



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:31 PM UTC

PDB ID : 6JRR / pdb_00006jrr
EMDB ID : EMD-9879
Title : Structure of RyR2 (*F/A/C/L-Ca²⁺ dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-04-05
Resolution : 3.90 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:

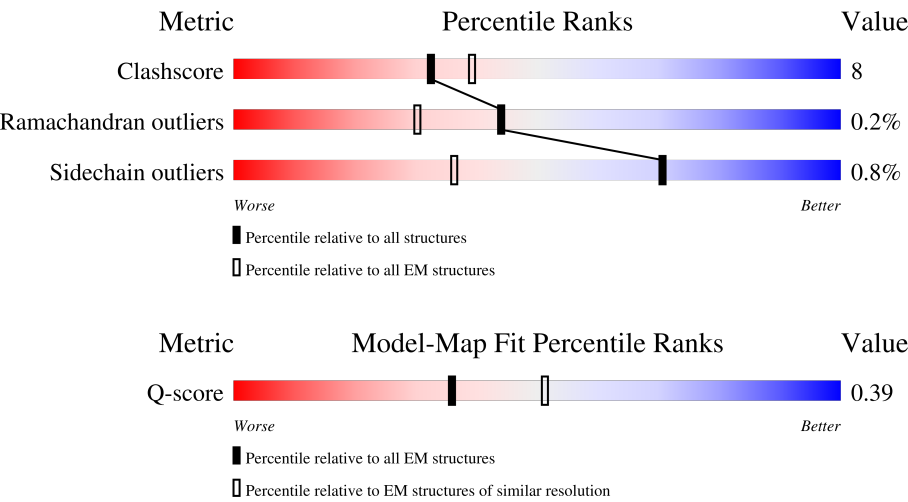
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	4968	9% 57% 13% 30%
1	C	4968	9% 57% 13% 30%
1	E	4968	9% 57% 13% 30%
1	G	4968	9% 57% 12% 30%

Continued on next page...

Mol	Chain	Length	Quality of chain
2	B	108	 72%26%..
2	D	108	 74%24%..
2	F	108	 73%25%..
2	H	108	 75%23%..

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CFF	A	6003	-	X	-	-
6	CFF	C	6003	-	X	-	-
6	CFF	E	6003	-	X	-	-
6	CFF	G	6003	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 109132 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		
1	C	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		
1	E	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		
1	G	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	D	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	F	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

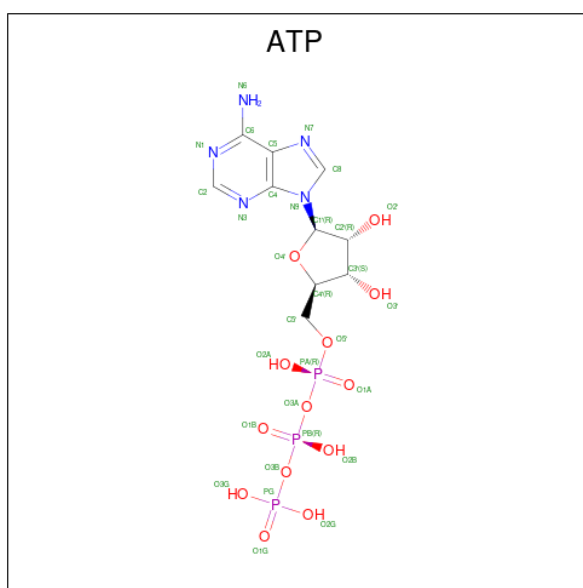
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	

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

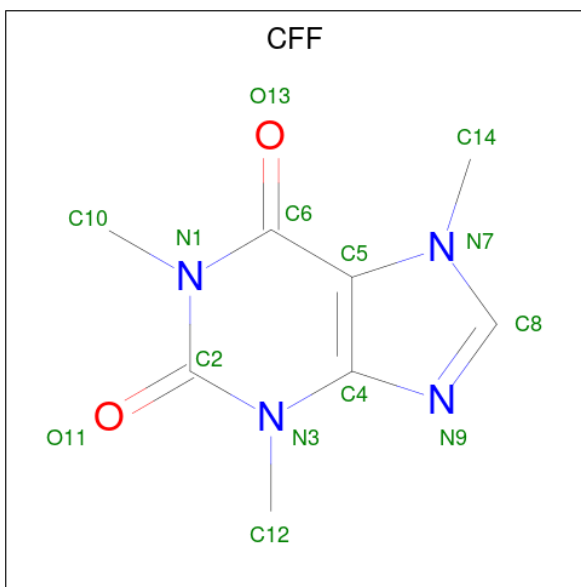
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	E	1	Total	Ca	0
			1	1	
4	G	1	Total	Ca	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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



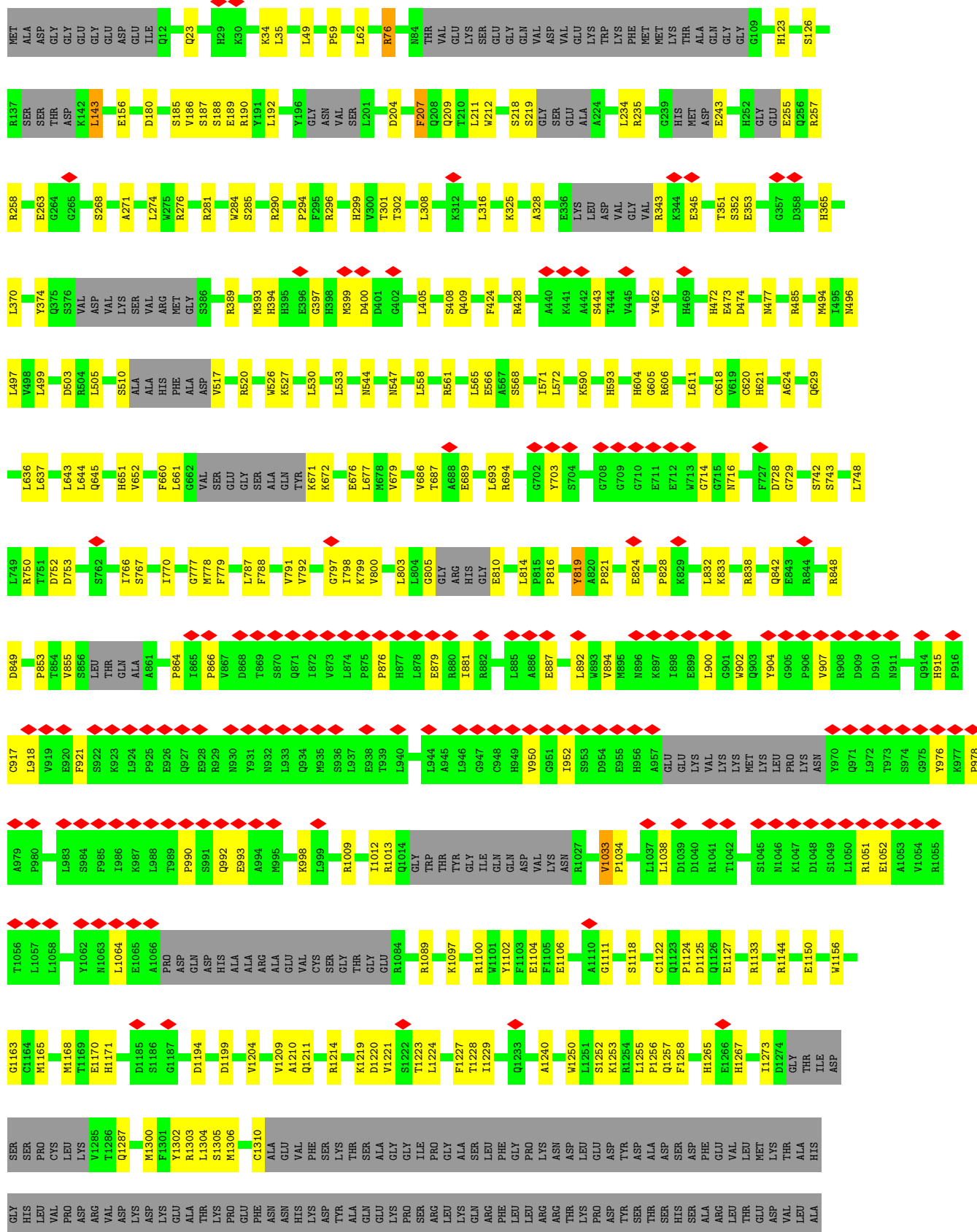
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	



