



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:01 PM UTC

PDB ID : 8UQ2 / pdb_00008uq2
EMDB ID : EMD-42458
Title : Structure of human RyR2-S2808D in the subprimed state
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-10-23
Resolution : 2.98 Å (reported)
Based on initial model : 7UA5

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

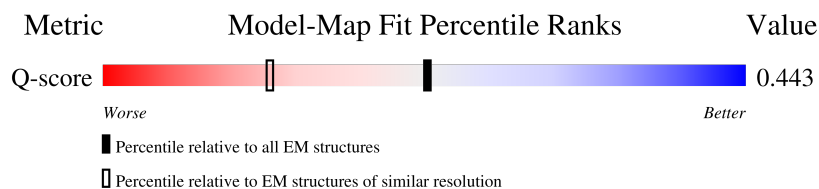
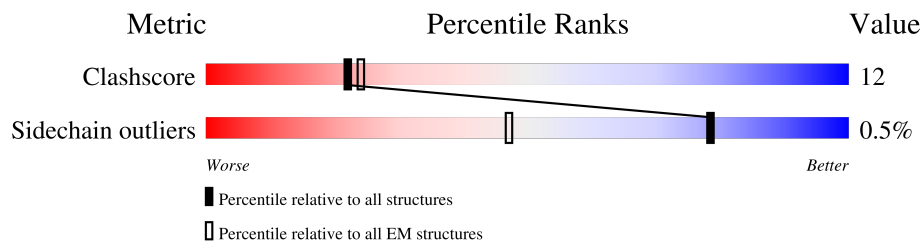
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13236 (2.48 - 3.48)

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	4967	9% 63% 22% 15%
1	B	4967	9% 63% 21% 15%
1	C	4967	9% 63% 21% 15%
1	D	4967	9% 63% 21% 15%
2	E	108	66% 32% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	108	 69%30%..
2	G	108	 66%32%..
2	H	108	 66%32%..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 138608 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	B	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	C	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	D	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2808	ASP	SER	engineered mutation	UNP Q92736
B	2808	ASP	SER	engineered mutation	UNP Q92736
C	2808	ASP	SER	engineered mutation	UNP Q92736
D	2808	ASP	SER	engineered mutation	UNP Q92736

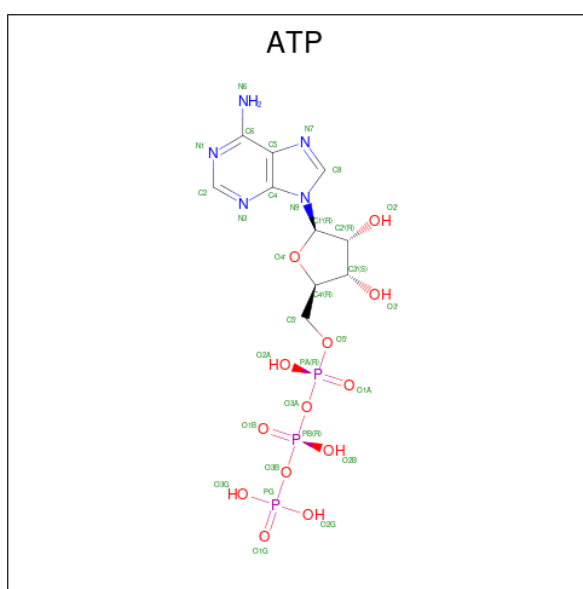
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

