



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 12:26 AM UTC

PDB ID : 7M6A / pdb_00007m6a
EMDB ID : EMD-23692
Title : High resolution structure of the membrane embedded skeletal muscle ryanodine receptor
Authors : Melville, Z.; Kim, K.; Clarke, O.B.; Marks, A.R.
Deposited on : 2021-03-25
Resolution : 3.36 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

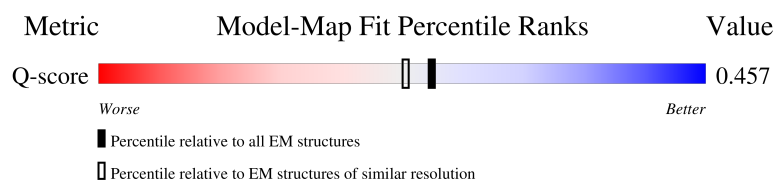
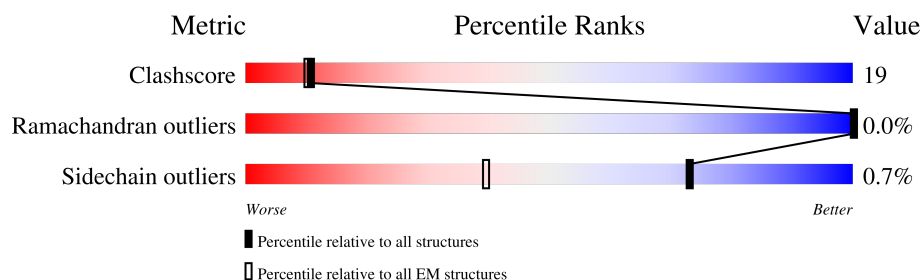
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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.



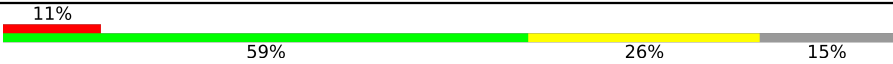
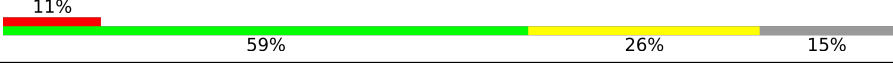
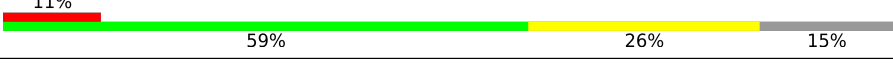
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14332 (2.86 - 3.86)

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	F	108	 64% 29% 6% ..
1	H	108	 64% 29% 6% .
1	J	108	 66% 27% 6% .
1	O	108	 65% 28% 6% ..

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Mol	Chain	Length	Quality of chain
2	A	5037	
2	B	5037	
2	G	5037	
2	I	5037	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 140632 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

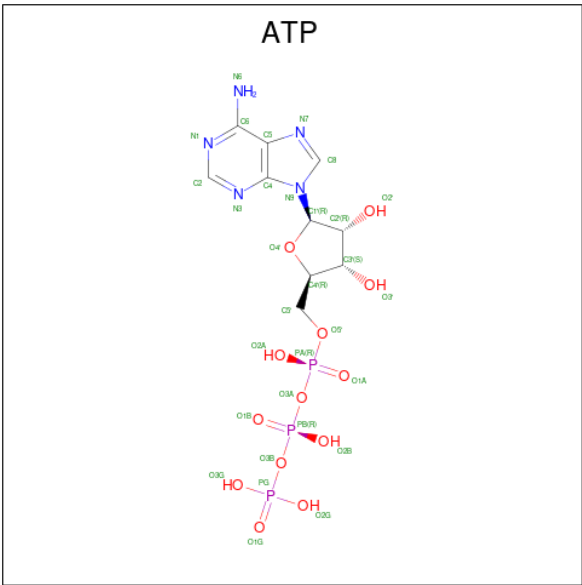
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4306	Total	C	N	O	S	0	0
			34293	21843	5903	6312	235		
2	G	4306	Total	C	N	O	S	0	0
			34293	21843	5903	6312	235		
2	B	4306	Total	C	N	O	S	0	0
			34293	21843	5903	6312	235		
2	I	4306	Total	C	N	O	S	0	0
			34293	21843	5903	6312	235		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

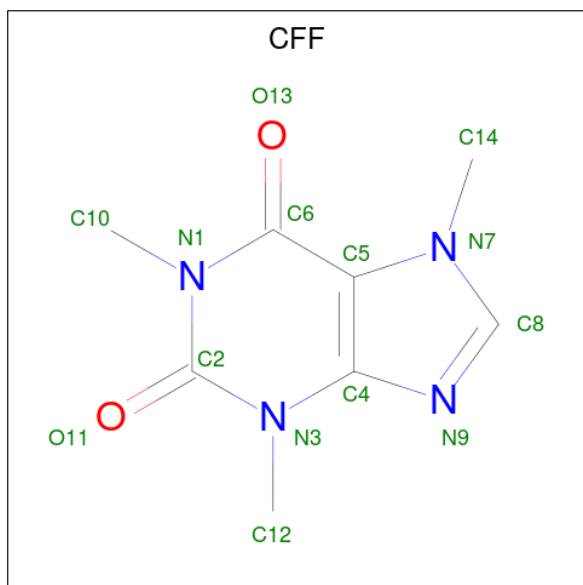
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).

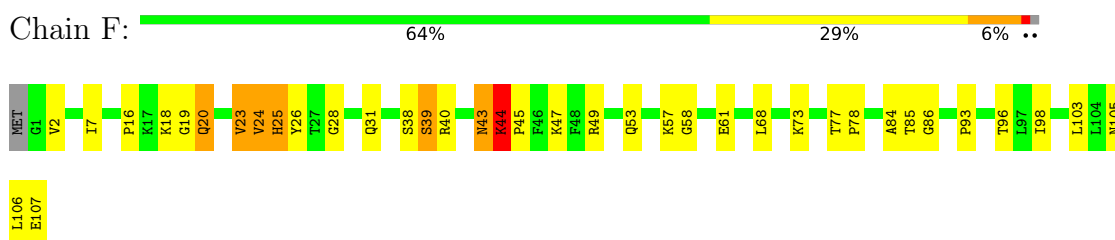


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	I	1	Total	C	N	O	0
			14	8	4	2	

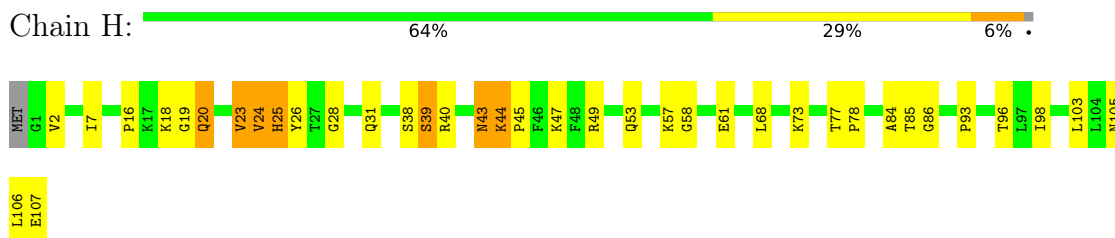
3 Residue-property plots [i](#)

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

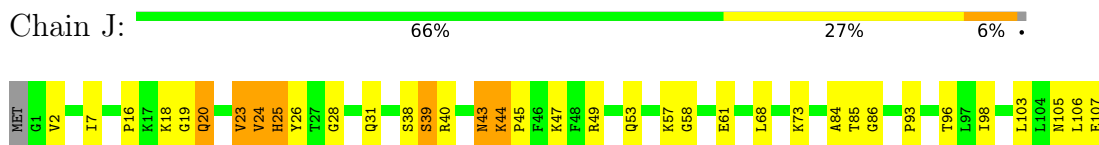
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



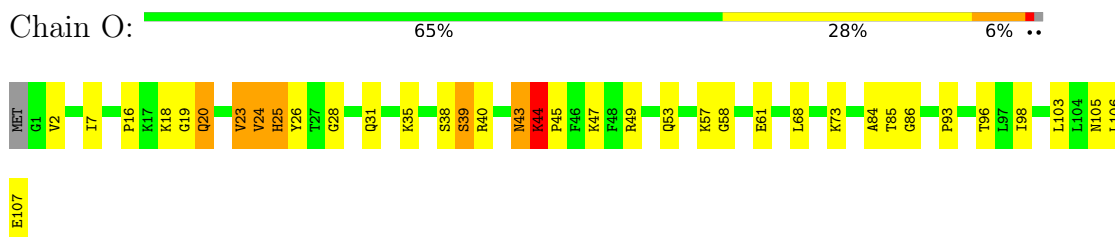
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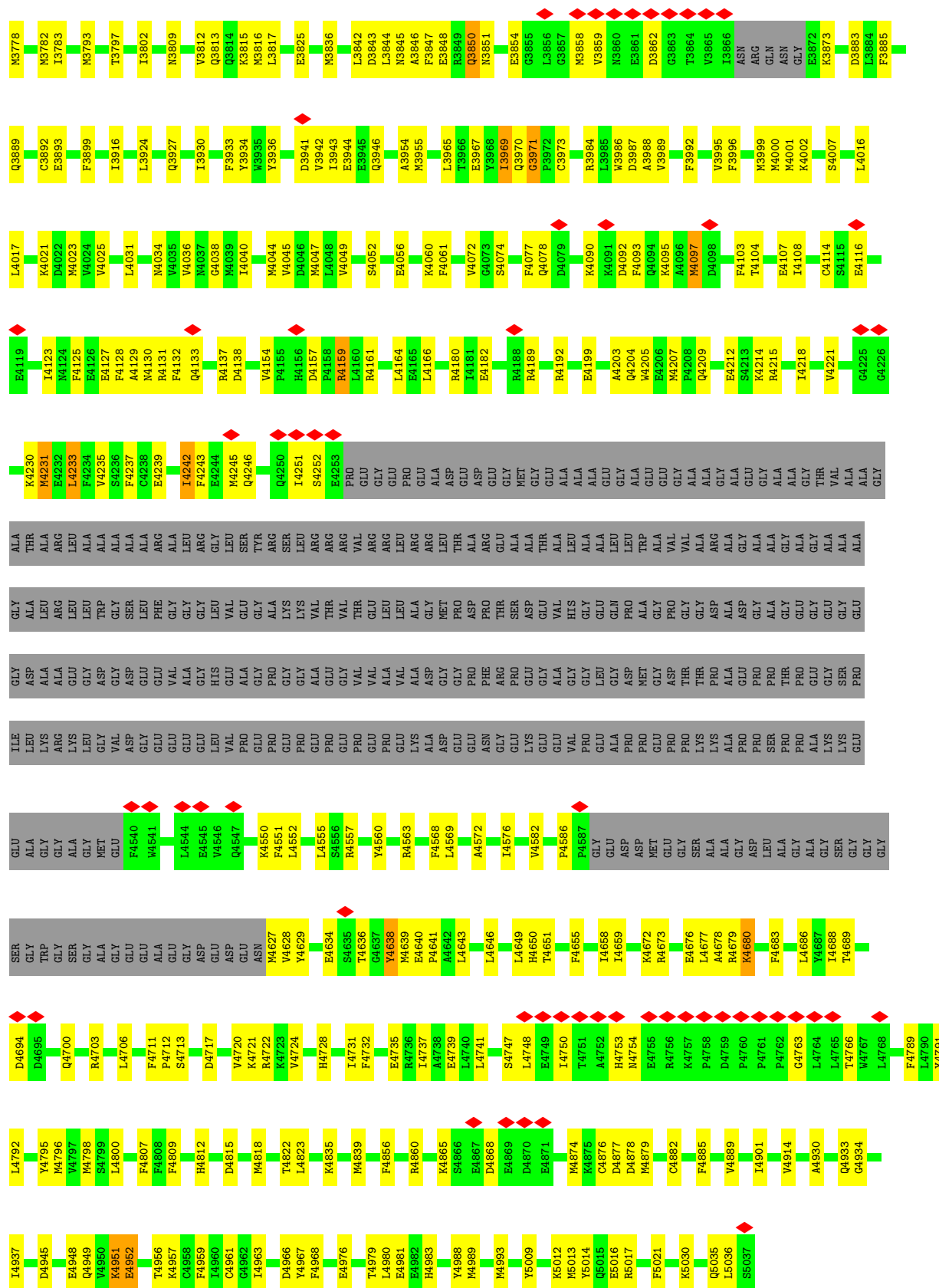