VAL	LYS	TRP	ARG	GLY	V3046	LYS	A2843	T2762	I2722	A2652	L2526	R2425	V2321
LYS	GLN	GLY	GLU	ASP	T3049	PHE	E2844	M2763	M2723	L2653	L2526	R2426	V2322
LEU	ALA	ASP	ALA	ASP	M2845	ALA	M2844	L2764	K2724	SER	L2529	S2426	R2323
LEU	VAL	LEU	M2845	A2765	M2845	LYS	M2845	A2765	Y2725	LYS	THR	L2427	L2324
VAL	VAL	LEU	E2846	M2766	E2846	VAL	E2846	M2766	A2726	LYS	ARG	L2433	L2325
PRO	PRO	LEU	E2847	M2767	E2847	LEU	E2847	M2767	E2727	ALA	CYS	V2436	L2326
LEU	LEU	LEU	N2848	M2768	N2848	LEU	N2848	M2768	H2728	ALA	PRO	L2439	R2327
LEU	LEU	LEU	Y2849	M2769	Y2849	LEU	Y2849	M2769	S2729	ALA	ALA	A2440	R2328
ASP	ASP	LEU	H2850	E2790	H2850	LEU	H2850	E2790	D2730	ALA	ALA	A2441	P2329
GLN	GLN	LEU	N2851	E2791	N2851	LEU	N2851	E2791	H2731	ALA	ALA	F2442	E2330
TYR	TYR	LEU	I2852	R2792	I2852	LEU	I2852	R2792	K2732	ALA	ALA	Q2443	P2339
PHE	PHE	LEU	V2853	R2793	V2853	LEU	V2853	R2793	M2733	ALA	ALA	Q2444	E2330
LYS	LYS	LEU	A2854	E2794	A2854	LEU	A2854	E2794	S2734	ALA	ALA	Q2445	CYS
ASN	ASN	LEU	K2855	E2795	K2855	LEU	K2855	E2795	M2735	ALA	ALA	Q2446	PHE
HIS	HIS	LEU	K2856	G2796	K2856	LEU	K2856	G2796	D2736	ALA	ALA	Q2447	GLY
ARG	ARG	LEU	K2857	D2797	K2857	LEU	K2857	D2797	K2737	ALA	ALA	Q2448	GLY
ALA	ALA	LEU	K2858	SER	K2858	LEU	K2858	SER	L2738	ALA	ALA	Q2449	ASN
TYR	TYR	LEU	L2859	ALA	L2859	LEU	L2859	ALA	A2739	ALA	ALA	Q2450	C2343
SER	SER	LEU	E2860	LEU	E2860	LEU	E2860	LEU	M2740	ALA	ALA	Q2451	T2384
LEU	LEU	LEU	E2861	TYR	E2861	LEU	E2861	TYR	G2741	ALA	ALA	Q2452	ALA
LEU	LEU	LEU	E2862	ASN	E2862	LEU	E2862	ASN	M2742	ALA	ALA	Q2453	GLU
LEU	LEU	LEU	S2863	ARG	S2863	LEU	S2863	ARG	L2743	ALA	ALA	Q2454	PRO
LEU	LEU	LEU	K2864	THR	K2864	LEU	K2864	THR	L2744	ALA	ALA	Q2455	ASP
LEU	LEU	LEU	G2865	ARG	G2865	LEU	G2865	ARG	Y2744	ALA	ALA	Q2456	PRO
LEU	LEU	LEU	G2866	ILE	G2866	LEU	G2866	ILE	G2745	ALA	ALA	Q2457	PRO
LEU	LEU	LEU	G2867	GLN	G2867	LEU	G2867	GLN	E2746	ALA	ALA	Q2458	SER
LEU	LEU	LEU	N2868	THR	N2868	LEU	N2868	THR	L2747	ALA	ALA	Q2459	ASP
LEU	LEU	LEU	H2869	SER	H2869	LEU	H2869	SER	Y2748	ALA	ALA	Q2460	GLY
LEU	LEU	LEU	P2870	GLN	P2870	LEU	P2870	GLN	S2749	ALA	ALA	Q2461	PRO
LEU	LEU	LEU	L2871	VAL	L2871	LEU	L2871	VAL	D2750	ALA	ALA	Q2462	SER
LEU	LEU	LEU	L2872	SER	L2872	LEU	L2872	SER	S2751	ALA	ALA	Q2463	PRO
LEU	LEU	LEU	V2873	ASP	V2873	LEU	V2873	ASP	G2752	ALA	ALA	Q2464	THR
LEU	LEU	LEU	P2874	A2818	P2874	LEU	P2874	A2818	M2753	ALA	ALA	Q2465	SER
LEU	LEU	LEU	Y2875	A2819	Y2875	LEU	Y2875	A2819	K2754	ALA	ALA	Q2466	GLY
LEU	LEU	LEU	D2876	H2820	D2876	LEU	D2876	H2820	Q2755	ALA	ALA	Q2467	PRO
LEU	LEU	LEU	T2877	G2821	T2877	LEU	T2877	G2821	P2756	ALA	ALA	Q2468	SER
LEU	LEU	LEU	L2878	Y2822	L2878	LEU	L2878	Y2822	L2757	ALA	ALA	Q2469	PRO
LEU	LEU	LEU	T2879	S2823	T2879	LEU	T2879	S2823	M2758	ALA	ALA	Q2470	THR
LEU	LEU	LEU	A2880	P2824	A2880	LEU	A2880	P2824	K2759	ALA	ALA	Q2471	ASP
LEU	LEU	LEU	K2881	A2826	K2881	LEU	K2881	A2826	P2760	ALA	ALA	Q2472	GLY
LEU	LEU	LEU	E2882	T2827	E2882	LEU	E2882	T2827	T2761	ALA	ALA	Q2473	GLU
LEU	LEU	LEU	K2883	D2828	K2883	LEU	K2883	D2828	K2762	ALA	ALA	Q2474	THR
LEU	LEU	LEU	A2884	M2829	A2884	LEU	A2884	M2829	L2763	ALA	ALA	Q2475	ASP
LEU	LEU	LEU	K2885	S2830	K2885	LEU	K2885	S2830	L2764	ALA	ALA	Q2476	ASP
LEU	LEU	LEU	D2886	N2831	D2886	LEU	D2886	N2831	S2765	ALA	ALA	Q2477	GLU
LEU	LEU	LEU	R2887	V2832	R2887	LEU	R2887	V2832	E2766	ALA	ALA	Q2478	THR
LEU	LEU	LEU	E2888	N2833	E2888	LEU	E2888	N2833	K2767	ALA	ALA	Q2479	GLY
LEU	LEU	LEU	K2889	T2833	K2889	LEU	K2889	T2833	E2768	ALA	ALA	Q2480	THR
LEU	LEU	LEU	A2890	L2834	A2890	LEU	A2890	L2834	E2769	ALA	ALA	Q2481	ASP
LEU	LEU	LEU	Q2891	S2835	Q2891	LEU	Q2891	S2835	E2770	ALA	ALA	Q2482	GLU
LEU	LEU	LEU	D2892	K2836	D2892	LEU	D2892	K2836	L2771	ALA	ALA	Q2483	THR
LEU	LEU	LEU	L2893	D2837	L2893	LEU	L2893	D2837	Y2772	ALA	ALA	Q2484	ASP
LEU	LEU	LEU	L2894	L2838	L2894	LEU	L2894	L2838	K2773	ALA	ALA	Q2485	GLU
LEU	LEU	LEU	K2895	H2839	K2895	LEU	K2895	H2839	M2774	ALA	ALA	Q2486	THR
LEU	LEU	LEU	F2896	A2840	F2896	LEU	F2896	A2840	P2775	ALA	ALA	Q2487	ASP
LEU	LEU	LEU	L2897	M2841	L2897	LEU	L2897	M2841	I2776	ALA	ALA	Q2488	GLU
LEU	LEU	LEU	Q2898	S2836	Q2898	LEU	Q2898	S2836	K2777	ALA	ALA	Q2489	THR
LEU	LEU	LEU	I2899	K2837	I2899	LEU	I2899	K2837	E2778	ALA	ALA	Q2490	ASP
LEU	LEU	LEU	N2900	L2838	N2900	LEU	N2900	L2838	M2779	ALA	ALA	Q2491	GLU
LEU	LEU	LEU	G2901	H2839	G2901	LEU	G2901	H2839	K2779	ALA	ALA	Q2492	THR
LEU	LEU	LEU		A2840		LEU		A2840	L2780	ALA	ALA	Q2493	ASP
LEU	LEU	LEU		M2841		LEU		M2841	K2781	ALA	ALA	Q2494	GLU
LEU	LEU	LEU		S2836		LEU		S2836		ALA	ALA	Q2495	THR
LEU	LEU	LEU		D2837		LEU		D2837		ALA	ALA	Q2496	ASP
LEU	LEU	LEU		L2838		LEU		L2838		ALA	ALA	Q2497	GLU
LEU	LEU	LEU		H2839		LEU		H2839		ALA	ALA	Q2498	THR
LEU	LEU	LEU		A2840		LEU		A2840		ALA	ALA	Q2499	ASP
LEU	LEU	LEU		M2841		LEU		M2841		ALA	ALA	Q2500	GLU
LEU	LEU	LEU		S2836		LEU		S2836		ALA	ALA	Q2501	THR
LEU	LEU	LEU		D2837		LEU		D2837		ALA	ALA	Q2502	ASP
LEU	LEU	LEU		L2838		LEU		L2838		ALA	ALA	Q2503	GLU
LEU	LEU	LEU		H2839		LEU		H2839		ALA	ALA	Q2504	THR
LEU	LEU	LEU		A2840		LEU		A2840		ALA	ALA	Q2505	ASP
LEU	LEU	LEU		M2841		LEU		M2841		ALA	ALA	Q2506	GLU
LEU	LEU	LEU		S2836		LEU		S2836		ALA	ALA	Q2507	THR
LEU	LEU	LEU		D2837		LEU		D2837		ALA	ALA	Q2508	ASP
LEU	LEU	LEU		L2838		LEU		L2838		ALA	ALA	Q2509	GLU
LEU	LEU	LEU		H2839		LEU		H2839		ALA	ALA	Q2510	THR
LEU	LEU	LEU		A2840		LEU		A2840		ALA	ALA	Q2511	ASP
LEU	LEU	LEU		M2841		LEU		M2841		ALA	ALA	Q2512	GLU
LEU	LEU	LEU		S2836		LEU		S2836		ALA	ALA	Q2513	THR
LEU	LEU	LEU		D2837		LEU		D2837		ALA	ALA	Q2514	ASP
LEU	LEU	LEU		L2838		LEU		L2838		ALA	ALA	Q2515	GLU
LEU	LEU	LEU		H2839		LEU		H2839		ALA	ALA	Q2516	THR
LEU	LEU	LEU		A2840		LEU		A2840		ALA	ALA	Q2517	ASP
LEU	LEU	LEU		M2841		LEU		M2841		ALA	ALA	Q2518	GLU
LEU	LEU	LEU		S2836		LEU		S2836		ALA	ALA	Q2519	THR
LEU	LEU	LEU		D2837		LEU		D2837		ALA	ALA	Q2520	ASP
LEU	LEU	LEU		L2838		LEU		L2838		ALA	ALA	Q2521	GLU
LEU	LEU	LEU		H2839		LEU		H2839		ALA	ALA	Q2522	THR
LEU	LEU	LEU		A2840		LEU		A2840		ALA	ALA	Q2523	ASP
LEU	LEU	LEU		M2841		LEU		M2841		ALA	ALA	Q2524	GLU
LEU	LEU	LEU		S2836		LEU		S2836		ALA	ALA	Q2525	THR
LEU	LEU	LEU		D2837		LEU		D2837		ALA	ALA	Q2526	ASP
LEU	LEU	LEU		L2838		LEU		L2838		ALA	ALA	Q2527	GLU
LEU	LEU	LEU		H2839		LEU		H2839		ALA	ALA	Q2528	THR
LEU	LEU	LEU		A2840		LEU		A2840		ALA	ALA	Q2529	ASP
LEU	LEU	LEU		M2841		LEU		M2841		ALA	ALA	Q2530	GLU
LEU	LEU	LEU		S2836		LEU		S2836		ALA	ALA	Q2531	THR
LEU	LEU	LEU		D2837		LEU		D2837		ALA	ALA	Q2532	ASP
LEU	LEU	LEU		L2838		LEU		L2838		ALA	ALA	Q2533	GLU
LEU	LEU	LEU		H2839		LEU		H2839		ALA	ALA	Q2534	THR
LEU	LEU	LEU		A2840		LEU		A2840		ALA	ALA	Q2535	ASP
LEU	LEU	LEU		M2841		LEU		M2841		ALA	ALA	Q2536	GLU
LEU	LEU	LEU		S2836		LEU		S2836		ALA	ALA	Q2537	THR
LEU	LEU	LEU		D2837		LEU		D2837		ALA	ALA	Q2538	ASP
LEU	LEU	LEU		L2838		LEU		L2838		ALA	ALA	Q2539	GLU
LEU	LEU	LEU		H2839		LEU		H2839		ALA	ALA	Q2540	THR
LEU	LEU	LEU		A2840		LEU		A2840		ALA	ALA	Q2541	ASP
LEU	LEU	LEU		M2841		LEU		M2841		ALA	ALA	Q2542	GLU
LEU	LEU	LEU		S2836		LEU		S2836		ALA	ALA	Q2543	THR
LEU	LEU	LEU		D2837		LEU		D2837		ALA	ALA	Q2544	ASP
LEU	LEU	LEU		L2838		LEU		L2838		ALA	ALA	Q2545	GLU
LEU	LEU	LEU		H2839		LEU		H2839		ALA	ALA	Q2546	THR
LEU	LEU	LEU		A2840		LEU		A2840		ALA	ALA	Q2547	ASP
LEU	LEU	LEU		M2841		LEU		M2841		ALA	ALA	Q2548	GLU
LEU	LEU	LEU		S2836		LEU		S2836		ALA	ALA	Q2549	THR
LEU	LEU	LEU		D2837		LEU		D2837		ALA			

