



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 05:05 PM EST

PDB ID : 7JMG
EMDB ID : EMD-22393
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots
- Frame 22 - State 2 (S2)
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

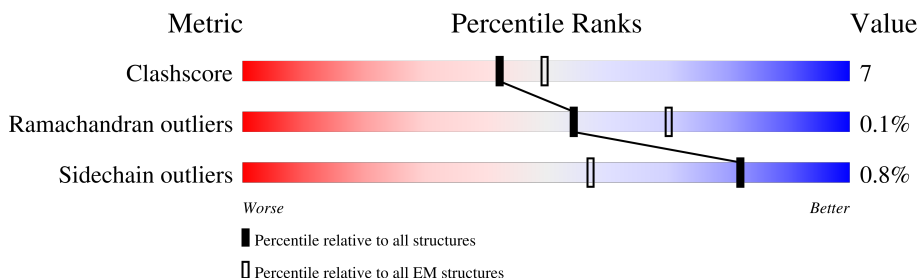
1 Overall quality at a glance

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	B	4687	
1	E	4687	
1	G	4687	
1	I	4687	
2	A	107	
2	F	107	
2	H	107	
2	J	107	

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 ryanodine receptor type 1.

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

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

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

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

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

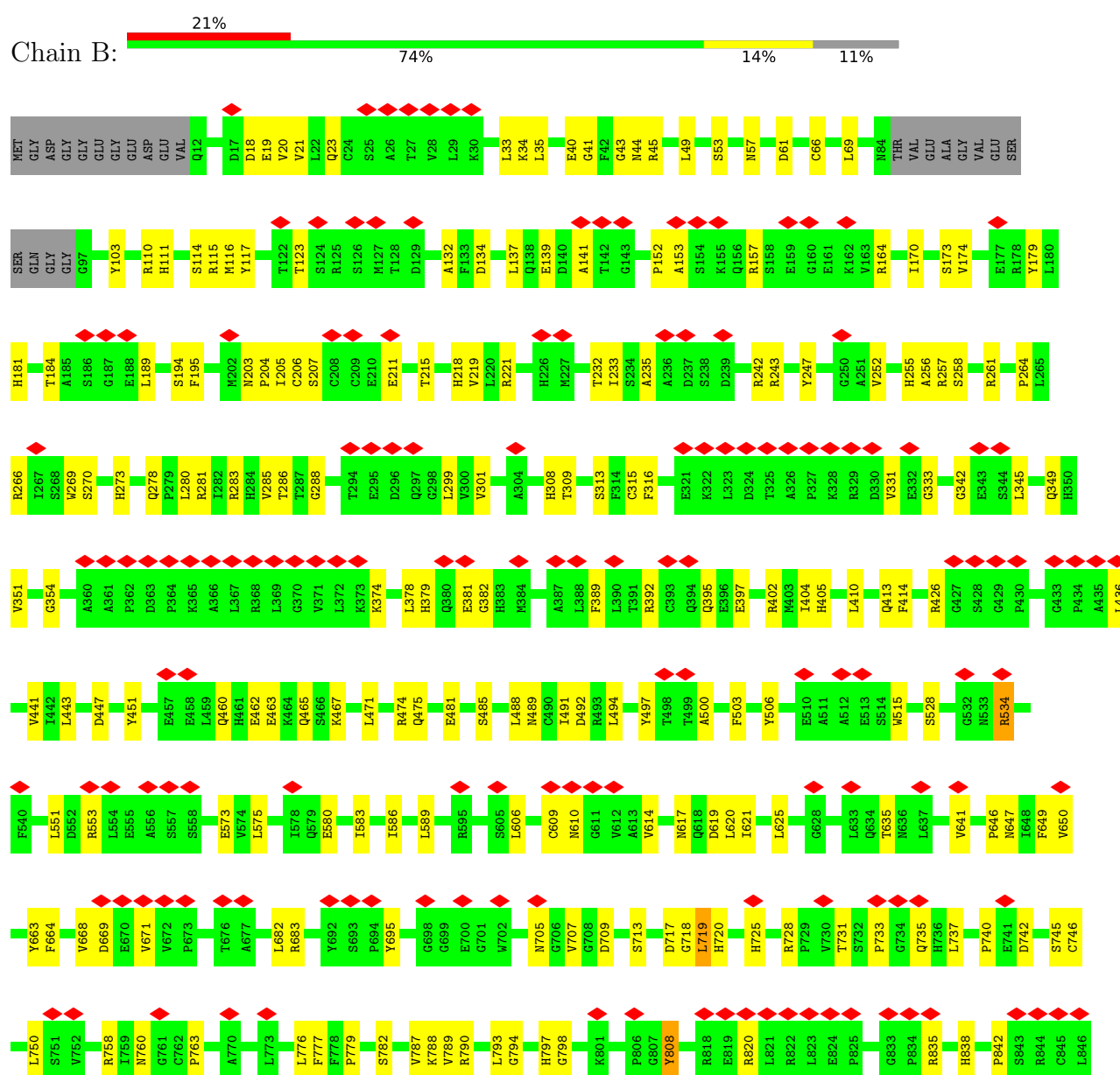
Interest" by depositor).

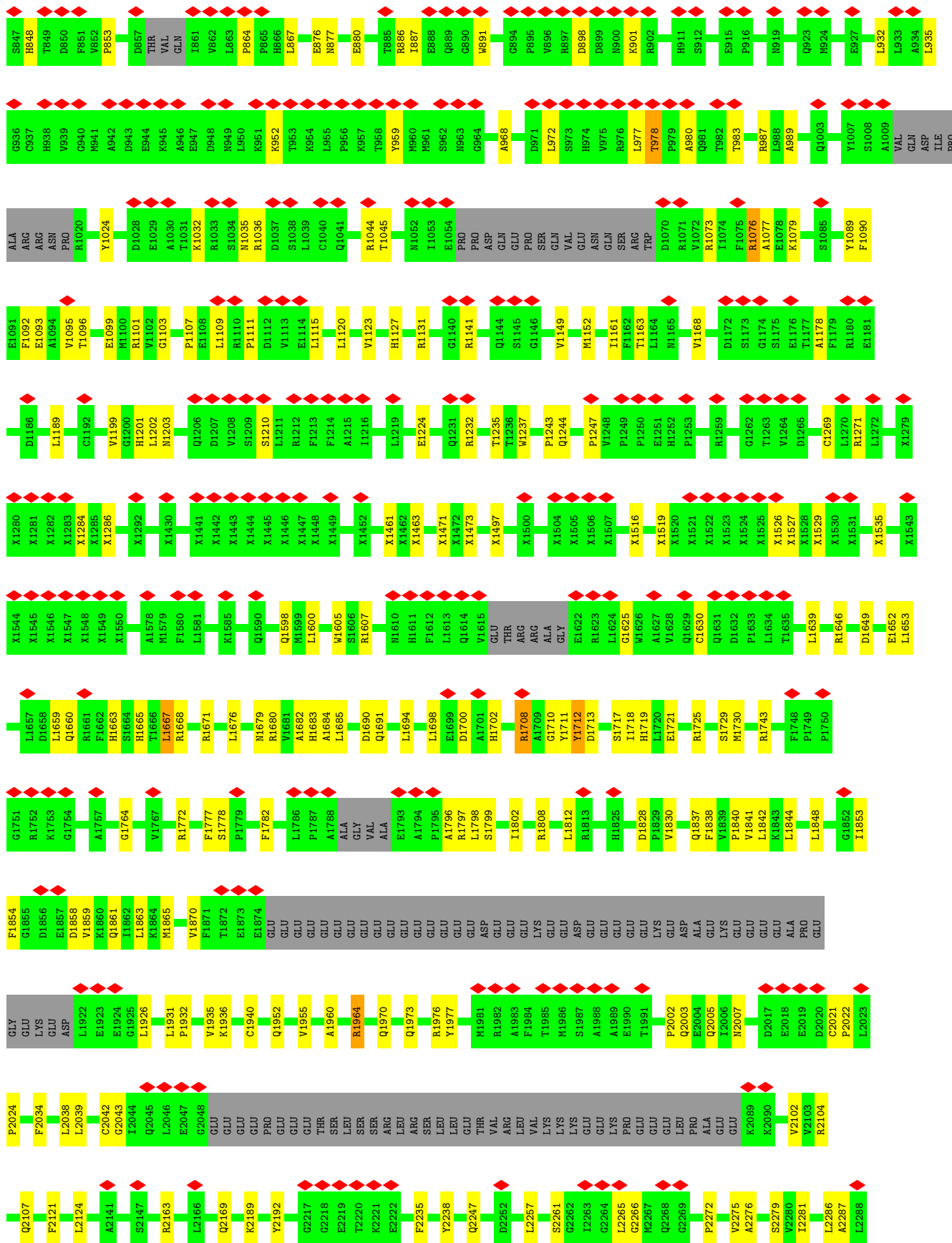
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0