- Molecule 2: Ryanodine receptor 1







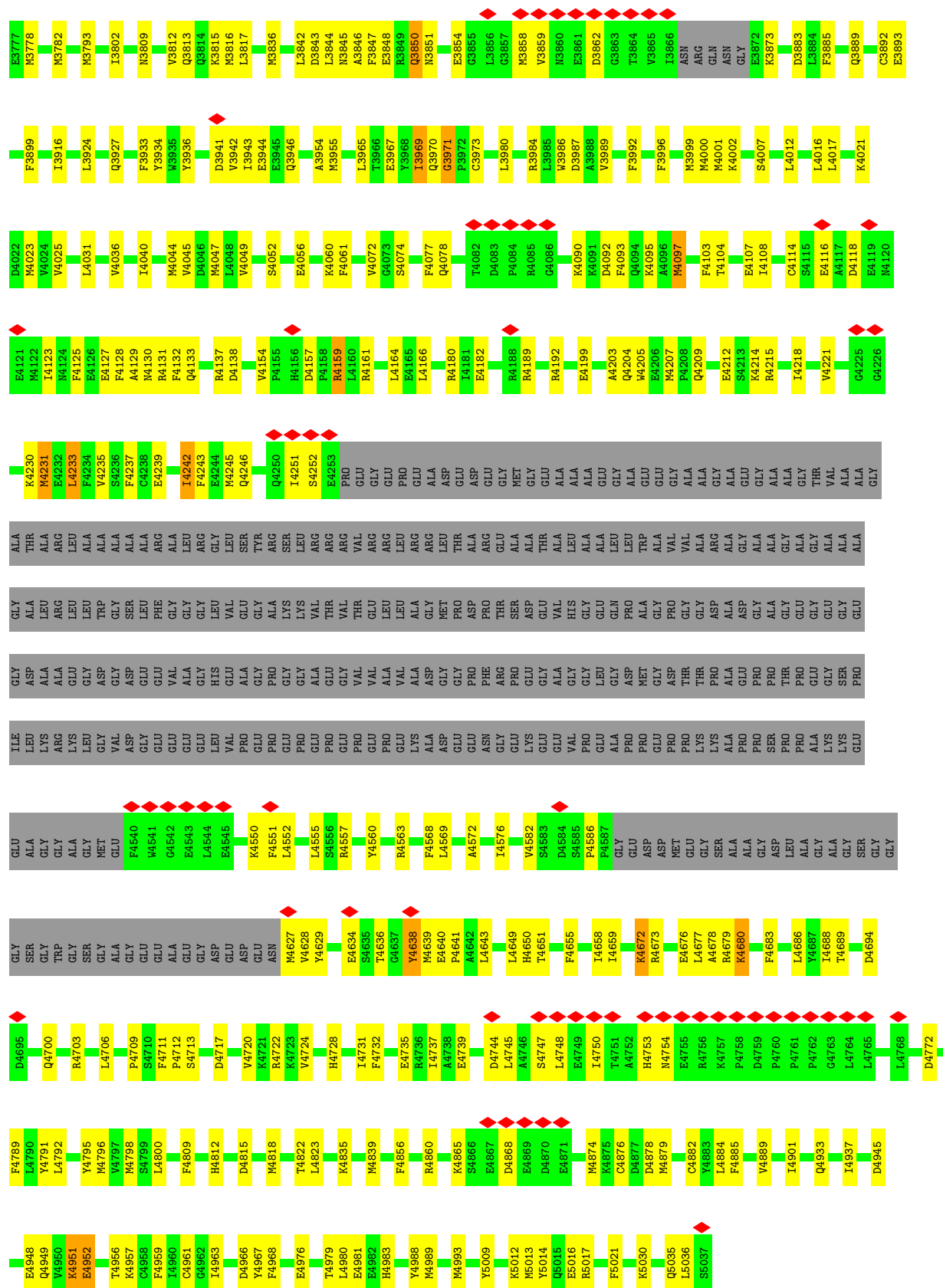




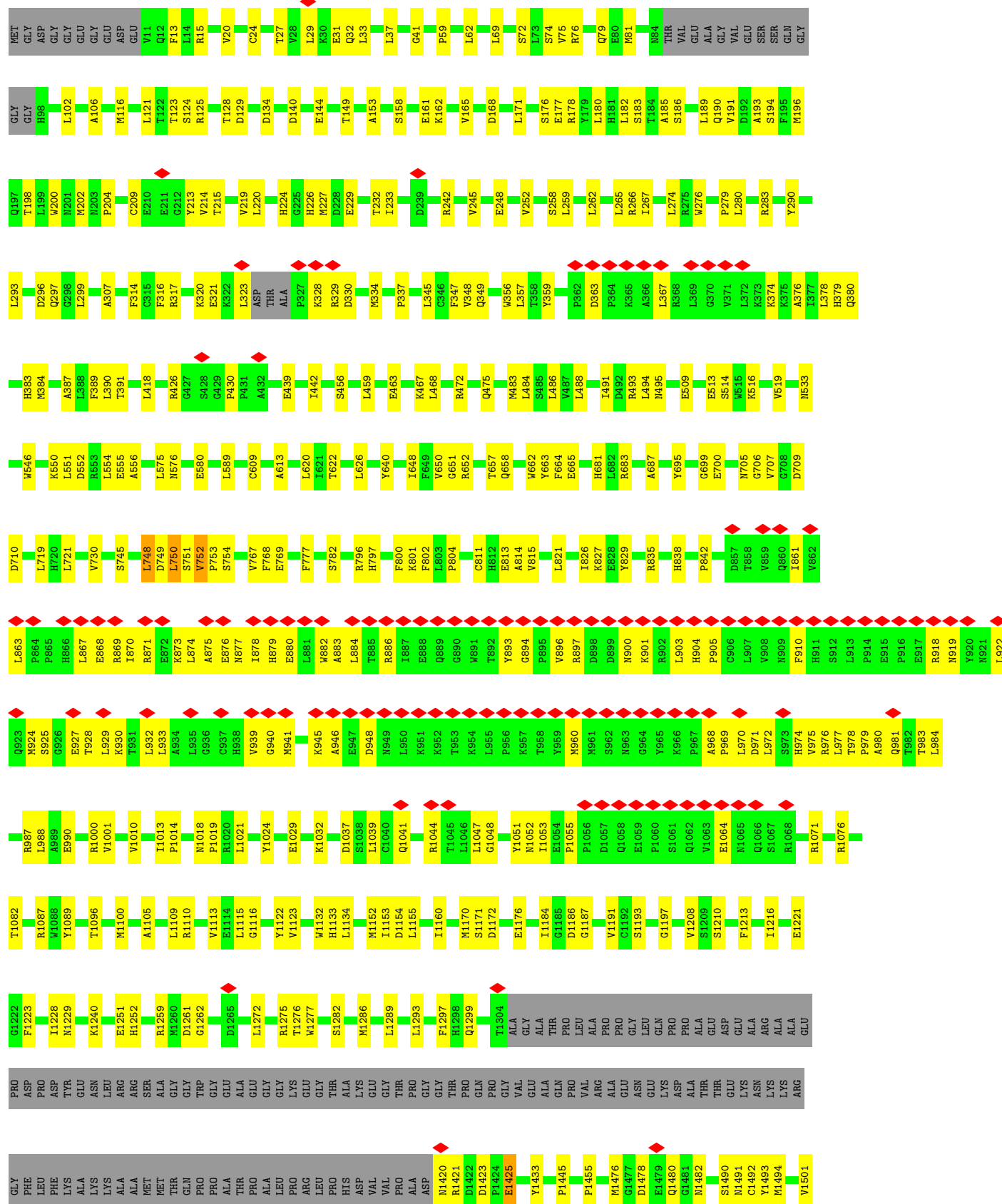
MET	L198	L199	L200	L201	L202	L203	L204	L205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1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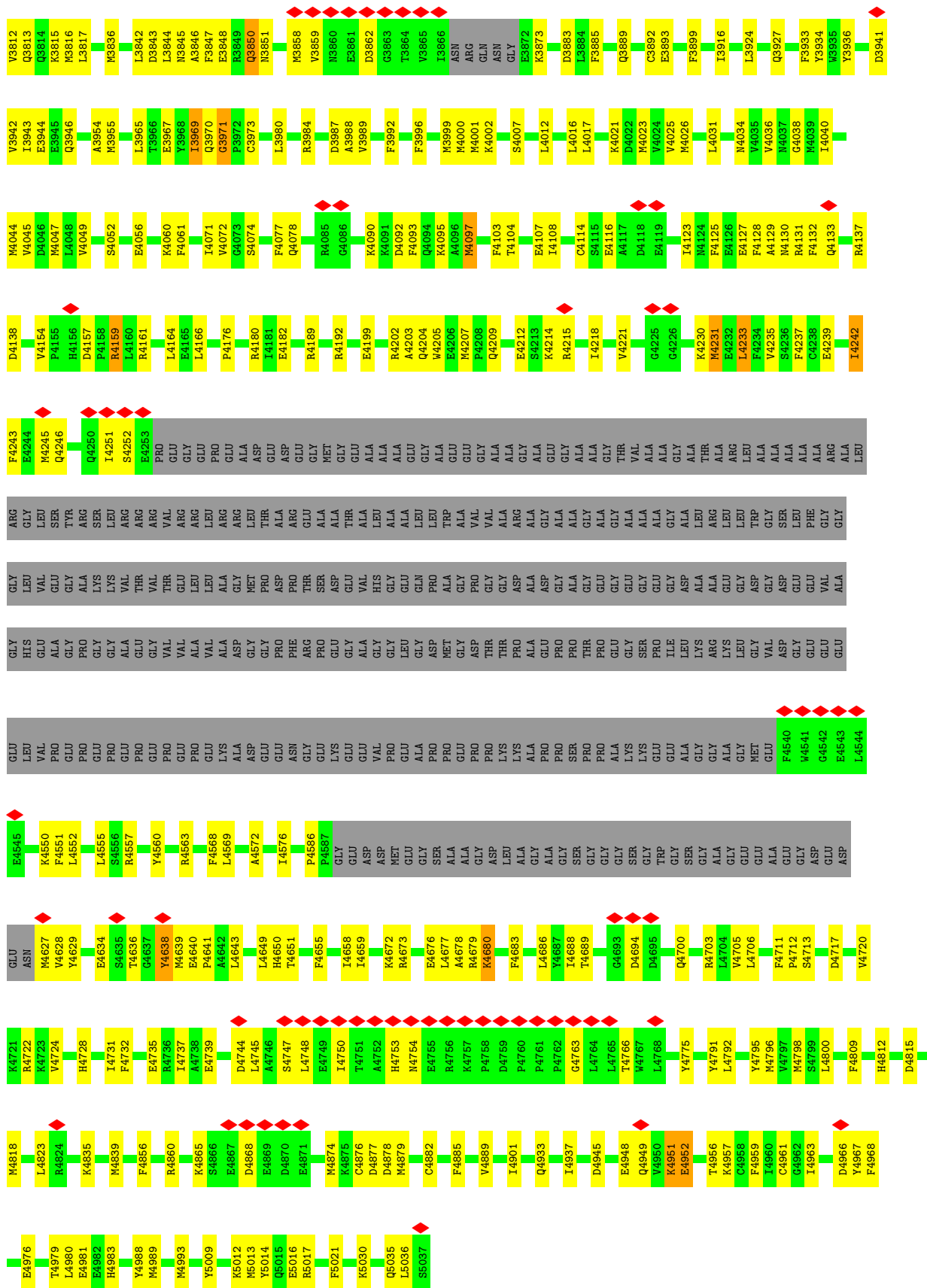


Chain B:



R2738	T2667	R2591	L2518	E2439	S2345	I1E	G1925	F1854	A1692	SER
P2739	S2668	L2595	L2519	M2440	V2346	GLY	L1926	F1854	Q1693	PRO
V2740	E2670	L2599	H2521	Q2444	E2347	LEU	L1927	V1859	GLN	GLY
E2741	E2671	Q2599	V2524	E2449	E2348	MET	Q1928	E1699	GLN	GLY
T2742	L2672	E2604	G2525	E2452	N2349	GLU	M1939	E1733	GLY	R1508
L2743	T2675	D2605	G2526	R2453	A2350	GLU	L1943	Y1734	GLY	R1508
N2744	R2676	C2606	F2527	R2458	R2359	PRO	L1943	P1737	GLU	V1520
V2745	L2677	M2608	P2528	I2453	L2377	GLU	C1947	F1748	GLU	G1525
L2746	F2679	M2610	P2529	R2458	E2362	THR	D1948	F1748	GLU	G1525
I2747	L2679	M2613	M2530	P2462	C2363	LEU	N1972	G1751	GLU	L1526
P2748	L2680	L2614	R2531	D2465	R2369	SER	Q1973	ARG	GLU	M1527
E2749	L2682	R2615	L2536	D2465	L2377	SER	Q1974	GLY	GLU	F1549
L2750	L2686	M2618	T2537	L2466	L2377	SER	R1976	GLY	GLU	F1553
L2751	L2619	T2538	T2538	L2466	L2377	ARG	R1976	GLY	GLU	F1553
D2752	L2620	A2539	L2380	V2467	L2380	LEU	M1981	ALA	GLU	Q1559
S2753	H2621	T2540	E2381	G2468	E2381	SER	R1982	ALA	GLU	Q1559
F2754	L2622	F2541	F2541	I2469	E2382	LEU	A1983	R1768	GLU	N1560
L2755	L2623	S2542	S2542	L2470	A2383	LEU	F1984	V1561	GLU	V1561
F2756	L2623	L2623	L2623	L2471	I2384	LEU	T1985	H1760	GLU	I1562
N2757	Y2696	R2624	F2545	L2472	R2385	THR	M1985	L1771	GLU	A1578
N2758	R2697	R2625	M2546	P2473	I2386	VAL	M1986	GLU	GLU	A1578
K2757	M2698	L2626	A2547	L2474	G2394	ARG	S1987	GLU	GLU	C1591
F2758	L2627	V2627	L2551	Q2475	P2395	ARG	A1988	ASP	GLU	C1591
A2759	F2628	V2627	R2552	I2476	G2395	LEU	F1782	GLU	GLU	R1594
E2760	V2630	V2630	Y2553	L2476	GLY	VAL	V1783	GLU	GLU	L1595
Y2761	N2634	E2635	L2554	L2479	ARG	LYS	R1993	LYS	GLU	R1607
T2762	E2636	F2636	C2555	G2480	ASP	LYS	R1994	GLU	GLU	M1608
H2763	L2637	L2637	L2556	K2481	ASP	GLU	T1995	GLU	GLU	R1607
E2764	K2638	M2639	L2559	D2482	ARG	GLU	R1996	ALA	GLU	R1619
K2765	P2646	L2641	L2562	L2485	ARG	GLU	E1997	GLY	GLU	L1634
W2766	L2642	L2642	T2563	L2485	GLU	THR	Q2003	VAL	GLU	L1634
A2767	L2643	T2645	A2566	P2488	HIS	GLY	I2006	ALA	GLU	M1637
F2768	L2644	L2645	P2567	K2489	GLY	LYS	L2009	ALA	GLU	A1638
D2769	L2645	T2645	L2568	M2490	GLU	LYS	L2009	GLU	GLU	A1638
K2770	L2646	N2646	F2569	F2494	PRO	ALA	L2009	GLU	GLU	I1641
I2771	L2647	N2646	A2570	V2495	PRO	GLU	D2014	ASP	GLU	C1647
Q2772	Y2648	Y2648	E2573	P2496	GLU	GLU	E2015	GLU	GLU	M1648
N2773	E2649	H2498	H2574	D2497	N2414	LYS	D2015	GLU	GLU	M1648
N2774	R2650	K2499	R2575	H2498	N2324	LYS	E2016	GLU	GLU	D1649
W2775	C2651	A2500	L2575	A2500	P2325	LYS	A2016	GLU	GLU	L1650
S2776	K2652	M2501	V2578	S2501	C2326	LYS	E2019	GLU	GLU	E1652
Y2777	L2653	M2502	V2579	M2502	G2327	LYS	P2022	GLU	GLU	L1653
G2778	Y2654	L2506	L2579	L2506	G2328	LYS	L2023	ALA	GLU	S1654
E2779	Y2655	L2507	M2582	D2507	E2329	LYS	P2024	PRO	GLU	E1655
N2780	C2656	R2508	H2584	R2508	R2330	LYS	I2027	GLY	GLU	Q1660
V2781	L2657	V2509	T2585	V2509	Y2331	LYS	R2028	GLY	GLU	L1676
D2782	L2657	V2509	L2429	L2429	L2332	LYS	Q2029	GLY	GLU	A1826
E2783	G2660	E2513	D2431	D2431	E2333	LYS	D2030	GLY	GLU	R1827
E2784	W2661	M2514	R2435	R2435	F2334	LYS	L2031	GLY	GLU	D1828
L2785	F2664	S2515	C2436	C2436	P2337	LYS	Q2032	GLY	GLU	V1689
K2786	F2735	F2735	L2589	L2589	A2338	LYS	D2033	GLY	GLU	P1829
T2787	D2736	D2736	L2590	L2590	GLY	LYS	I2044	GLY	GLU	Q1691
H2788	F2737	F2737	L2590	L2590	GLY	LYS	I2044	GLY	GLU	Q1691
P2789	F2737	F2737	L2590	L2590	GLY	LYS	I2044	GLY	GLU	Q1691
M2790	F2737	F2737	L2590	L2590	GLY	LYS	I2044	GLY	GLU	Q1691
L2791	F2737	F2737	L2590	L2590	GLY	LYS	I2044	GLY	GLU	Q1691
R2792	F2737	F2737	L2590	L2590	GLY	LYS	I2044	GLY	GLU	Q1691
P2793	F2737	F2737	L2590	L2590	GLY	LYS	I2044	GLY	GLU	Q1691
Y2794	F2737	F2737	L2590	L2590	GLY	LYS	I2044	GLY	GLU	Q1691
K2795	F2737	F2737	L2590	L2590	GLY	LYS	I2044	GLY	GLU	Q1691
T2796	F2737	F2737	L2590	L2590	GLY	LYS	I2044	GLY	GLU	Q1691
F2797	F2737	F2737	L2590	L2590	GLY	LYS	I2044	GLY	GLU	Q1691

