 (0.0%)	0.59	19/33295 (0.1%)
1	C	0.33	2/24616 (0.0%)	0.59	19/33295 (0.1%)
1	E	0.33	2/24616 (0.0%)	0.59	19/33295 (0.1%)
1	G	0.33	2/24616 (0.0%)	0.59	19/33295 (0.1%)
2	B	0.26	0/851	0.45	0/1146
2	D	0.26	0/851	0.45	0/1146
2	F	0.26	0/851	0.45	0/1146
2	H	0.26	0/851	0.45	0/1146
All	All	0.33	8/101868 (0.0%)	0.59	76/137764 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	3
1	E	0	3
1	G	0	3
All	All	0	12

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

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

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

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

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1253	PRO	Peptide
1	A	1867	GLU	Peptide
1	A	646	PRO	Peptide
1	C	1253	PRO	Peptide
1	C	646	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	26957	0	23849	1705	0
1	C	26957	0	23849	1709	0
1	E	26957	0	23849	1698	0
1	G	26957	0	23849	1714	0
2	B	832	0	831	41	0
2	D	832	0	831	42	0
2	F	832	0	831	42	0
2	H	832	0	831	43	0
3	A	1	0	0	2	0
3	C	1	0	0	2	0
3	E	1	0	0	2	0
3	G	1	0	0	2	0
All	All	111160	0	98720	6845	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

The worst 5 of 6845 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:554:LEU:HD11	1:E:593:HIS:CE1	1.12	1.64
1:G:554:LEU:HD11	1:G:593:HIS:CE1	1.12	1.63
1:A:554:LEU:HD11	1:A:593:HIS:CE1	1.12	1.62
1:C:554:LEU:HD11	1:C:593:HIS:CE1	1.12	1.61
1:G:1961:PHE:CZ	1:G:2063:LEU:HD23	1.36	1.60

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2991/4599 (65%)	2776 (93%)	155 (5%)	60 (2%)	7	41
1	C	2991/4599 (65%)	2776 (93%)	155 (5%)	60 (2%)	7	41
1	E	2991/4599 (65%)	2776 (93%)	155 (5%)	60 (2%)	7	41
1	G	2991/4599 (65%)	2776 (93%)	155 (5%)	60 (2%)	7	41
2	B	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
2	D	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
2	F	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
2	H	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
All	All	12384/18824 (66%)	11492 (93%)	652 (5%)	240 (2%)	11	42

5 of 240 Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2507/3406 (74%)	2439 (97%)	68 (3%)	44 69
1	C	2507/3406 (74%)	2439 (97%)	68 (3%)	44 69
1	E	2507/3406 (74%)	2439 (97%)	68 (3%)	44 69
1	G	2507/3406 (74%)	2439 (97%)	68 (3%)	44 69
2	B	89/89 (100%)	88 (99%)	1 (1%)	73 85
2	D	89/89 (100%)	88 (99%)	1 (1%)	73 85
2	F	89/89 (100%)	88 (99%)	1 (1%)	73 85
2	H	89/89 (100%)	88 (99%)	1 (1%)	73 85
All	All	10384/13980 (74%)	10108 (97%)	276 (3%)	48 69

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

Mol	Chain	Res	Type
1	G	851	PHE
1	G	1055	PRO
1	G	4006	ASP
1	C	979	PRO
1	C	865	PRO

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

Mol	Chain	Res	Type
1	E	156	GLN
1	E	2100	HIS
2	H	25	HIS

Continued on next page...

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Mol	Chain	Res	Type
1	G	2196	ASN
1	E	278	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	36

Continued on next page...

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Mol	Chain	Number of breaks
1	C	36
1	E	36
1	G	36

The worst 5 of 144 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3572:UNK	C	3645:PRO	N	56.50
1	C	3572:UNK	C	3645:PRO	N	56.50
1	E	3572:UNK	C	3645:PRO	N	56.50
1	G	3572:UNK	C	3645:PRO	N	56.50
1	A	2712:UNK	C	2734:ASN	N	35.36

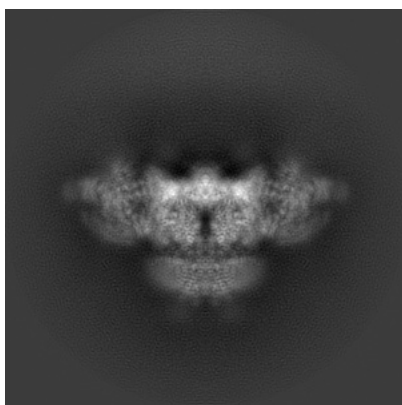
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2807. These allow visual inspection of the internal detail of the map and identification of artifacts.