3 Residue-property plots

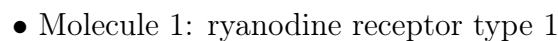
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 type 1





Q3960	N3963	T3966	G3971	F3972	C3973	N3976	H3982	S3983	H3984	V3990	G3991	F3992	L3993	H3994	V3995	F3996	A3997	H3998	K4002	L4003	L4013	N3896	N3897	L4027	N4034	N3901	T3905	Q3906	T3907	T3910	T3911	T3912	Q3927	T3930	S3931	D3932	V3935	V3936	V3937	S3938	G3939	K3940	D3941	Q3946	N3950	F3951													
X3609	X3610	X3611	X3612	X3613	Y3642	T3646	C3650	K3658	A3659	A3660	W3661	L3662	L3663	T3664	E3665	D3666	H3667	D3676	K3679	E3682	Q3683	L3780	Q3781	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	L3710	K3713	S3714	K3715	L3716	D3717	E3718	D3719	Y3720	Y3725	K3731	L3735	E3736	E3737	G3738	G3739	E3740											
X3432	X3467	X3468	X3511	X3512	X3516	X3517	X3520	X3523	X3524	X3534	X3539	X3540	X3543	X3546	X3547	X3552	X3556	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3571	X3572	X3576	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3591	X3606																
X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3273	X3280	X3284	X3285	X3286	X3311	X3312	X3313	X3314	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3387	X3390	X3391	X3392	X3393	X3394	X3419	X3423	X3424	X3427	X3430	X3431											
X2947	X2948	X2995	X3010	X3013	X3014	X3015	X3016	X3017	X3020	X3021	X3022	X3023	X3045	X3046	X3047	X3048	X3049	X3050	X3134	X3135	X3136	X3137	X3138	X3139	X3142	X3143	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3219	X3220	X3221	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249										
T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	D2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	W2932	N2933	G2934	Y2935	A2936	T2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946
K2765	W2766	A2767	F2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	S2776	L2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	F2789	L2790	R2791	R2792	T2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	W2818	W2819	E2820	W2821	T2822	I2823	E2824
X2586	X2618	X2619	X2620	X2625	X2649	X2650	X2651	X2652	X2653	X2673	X2674	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2700	X2701	X2702	X2703	N2734	P2735	D2736	P2737	K2738	P2739	V2740	E2741	K2800	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	T2754	I2755	K2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764					
VAL	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	PRO	GLU	GLU	N2414	H2420	H2441	A2445	G2446	K2447	R2452	L2457	L2460	L2463	D2464	S2471	L2472	I2476	L2479	X2487	X2488	X2493	X2512	X2513	X2514	X2515	X2516	X2517	X2521	X2562	X2563	X2564	F2395	GLY														



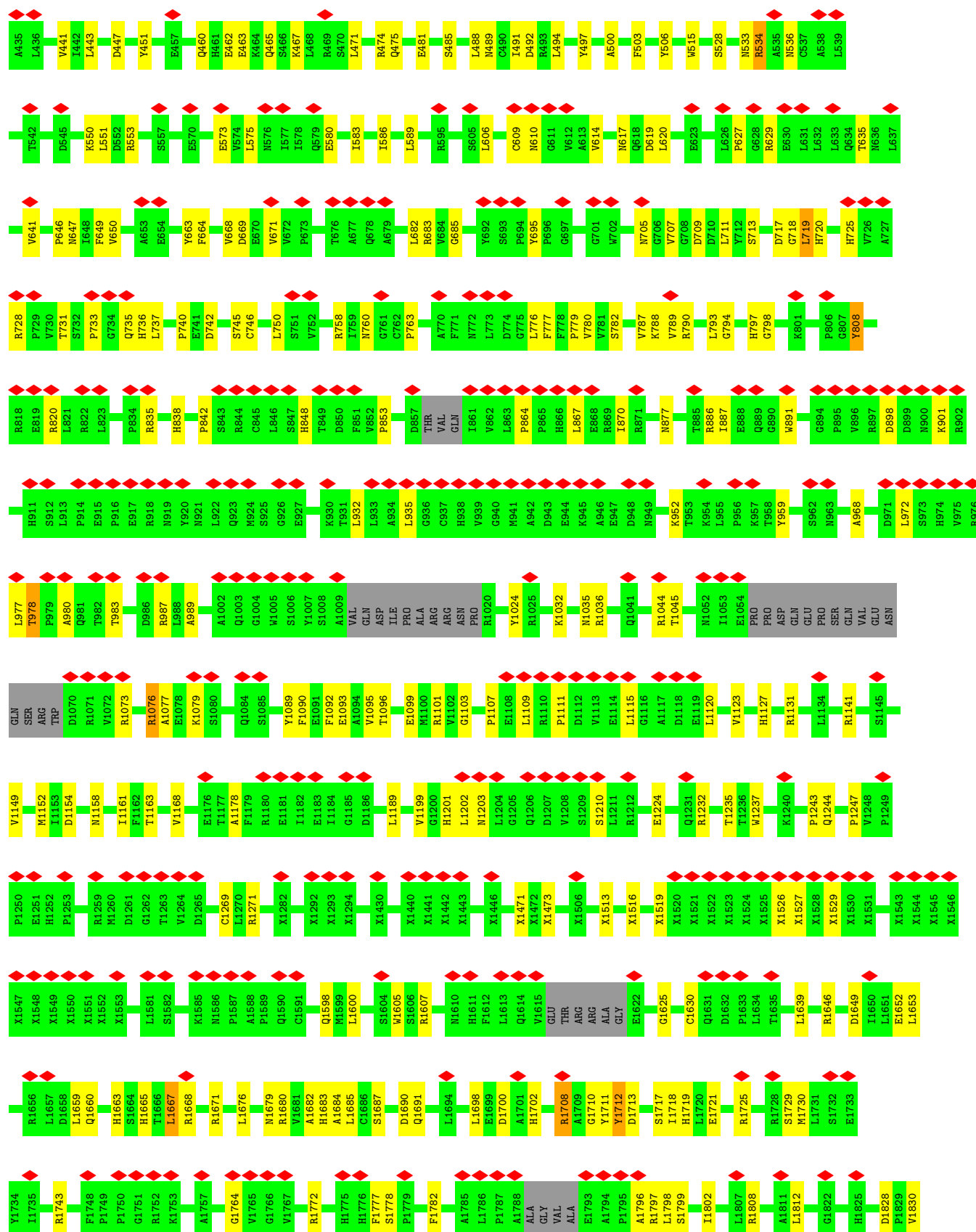
Protein	Residue	Score	Category
Protein 1	ALA	0.95	High
	GLY	0.90	High
	VAL	0.85	High
	GLU	0.80	High
	SER	0.75	High
	SER	0.70	High
	GLN	0.65	High
	GLY	0.60	High
	GLU	0.55	High
	ASP	0.50	High
	GLU	0.45	High
	VAL	0.40	High
	Q12	0.35	High
	D17	0.30	High
	D18	0.25	High
	E19	0.20	High
	V20	0.15	High
V21	0.10	High	
L22	0.05	High	
Q23	0.00	High	
C24	-0.05	High	
S25	-0.10	High	
A26	-0.15	High	
T27	-0.20	High	
V28	-0.25	High	
L29	-0.30	High	
K30	-0.35	High	
E31	-0.40	High	
Q32	-0.45	High	
L33	-0.50	High	
K34	-0.55	High	
L35	-0.60	High	
E40	-0.65	High	
G41	-0.70	High	
F42	-0.75	High	
G43	-0.80	High	
N44	-0.85	High	
R45	-0.90	High	
F48	-0.95	High	
L49	-1.00	High	
S53	-1.05	High	
N57	-1.10	High	
D61	-1.15	High	
L62	-1.20	High	
A63	-1.25	High	
C66	-1.30	High	
E70	-1.35	High	
Q71	-1.40	High	
N84	-1.45	High	
THR	-1.50	High	
GLU	-1.55	High	
Protein 2	GLY	0.95	High
	GLU	0.90	High
	VAL	0.85	High
	GLU	0.80	High
	SER	0.75	High
	SER	0.70	High
	GLN	0.65	High
	GLY	0.60	High
	GLU	0.55	High
	ASP	0.50	High
	G97	0.45	High
	H98	0.40	High
	Y103	0.35	High
	L108	0.30	High
	L109	0.25	High
	R110	0.20	High
	H111	0.15	High
S114	0.10	High	
R115	0.05	High	
M116	0.00	High	
Y117	-0.05	High	
L121	-0.10	High	
T122	-0.15	High	
T123	-0.20	High	
S124	-0.25	High	
R125	-0.30	High	
S126	-0.35	High	
M127	-0.40	High	
T128	-0.45	High	
D129	-0.50	High	
K130	-0.55	High	
L131	-0.60	High	
A132	-0.65	High	
F133	-0.70	High	
D134	-0.75	High	
L137	-0.80	High	
Q138	-0.85	High	
E139	-0.90	High	
D140	-0.95	High	
A141	-1.00	High	
T142	-1.05	High	
P152	-1.10	High	
A153	-1.15	High	
S154	-1.20	High	
K155	-1.25	High	
Q156	-1.30	High	
R157	-1.35	High	
R164	-1.40	High	
L170	-1.45	High	
L171	-1.50	High	
V172	-1.55	High	