S2798	Q2868	R2918	G2984	D3060	L3143	T3221	P3297	L3381	E3455	T3520	R3595	K3694
E2799	P2859	D2919	G2985	A3061	F3144	K3222	A3298	E3382	Q3456	G3521	V3596	P3695
K2800	P2860	R2920	V2986	V3064	Q3145	S3223	G3299	A3383	M3457	L3522	Q3597	H3699
D2801	D2861	E2921	E2987	C3067	I3147	P3224	A3300	K3384	F3458	N3523	K3598	H3699
K2802	L2862	E2922	V2988	C3068	I3148	R3225	A3301	K3385	V3459	M3524	V3599	L3701
E2803	S2863	A2923	S2989	H3069	Q3149	E3226	P3301	A3386	V3460	C3525	V3602	F3705
T2804	G2864	Q2924	P2990	L3070	H3150	R3227	T3305	E3387	Q3461	D3529	L3603	A3709
Y2805	V2865	E2925	H2991	L3071	Q3151	I3229	T3309	E3388	E3463	D3530	K3604	E3607
R2806	T2866	L2926	E2992	D3076	F3152	L3230	S3309	E3389	I3464	D3531	E3611	K3715
W2807	L2867	L2927	Q2993	D3077	D3155	G3231	L3312	E3390	N3465	K3532	K3612	E3718
P2808	S2868	K2928	I2994	R3078	I3156	L3232	M3313	E3391	N3466	L3533	P3613	K3723
T2809	R2869	F2929	K2996	T3079	I3157	P3233	N3318	E3392	K3467	K3534	K3614	K3725
K2810	E2870	L2930	F2997	V3080	D3158	S3235	L3319	L3392	S3468	K3537	S3615	A3729
E2811	R2871	Q2931	F2998	M3081	Q3160	V3236	L3320	V3394	F3469	A3541	L3616	K3729
S2812	L2871	M3082	A2999	P3085	V3161	E3237	I3321	R3395	L3470	L3542	L3617	L3735
L2813	Q2872	M2932	K3000	P3088	Q3162	E3238	I3322	D3396	ALA	K3543	ALA	L3735
K2814	A2873	M2933	L3001	V3088	I3166	E3239	V3324	E3397	ASP	T3544	VAL	L3735
A2815	M2874	Q2934	L3002	K3089	F3167	C3240	N3325	S3399	SER	D3545	TRP	L3735
M2816	A2875	Y2935	P3004	L3092	T3168	I3243	N3326	V3401	LYS	T3546	HIS	L3735
T2817	E2876	A2936	L3005	L3092	L3169	V3245	L3327	C3402	SER	E3547	LEU	L3735
W2819	Q2877	V2937	K3007	A3099	I3172	G3328	I3329	R4003	MET	E3548	GLY	L3735
E2820	L2878	T2938	Q3008	S3100	Q3173	L3246	D3330	R4004	ALA	V3549	ASN	L3735
W2821	E2880	L3015	C3014	E3104	S3174	R3248	E3331	L3405	LYS	E3551	LYS	L3735
T2822	N2881	L3016	Y3016	M3106	Q3176	M3250	A3332	Y3409	GLY	F3552	ALA	L3735
T2823	Y2882	L3016	A3022	V3107	T3177	I3253	V3334	L3412	ASP	Q3554	ASP	L3735
E2824	H2883	GLU	K3023	F3107	Y3182	G3260	I3345	R3414	GLN	N3555	GLN	L3735
K2825	N2884	LEU	V3024	N3108	K3185	A2861	T3346	Y3415	SER	L3556	SER	L3735
E2826	T2885	ASP	L3110	R3111	L3186	R3262	S3347	D3417	GLY	L3557	GLY	L3735
R2827	W2886	THR	G3026	L3112	P3188	P3267	G3348	N3418	ASP	Q3560	ASP	L3735
E2828	S2949	LYS	S3027	G3113	G3193	H3268	A3349	R3420	GLN	V3563	GLN	L3735
Q2829	T2951	L2951	N3033	VAL	L3194	V3269	R3350	R3425	ARG	E3564	ARG	L3735
E2830	E2952	K2953	K3034	GLN	L3197	I3270	H3357	T3425	THR	P3567	THR	L3735
GLU	K2890	K2953	E3035	ALA	A3198	E3271	T3361	E3426	LYS	K3570	LYS	L3735
GLU	Q2892	F2959	E3036	ARG	A3199	T3272	T3362	P3427	LYS	L3570	LYS	L3735
THR	E2893	Q2961	E3037	THR	A3199	L3274	I3363	N3428	ARG	L3575	ARG	L3735
GLU	L2894	L2962	M3038	GLN	A3200	P3275	G3363	E3432	ARG	Y3576	ARG	L3735
LYS	E2895	L2963	T3039	VAL	K3201	M3276	R3364	E3433	ASP	L3579	ASP	L3735
LYS	A2896	L2964	S3041	VAL	P3202	L3277	R3367	M3437	ARG	P3580	ARG	L3735
THR	K2897	R2965	L3042	K3123	V3203	C3278	R3368	F3442	LYS	G3581	LYS	L3735
ARG	G2898	W2966	F3043	Q3124	A3204	G3279	R3369	I3443	LYS	R3582	LYS	L3735
LYS	G2899	K3045	C3044	V3125	F3205	Y3280	G3370	T3444	LYS	E3583	LYS	L3735
ILE	G2900	L2969	L3046	G3126	L3206	L3281	K3371	Y3445	LYS	D3584	LYS	L3735
SER	G2901	T2969	L3046	T3130	E3207	P3282	V3372	W3445	LYS	T3507	LYS	L3735
GLN	T2901	Q2971	L3049	L3136	K3215	R3283	E3375	S3448	LYS	S3508	LYS	L3735
THR	H2902	E2972	V3050	V3139	C3216	Y3284	E3376	H3449	LYS	L3509	LYS	L3735
ALA	P2903	F2973	R3051	T3140	S3217	E3290	E3377	N3450	LYS	I3510	LYS	L3735
GLN	T2904	T2974	H3052	T3141	Y3218	L3296	Q3378	F3451	LYS	V3511	LYS	L3735
THR	L2905	A2975	L3056	T3142	T3219		L3379	K3452	LYS	M3517	LYS	L3735
TYR	V2906	H2976	F3057				R3380	R3453	LYS	K3593	LYS	L3735
ASP	L2977	E2978						E3454	LYS	R3594	LYS	L3735
PRO	P2907								LYS		LYS	L3735
ARG	Y2908								LYS		LYS	L3735
GLU	D2909								LYS		LYS	L3735
GLY	T2910								LYS		LYS	L3735
	L2911								LYS		LYS	L3735
	T2912								LYS		LYS	L3735
	A2913								LYS		LYS	L3735
	E2914								LYS		LYS	L3735
	K2915								LYS		LYS	L3735
	K2916								LYS		LYS	L3735
	A2917								LYS		LYS	L3735