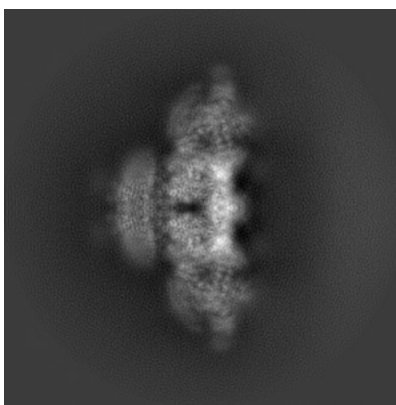
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

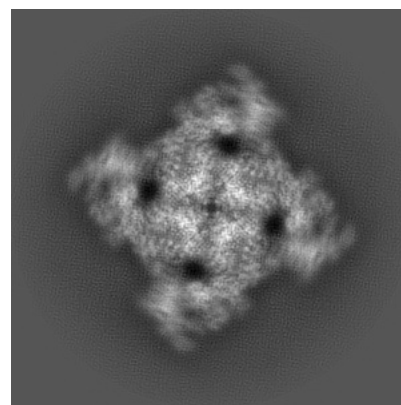
6.1.1 Primary map



X



Y

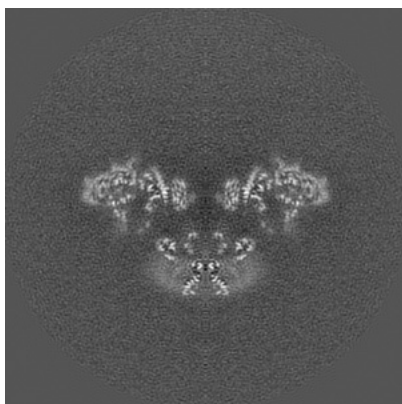


Z

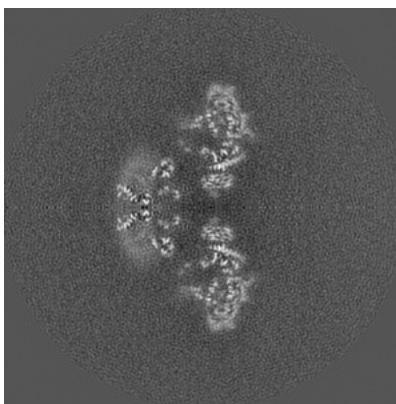
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

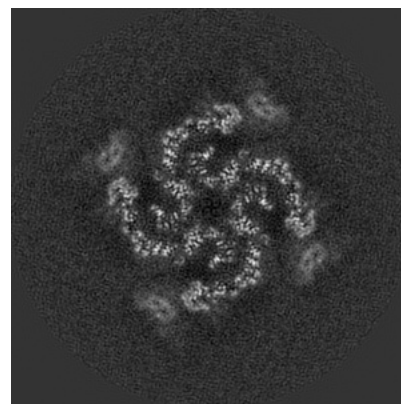
6.2.1 Primary map



X Index: 180



Y Index: 180

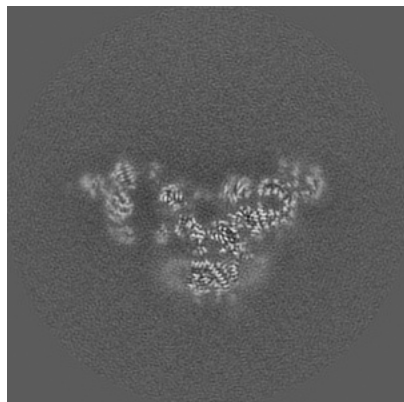


Z Index: 180

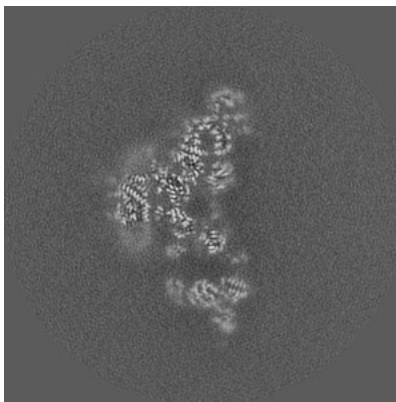
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