P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	V2761	T2762	H2763	E2764	K2765	K2766	A2767	F2768	D2769	K2770	I2771	K2772	N2773	K2774	K2775	S2776	T2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	K2786	T2787	R2788	P2789	K2790	L2791	D2792	P2793	V2794	K2795	T2796	F2797	S2798	E2799	K2800	L2801	D2802	E2803	I2804	Y2805	R2806	W2807
X2557	X2561	X2562	X2563	X2564	X2583	X2586	X2610	X2613	X2614	X2624	X2625	X2626	X2641	X2645	X2646	X2649	X2650	X2651	X2674	X2675	X2683	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	D2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747											
E2388	D2389	P2390	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	HIS	PHE	GLY	GLU	GLU	PRO	PRO	GLU	N2414	R2415	H2441	L2442	A2445	G2446	K2447	L2457	L2460	L2463	D2464	L2472	T2478	L2479	X2487	X2512	X2513	X2514	X2515	X2516	X2517	X2521	X2533	X2536																
I2281	N2284	E2285	L2286	A2287	L2288	A2289	L2290	Q2291	E2292	Q2293	K2297	Y2301	M2312	A2315	Y2318	P2319	D2320	I2321	C2326	G2327	G2328	E2329	R2330	F2340	V2341	N2342	G2343	E2344	S2345	V2346	E2347	N2351	R2355	R2359	C2363	F2364	L2368	E2371	G2372	G2373	F2380	E2381	I2384															
R2140	A2141	P2146	S2147	E2150	R2163	L2166	Q2169	N2187	N2188	K2189	Y2192	Q2193	G2217	G2218	E2219	T2220	K2221	K2227	R2234	F2235	Y2238	R2241	I2242	Q2247	R2248	L2257	S2261	G2262	I2263	G2264	L2265	G2266	M2267	Q2268	G2269	L2272	P2272	L2273	D2274	A2275	S2279	V2280																
E2047	G2048	GLU	GLU	GLU	PRO	GLU	GLU	GLU	THR	SER	LEU	SER	ARG	LEU	ARG	LEU	SER	ARG	GLU	THR	VAL	ARG	LEU	VAL	LYS	LYS	GLU	GLU	PRO	GLU	GLU	GLU	LEU	PRO	ALA	GLU	K2089	K2090	V2102	V2103	R2104	Q2107	V2111	F2121	L2124	H2125	R2126	P2139										
P1932	V1935	K1936	C1940	Q1952	V1955	A1960	R1964	Q1970	Q1973	R1974	S1975	R1976	Y1977	M1981	R1982	A1983	F1984	T1985	M1986	S1987	A1988	A1989	P2002	Q2003	E2004	Q2005	I2006	N2007	A2016	D2017	E2018	E2019	D2020	C2021	P2022	L2023	P2024	E2025	F2034	L2038	C2042	Q2043	I2044	Q2045	L2046													
V1870	F1871	T1872	E1873	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	LYS	ASP	ALA	GLU	PRO	GLU	GLY	LYS	GLU	ASP	L1922	E1923	E1924	G1925	L1926	L1931															
V1783	A1784	A1785	L1786	P1787	A1788	ALA	GLY	VAL	ALA	E1793	A1794	P1795	A1796	R1797	L1798	S1799	P1800	A1801	I1802	P1803	L1804	E1805	A1806	L1807	R1808	D1809	L1812	R1813	D1828	P1829	V1830	Q1837	V1838	V1839	P1840	V1841	L1842	K1843	L1844	L1848	G1852	I1853	F1854	R1855	D1856	E1857	G1858	V1859	K1860	I1861	L1862	K1863	A1864	M1865				
L1695	H1696	A1697	L1698	E1699	D1700	A1701	H1702	R1708	A1709	G1710	Y1711	Y1712	D1713	S1717	I1718	H1719	L1720	E1721	R1725	S1729	M1730	L1738	T1739	P1740	R1743	A1744	F1748	P1749	P1750	G1751	R1752	K1753	G1754	A1757	G1764	V1765	G1766	N1767	V1767	R1772	P1773	P1774	H1775	H1776	F1777	S1778	P1779	P1780	C1781	F1782								
Q1614	V1615	GLU	THR	ARG	ALA	GLY	E1622	R1623	L1624	W1625	A1627	V1628	Q1629	C1630	Q1631	D1632	P1633	L1634	T1635	L1639	R1646	D1649	E1652	L1653	L1659	Q1660	H1663	S1664	H1665	T1666	L1667	R1668	L1669	Y1670	R1671	L1676	G1677	N1678	M1679	R1680	V1681	A1682	H1683	L1684	L1685	D1690	Q1691	A1692										
X1507	X1513	X1516	X1519	X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1534	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1549	X1550	X1564	A1578	M1579	F1580	L1581	S1582	E1583	R1584	K1585	Q1588	M1599	L1600	W1605	S1606	R1607	N1610	H1611	F1612	L1613														
P1243	Q1244	F1245	E1246	P1247	V1248	P1249	P1250	E1251	V1255	E1256	V1257	D1261	G1262	T1263	V1264	D1265	C1269	L1270	R1271	L1272	X1279	X1280	X1281	X1282	X1292	X1293	X1294	X1430	X1431	X1441	X1442	X1443	X1444	X1445	X1446	X1449	X1450	X1451	X1452	X1471	X1472	X1473	X1500	X1501	X1502	X1503	X1504	X1505	X1506									