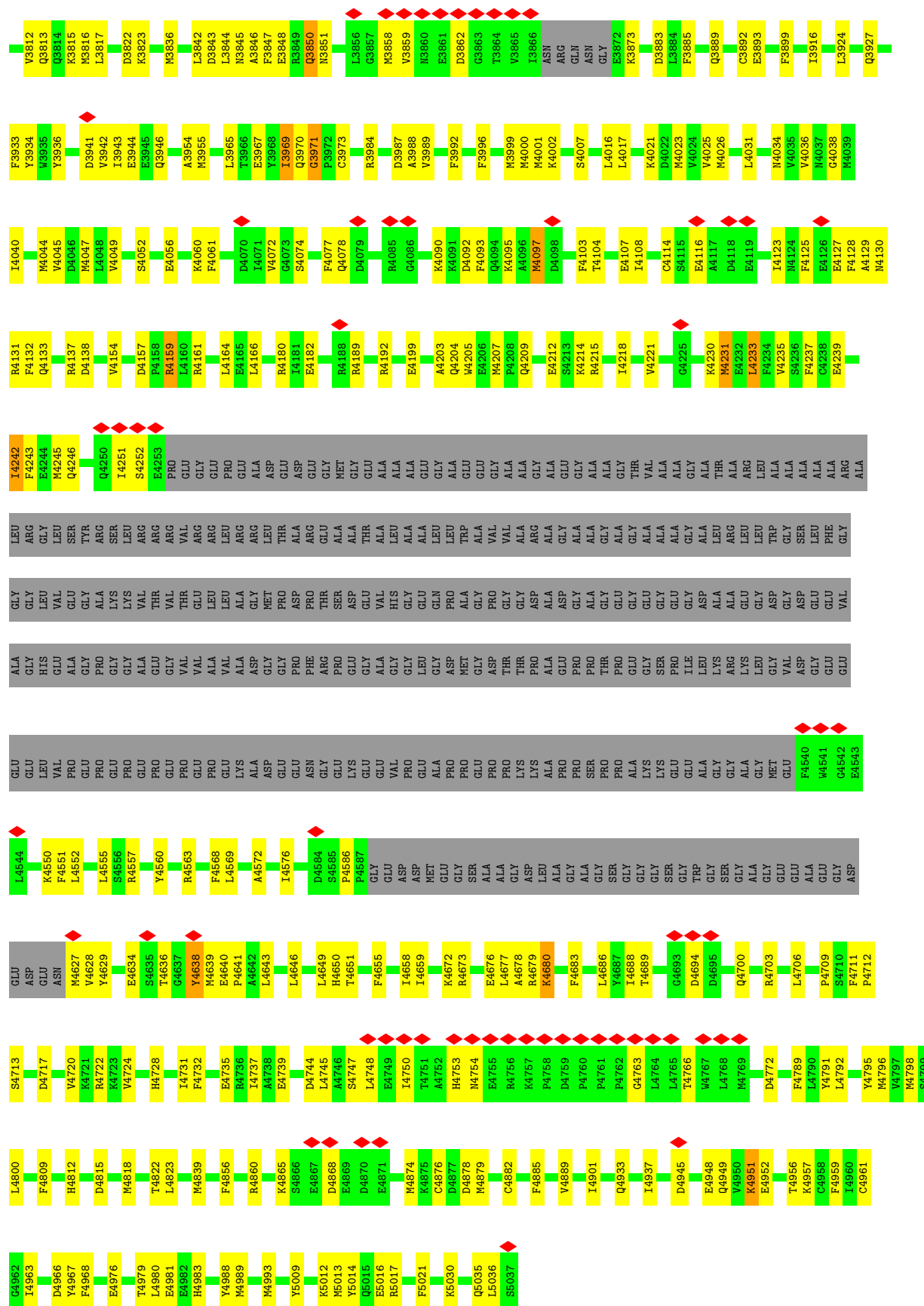


- Molecule 2: Ryanodine receptor 1



P2739	S2668	R2591	L2519	E2439	E2348	RET	R2136	GLU	L1943	T1872	Y1734	Y1520
V2740	E2669	L2595	H2520	M2440	D2349	Q2268	A2137	GLU	C1947	GLU	P1737	G1525
E2741	E2670	L2595	V2521	Q2444	A2350	G2269	L2155	PRO	D1948	GLU	F1748	L1526
L2742	L2672	Q2599	V2524	Q2444	R2359	L2273	L2165	GLU	N1972	GLU	G1751	M1527
L2743	T2675	E2604	G2525	E2449	R2359	A2277	L2166	THR	Q1974	GLU	ARG	F1549
N2744	R2676	D2605	F2526	R2452	E2362	L2278	L2167	GLU	S1976	GLU	GLY	F1559
V2745	R2677	R2528	L2527	I2453	C2363	S2279	Q2169	LEU	R1759	GLU	LYS	F1553
I2746	L2678	L2607	D2529	R2458	R2369	N2283	Q2169	SER	S1976	GLU	GLY	Q1559
I2747	F2679	M2608	M2530	R2458	R2369	N2283	M2178	ARG	M1981	GLU	ASN	N1560
L2748	M2680	R2531	R2531	R2458	I2386	K2297	M2178	ARG	M1981	GLU	ALA	V1561
P2749	G2681	Y2613	S2535	P2462	L2377	L2286	T2185	ARG	R1982	GLU	ALA	V1561
E2749	I2682	I2614	L2536	D2465	I2380	L2290	T2185	ARG	R1982	GLU	ALA	I1562
K2750	L2686	R2615	L2536	L2466	E2381	Q2291	M2186	SER	F1984	GLU	H1760	A1578
L2751	L2686	R2615	D2537	E2467	E2382	Y2191	F2191	LEU	F1984	GLU	H1760	A1578
D2752	D2682	M2618	T2538	Q2468	A2383	D2294	F2191	LEU	T1985	GLU	L1771	C1591
S2753	Q2693	D2670	A2539	I2469	I2384	L2295	M2198	THR	M1986	GLU	S1778	R1594
F2754	E2694	H2621	T2540	I2470	I2384	L2295	M2198	THR	S1987	GLU	S1778	R1594
I2755	L2695	L2622	F2541	I2470	R2385	E2296	M2198	VAL	A1988	ASP	C1781	L1595
N2756	Y2696	L2623	S2542	S2471	I2386	K2297	L2201	ARG	A1988	GLU	F1782	R1607
N2757	R2697	R2624	E2545	P2473	G2394	Y2301	M2203	VAL	E1990	GLU	V1783	M1608
R2758	M2698	R2625	M2546	Q2475	P2395	L2302	M2203	LYS	T1991	LYS	L1786	R1619
A2759	A2699	V2627	A2547	I2476	GLY	L2302	T2206	LYS	A1992	GLU	PRO	R1619
Z2760	H2700	F2628	N2551	L2479	VAL	C2305	G2207	GLU	R1993	GLU	ALA	L1634
P2761	C2702	D2629	R2552	Q2480	ARG	G2306	M2208	GLU	R1994	ASP	ALA	L1634
Y2761	V2630	V2630	Y2553	K2481	ASP	Q2308	V2212	LYS	T1995	GLU	GLY	M1637
T2762	D2634	D2634	C2555	D2482	ARG	S2309	V2212	PRO	R1996	GLU	VAL	A1638
H2763	E2635	E2635	L2559	L2485	ARG	P2311	G2216	GLU	E1997	GLU	ALA	T1641
E2764	F2636	F2636	L2562	A2484	GLU	M2312	GLY	GLU	Q2003	GLU	GLU	T1641
K2765	A2637	A2637	T2563	L2488	GLU	L2314	T2223	LYS	I2006	LYS	A1794	C1647
Y2766	M2638	M2638	T2563	P2488	GLU	A2315	M2228	PRO	N2007	GLU	R1808	M1648
A2767	P2640	P2640	T2563	M2490	PRO	K2316	M2228	ALA	D1809	ASP	D1808	D1649
F2768	L2641	L2641	A2566	F2494	GLU	P2319	C2237	LYS	L2009	GLU	K1810	I1650
D2769	K2642	K2642	P2567	V2495	GLU	D2320	C2237	LYS	A2016	GLU	R1813	L1651
K2770	L2643	L2643	L2568	P2496	GLU	T2321	C2237	GLU	E2019	GLU	M1814	L1653
L2771	T2645	T2645	F2569	D2497	GLU	G2322	C2237	GLU	E2019	GLU	E1817	L1654
Q2772	Y2648	Y2648	E2570	P2496	N2414	G2322	C2237	GLU	E2019	GLU	E1817	L1654
S2773	E2649	E2649	E2573	D2497	R2415	G2322	C2237	GLU	E2019	GLU	E1817	L1654
N2774	R2650	R2650	H2574	H2498	V2416	G2322	C2237	GLU	E2019	GLU	E1817	L1654
W2775	C2651	C2651	R2575	A2500	H2417	G2322	C2237	GLU	E2019	GLU	E1817	L1654
S2776	W2652	W2652	R2575	S2501	A2421	G2327	C2237	GLU	E2019	GLU	E1817	L1654
Y2777	K2653	K2653	M2578	M2502	I2422	G2328	C2237	GLU	E2019	GLU	E1817	L1654
E2778	Y2654	Y2654	V2579	L2506	M2423	E2329	C2237	GLU	E2019	GLU	E1817	L1654
G2779	Y2655	Y2655	D2580	D2507	L2429	R2330	C2237	GLU	E2019	GLU	E1817	L1654
N2780	C2656	C2656	S2581	R2508	I2430	Y2331	C2237	GLU	E2019	GLU	E1817	L1654
V2781	L2657	L2657	M2582	V2509	D2431	G2332	C2237	GLU	E2019	GLU	E1817	L1654
D2782	G2660	G2660	L2583	L2433	L2433	D2333	C2237	GLU	E2019	GLU	E1817	L1654
E2783	W2661	W2661	H2584	L2433	L2433	D2333	C2237	GLU	E2019	GLU	E1817	L1654
E2784	W2661	W2661	T2585	G2434	G2434	F2337	C2237	GLU	E2019	GLU	E1817	L1654
L2785	F2664	F2664	Y2587	R2435	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654
K2786	T2667	T2667	R2588	I2514	C2436	K2337	C2237	GLU	E2019	GLU	E1817	L1654
T2787	F2735	F2735	L2589	I2514	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654
H2788	D2736	D2736	S2590	I2514	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654
P2789	R2737	R2737	S2590	I2514	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654
M2790	P2738	P2738	S2590	I2514	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654
L2791	M2790	M2790	S2590	I2514	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654
R2792	L2791	L2791	S2590	I2514	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654
P2793	R2792	R2792	S2590	I2514	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654
Y2794	P2793	P2793	S2590	I2514	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654
K2795	Y2794	Y2794	S2590	I2514	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654
T2796	K2795	K2795	S2590	I2514	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654
T2797	T2796	T2796	S2590	I2514	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654
S2798	F2797	F2797	S2590	I2514	C2436	A2338	C2237	GLU	E2019	GLU	E1817	L1654





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	53882	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.34	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.119	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.121	Depositor
Map size (Å)	425.472, 425.472, 425.472	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.831, 0.831, 0.831	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, CFF, 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	F	1.07	4/834 (0.5%)	0.84	4/1123 (0.4%)
1	H	1.07	4/834 (0.5%)	0.84	4/1123 (0.4%)
1	J	1.07	4/834 (0.5%)	0.84	4/1123 (0.4%)
1	O	1.07	4/834 (0.5%)	0.84	4/1123 (0.4%)
2	A	0.44	10/35070 (0.0%)	0.59	43/47504 (0.1%)
2	B	0.45	10/35070 (0.0%)	0.59	41/47504 (0.1%)
2	G	0.44	10/35070 (0.0%)	0.59	43/47504 (0.1%)
2	I	0.44	10/35070 (0.0%)	0.59	43/47504 (0.1%)
All	All	0.47	56/143616 (0.0%)	0.60	186/194508 (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
2	A	0	1
2	B	0	1
2	G	0	1
2	I	0	1
All	All	0	4

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	752	VAL	CA-C	-11.19	1.42	1.52
2	I	752	VAL	CA-C	-11.11	1.43	1.52
2	G	752	VAL	CA-C	-11.09	1.43	1.52
2	B	752	VAL	CA-C	-11.09	1.43	1.52
2	A	3188	PRO	N-CD	-8.36	1.36	1.47

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	752	VAL	CA-C-N	-25.72	92.21	119.99
2	G	752	VAL	C-N-CA	-25.72	92.21	119.99
2	B	752	VAL	CA-C-N	-25.72	92.21	119.99
2	B	752	VAL	C-N-CA	-25.72	92.21	119.99
2	A	752	VAL	CA-C-N	-25.71	92.23	119.99

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	4638	TYR	Peptide
2	B	4638	TYR	Peptide
2	G	4638	TYR	Peptide
2	I	4638	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	F	818	0	824	36	0
1	H	818	0	824	35	0
1	J	818	0	824	34	0
1	O	818	0	824	36	0
2	A	34293	0	33897	1283	0
2	B	34293	0	33897	1271	0
2	G	34293	0	33897	1282	0
2	I	34293	0	33897	1268	0
3	A	31	0	12	2	0
3	B	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	A	14	0	10	0	0
6	B	14	0	10	0	0
6	G	14	0	10	0	0
6	I	14	0	10	0	0
All	All	140632	0	138972	5189	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 19.

The worst 5 of 5189 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2469:ILE:CG2	2:G:2502:MET:HE1	1.38	1.53
2:I:3989:VAL:HG23	2:I:4023:MET:CE	1.38	1.52
2:B:3989:VAL:HG23	2:B:4023:MET:CE	1.38	1.51
2:B:2469:ILE:CG2	2:B:2502:MET:HE1	1.38	1.50
2:B:3989:VAL:CG2	2:B:4023:MET:HE2	1.42	1.50

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	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	J	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	O	105/108 (97%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	4260/5037 (85%)	4079 (96%)	179 (4%)	2 (0%)	100	100
2	B	4260/5037 (85%)	4078 (96%)	180 (4%)	2 (0%)	100	100
2	G	4260/5037 (85%)	4080 (96%)	178 (4%)	2 (0%)	100	100
2	I	4260/5037 (85%)	4079 (96%)	179 (4%)	2 (0%)	100	100
All	All	17460/20580 (85%)	16720 (96%)	732 (4%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	801	LYS
2	G	801	LYS
2	B	801	LYS
2	I	801	LYS
2	A	3267	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	F	88/89 (99%)	77 (88%)	11 (12%)	4	17
1	H	88/89 (99%)	77 (88%)	11 (12%)	4	17
1	J	88/89 (99%)	77 (88%)	11 (12%)	4	17
1	O	88/89 (99%)	77 (88%)	11 (12%)	4	17
2	A	3738/4276 (87%)	3722 (100%)	16 (0%)	84	82
2	B	3738/4276 (87%)	3721 (100%)	17 (0%)	81	80
2	G	3738/4276 (87%)	3722 (100%)	16 (0%)	84	82
2	I	3738/4276 (87%)	3721 (100%)	17 (0%)	81	80
All	All	15304/17460 (88%)	15194 (99%)	110 (1%)	73	77

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	43	ASN
2	G	4672	LYS
2	I	5016	GLU
2	I	4026	MET
1	O	107	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 160 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	4650	HIS
2	I	2931	GLN
2	B	4973	HIS
2	I	1203	ASN
2	I	3882	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CFF	B	5304	-	15,15,15	1.60	4 (26%)	23,23,23	1.73	7 (30%)
3	ATP	B	5301	-	32,33,33	1.30	5 (15%)	48,52,52	1.74	8 (16%)
6	CFF	G	5304	-	15,15,15	1.58	4 (26%)	23,23,23	1.72	7 (30%)
3	ATP	A	5301	-	32,33,33	1.30	5 (15%)	48,52,52	1.75	8 (16%)
3	ATP	G	5301	-	32,33,33	1.30	5 (15%)	48,52,52	1.75	8 (16%)
3	ATP	I	5301	-	32,33,33	1.30	5 (15%)	48,52,52	1.74	8 (16%)
6	CFF	A	5304	-	15,15,15	1.60	4 (26%)	23,23,23	1.73	7 (30%)
6	CFF	I	5304	-	15,15,15	1.60	4 (26%)	23,23,23	1.74	7 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CFF	B	5304	-	-	-	0/2/2/2
3	ATP	B	5301	-	-	4/22/38/38	0/3/3/3
6	CFF	G	5304	-	-	-	0/2/2/2
3	ATP	A	5301	-	-	4/22/38/38	0/3/3/3
3	ATP	G	5301	-	-	4/22/38/38	0/3/3/3
3	ATP	I	5301	-	-	4/22/38/38	0/3/3/3
6	CFF	A	5304	-	-	-	0/2/2/2
6	CFF	I	5304	-	-	-	0/2/2/2

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	5301	ATP	C5-C4	4.16	1.46	1.39
3	A	5301	ATP	C5-C4	4.15	1.46	1.39
3	G	5301	ATP	C5-C4	4.13	1.46	1.39
3	B	5301	ATP	C5-C4	4.13	1.46	1.39
6	A	5304	CFF	C4-N3	-3.37	1.32	1.38

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5301	ATP	C5-C4-N3	-5.69	118.88	126.72
3	A	5301	ATP	C5-C4-N3	-5.69	118.88	126.72
3	B	5301	ATP	C5-C4-N3	-5.67	118.91	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5301	ATP	C5-C4-N3	-5.65	118.93	126.72
3	A	5301	ATP	N3-C4-N9	4.55	134.91	127.17

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

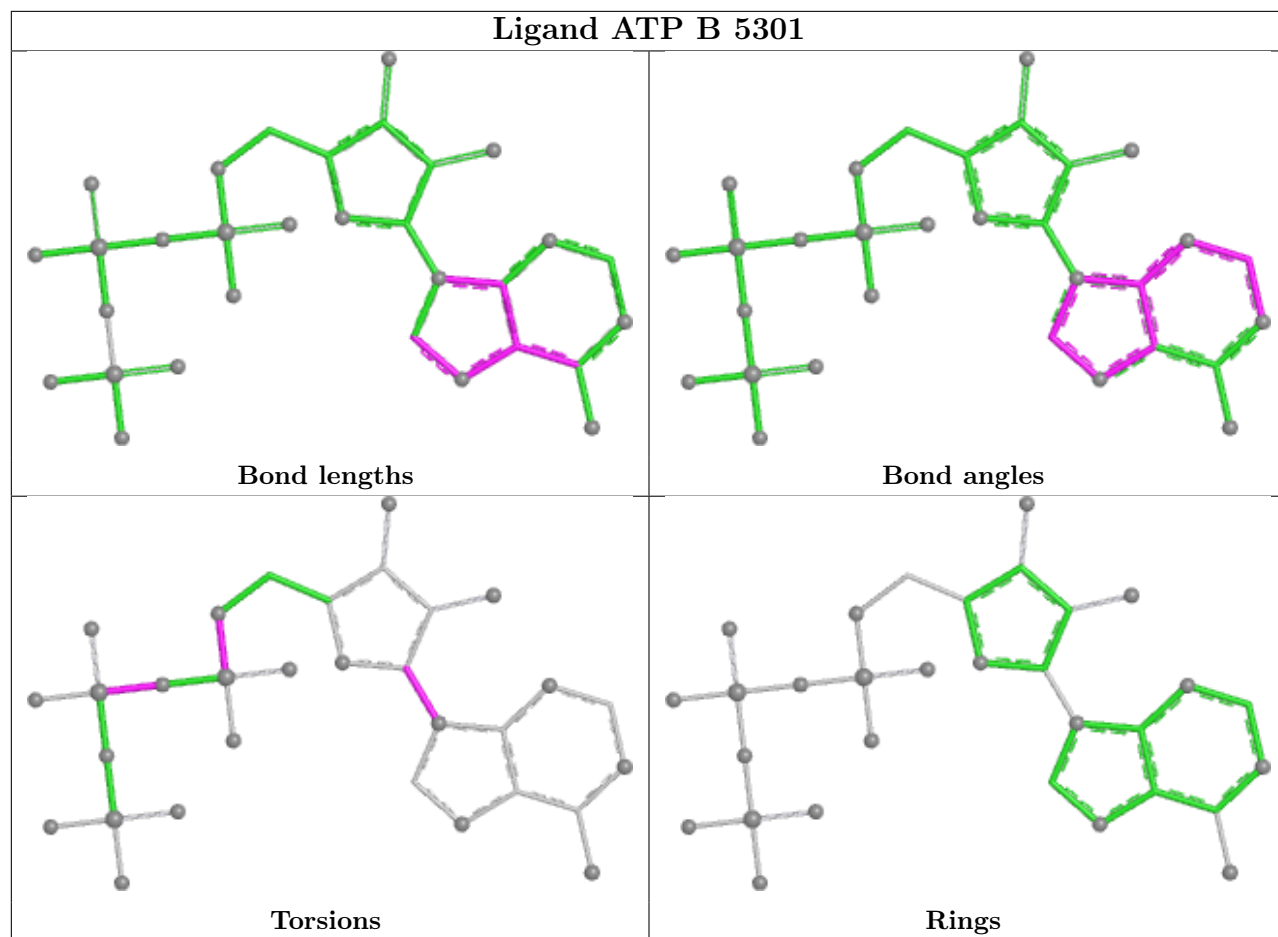
Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O3A
3	G	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	C5'-O5'-PA-O3A
3	I	5301	ATP	C5'-O5'-PA-O3A
3	A	5301	ATP	O4'-C1'-N9-C4