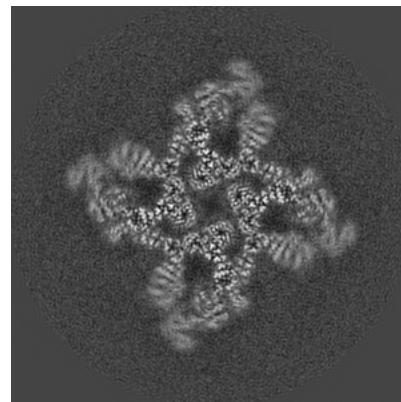
6.3.1 Primary map



X Index: 169



Y Index: 191

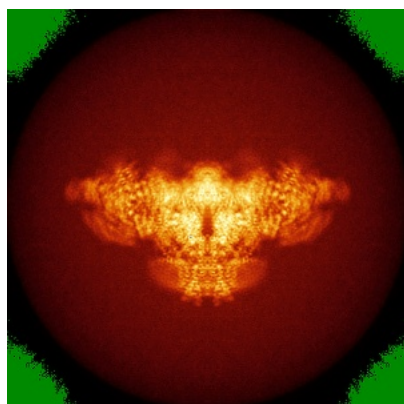


Z Index: 193

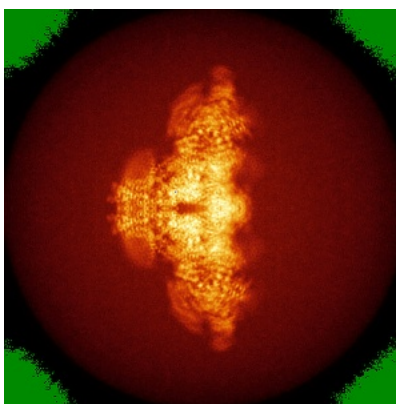
The images above show the largest variance slices of the map in three orthogonal directions.

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

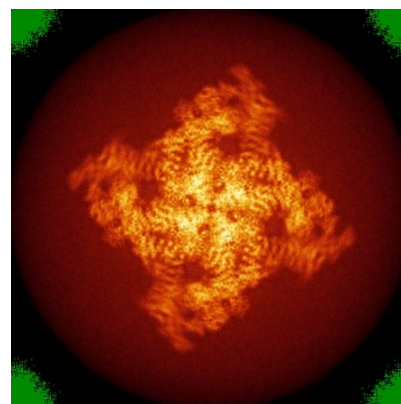
6.4.1 Primary map



X



Y

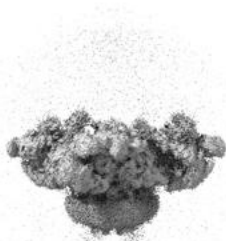


Z

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](#)

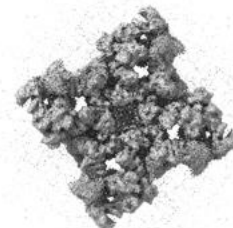
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