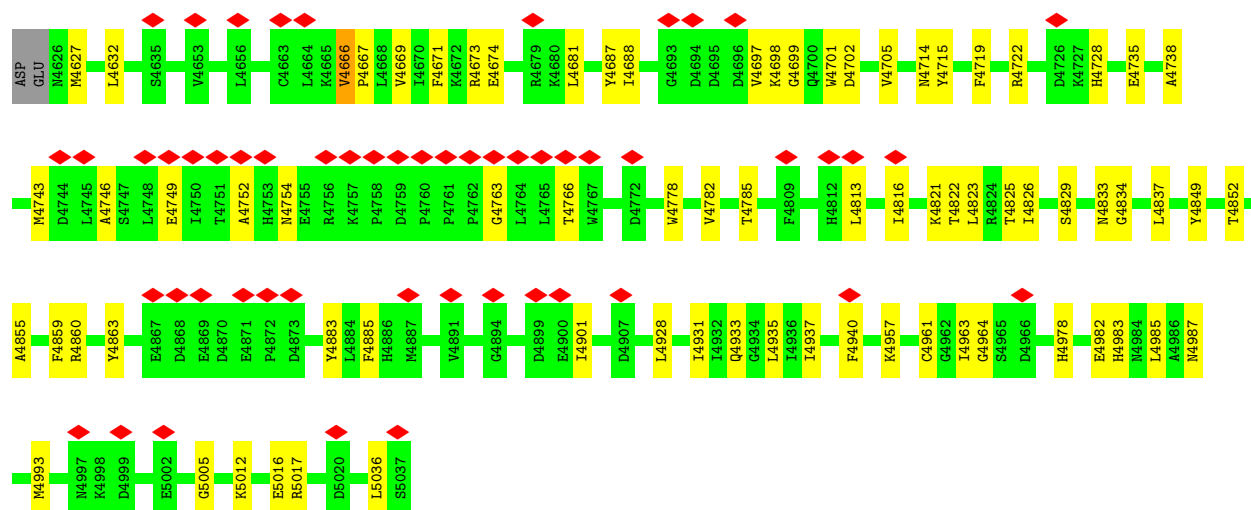
MET	R4159	E3945	K4069	E3859	L3764	E3684	X3559	X3336	X3192	K2928	S2868	GLY	F2808
GLY	L4160	Q3946	D4070	N3860	Q3767	E3685	X3560	X3345	X3193	F2929	R2869	GLU	T2809
ALA		N3950		E3861	L3770	E3686	X3561	X3346	X3194	L2930	E2870	ALA	K2810
ALA	I4170	F3951	G4073	D3862		E3687	X3562	X3347	X3195	Q2931	L2871	ALA	E2811
GLY	R4175	Q3960	S4074	T3864	R3773	E3688	X3564	X3348	X3196	L2932	Q2872	GLY	S2812
ALA	P4176	N3963	E4075	T3865	G3774	E3689	X3565	X3349	X3197	M2933	L2873	ALA	L2813
GLY	Y4177	T3966	Q4078	T3866	A3775	V3690	X3566	X3350	X3216	G2934	M2874	GLY	K2814
GLY	L4178		D4079	I3867		E3691	X3567	X3351	X3217	Y2935	A2875	GLY	A2815
ALA	R4180	T3966	D4079	N3867	V3779	E3692	X3568	X3352	X3218	Q2877	L2877	GLY	M2816
ALA	I4183	G3971	T4082	Q3868	Q3781	H3704	X3569	X3353	X3219	T2938	L2878	ALA	A2818
GLY	M4184	C3973	P4083	N3870	S3784		X3576	X3354	X3220	R2939	A2879	GLY	W2819
ALA	R4189	N3976	D4084	G3871	A3785	T3708		X3355	X3235	R2942	E2880	ALA	W2820
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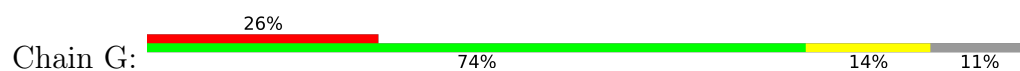


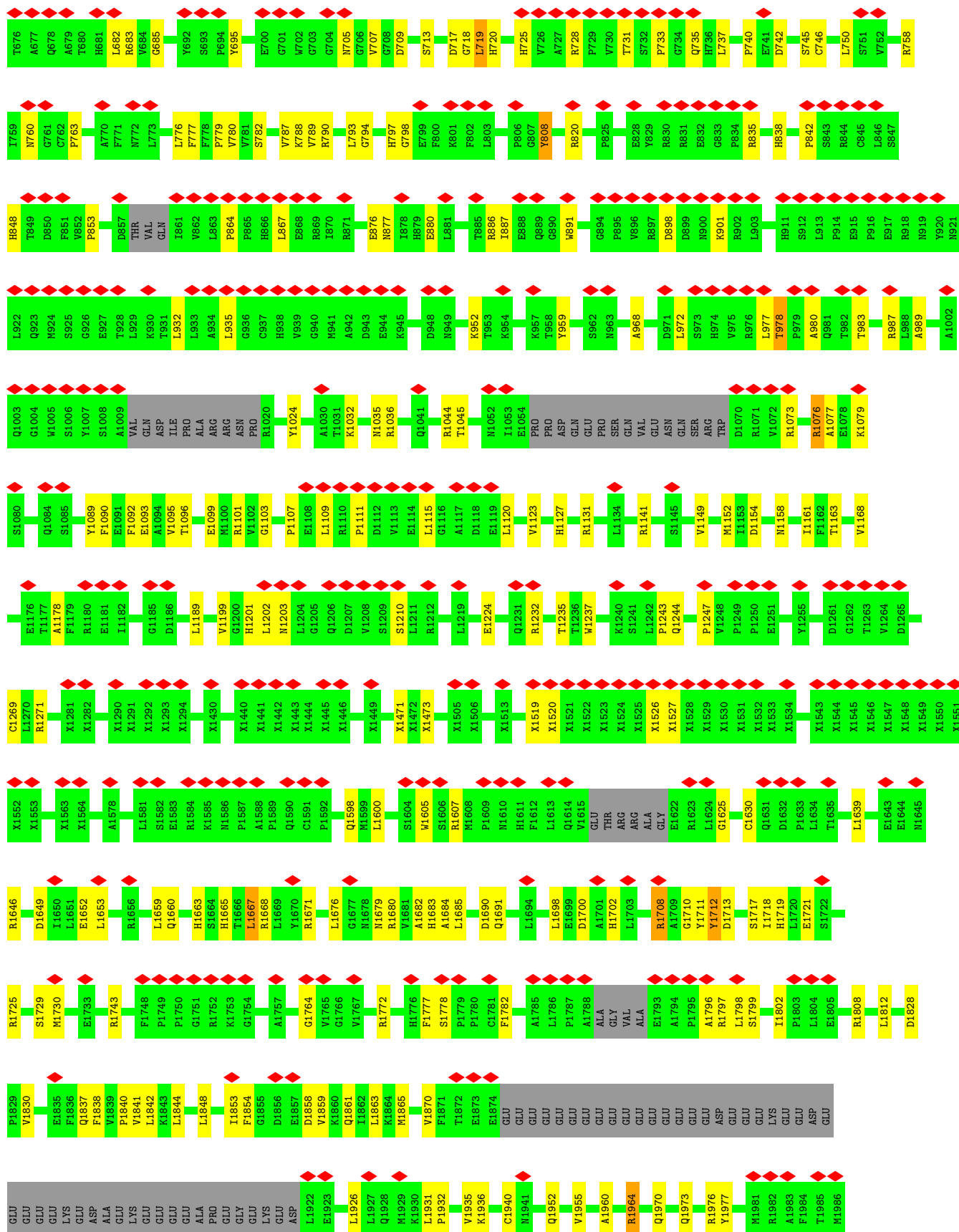






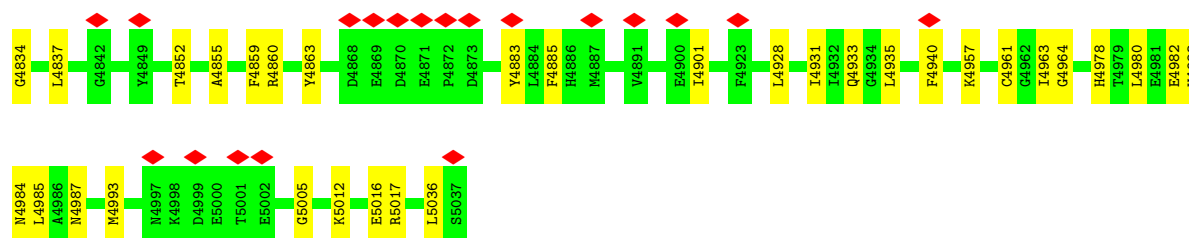
• Molecule 1: ryanodine receptor type 1



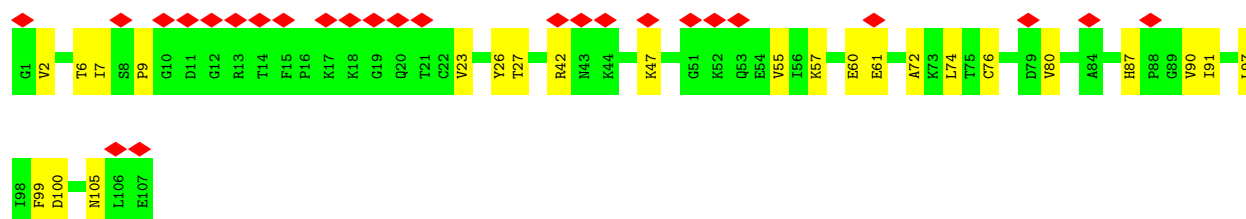
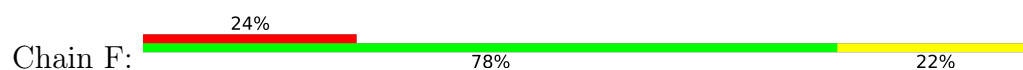