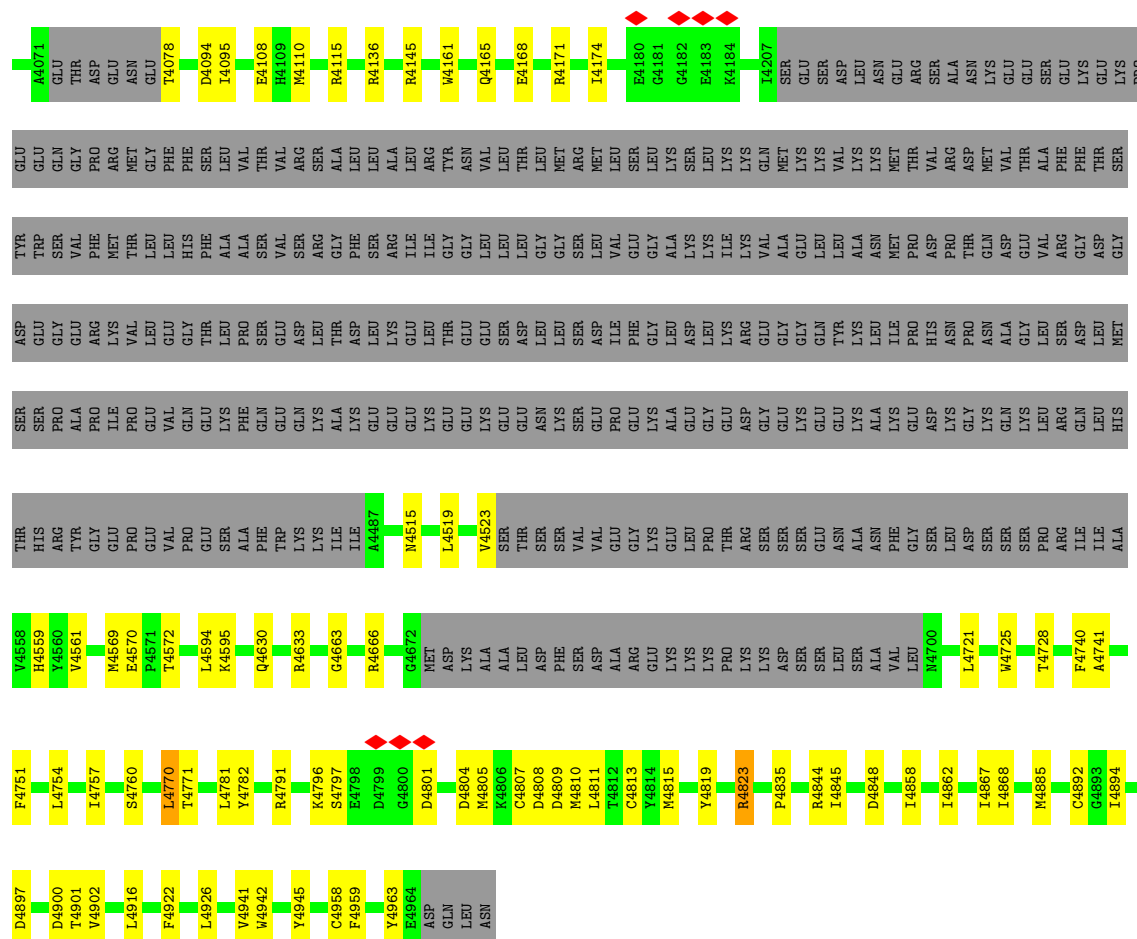
I4868	F4740	ARG	ARG	ARG	GLN	GLY	THR	PHE	LYS	S4055	A3910	S3748	S3628	ALA	PHE	TYR
M4885	A4741	ILE	ILE	THR	LEU	ASP	GLY	PHE	LYS	H4056	A3910	M3755	W3629	LEU	LEU	PRO
F4888	L4744	ALA	MET	SER	HIS	ASP	GLY	THR	PRO	E4065	N3919	N3771	H3635	ASN	THR	ILE
C4892	F4751	ARG	SER	TRP	HIS	GLU	GLY	TRP	GLU	L4068	L3921	Q3775	L3641	ARG	THR	ARG
I4894	L4754	ALA	PRO	VAL	ARG	GLY	GLY	SER	GLN	A4071	T3922	Q3776	I3642	PHE	LYS	PHE
D4897	I4757	ILE	ALA	PHE	ILE	ASP	THR	PHE	GLY	GLU	E3923	K3777	P3648	ASP	VAL	ASP
D4900	S4760	GLU	GLU	LEU	GLU	ASP	GLY	LEU	MET	THR	G3927	S3793	GLY	LYS	TYR	TYR
T4901	L4770	VAL	PRO	HIS	VAL	GLY	GLY	LEU	PHE	ASN	P3928	L3794	ALA	ARG	ASN	ASN
V4902	T4771	GLN	GLU	PHE	GLU	THR	THR	PHE	SER	GLU	C3929	L3797	VAL	ALA	ALA	ALA
L4911	L4781	LYS	SER	ALA	LEU	LEU	ALA	PHE	LEU	T4078	S3939	Q3798	PRO	GLU	LYS	LYS
N4915	R4791	THR	PHE	VAL	VAL	SER	SER	VAL	VAL	D4094	R3940	Q3799	PRO	VAL	THR	THR
L4916	K4796	GLN	GLY	ARG	ARG	ASP	GLY	ARG	ARG	I4095	R3943	S3800	GLY	ARG	LYS	LYS
F4922	S4797	ILE	ILE	PHE	GLY	ASP	GLY	THR	LEU	M4110	Q3956	F3809	GLU	ASN	ALA	ALA
L4926	E4798	ILE	ILE	THR	ILE	LEU	GLY	THR	LEU	R4115	K3957	V3803	GLY	ILE	GLU	GLU
V4941	D4799	GLU	GLU	LEU	ARG	LYS	LEU	ARG	ALA	R4145	S3960	N3813	L3661	HIS	PRO	ASN
W4942	G4800	LYS	LYS	ILE	ILE	ASN	GLY	ILE	LEU	W4161	Q3962	G3819	V3662	GLY	ASN	PRO
Y4945	D4801	MET	GLU	GLY	GLY	GLY	GLY	GLY	ARG	Q4165	Q3965	VAL	Q3667	ARG	LYS	LYS
C4958	D4804	ASP	GLU	SER	LEU	GLY	LEU	LEU	LEU	E4168	K3973	GLU	L3670	LEU	ARG	LEU
F4959	M4805	LYS	THR	THR	SER	ASP	LEU	LEU	LEU	R4171	V3980	GLY	L3683	ALA	ALA	GLU
Y4963	D4808	ALA	SER	VAL	VAL	LEU	GLY	GLY	LEU	I4174	K3982	GLY	I3695	PRO	THR	VAL
E4964	M4810	ASP	VAL	VAL	VAL	GLU	SER	SER	MET	Q4171	V3981	SER	G3700	LEU	ILE	ILE
GLN	L4811	PHE	GLU	GLY	GLY	ASP	LEU	LEU	LEU	I4174	L3983	G3827	ALA	ARG	ARG	ARG
LEU	T4812	ASP	GLY	ILE	ILE	ILE	VAL	VAL	LEU	E4180	V3991	V3630	VAL	TRP	TRP	TRP
ASN	C4813	ALA	LYS	GLY	GLY	PHE	GLY	GLY	SER	G4181	V3992	F3841	HIS	GLN	SER	SER
	T4814	ARG	GLU	ALA	ALA	GLY	ALA	ALA	LEU	C4182	N3993	Q3845	GLU	MET	ALA	LYS
	M4815	GLU	LEU	LYS	LYS	ASP	LYS	LYS	SER	E4183	T4028	Q3845	ASP	ALA	LEU	HIS
	M4818	LYS	PRO	PRO	PRO	LEU	LEU	ILE	LEU	K4184	V4005	N3852	ASP	TYR	ASN	ASN
	Y4819	LYS	ARG	THR	THR	ARG	LYS	LYS	LYS	I4207	I4014	N3852	GLY	LYS	ARG	PHE
	R4823	PRO	SER	SER	VAL	GLU	VAL	VAL	GLN	SER	D4026	I3871	LEU	ASP	LEU	LYS
	G4826	LYS	SER	SER	ALA	GLY	GLU	GLU	MET	GLU	L4027	T3875	GLU	PRO	GLU	ARG
	P4835	ASP	GLU	GLU	GLN	GLY	GLY	LEU	LYS	SER	T4028	L3875	VAL	ILE	ILE	GLY
	R4844	SER	LYS	LYS	ALA	LYS	LYS	ALA	VAL	ASP	S4029	L3880	LYS	ASN	LEU	ASN
	I4845	LEU	ALA	ASN	ASN	LEU	ASN	ASN	LYS	LEU	T4032	R3881	VAL	ILE	VAL	VAL
	D4848	ALA	PHE	PHE	LYS	ILE	MET	MET	LYS	ASN	F4033	V3882	Q3729	THR	CYS	VAL
	I4858	VAL	GLY	GLY	GLY	PRO	THR	THR	THR	ARG	Q3883	Q3883	ALA	ALA	ALA	GLN
	T4862	LEU	SER	SER	SER	HIS	ASP	ASP	VAL	SER	E3884	E3884	PHE	PRO	ASN	ASN
	I4867	LEU	ASP	ASP	ASP	ASN	PRO	PRO	ARG	ALA	Y4036	S3885	ARG	GLY	GLY	GLY
			R4700	LEU	LEU	ASN	THR	THR	ASN	ASN	S4045	Y3892	R3735	LYS	ASN	ILE
			W4725	SER	SER	LYS	GLN	GLN	MET	LYS	K4051	K3896	E3739	THR	GLN	ASN
			T4728	GLY	GLY	LYS	GLY	GLY	VAL	GLU	A4052		Q3743	VAL	LEU	GLU
				SER	SER	LYS	THR	THR	ALA	SER				GLU	VAL	MET
				PRO	PRO	PRO	VAL	VAL	ALA	GLU				SER	ILE	SER