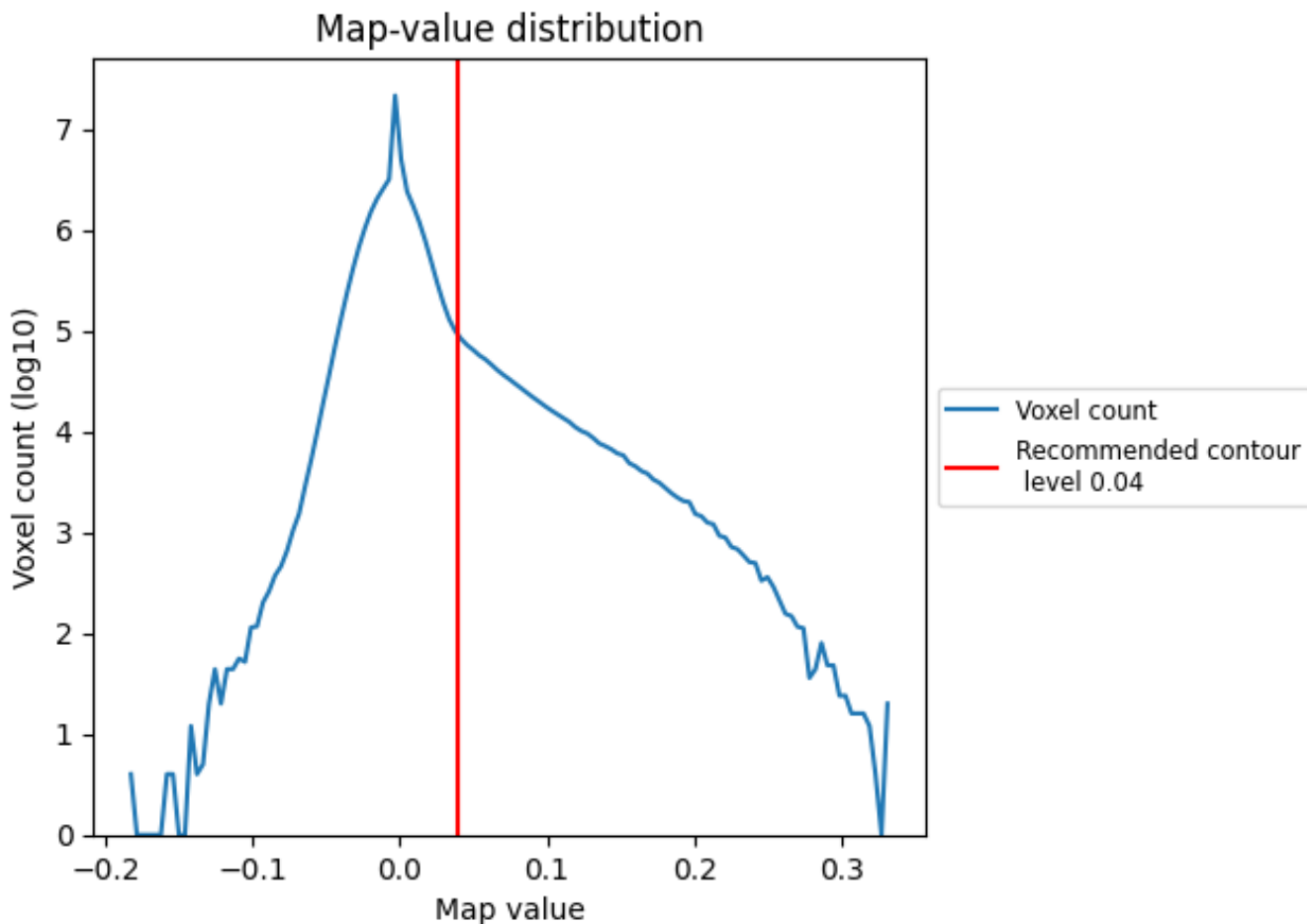
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