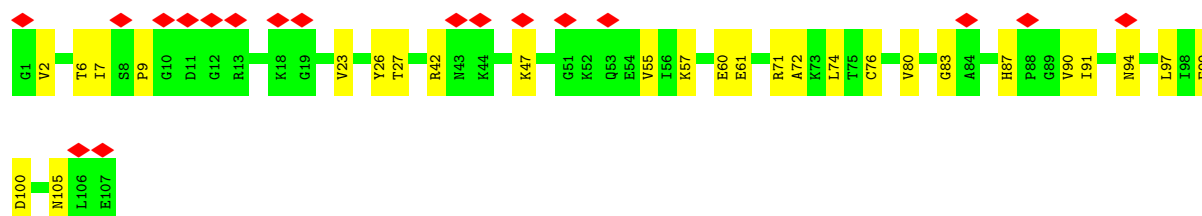
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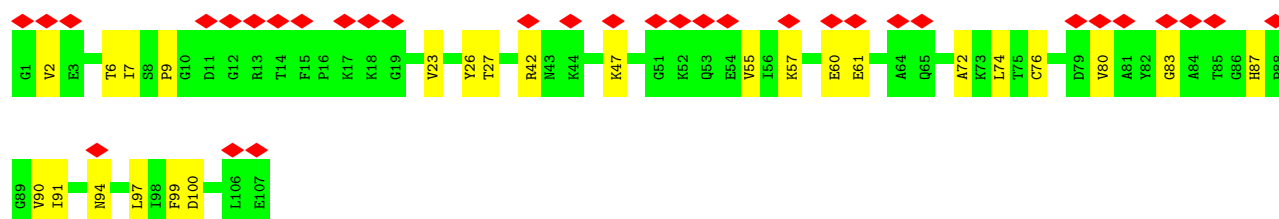
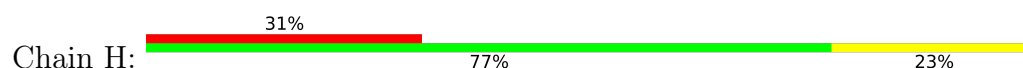
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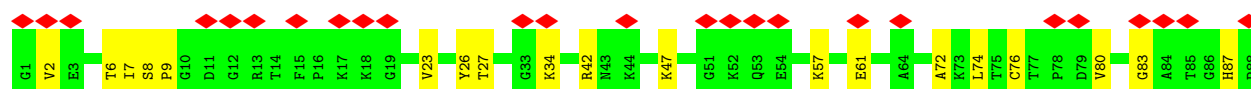
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

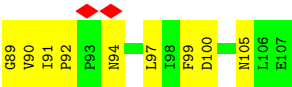


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B





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	0.555	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	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	B	0.33	0/25428	0.56	5/34534 (0.0%)
1	E	0.33	0/25428	0.56	6/34534 (0.0%)
1	G	0.33	0/25428	0.56	5/34534 (0.0%)
1	I	0.33	0/25428	0.56	5/34534 (0.0%)
2	A	0.33	0/834	0.56	0/1123
2	F	0.33	0/834	0.56	0/1123
2	H	0.33	0/834	0.56	0/1123
2	J	0.33	0/834	0.56	0/1123
All	All	0.33	0/105048	0.56	21/142628 (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
1	B	0	12
1	E	0	12
1	G	0	12
1	I	0	12
All	All	0	48

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	719	LEU	CA-CB-CG	6.77	130.87	115.30
1	E	719	LEU	CA-CB-CG	6.76	130.85	115.30
1	G	719	LEU	CA-CB-CG	6.75	130.81	115.30
1	B	719	LEU	CA-CB-CG	6.74	130.79	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3764	LEU	CA-CB-CG	6.40	130.03	115.30

There are no chirality outliers.

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1676	LEU	Peptide
1	B	1690	ASP	Peptide
1	B	1712	TYR	Peptide
1	B	1828	ASP	Peptide
1	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	B	29369	0	24714	390	0
1	E	29369	0	24715	385	0
1	G	29369	0	24713	387	0
1	I	29369	0	24715	388	0
2	A	818	0	824	16	0
2	F	818	0	824	14	0
2	H	818	0	824	14	0
2	J	818	0	824	20	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	102153	1593	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 7.

The worst 5 of 1593 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:4674:GLU:HG3	1:E:4714:ASN:HB3	1.69	0.75
1:G:4674:GLU:HG3	1:G:4714:ASN:HB3	1.69	0.74
1:B:4674:GLU:HG3	1:B:4714:ASN:HB3	1.69	0.73
1:I:4674:GLU:HG3	1:I:4714:ASN:HB3	1.69	0.73
1:G:788:LYS:HG2	1:G:1630:CYS:H	1.56	0.71

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	B	3235/4687 (69%)	2897 (90%)	334 (10%)	4 (0%)	51	85
1	E	3235/4687 (69%)	2895 (90%)	336 (10%)	4 (0%)	51	85
1	G	3235/4687 (69%)	2896 (90%)	335 (10%)	4 (0%)	51	85
1	I	3235/4687 (69%)	2895 (90%)	336 (10%)	4 (0%)	51	85
2	A	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	F	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	H	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	J	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
All	All	13360/19176 (70%)	11963 (90%)	1381 (10%)	16 (0%)	54	85

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1708	ARG
1	E	1708	ARG
1	I	1708	ARG
1	G	1708	ARG

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Mol	Chain	Res	Type
1	B	1932	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	2493/3209 (78%)	2473 (99%)	20 (1%)	81	89
1	E	2493/3209 (78%)	2473 (99%)	20 (1%)	81	89
1	G	2493/3209 (78%)	2473 (99%)	20 (1%)	81	89
1	I	2493/3209 (78%)	2473 (99%)	20 (1%)	81	89
2	A	88/88 (100%)	88 (100%)	0	100	100
2	F	88/88 (100%)	88 (100%)	0	100	100
2	H	88/88 (100%)	88 (100%)	0	100	100
2	J	88/88 (100%)	88 (100%)	0	100	100
All	All	10324/13188 (78%)	10244 (99%)	80 (1%)	82	89

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	4189	ARG
1	G	4034	ASN
1	I	4985	LEU
1	G	1964	ARG
1	G	4137	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 150 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	105	HIS
1	G	4120	ASN
1	G	273	HIS
1	G	1691	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	479	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
1	G	12
1	I	12

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	E	12
1	B	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	45.09
1	I	3613:UNK	C	3639:THR	N	45.04
1	E	3613:UNK	C	3639:THR	N	45.01
1	B	3613:UNK	C	3639:THR	N	44.86
1	G	3163:UNK	C	3170:UNK	N	16.51

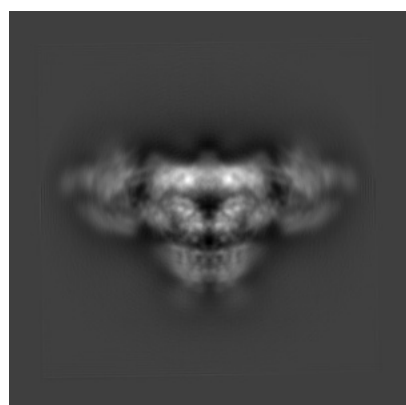
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22393. These allow visual inspection of the internal detail of the map and identification of artifacts.

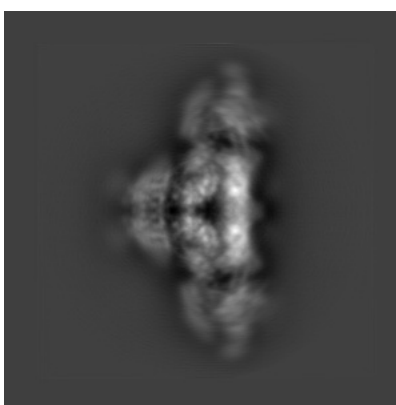
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

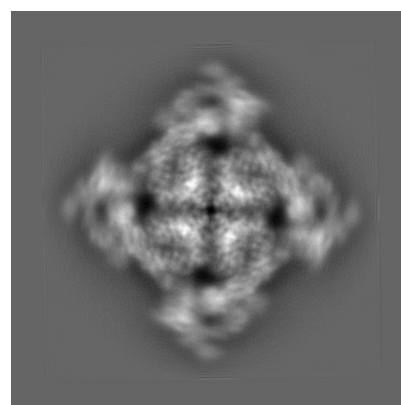
6.1.1 Primary map



X



Y

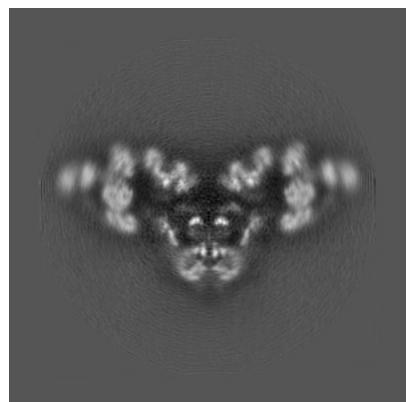


Z

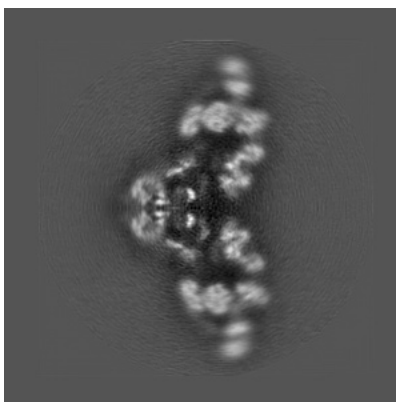
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