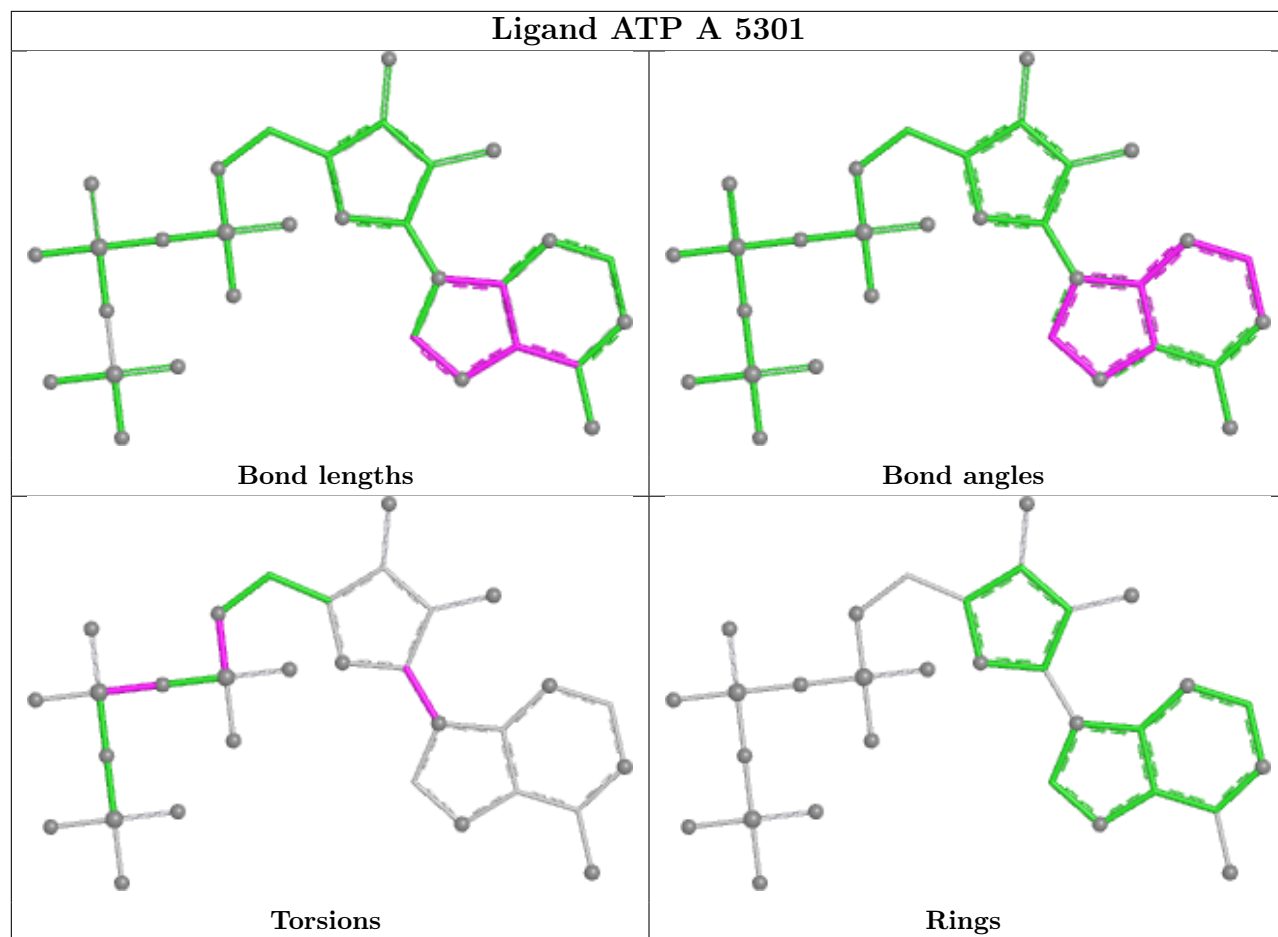
There are no ring outliers.

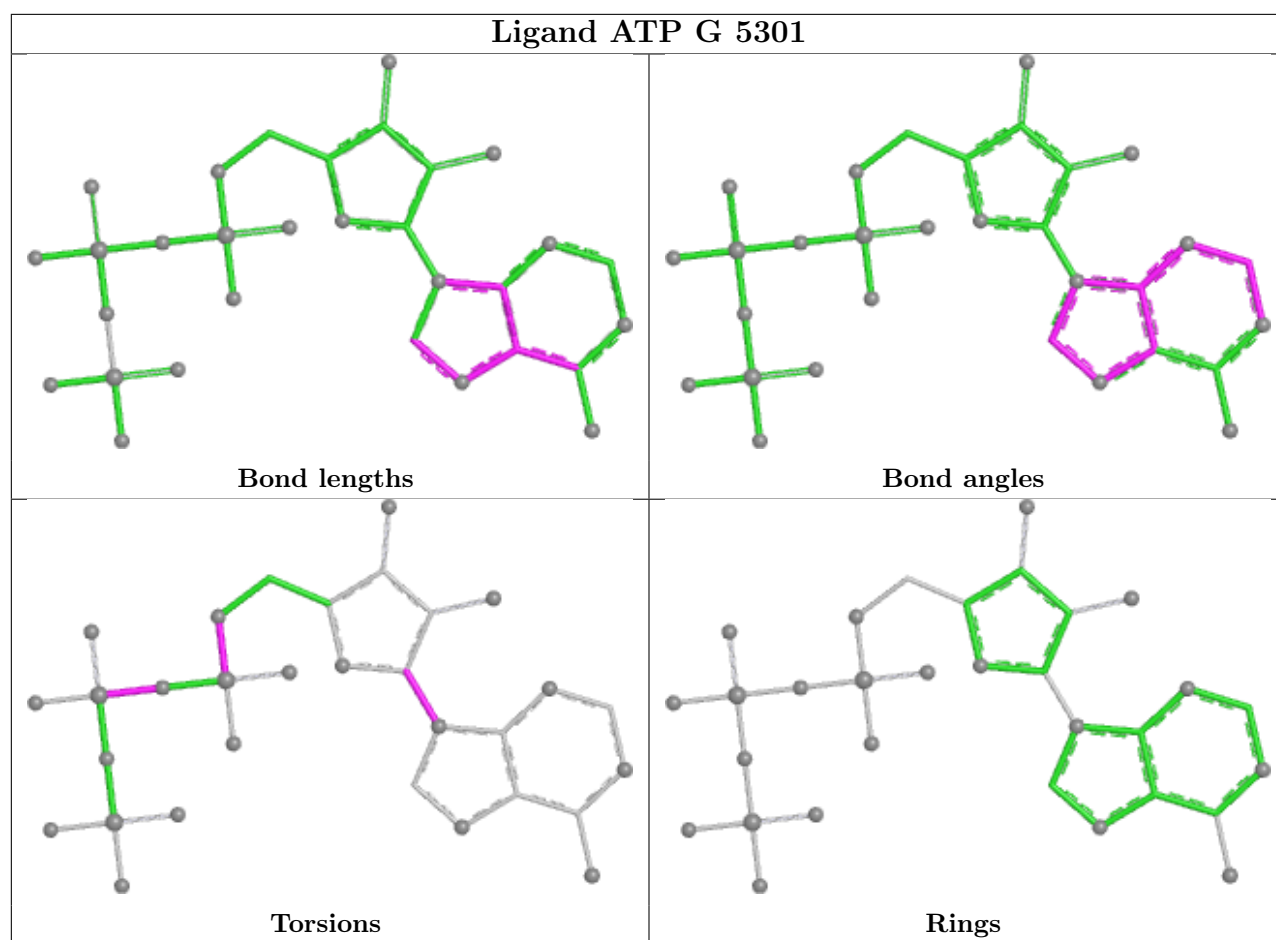
4 monomers are involved in 8 short contacts:

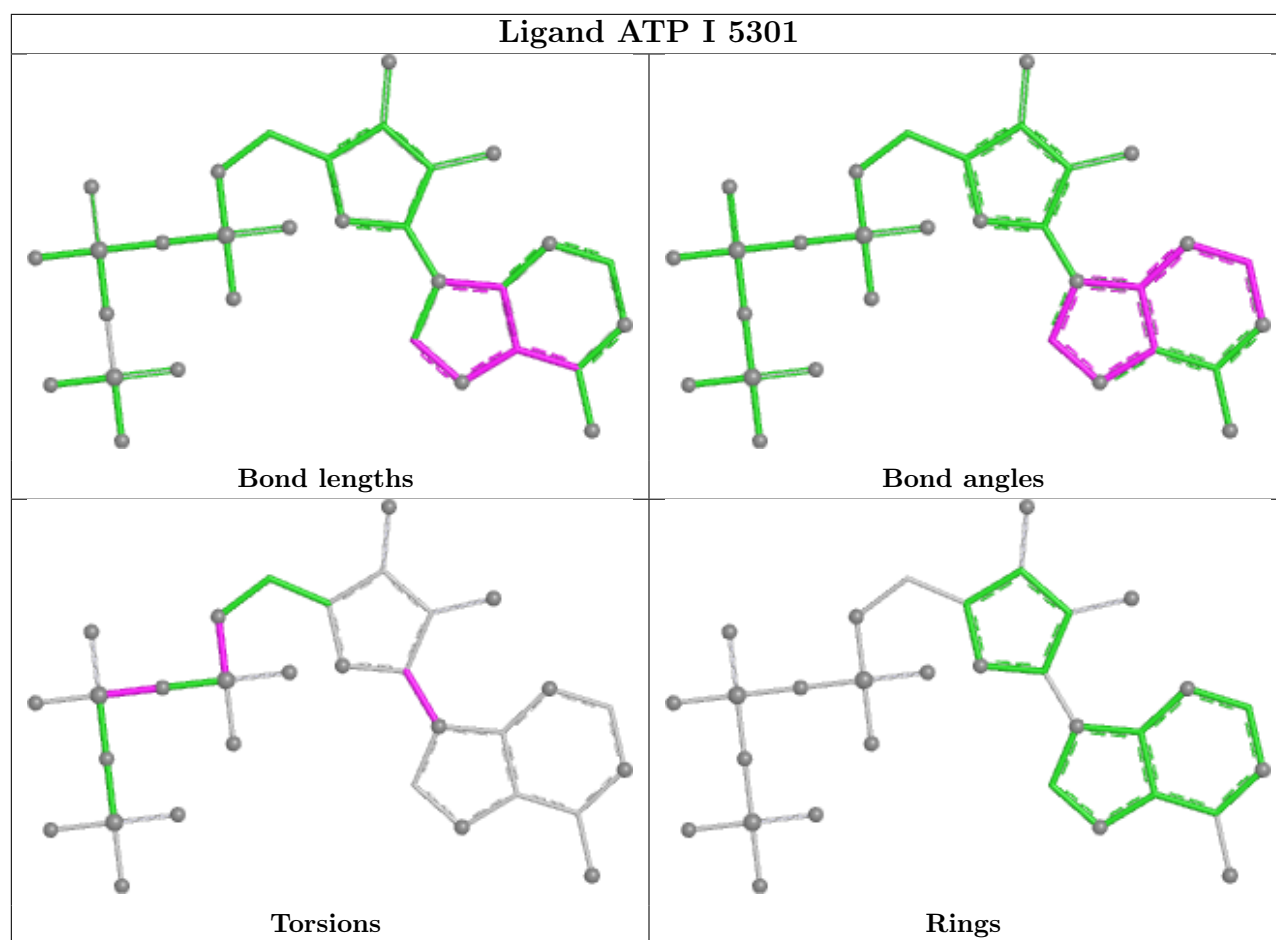
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5301	ATP	2	0
3	A	5301	ATP	2	0
3	G	5301	ATP	2	0
3	I	5301	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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.

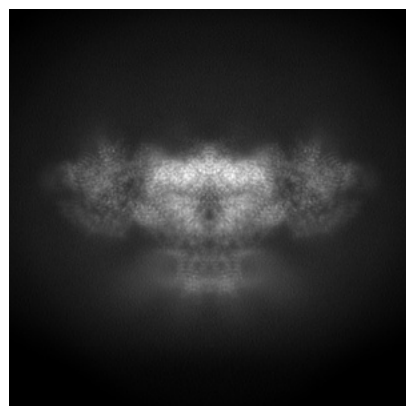
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23692. These allow visual inspection of the internal detail of the map and identification of artifacts.