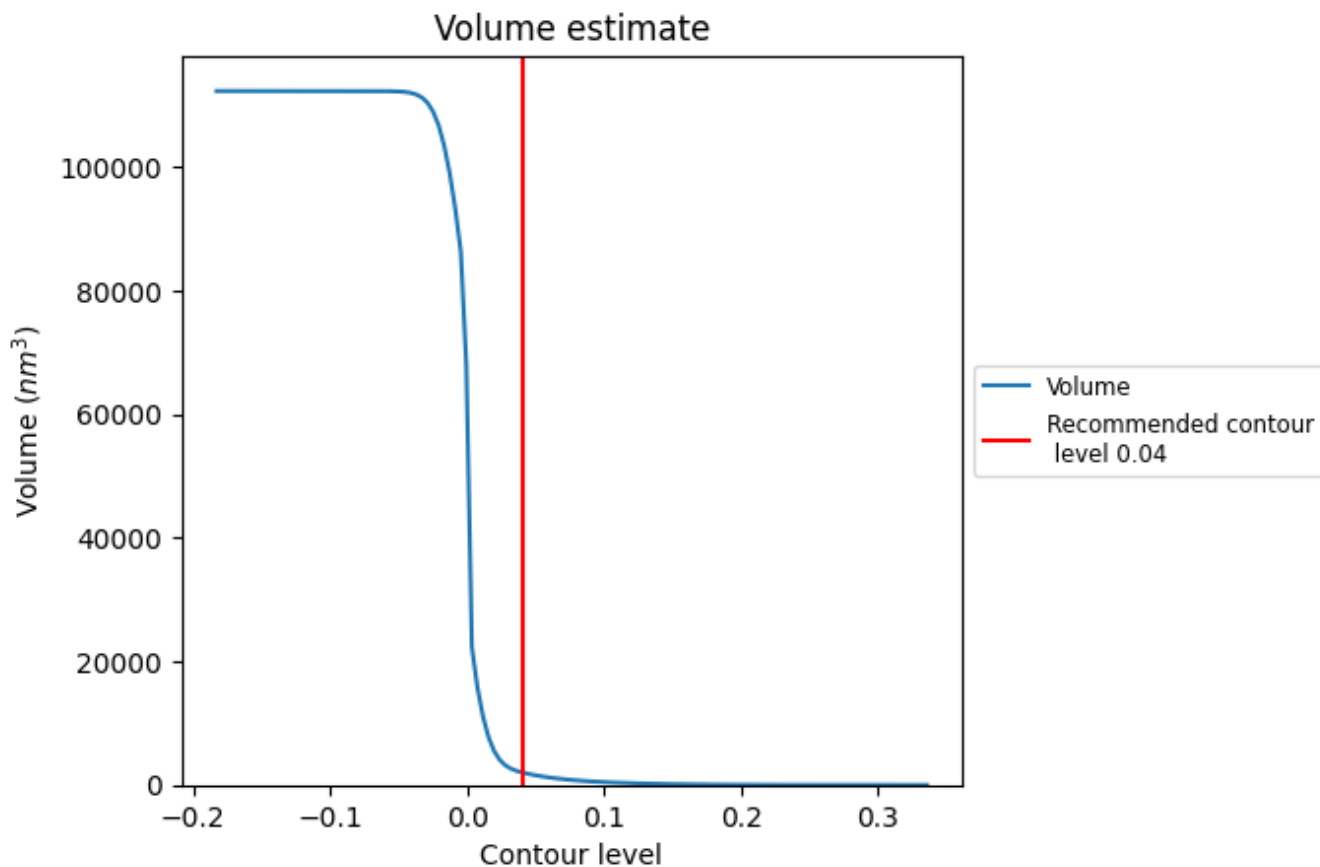
This section contains the results of statistical analysis of the map.

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.