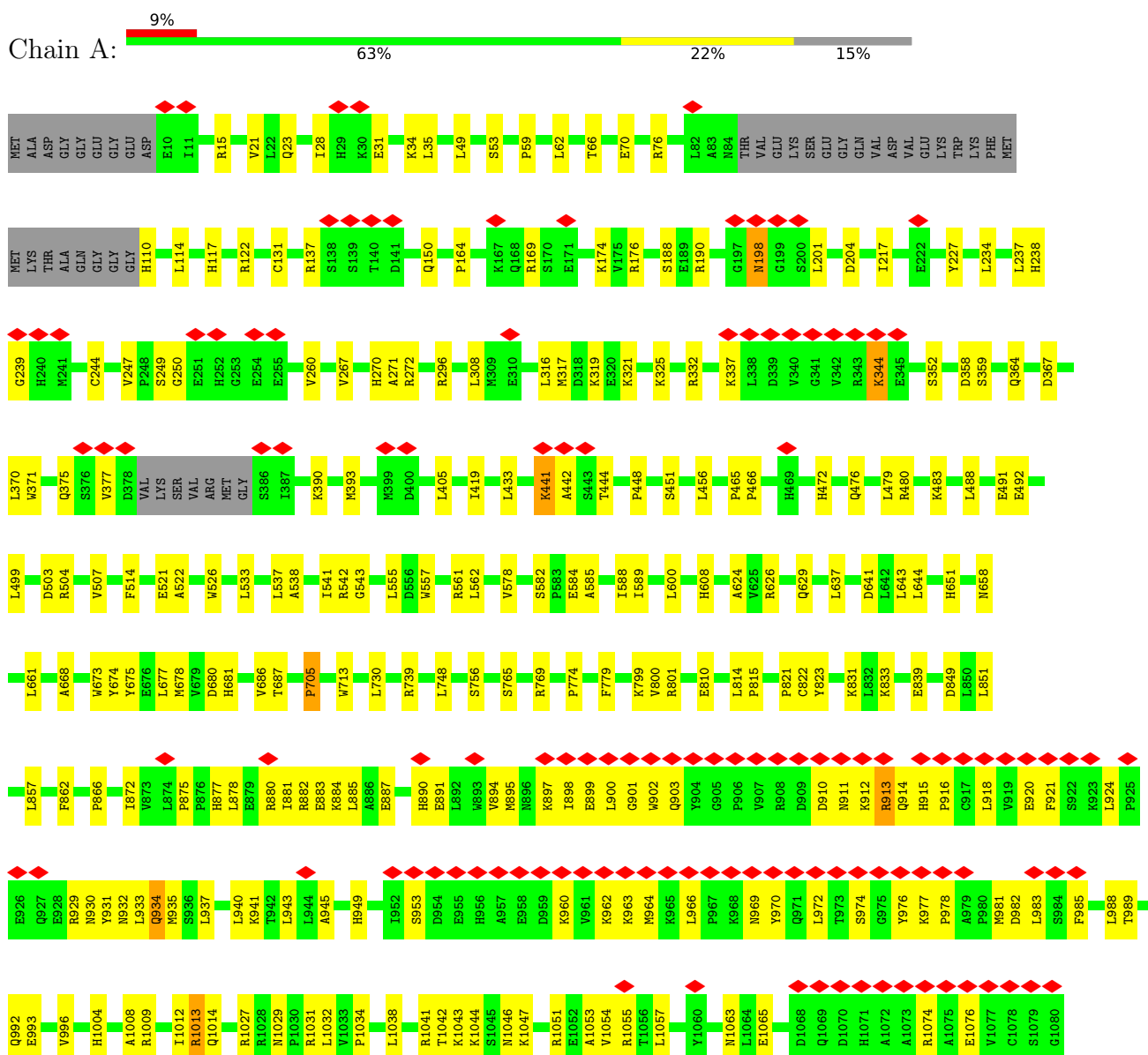
Continued from previous page...