● Molecule 1: RyR2

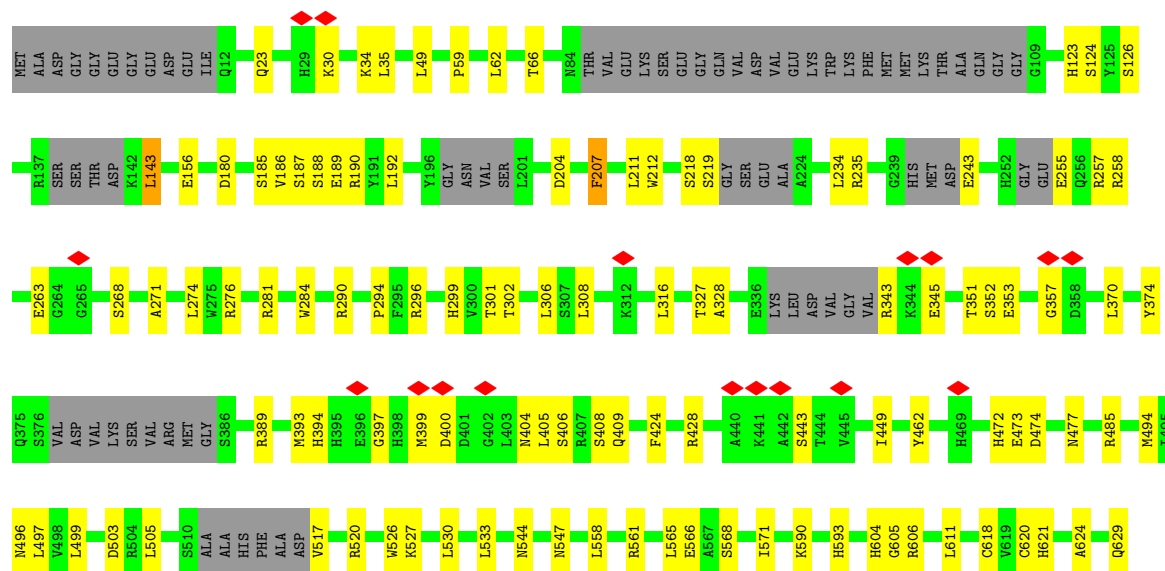


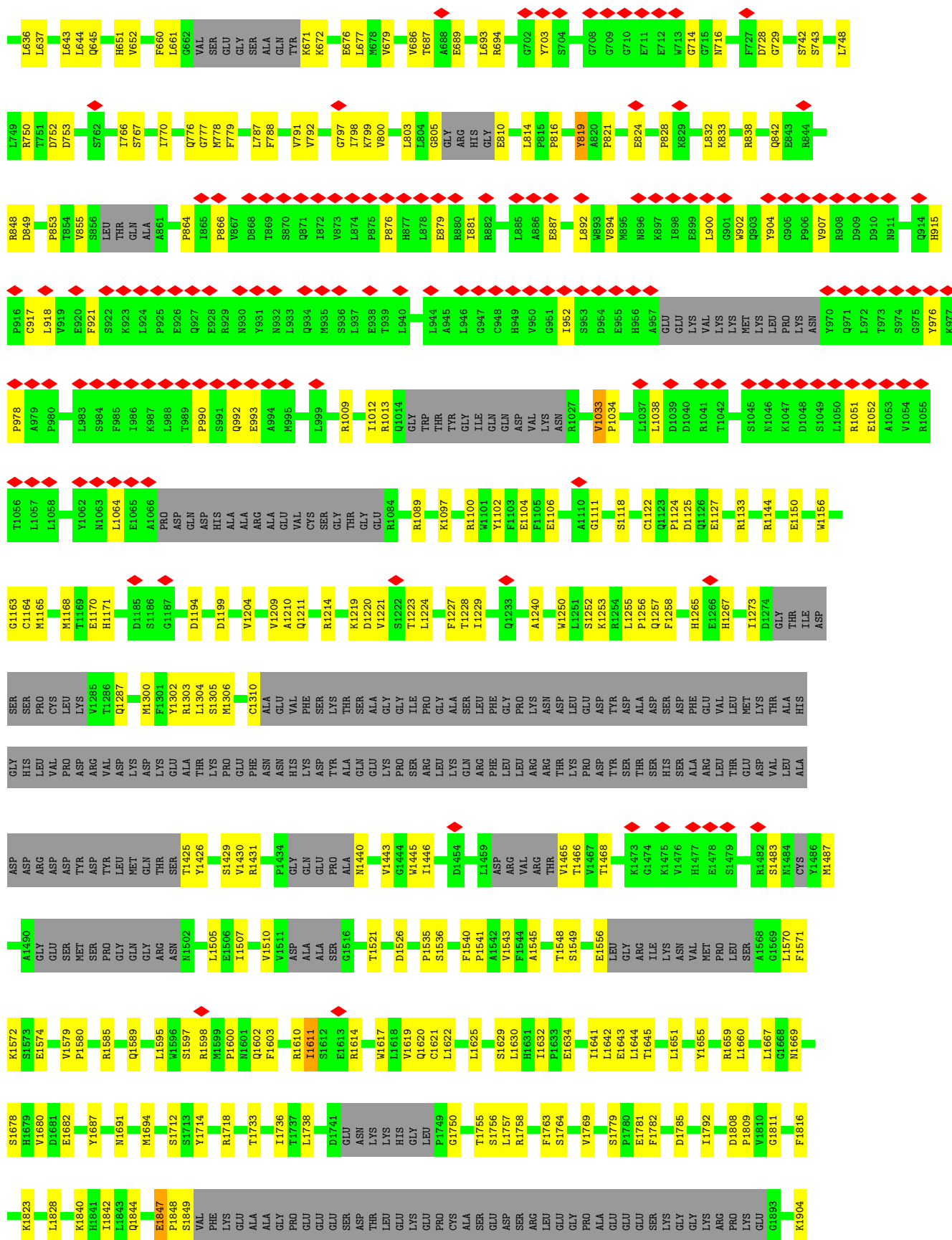
W2733	P2668	E2540	F2441	CYS	ARG	D2116	E1991	GLU	I1792	G1658	L1570	ASP
S2734	C2669	A2543	Q2442	PHE	GLY	D2116	D2013	G1893	D1808	N1669	F1571	ASP
W2735	A2672	V2553	THR	GLY	THR	L2120	GLU	K1904	P1809	S1678	K1572	ARG
K2737	P2678	TYR	ILE	ALA	ILE	R2128	ASP	L1905	H1679	H1679	E1574	ASP
L2738	ASP	ARG	ALA	ARG	ALA	L2131	LEU	Q1906	V1680	D1681	V1579	TYR
A2739	TYR	LEU	GLY	GLY	GLY	S2132	ASP	M1907	D1682	A1682	P1580	ASP
W2740	MET	GLY	GLY	GLY	GLY	V2133	ASN	A1925	Y1687	A1687	R1585	LEU
G2741	GLU	ASN	ASN	ASN	ASN	R2259	ASP	S1930	R1589	A1688	R1585	GLN
L2742	GLU	VAL	VAL	VAL	VAL	E2264	L2024	D1931	Q1589	F1689	Q1589	THR
L2743	ASN	ILE	VAL	GLY	GLY	K2265	ASP	D1932	I1842	F1690	Q1589	ASN
W2744	TYR	CYS	GLU	ALA	ALA	V2267	L2026	D1939	I1842	F1690	L1595	THR
G2745	VAL	GLN	ASP	ASP	ASP	R2268	T2025	R1942	I1842	F1690	L1595	GLN
E2746	SER	LEU	GLU	GLU	GLU	L2270	R2029	F1943	S1849	Y1714	L1595	GLN
G2747	MET	ARG	ASP	ASP	ASP	A2271	L2030	Q1950	VAL	R1718	P1600	THR
L2748	GLU	P2583	GLY	SER	SER	L2275	GLU	L1952	PHE	R1719	N1601	GLY
S2749	GLN	H2588	GLY	ASP	GLN	N2152	LEU	A1951	LYS	T1730	F1603	GLY
L2750	SER	L2589	THR	GLY	SER	N2153	LYS	L1952	ALA	E1731	F1603	GLN
S2751	MET	L2590	GLY	GLY	CYS	F2156	LYS	ASN	ALA	E1731	F1603	GLN
S2752	MET	R2591	ILE	THR	GLN	M2163	GLN	ALA	GLY	E1731	F1603	GLN
S2753	ASP	L2593	GLY	THR	VAL	M2168	LYS	ALA	GLY	E1731	F1603	GLN
K2754	SER	L2593	GLY	THR	SER	M2168	LYS	ALA	GLY	E1731	F1603	GLN
W2755	GLU	V2597	GLY	GLY	GLY	V2175	VAL	ALA	ASP	E1731	F1603	GLN
P2756	GLY	P2598	THR	SER	GLY	V2175	GLU	ARG	THR	E1731	F1603	GLN
L2757	GLY	L2599	ASP	SER	GLY	G2181	SER	ARG	THR	E1731	F1603	GLN
W2758	GLY	L2600	ASP	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2759	GLY	N2601	ASP	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
P2760	GLY	HIS	THR	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2761	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2762	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2763	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2764	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2765	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
E2766	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2767	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
E2768	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2769	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2770	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2771	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2772	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2773	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2774	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2775	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
P2776	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2777	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
E2778	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2779	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2780	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2781	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
T2782	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2783	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2784	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2785	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2786	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2787	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2788	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2789	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2790	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
E2791	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2792	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2793	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2794	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2795	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2796	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
T2797	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2798	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2799	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
E2800	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2801	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
T2802	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2803	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2804	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2805	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2806	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2807	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2808	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2809	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2810	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
T2811	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2812	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2813	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2814	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2815	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2816	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2817	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2818	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2819	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2820	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2821	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2822	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2823	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2824	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2825	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2826	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2827	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
T2828	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2829	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2830	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2831	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2832	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2833	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2834	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2835	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2836	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
T2837	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2838	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2839	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2840	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2841	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
T2842	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2843	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2844	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2845	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2846	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2847	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2848	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
L2849	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
K2850	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
T2851	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
W2852	ALA	K2605	ALA	GLY	GLY	G2181	GLY	THR	LEU	E1731	F1603	GLN
S2853	ALA	K2605	ALA									





• Molecule 1: RyR2









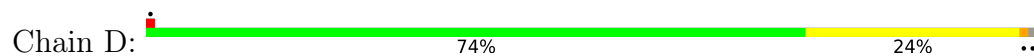








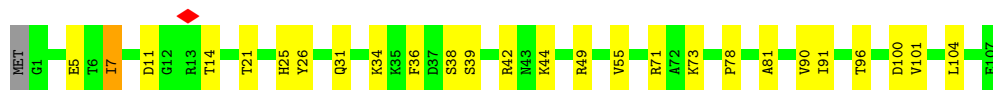
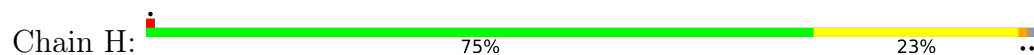
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- 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	149212	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 ($e^-/\text{\AA}^2$)	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	0.141	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.44	0/26913	0.67	4/36395 (0.0%)
1	C	0.43	0/26913	0.67	5/36395 (0.0%)
1	E	0.43	0/26913	0.67	5/36395 (0.0%)
1	G	0.43	0/26913	0.67	4/36395 (0.0%)
2	B	0.36	0/835	0.65	1/1123 (0.1%)
2	D	0.36	0/835	0.65	1/1123 (0.1%)
2	F	0.36	0/835	0.65	1/1123 (0.1%)
2	H	0.36	0/835	0.65	1/1123 (0.1%)
All	All	0.43	0/110992	0.67	22/150072 (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	A	0	15
1	C	0	15
1	E	0	15
1	G	0	15
All	All	0	60

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4771	THR	N-CA-C	11.30	123.68	111.36
1	C	4771	THR	N-CA-C	11.23	123.60	111.36
1	G	4771	THR	N-CA-C	8.26	121.86	111.69
1	A	4771	THR	N-CA-C	7.54	120.96	111.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4770	LEU	CB-CA-C	5.24	119.50	110.79

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	729	GLY	Peptide
1	A	791	VAL	Peptide
1	A	814	LEU	Peptide
1	A	816	PRO	Peptide
1	A	819	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	26417	0	24909	490	0
1	C	26417	0	24909	500	0
1	E	26417	0	24909	485	0
1	G	26417	0	24909	471	0
2	B	819	0	824	19	0
2	D	819	0	824	19	0
2	F	819	0	824	19	0
2	H	819	0	824	18	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	31	0	12	1	0
5	C	31	0	12	1	0
5	E	31	0	12	1	0
5	G	31	0	12	1	0
6	A	14	0	10	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	14	0	10	1	0
6	E	14	0	10	1	0
6	G	14	0	10	1	0
All	All	109132	0	103020	1803	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 8.

The worst 5 of 1803 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2427:LEU:HD13	1:G:143:LEU:CB	1.41	1.51
1:E:143:LEU:CB	1:G:2427:LEU:HD13	1.41	1.49
1:A:143:LEU:CB	1:C:2427:LEU:HD13	1.41	1.48
1:C:143:LEU:CB	1:E:2427:LEU:HD13	1.43	1.47
1:A:2427:LEU:CD1	1:G:143:LEU:HB3	1.48	1.42

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	3336/4968 (67%)	2981 (89%)	347 (10%)	8 (0%)	43	74
1	C	3336/4968 (67%)	2982 (89%)	345 (10%)	9 (0%)	36	69
1	E	3336/4968 (67%)	2980 (89%)	347 (10%)	9 (0%)	36	69
1	G	3336/4968 (67%)	2980 (89%)	348 (10%)	8 (0%)	43	74
2	B	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	D	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
All	All	13764/20304 (68%)	12323 (90%)	1407 (10%)	34 (0%)	44	74

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2328	ARG
1	A	4901	THR
1	C	2328	ARG
1	C	4901	THR
1	E	2328	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2650/4355 (61%)	2629 (99%)	21 (1%)	73	77
1	C	2650/4355 (61%)	2625 (99%)	25 (1%)	70	75
1	E	2648/4355 (61%)	2623 (99%)	25 (1%)	70	75
1	G	2650/4355 (61%)	2629 (99%)	21 (1%)	73	77
2	B	88/89 (99%)	88 (100%)	0	100	100
2	D	88/89 (99%)	88 (100%)	0	100	100
2	F	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
All	All	10950/17776 (62%)	10858 (99%)	92 (1%)	70	77

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2315	GLU
1	G	143	LEU
1	E	2323	ARG
1	E	3618	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	907	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 204 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	692	HIS
1	E	3961	GLN
1	G	4915	ASN
1	E	915	HIS
1	E	1836	ASN

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
5	ATP	A	6002	-	32,33,33	1.34	4 (12%)	48,52,52	1.67	8 (16%)
6	CFF	G	6003	-	15,15,15	2.28	8 (53%)	23,23,23	2.80	9 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ATP	E	6002	-	32,33,33	1.34	4 (12%)	48,52,52	1.67	8 (16%)
5	ATP	C	6002	-	32,33,33	1.34	4 (12%)	48,52,52	1.68	8 (16%)
6	CFF	E	6003	-	15,15,15	2.28	8 (53%)	23,23,23	2.80	10 (43%)
5	ATP	G	6002	-	32,33,33	1.34	4 (12%)	48,52,52	1.67	8 (16%)
6	CFF	A	6003	-	15,15,15	2.28	8 (53%)	23,23,23	2.80	9 (39%)
6	CFF	C	6003	-	15,15,15	2.28	8 (53%)	23,23,23	2.79	9 (39%)