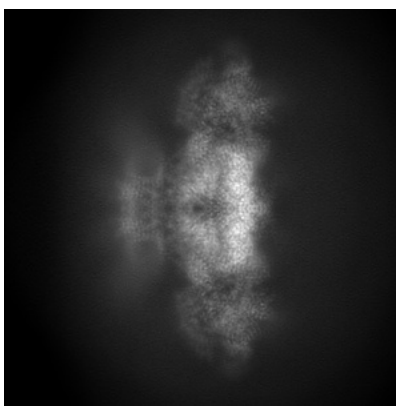
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

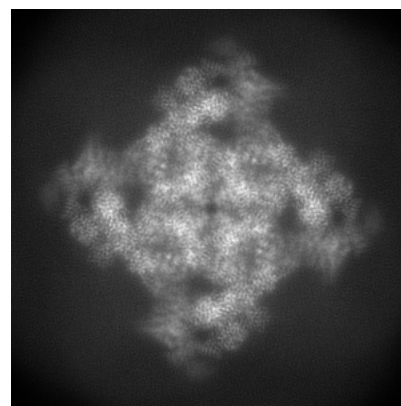
6.1.1 Primary map



X

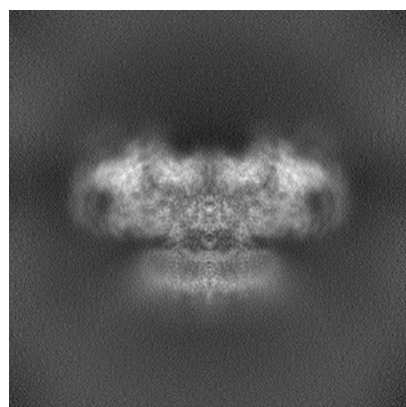


Y

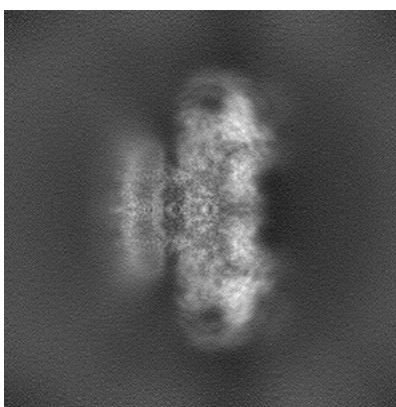


Z

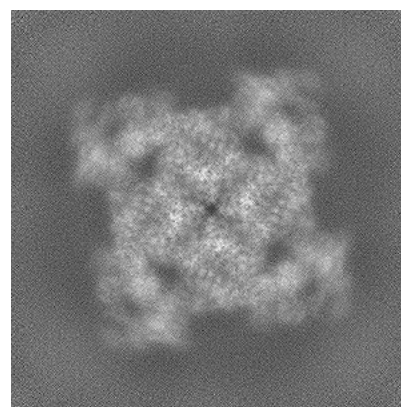
6.1.2 Raw map



X



Y

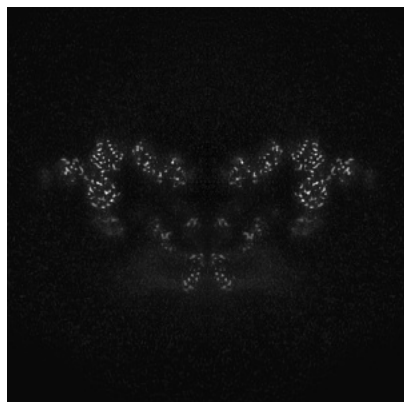


Z

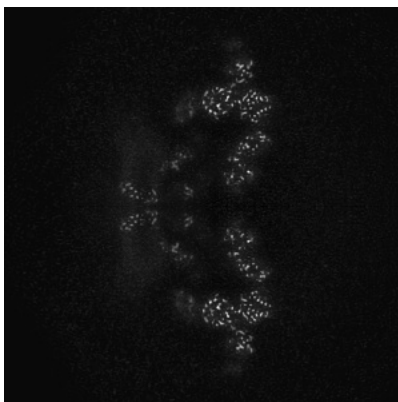
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

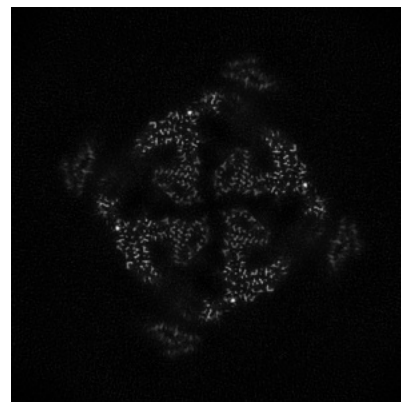
6.2.1 Primary map



X Index: 256

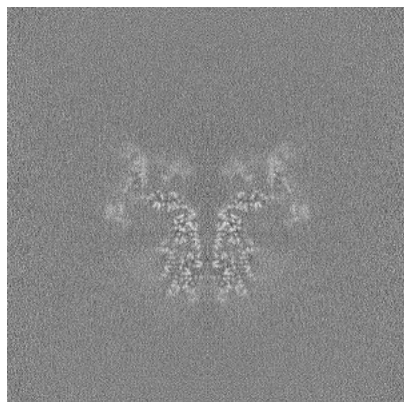


Y Index: 256

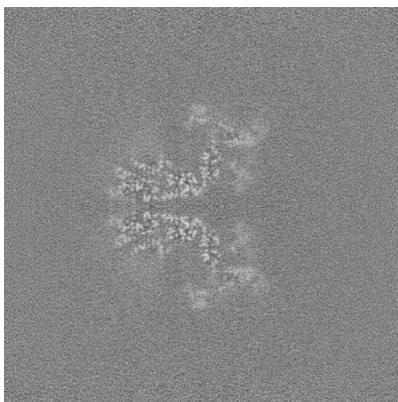


Z Index: 256

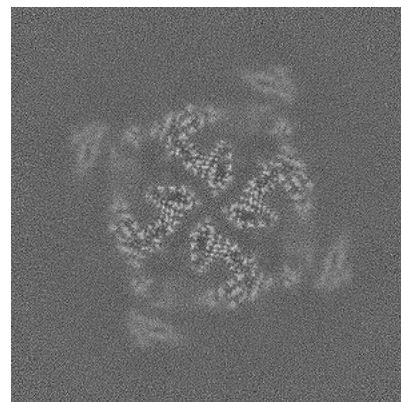
6.2.2 Raw map



X Index: 256



Y Index: 256

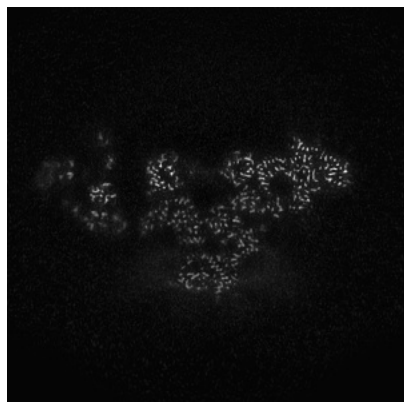


Z Index: 256

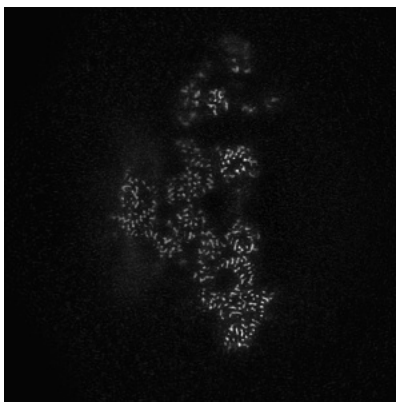
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

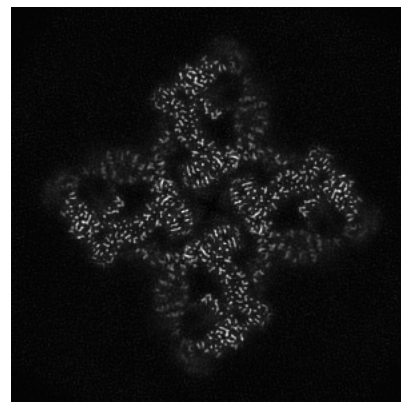
6.3.1 Primary map



X Index: 236

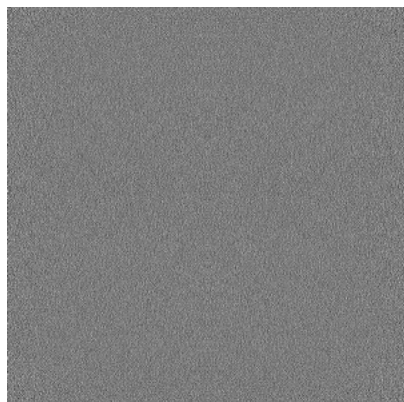


Y Index: 236

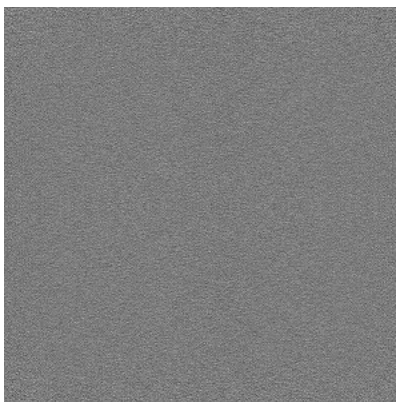


Z Index: 304

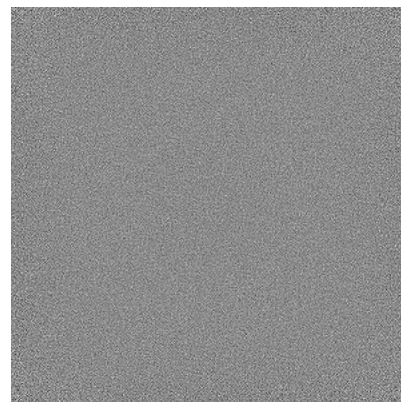
6.3.2 Raw map



X Index: 0



Y Index: 0

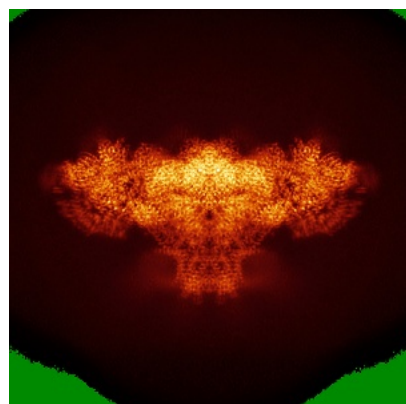


Z Index: 0

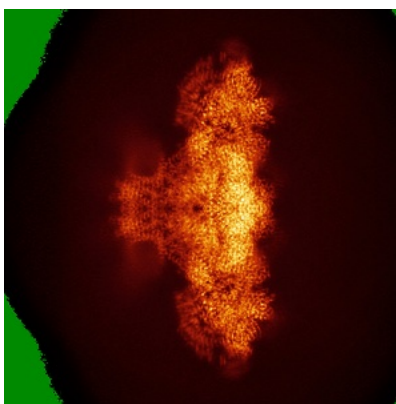
The images above show the largest variance slices of the map in three orthogonal directions.

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

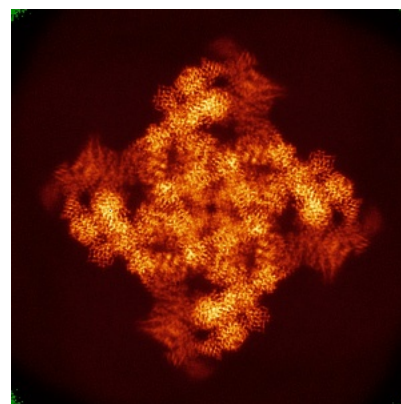
6.4.1 Primary map



X

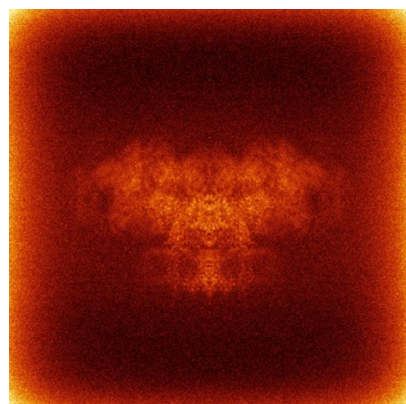


Y

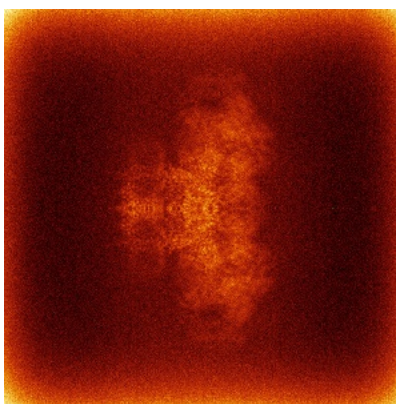


Z

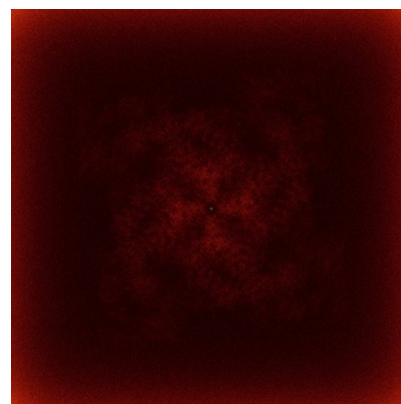
6.4.2 Raw map



X



Y

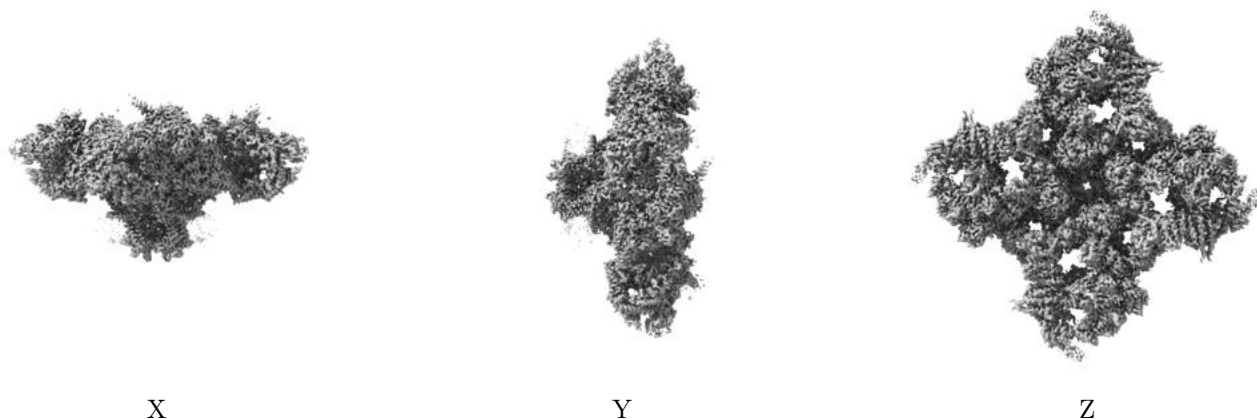


Z

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

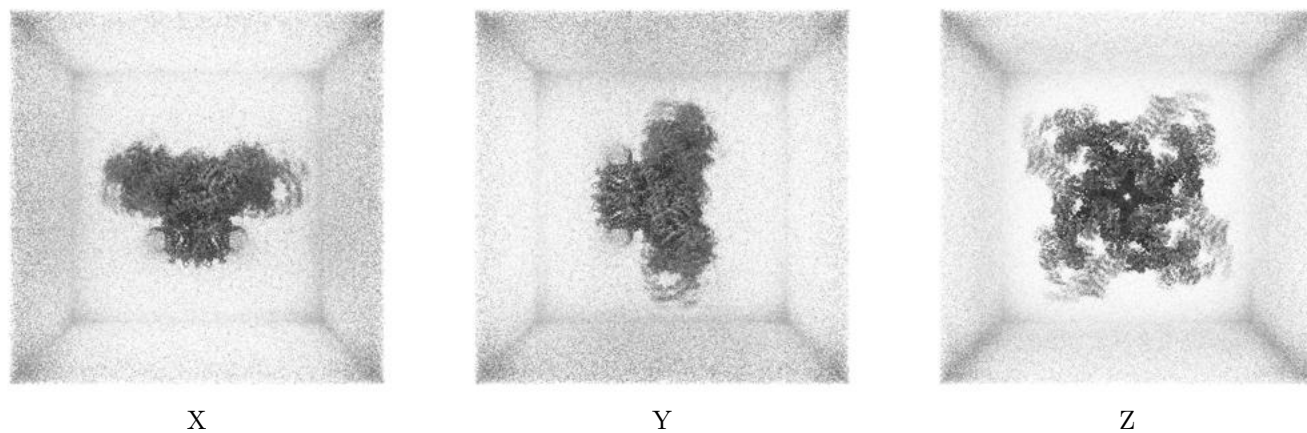
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.121. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