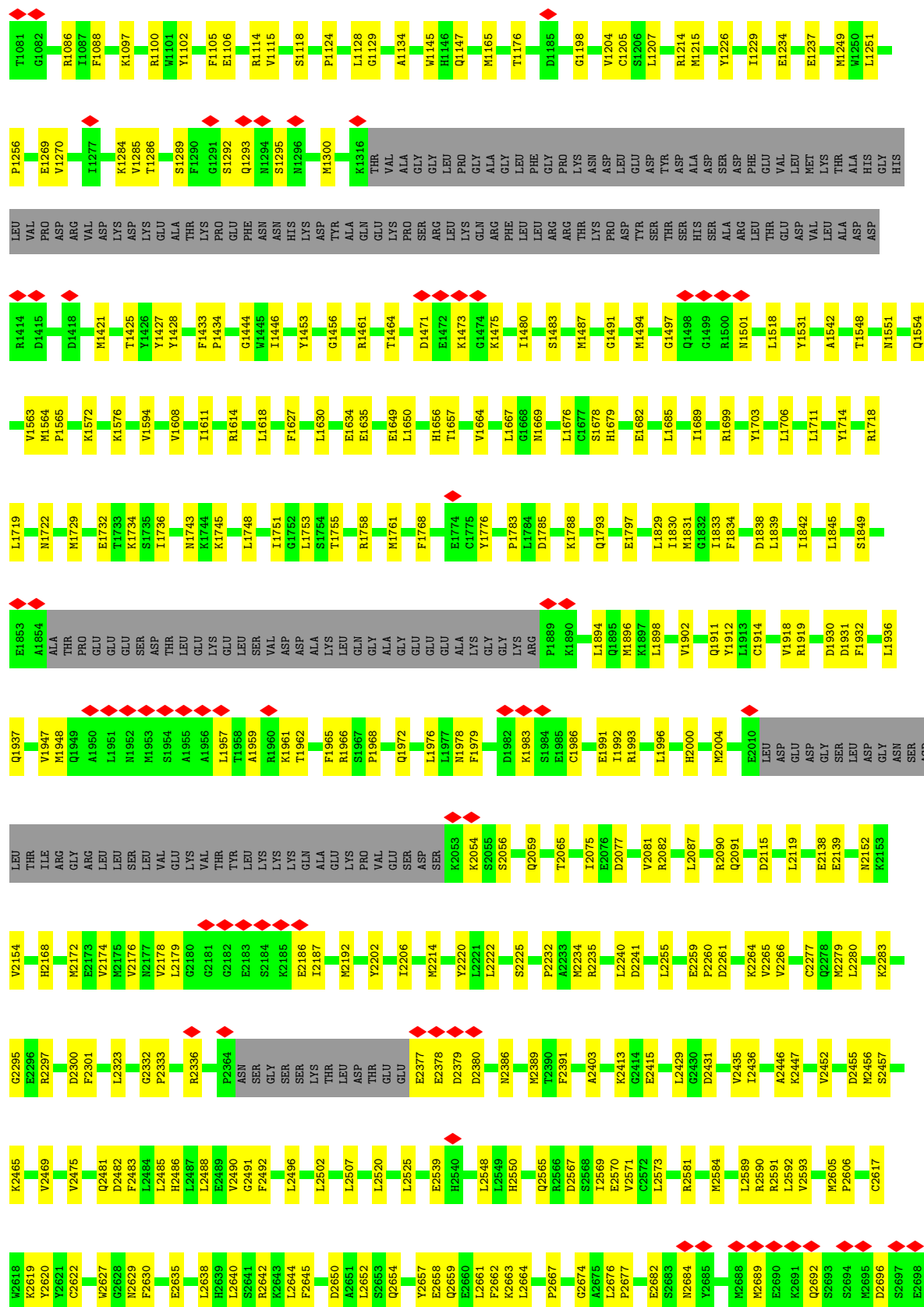
Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots