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
5	ATP	A	6002	-	-	5/22/38/38	0/3/3/3
6	CFF	G	6003	-	-	-	0/2/2/2
5	ATP	E	6002	-	-	5/22/38/38	0/3/3/3
5	ATP	C	6002	-	-	5/22/38/38	0/3/3/3
6	CFF	E	6003	-	-	-	0/2/2/2
5	ATP	G	6002	-	-	5/22/38/38	0/3/3/3
6	CFF	A	6003	-	-	-	0/2/2/2
6	CFF	C	6003	-	-	-	0/2/2/2

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	6003	CFF	C6-N1	-4.13	1.31	1.40
6	C	6003	CFF	C6-N1	-4.13	1.31	1.40
6	G	6003	CFF	C6-N1	-4.13	1.31	1.40
6	E	6003	CFF	C6-N1	-4.12	1.31	1.40
5	A	6002	ATP	C5-N7	-3.94	1.31	1.39

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	6003	CFF	C14-N7-C8	-7.81	111.67	126.28
6	G	6003	CFF	C14-N7-C8	-7.81	111.67	126.28
6	C	6003	CFF	C14-N7-C8	-7.79	111.70	126.28
6	E	6003	CFF	C14-N7-C8	-7.78	111.73	126.28
5	C	6002	ATP	C5-C4-N3	-5.37	119.32	126.72

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

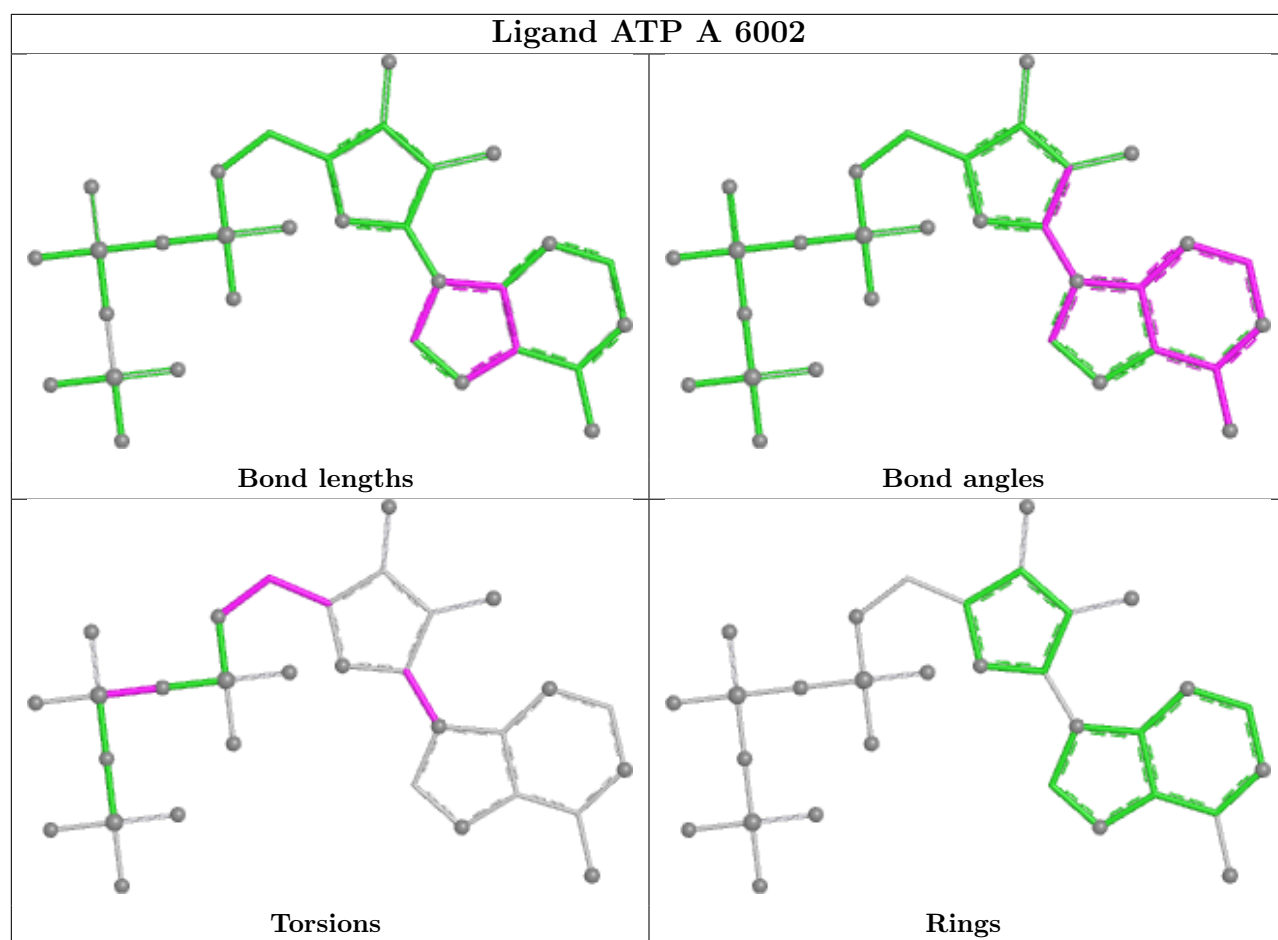
Mol	Chain	Res	Type	Atoms
5	A	6002	ATP	C3'-C4'-C5'-O5'
5	C	6002	ATP	C3'-C4'-C5'-O5'
5	E	6002	ATP	C3'-C4'-C5'-O5'
5	G	6002	ATP	C3'-C4'-C5'-O5'
5	A	6002	ATP	O4'-C4'-C5'-O5'

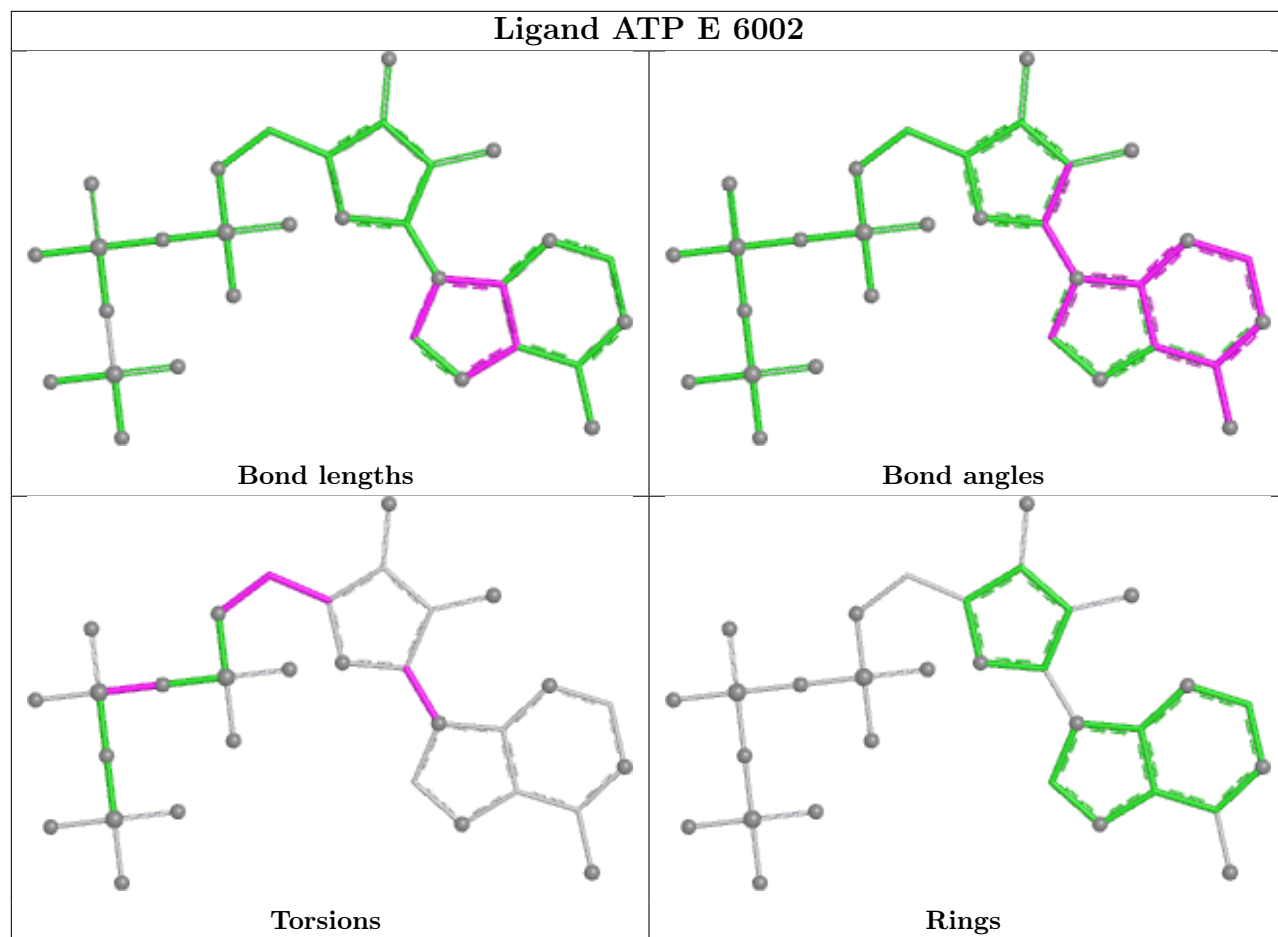
There are no ring outliers.

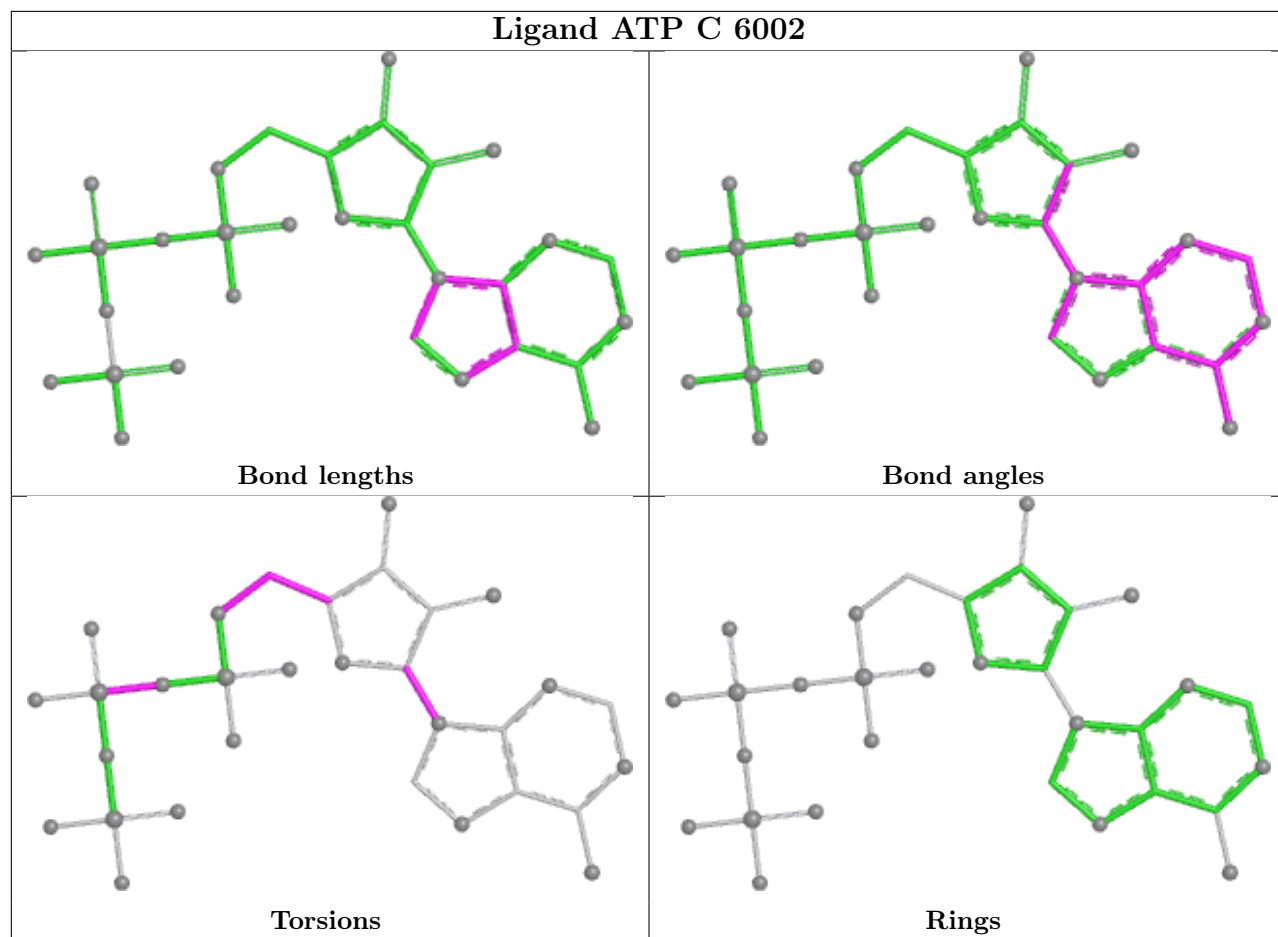
8 monomers are involved in 8 short contacts:

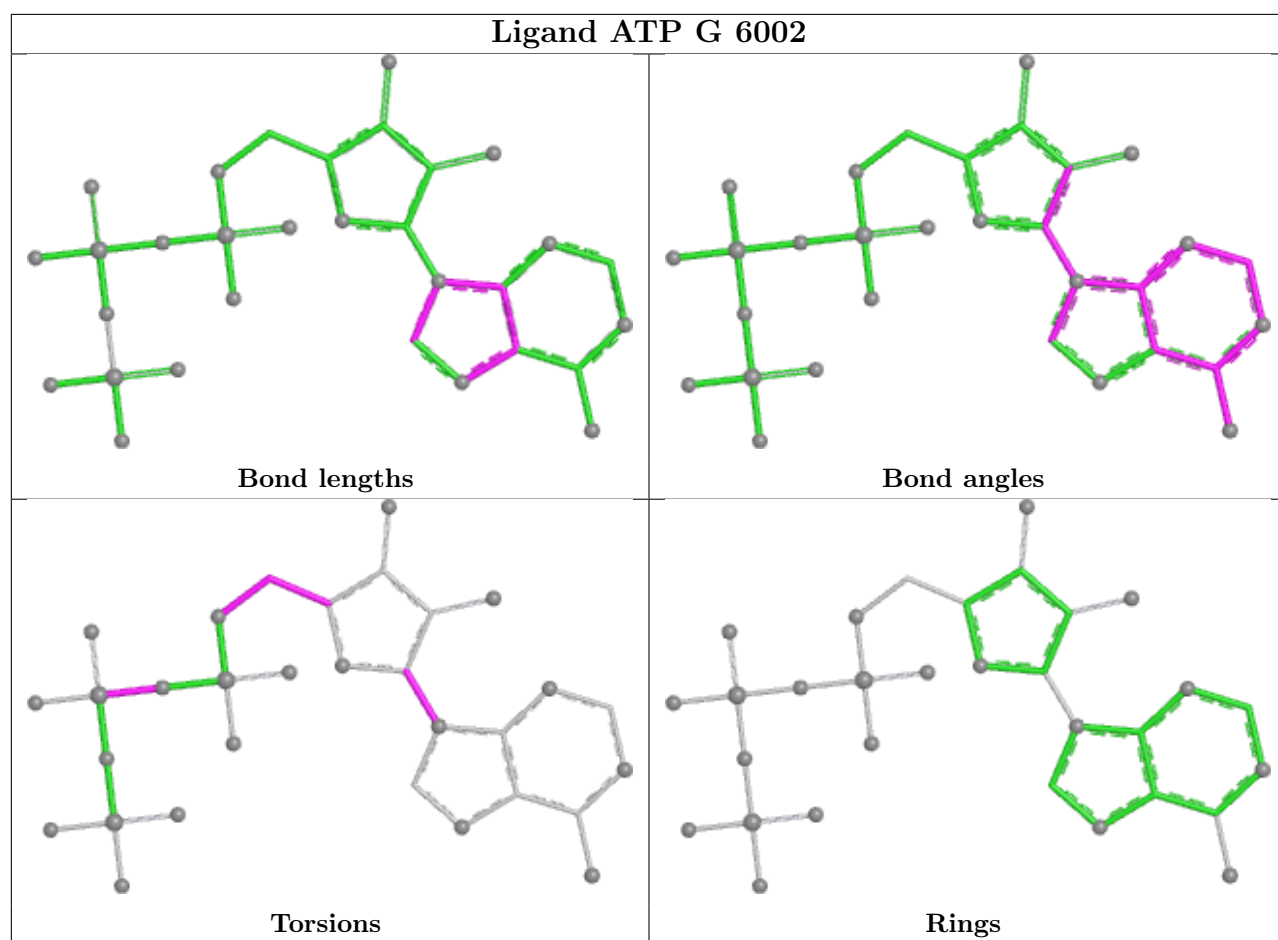
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	6002	ATP	1	0
6	G	6003	CFF	1	0
5	E	6002	ATP	1	0
5	C	6002	ATP	1	0
6	E	6003	CFF	1	0
5	G	6002	ATP	1	0
6	A	6003	CFF	1	0
6	C	6003	CFF	1	0

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.

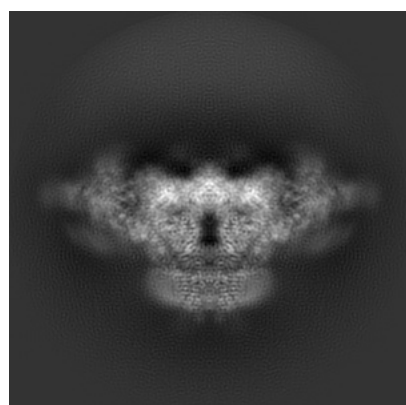
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9879. These allow visual inspection of the internal detail of the map and identification of artifacts.

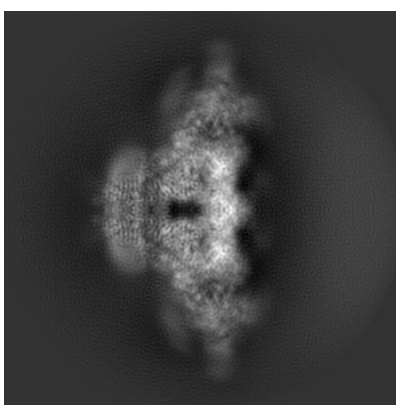
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

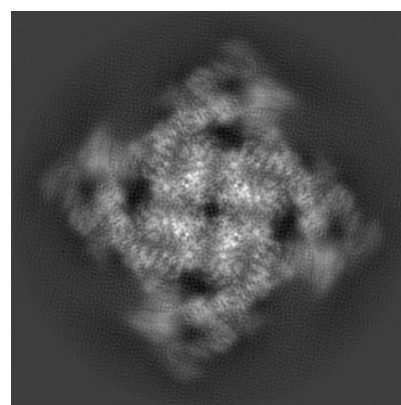
6.1.1 Primary map



X



Y

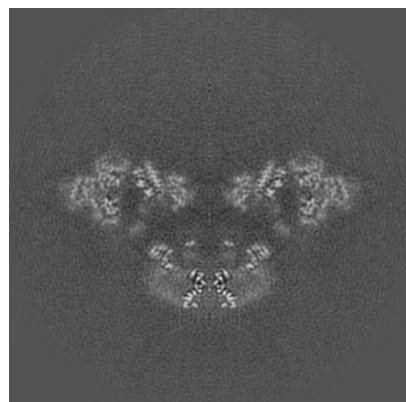


Z

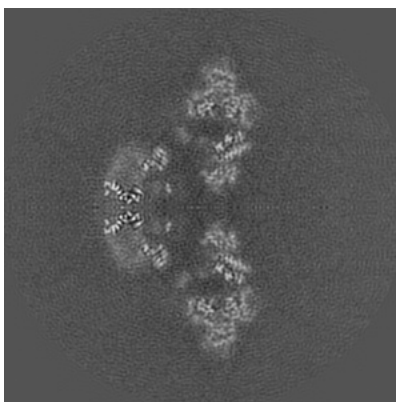
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

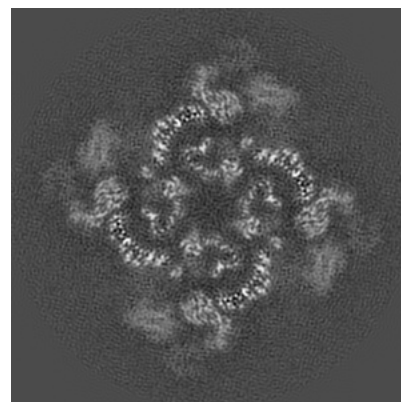
6.2.1 Primary map



X Index: 200



Y Index: 200

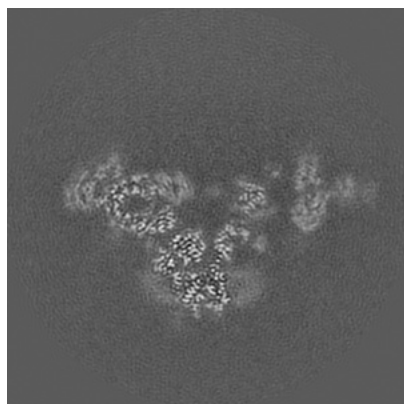


Z Index: 200

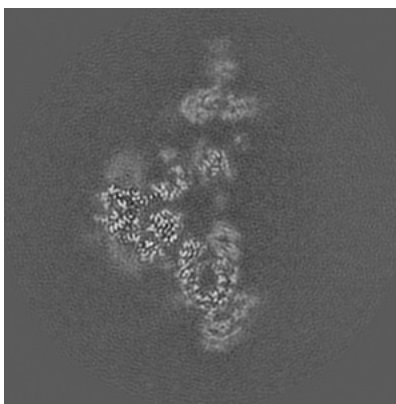
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

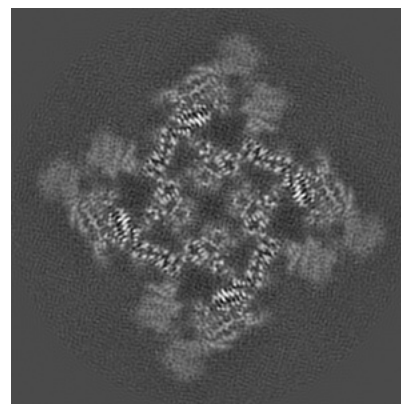
6.3.1 Primary map



X Index: 213



Y Index: 187

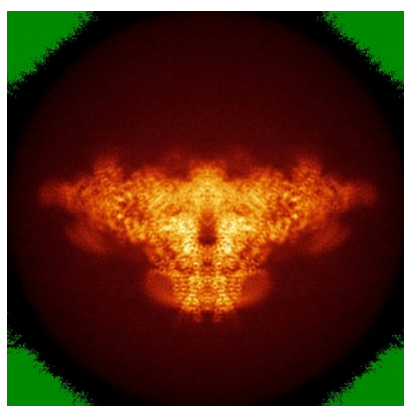


Z Index: 211

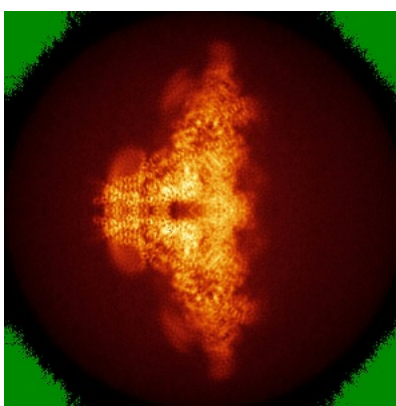
The images above show the largest variance slices of the map in three orthogonal directions.