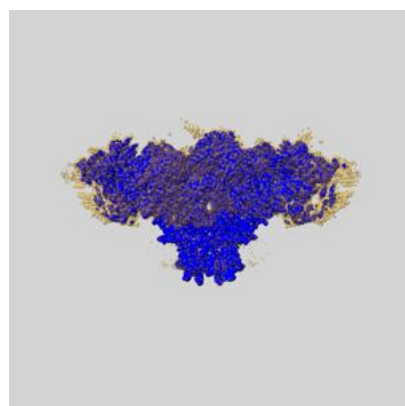
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

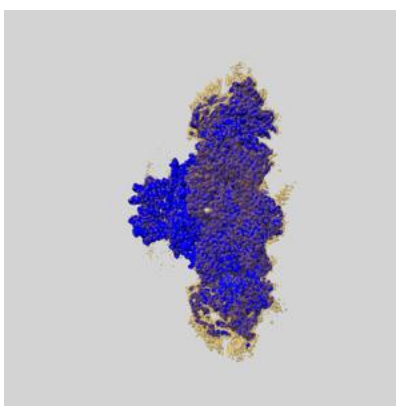
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

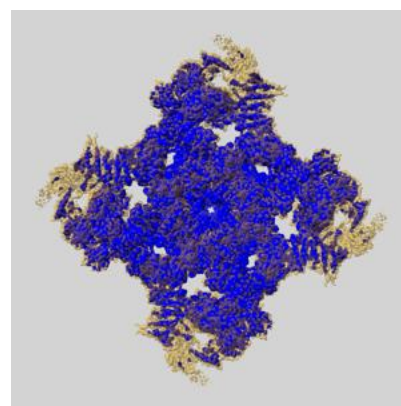
6.6.1 emd_23692_msk_1.map [i](#)



X



Y

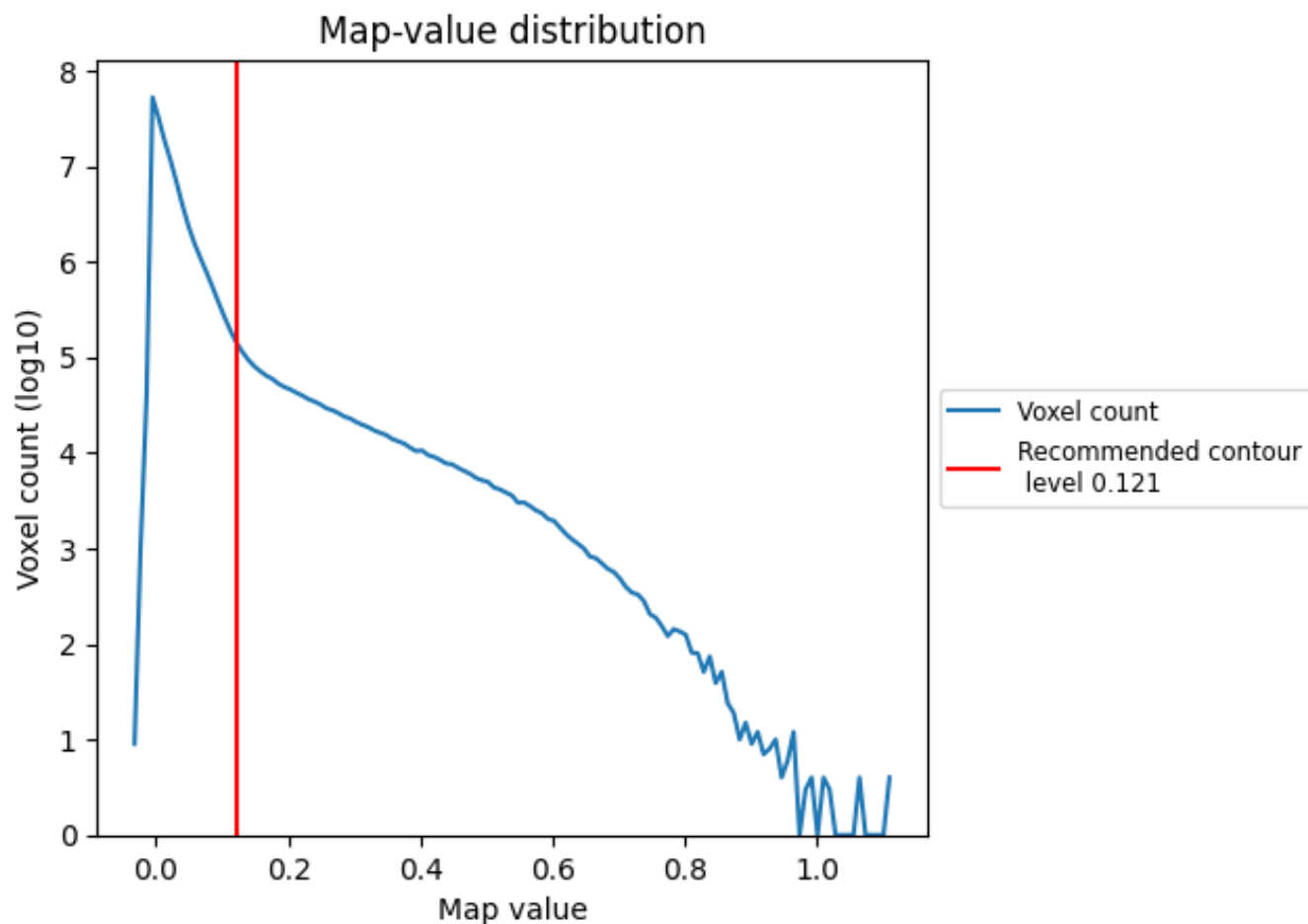


Z

7 Map analysis [i](#)

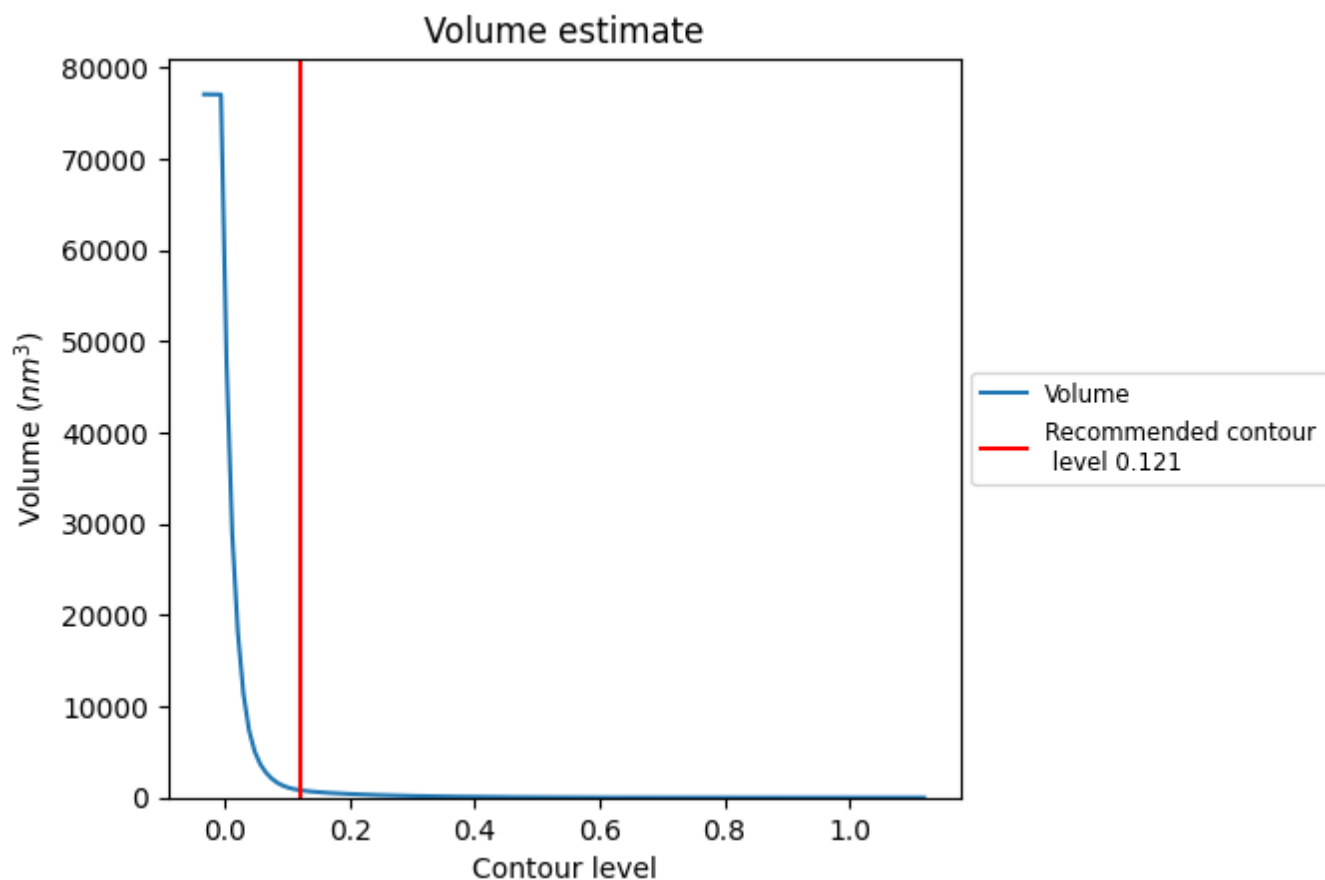
This section contains the results of statistical analysis of the map.

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.

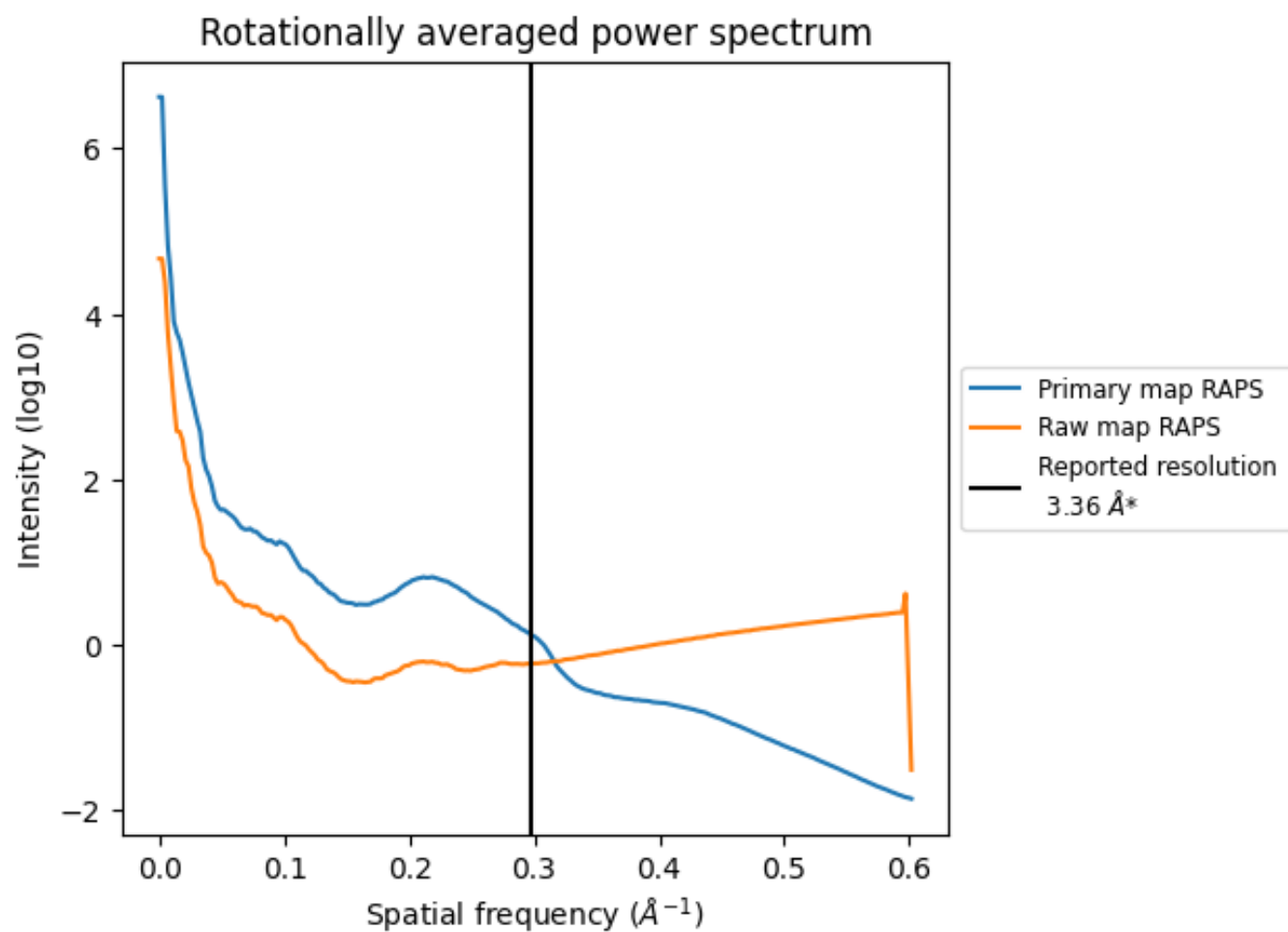
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 808 nm³; this corresponds to an approximate mass of 730 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