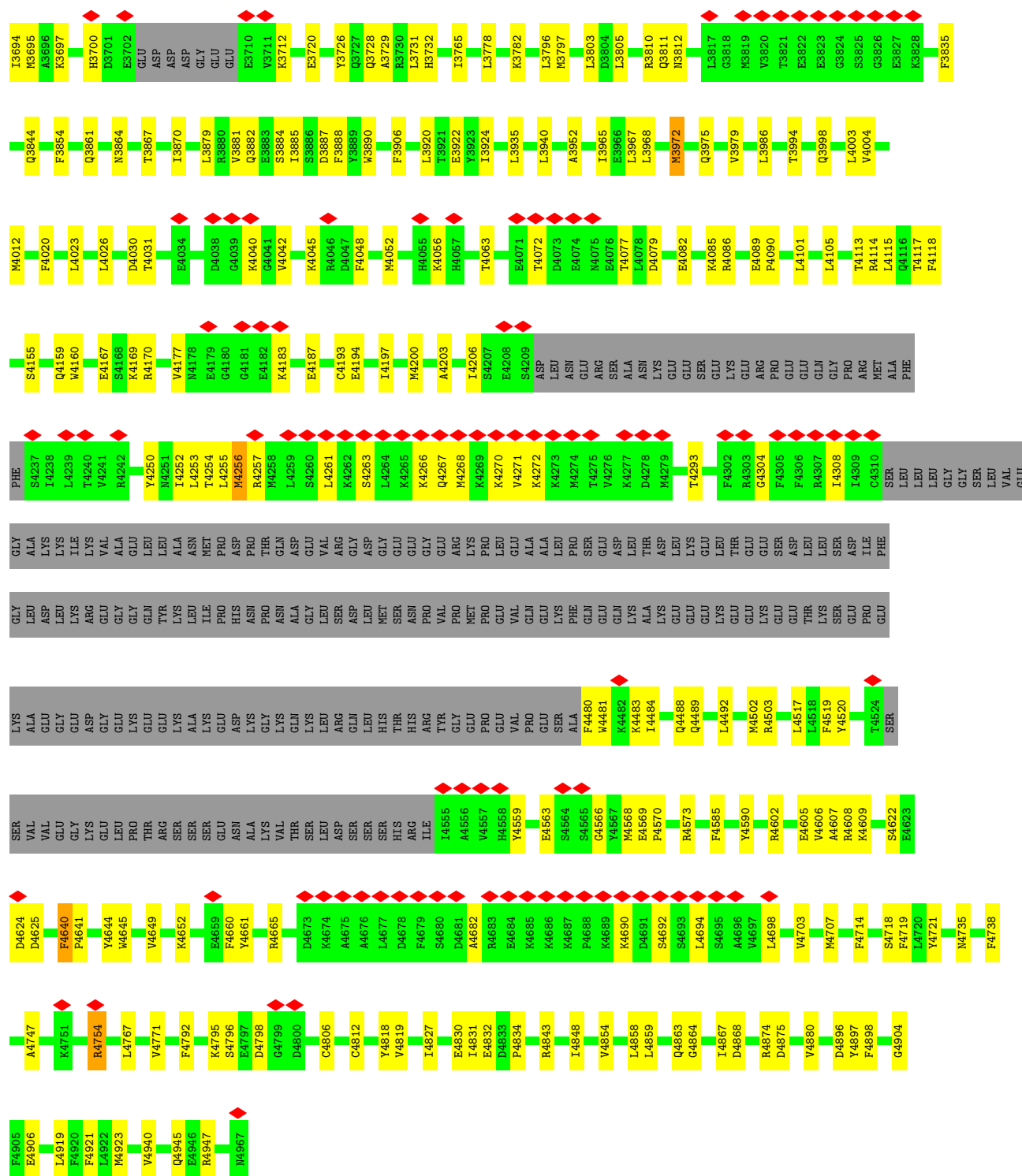
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ryanodine receptor 2