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

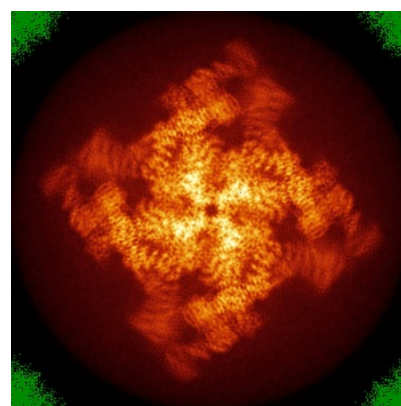
6.4.1 Primary map



X



Y

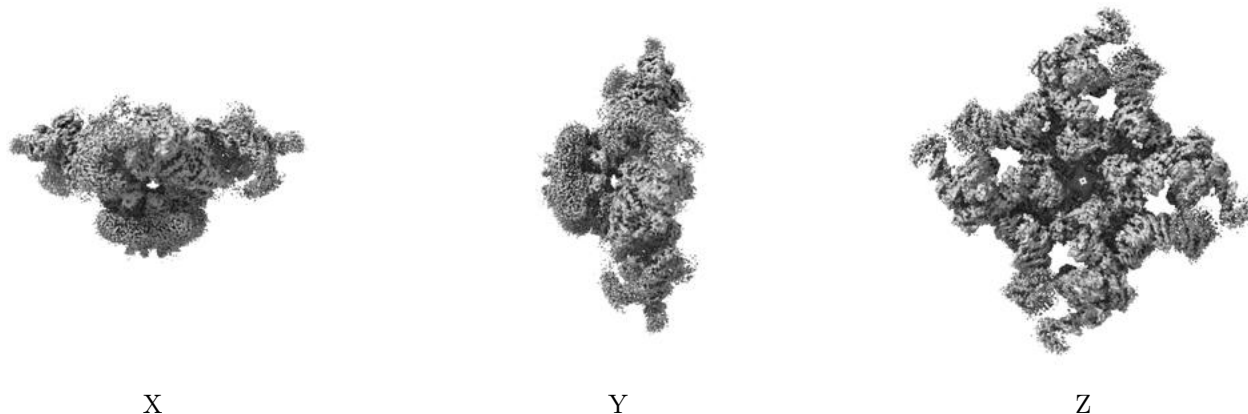


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

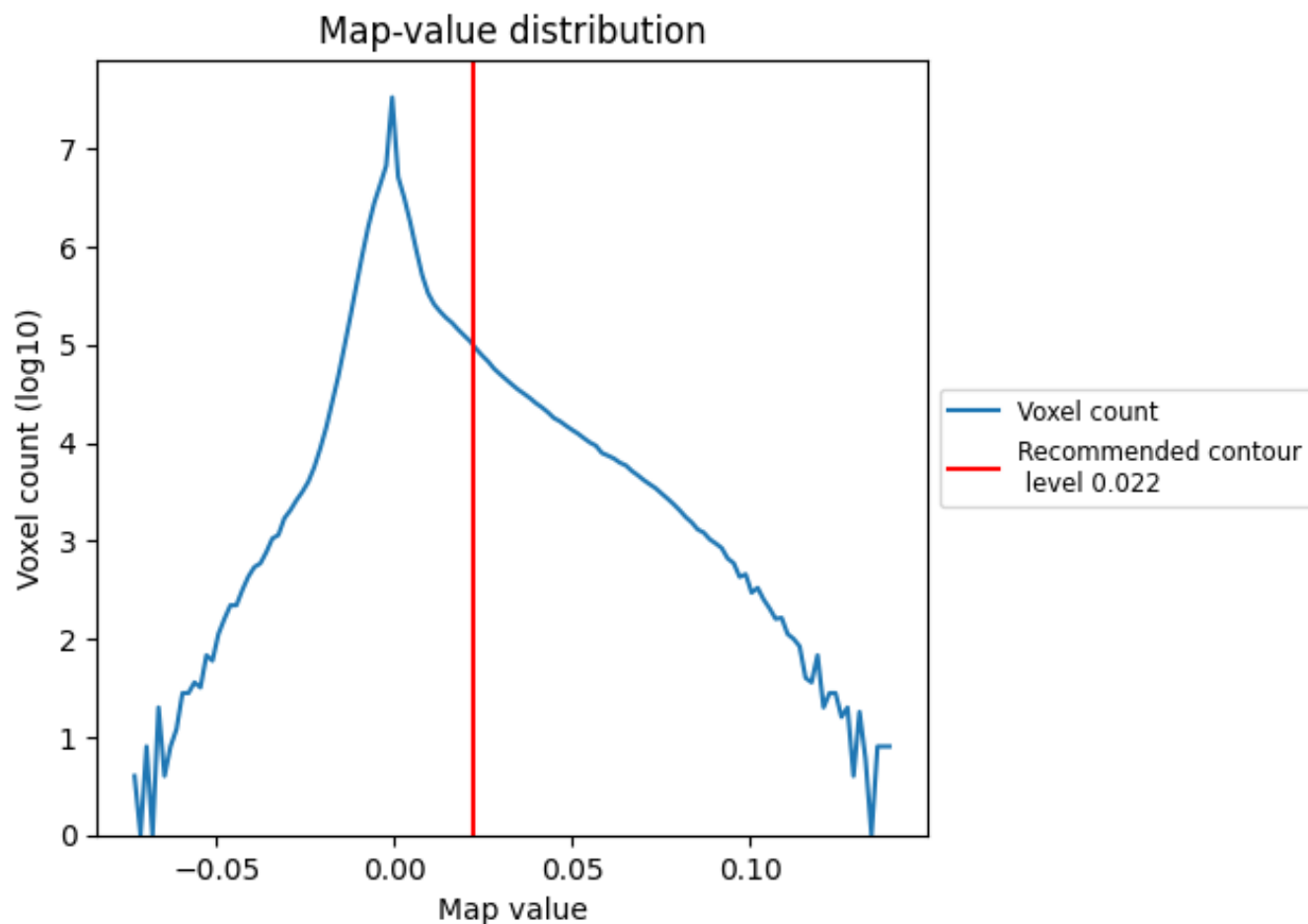
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

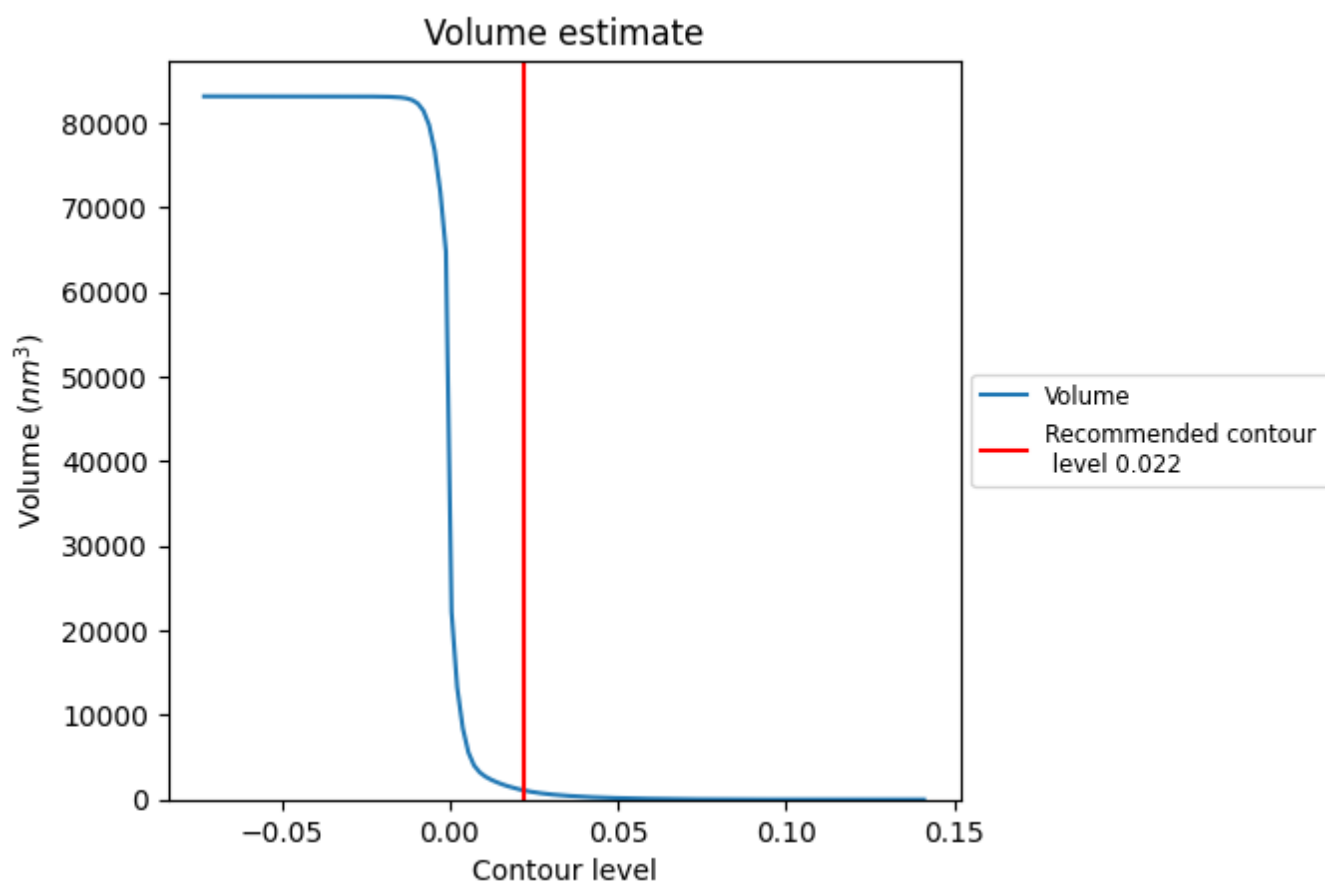
This section contains the results of statistical analysis of the map.

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.