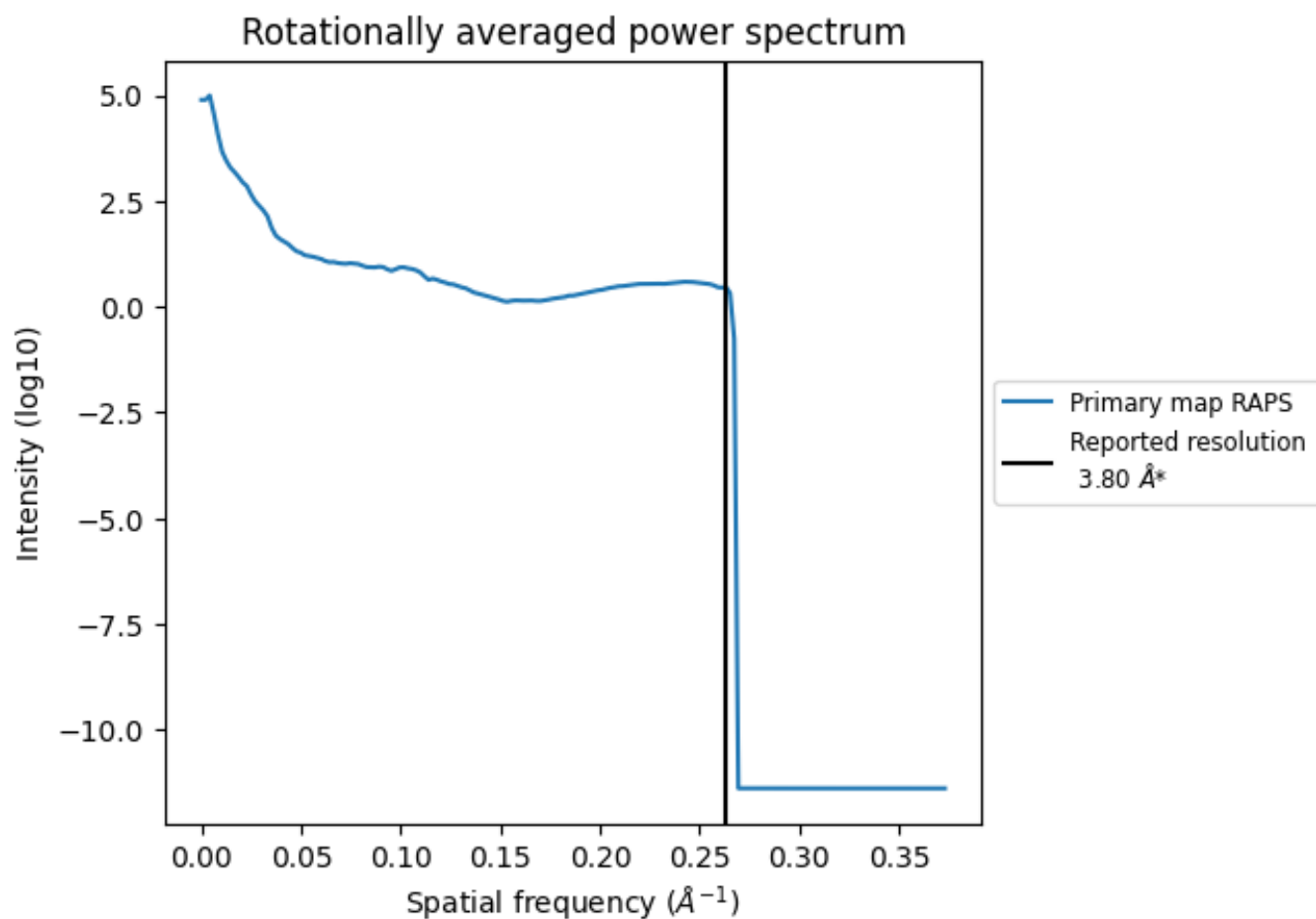
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2026 nm^3 ; this corresponds to an approximate mass of 1830 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 0.263 Å⁻¹

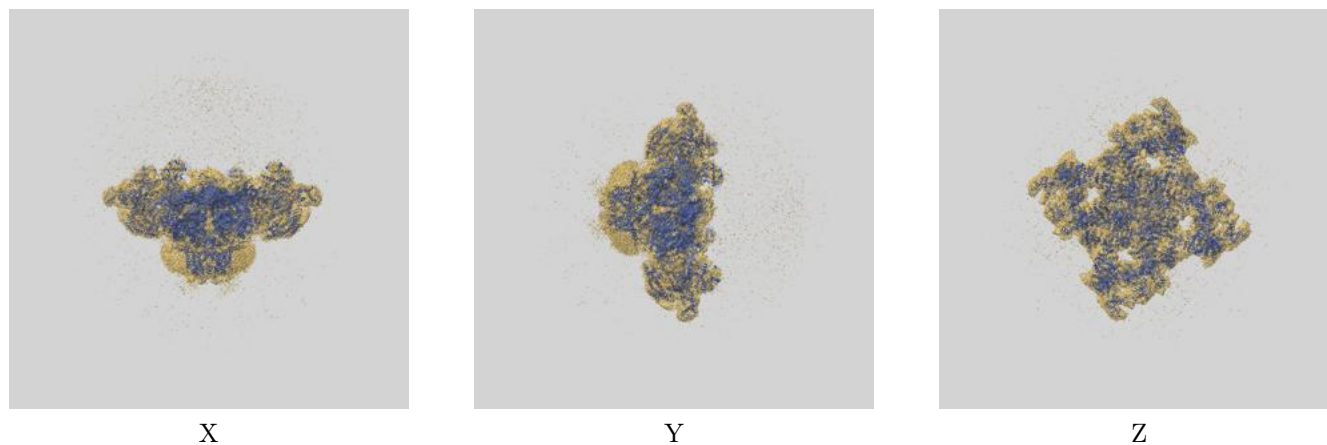
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