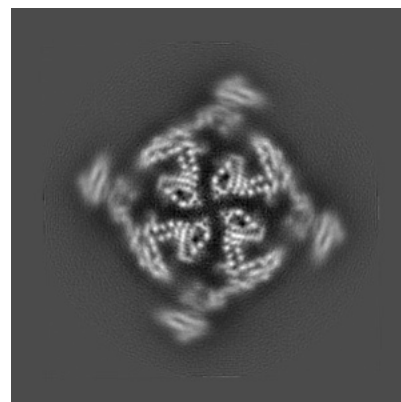
6.2.1 Primary map



X Index: 200



Y Index: 200

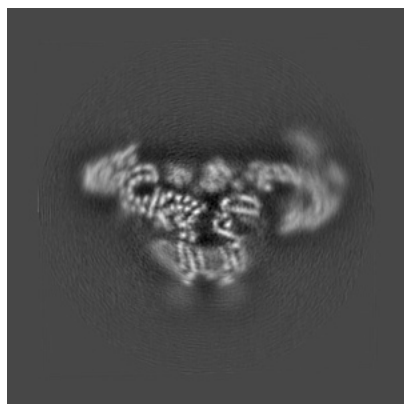


Z Index: 200

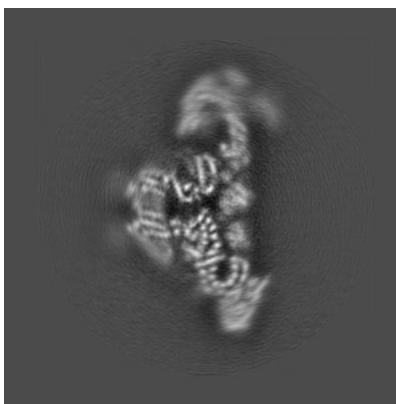
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

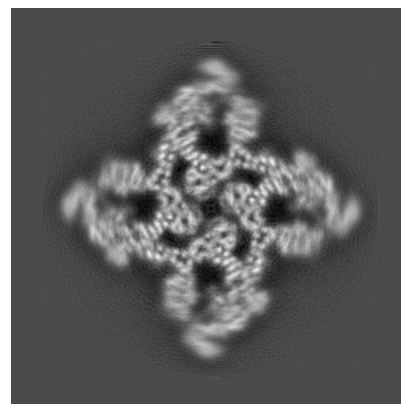
6.3.1 Primary map



X Index: 222



Y Index: 177



Z Index: 230

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

6.4 Orthogonal surface views [i](#)

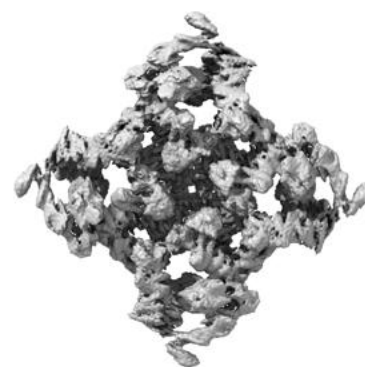
6.4.1 Primary map



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.