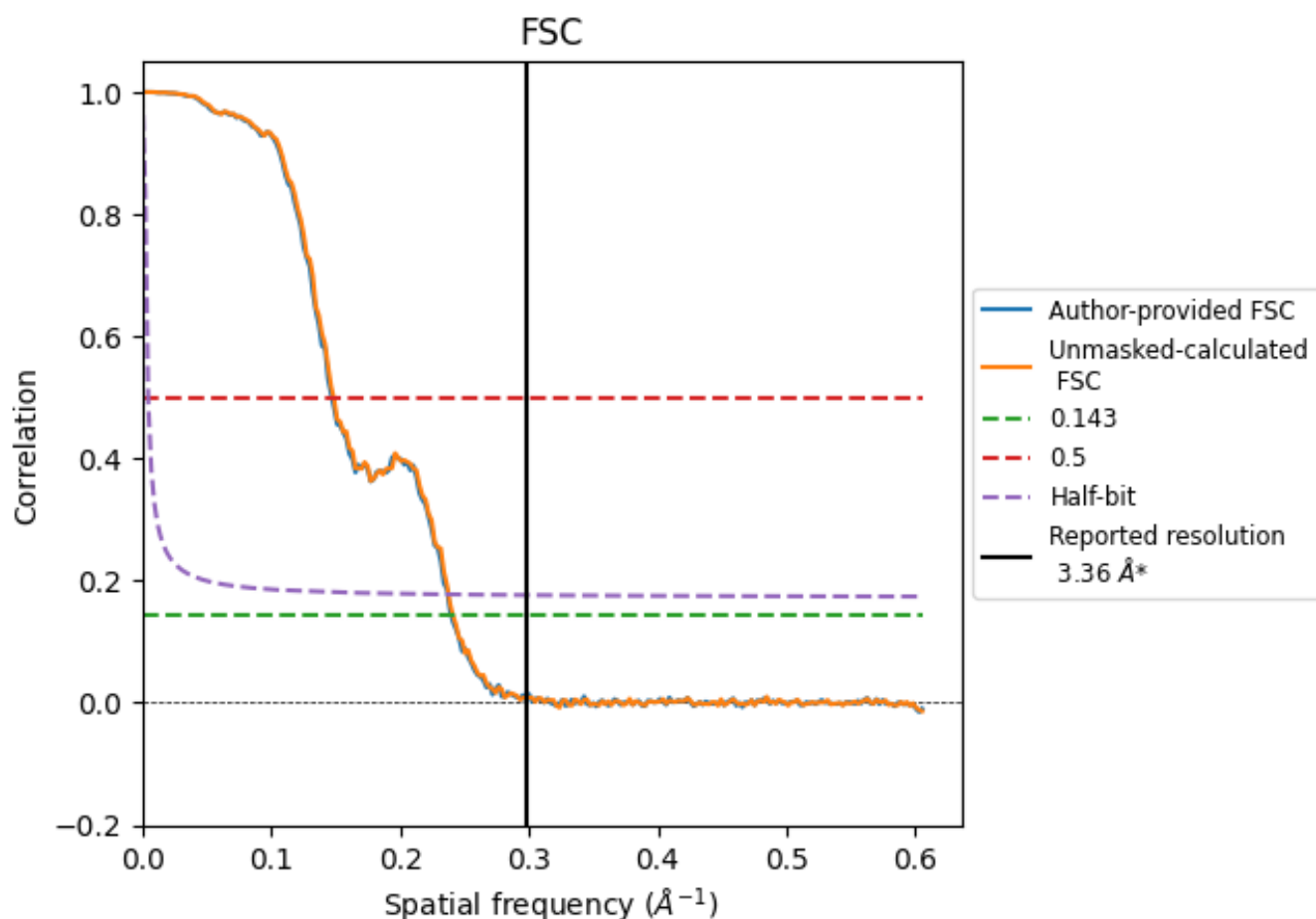


*Reported resolution corresponds to spatial frequency of $0.298 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.298 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	4.17	6.79	4.22
Unmasked-calculated*	4.15	6.73	4.21

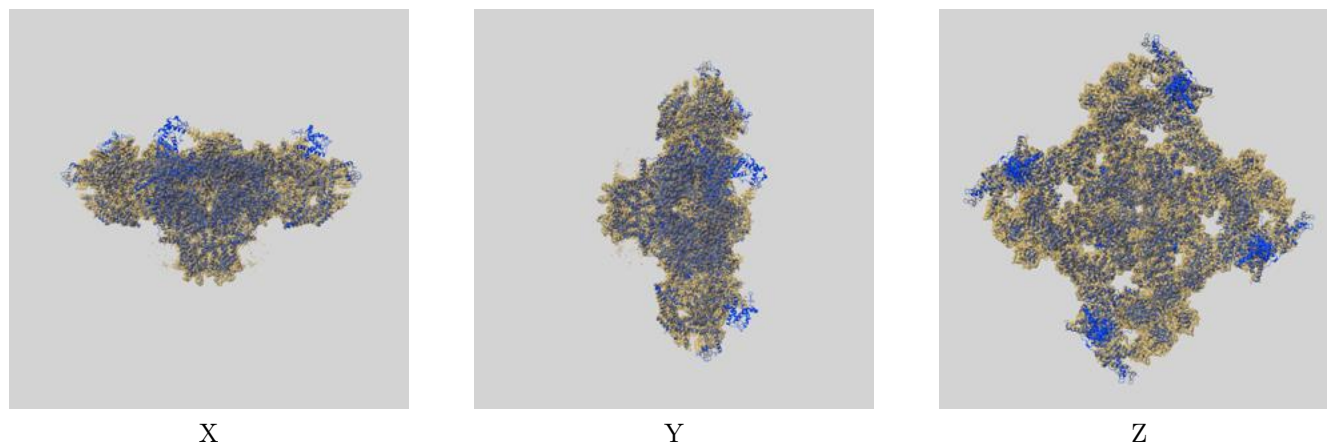
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.36 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.36 by more than 10 %

9 Map-model fit [i](#)

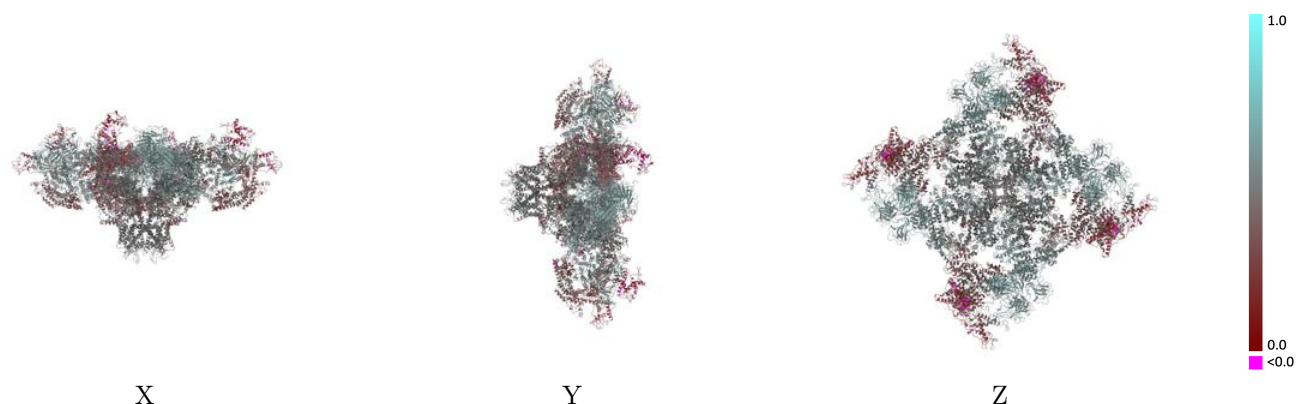
This section contains information regarding the fit between EMDB map EMD-23692 and PDB model 7M6A. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



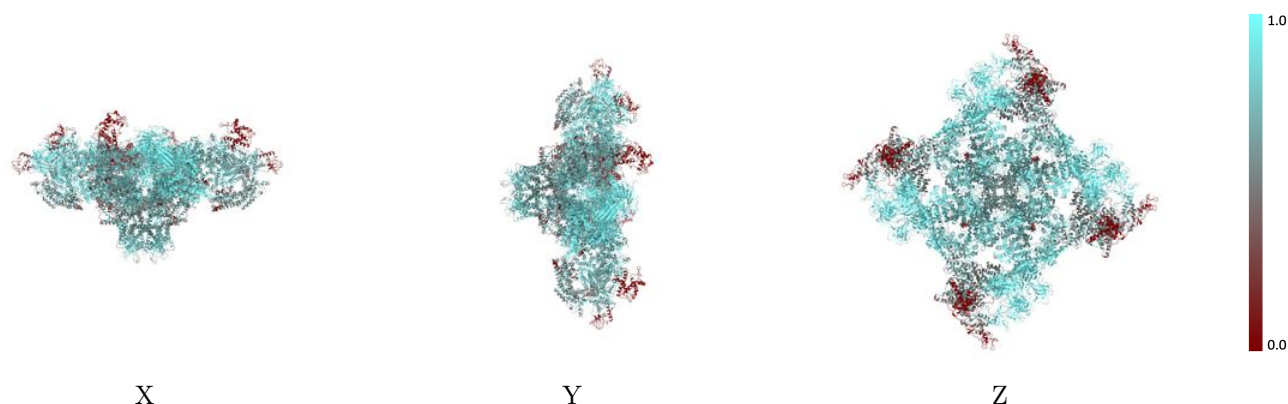
The images above show the 3D surface view of the map at the recommended contour level 0.121 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



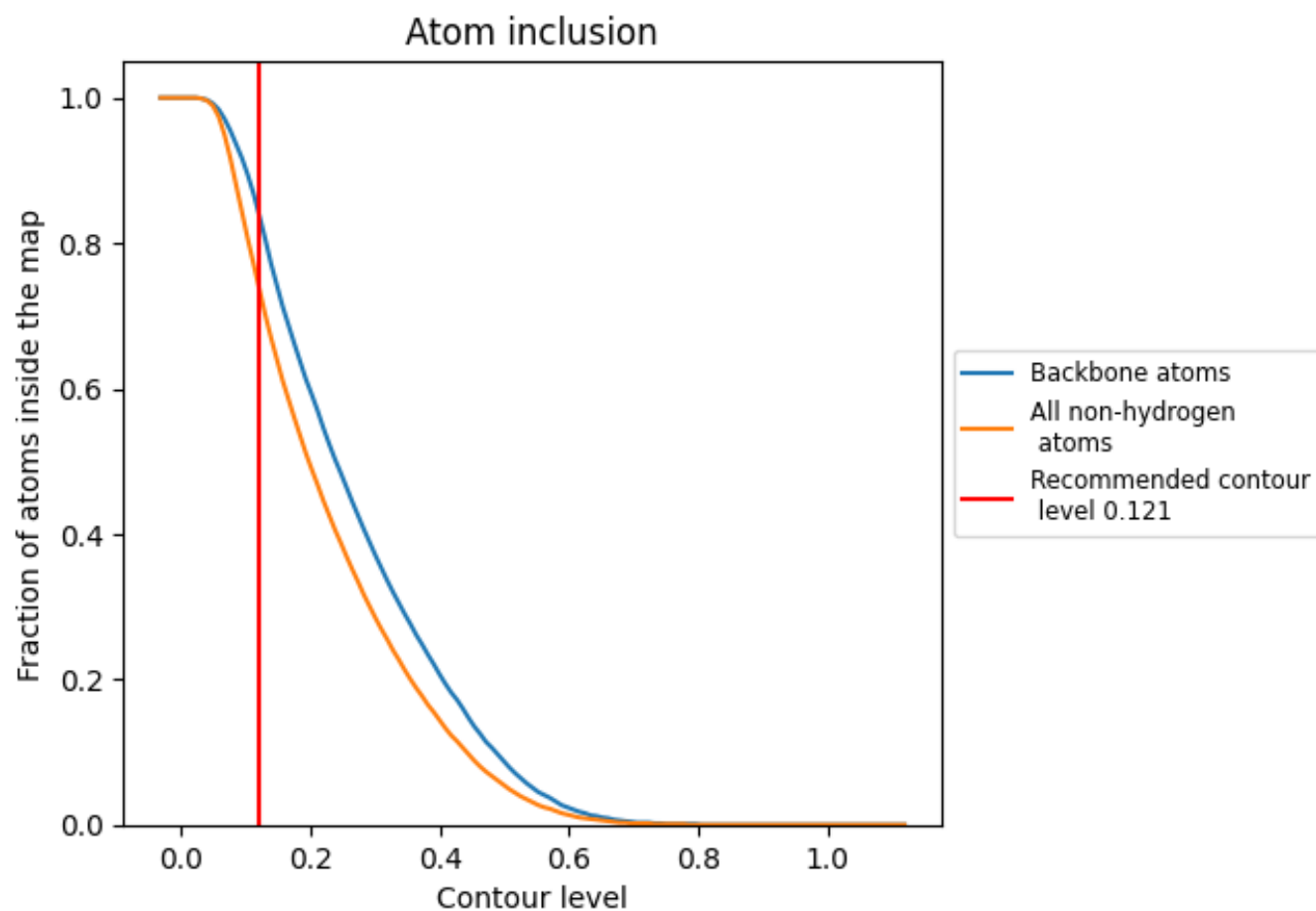
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.121).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.121) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7350	0.4570
A	0.7320	0.4580
B	0.7300	0.4530
F	0.8820	0.5530
G	0.7320	0.4540
H	0.8670	0.5530
I	0.7310	0.4530
J	0.8780	0.5500
O	0.8820	0.5520

1.0

0.0

<0.0