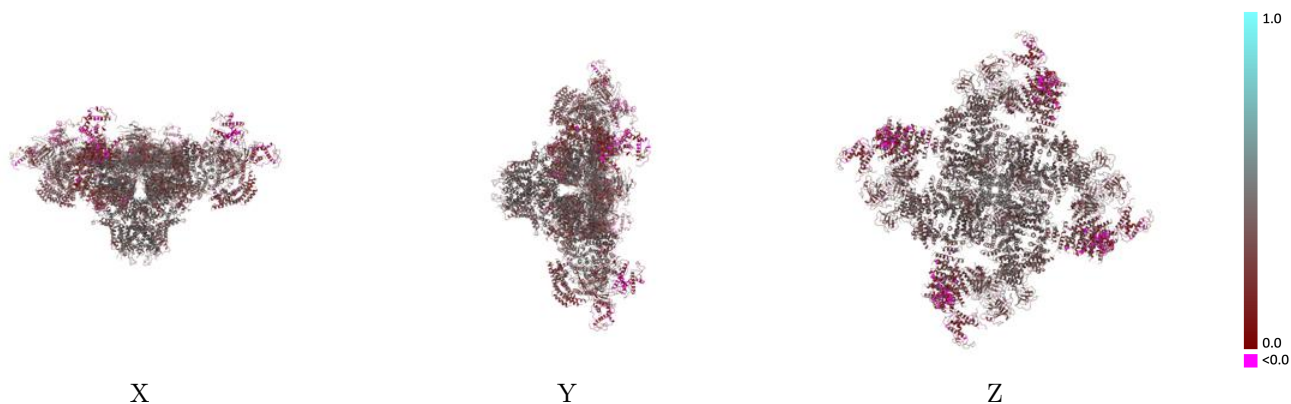
This section contains information regarding the fit between EMDB map EMD-2807 and PDB model 3J8H. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



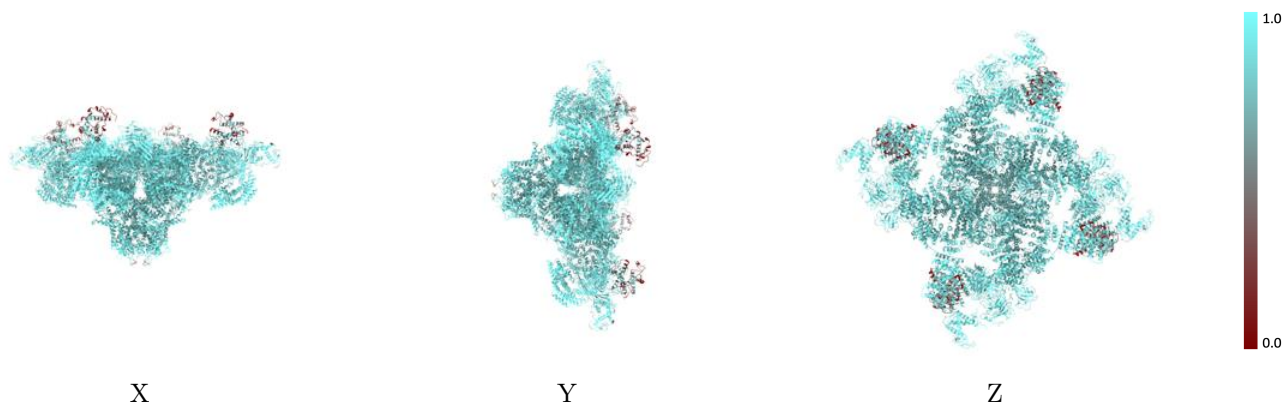
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