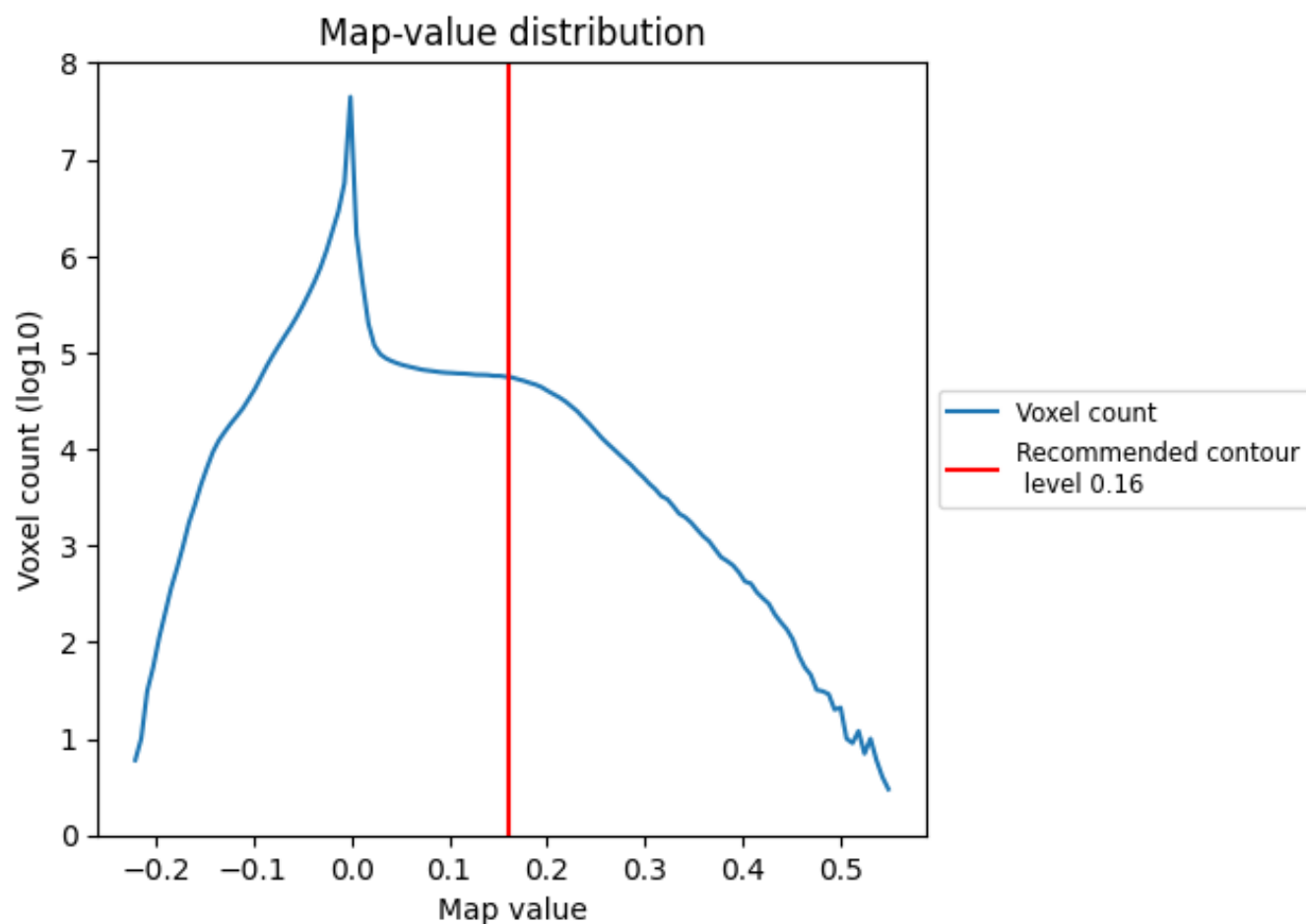
6.5 Mask visualisation

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

7 Map analysis [i](#)

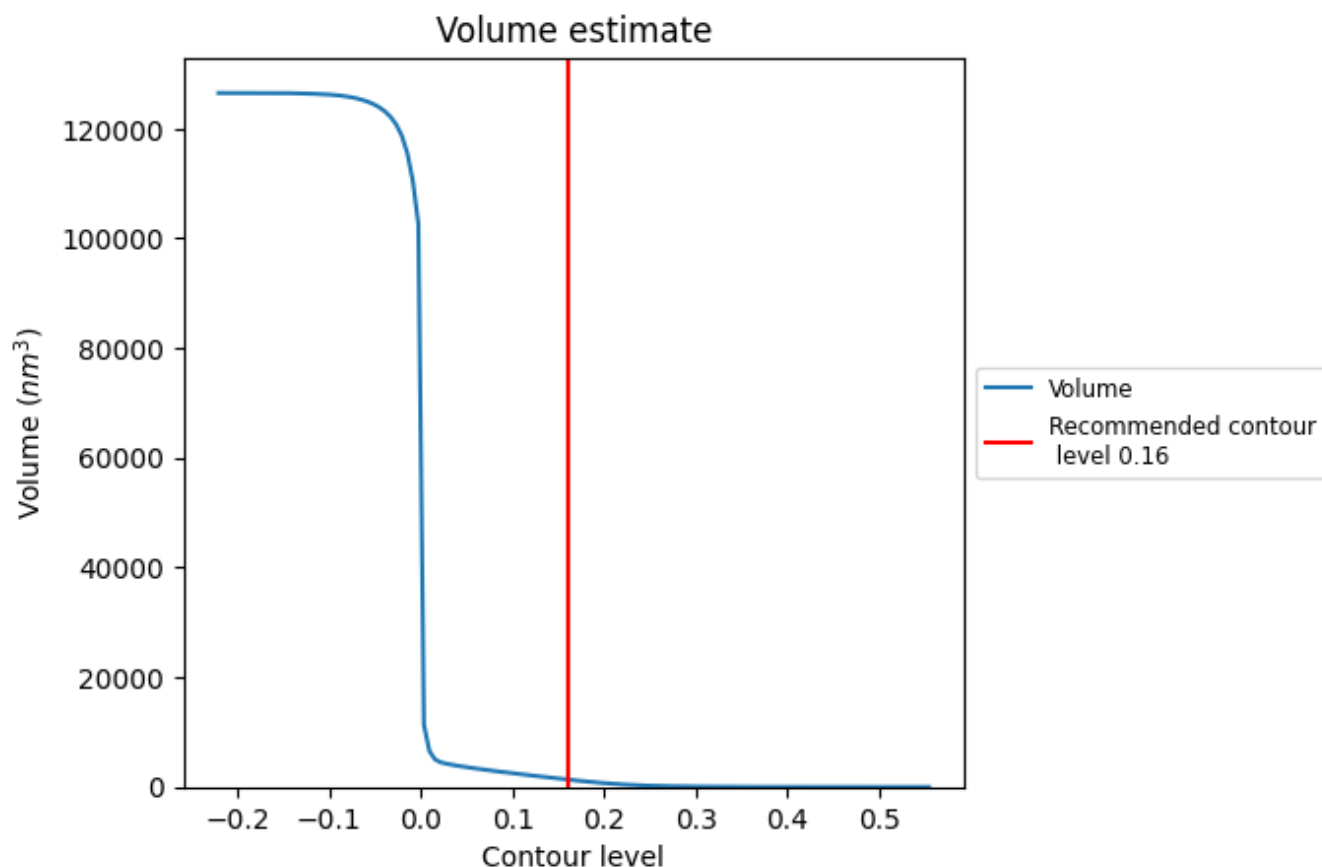
This section contains the results of statistical analysis of the map.

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.

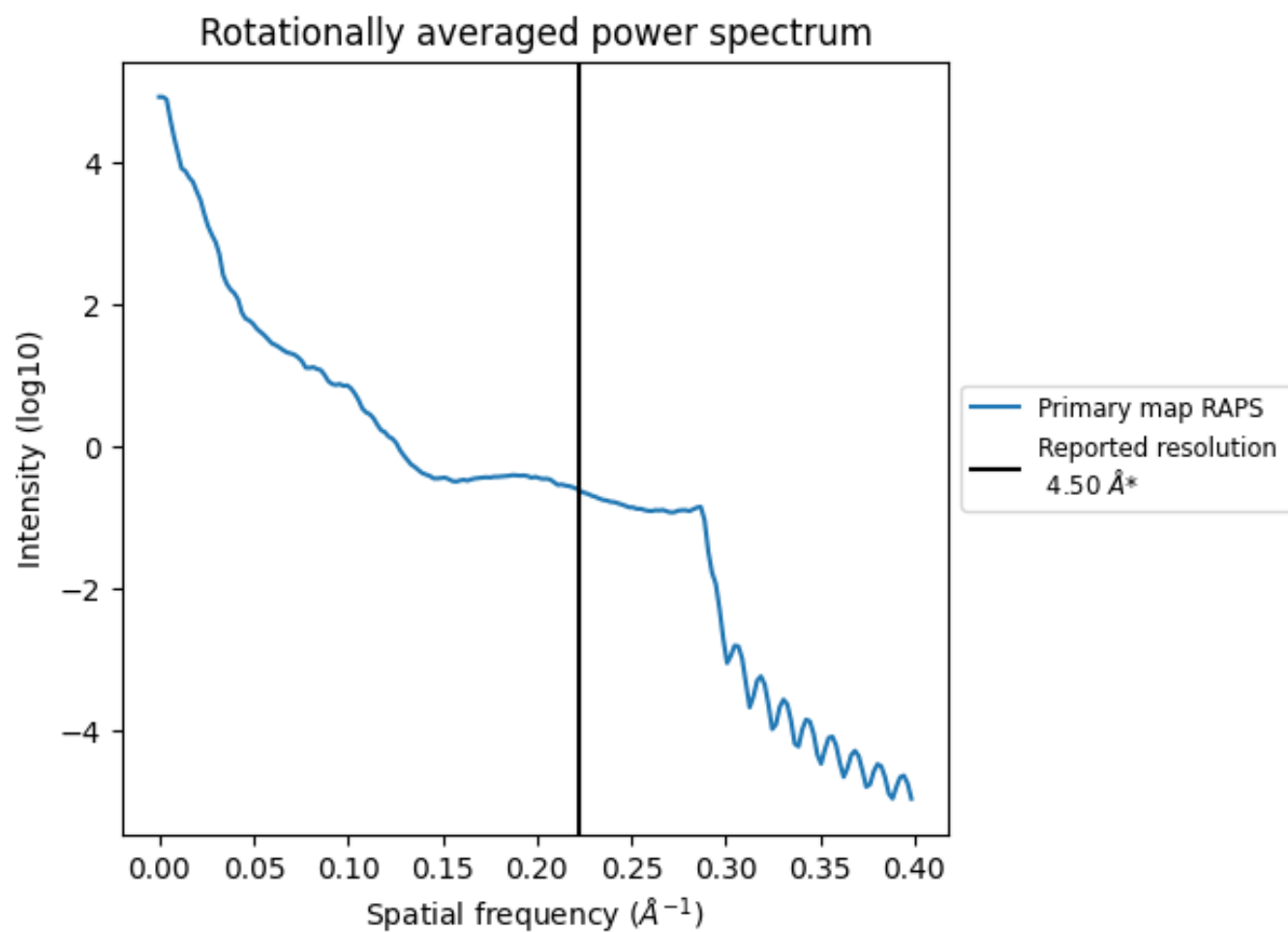
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1358 nm³; this corresponds to an approximate mass of 1227 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 0.222 Å⁻¹

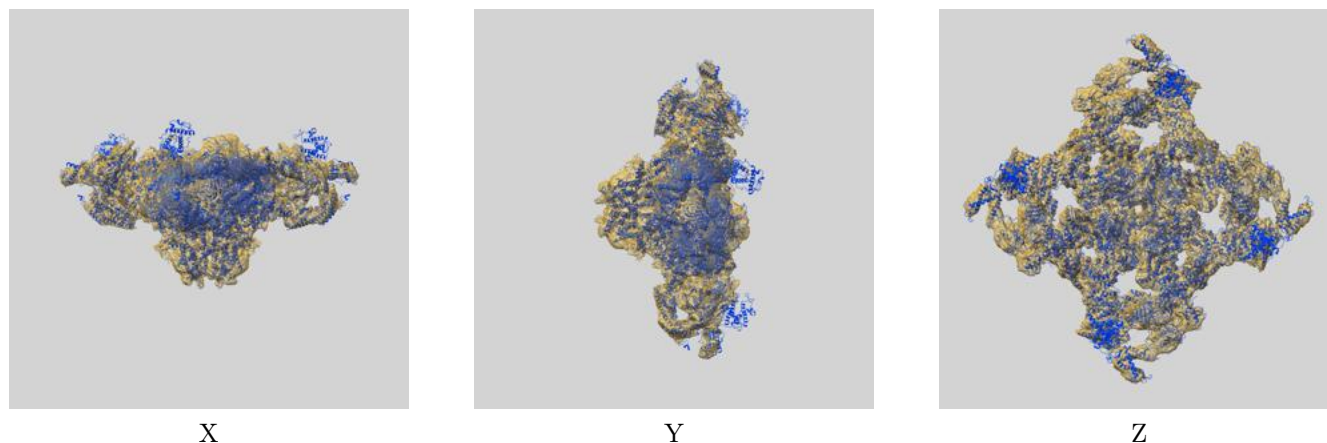
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