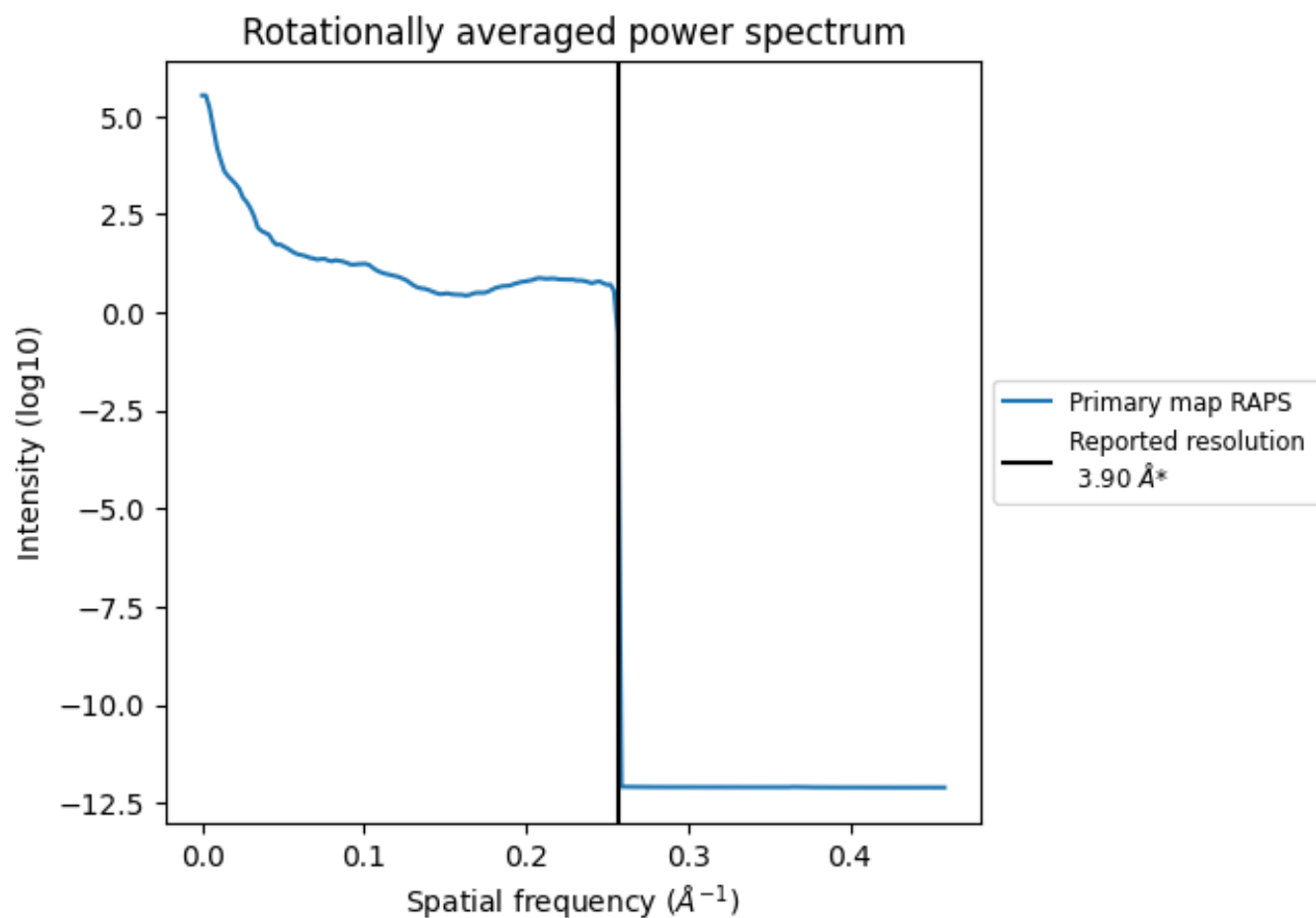
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1096 nm³; this corresponds to an approximate mass of 990 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 ⓘ

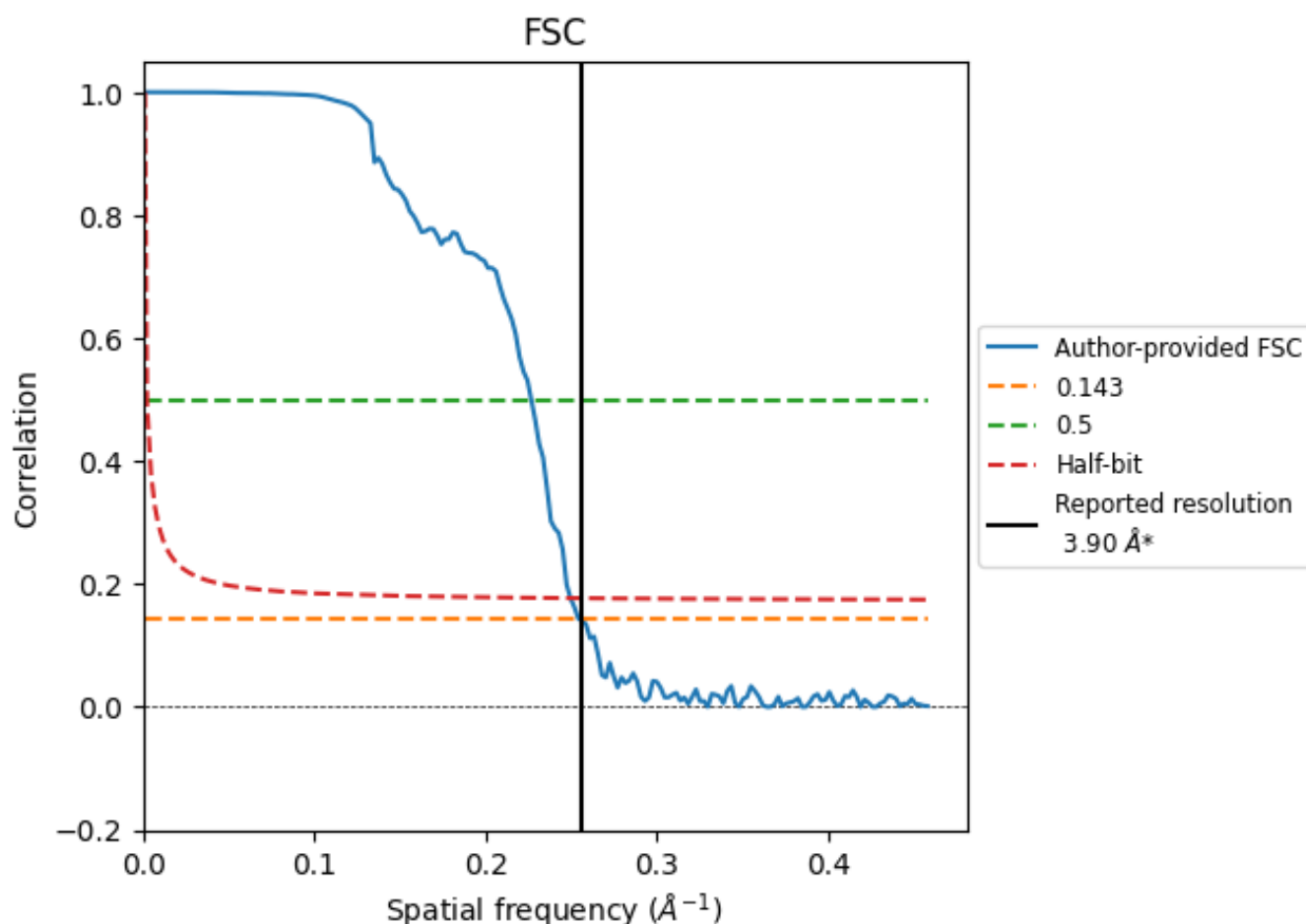


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.93	4.41	4.00
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

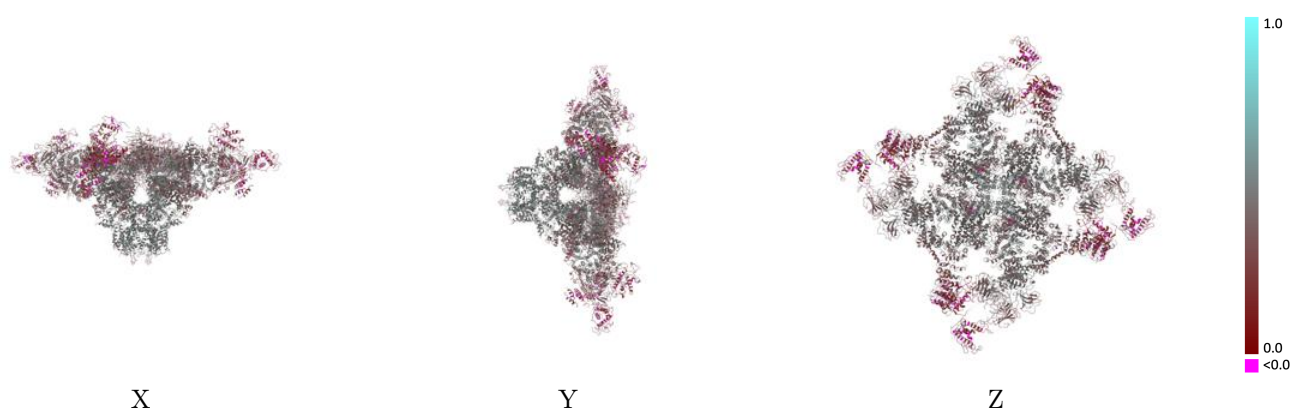
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9879 and PDB model 6JRR. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

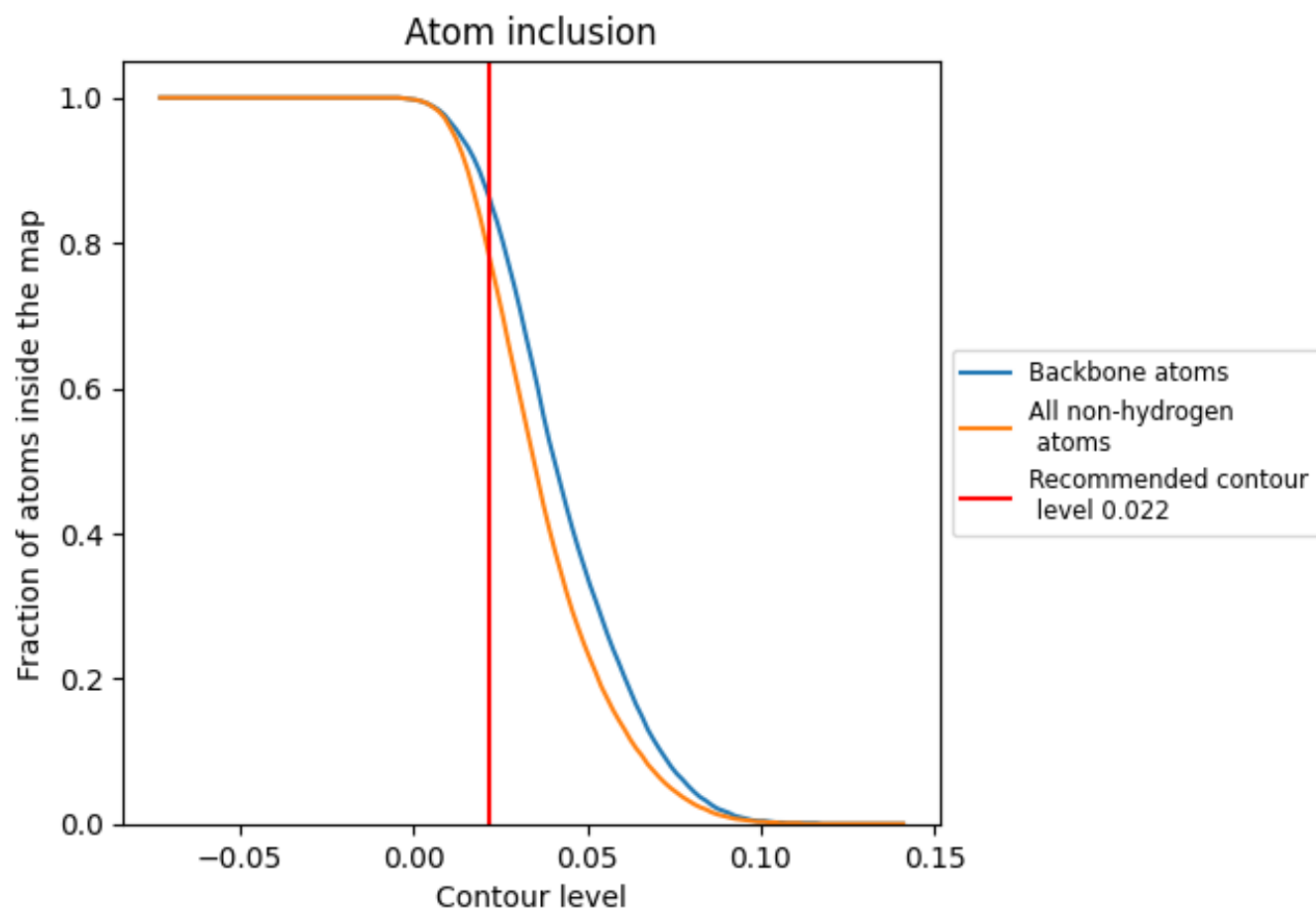


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7780	0.3900
A	0.7770	0.3900
B	0.8140	0.4170
C	0.7770	0.3890
D	0.8150	0.4160
E	0.7770	0.3890
F	0.8180	0.4170
G	0.7770	0.3890
H	0.8150	0.4160

1.0

0.0

<0.0