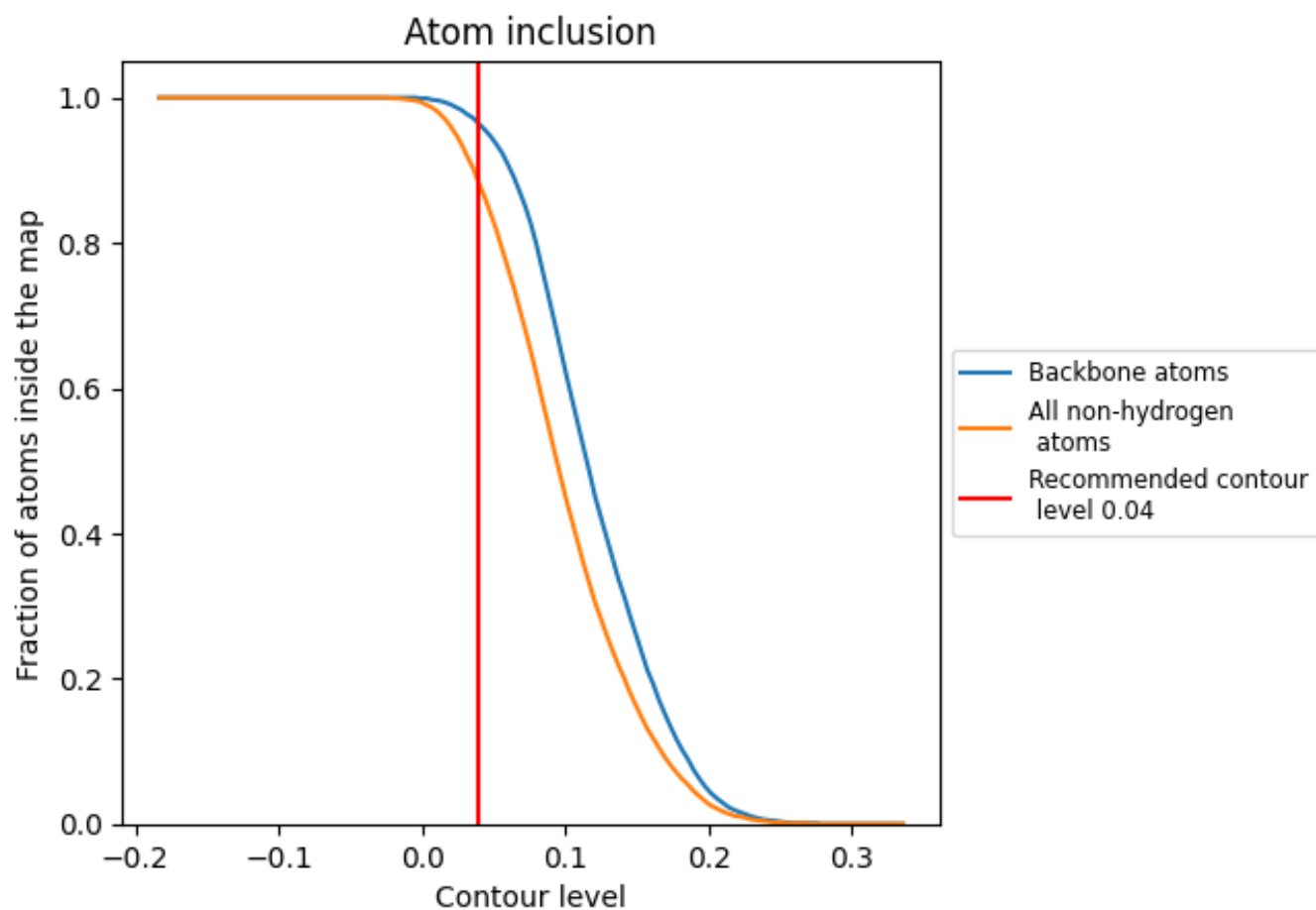
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 88% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8820	 0.3380
A	 0.8810	 0.3380
B	 0.9190	 0.3580
C	 0.8810	 0.3380
D	 0.9190	 0.3570
E	 0.8810	 0.3380
F	 0.9190	 0.3540
G	 0.8810	 0.3380
H	 0.9190	 0.3590