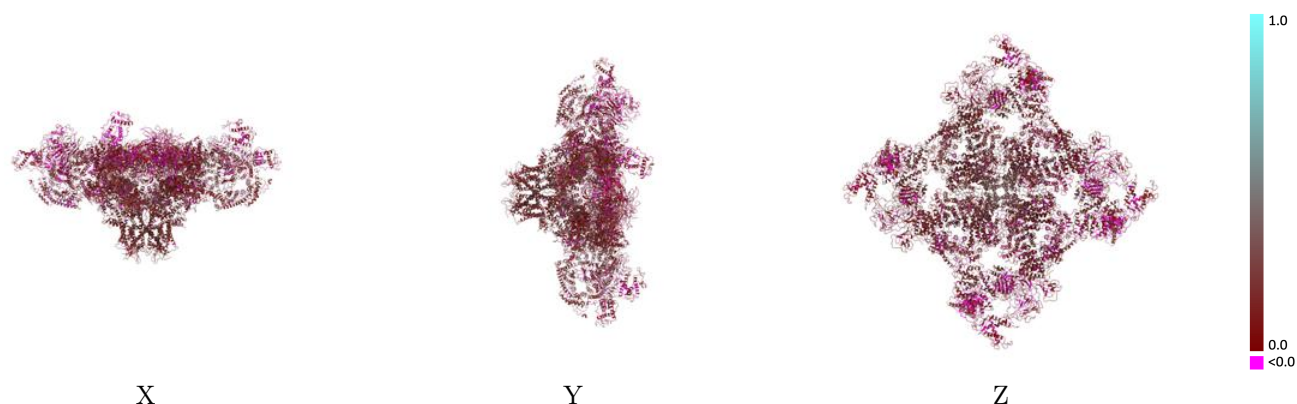
This section contains information regarding the fit between EMDB map EMD-22393 and PDB model 7JMG. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



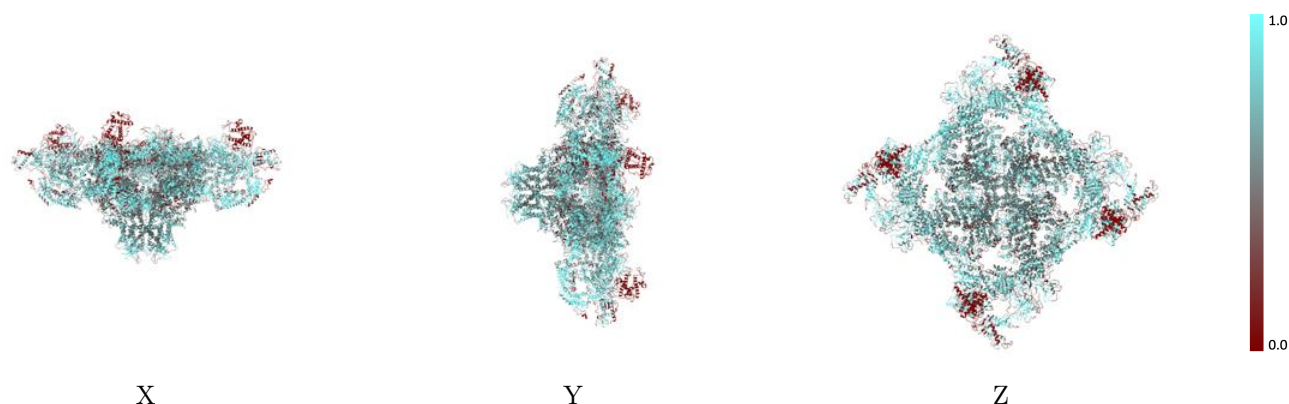
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



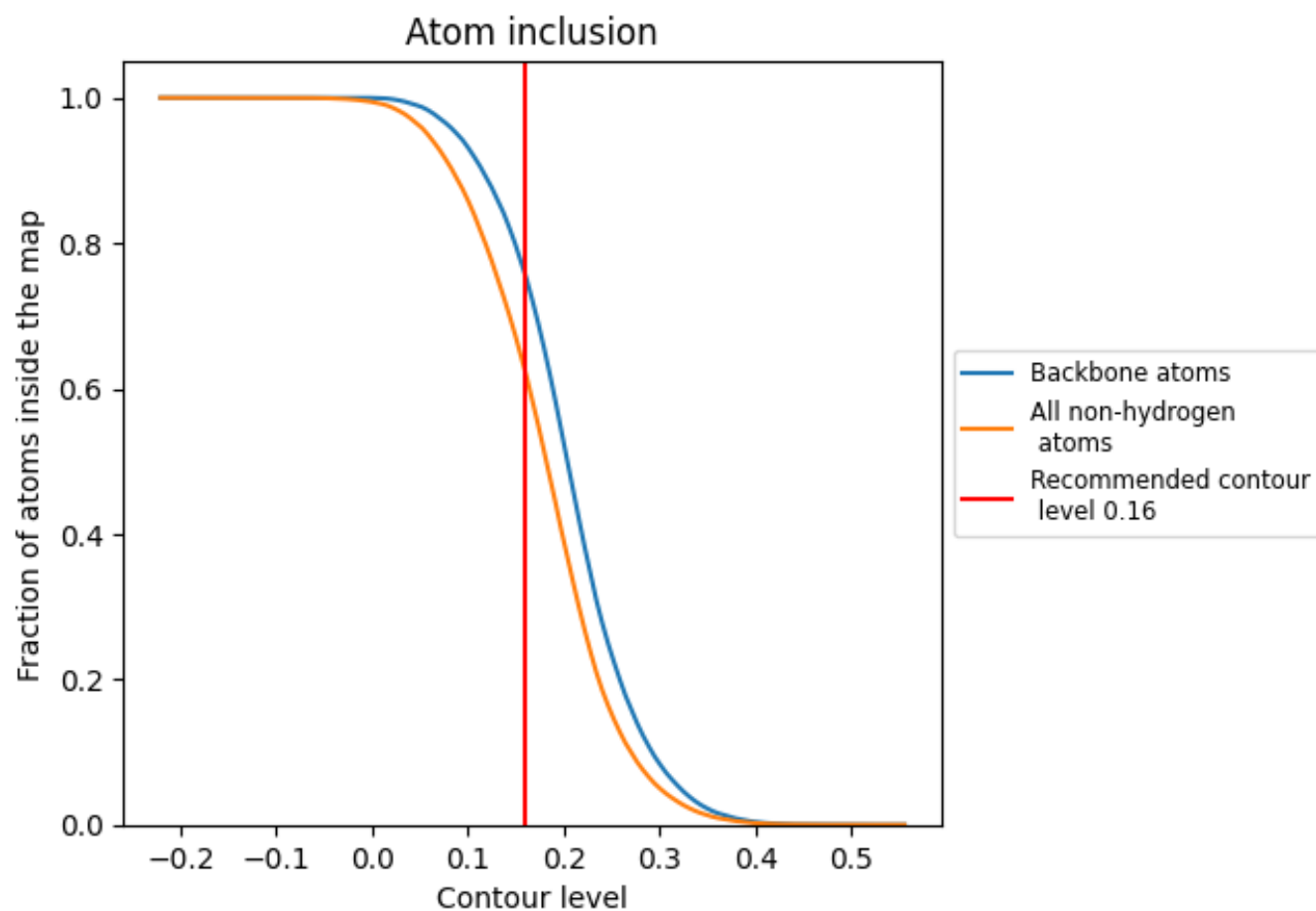
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 62% 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> 0.6216	<div></div> 0.1550
A	<div></div> 0.7060	<div></div> 0.1500
B	<div></div> 0.6410	<div></div> 0.1760
E	<div></div> 0.6130	<div></div> 0.1450
F	<div></div> 0.6576	<div></div> 0.1250
G	<div></div> 0.6064	<div></div> 0.1410
H	<div></div> 0.6154	<div></div> 0.1140
I	<div></div> 0.6216	<div></div> 0.1600
J	<div></div> 0.6737	<div></div> 0.1360

1.0

0.0

<0.0