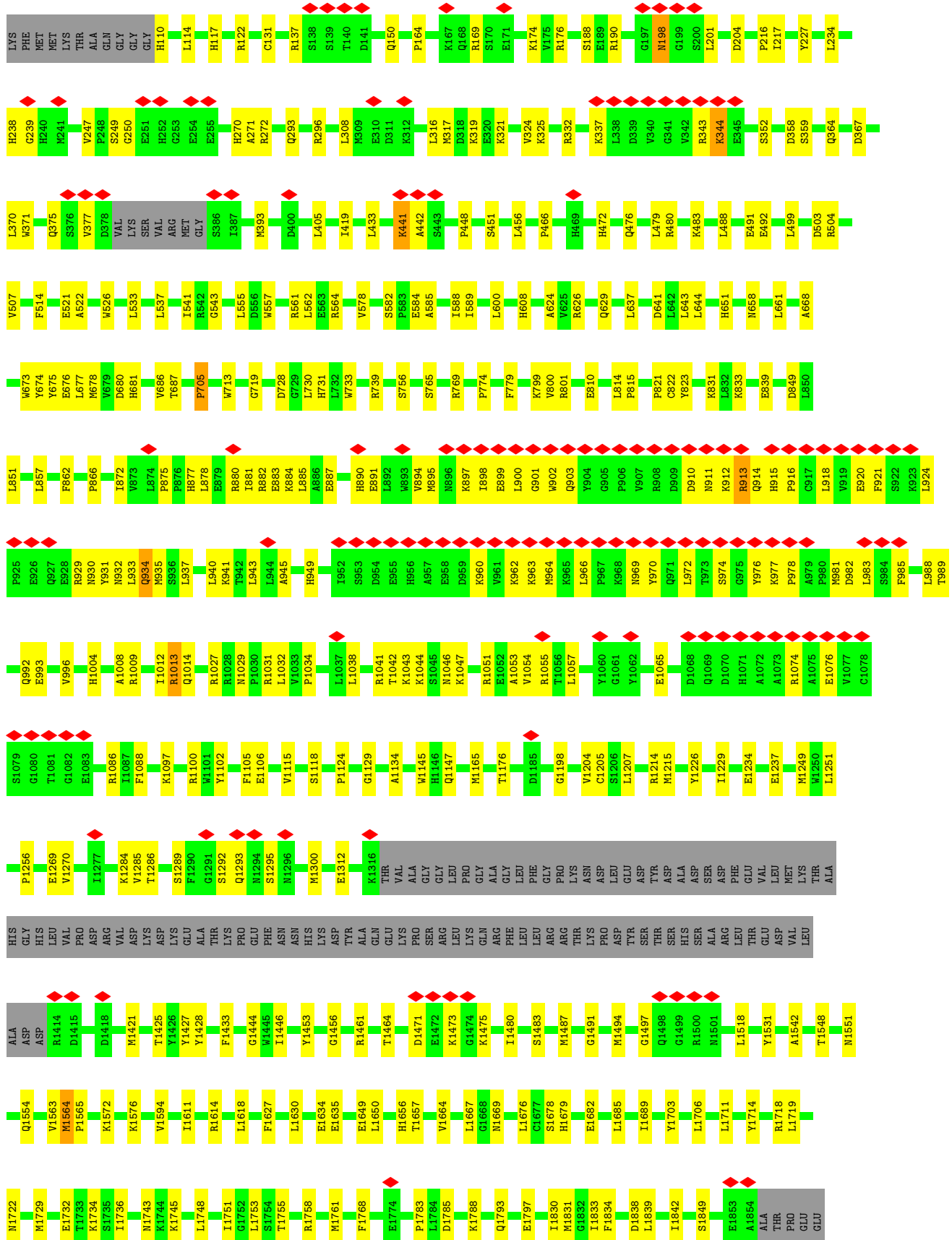






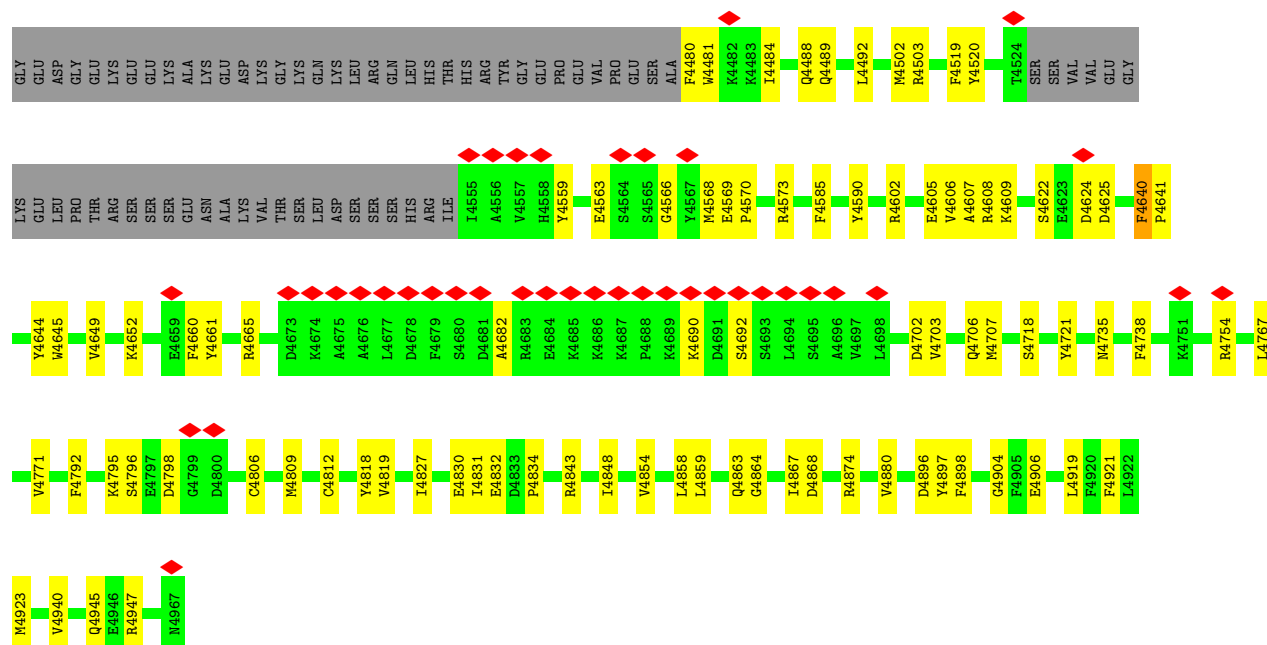
● Molecule 1: Ryanodine receptor 2



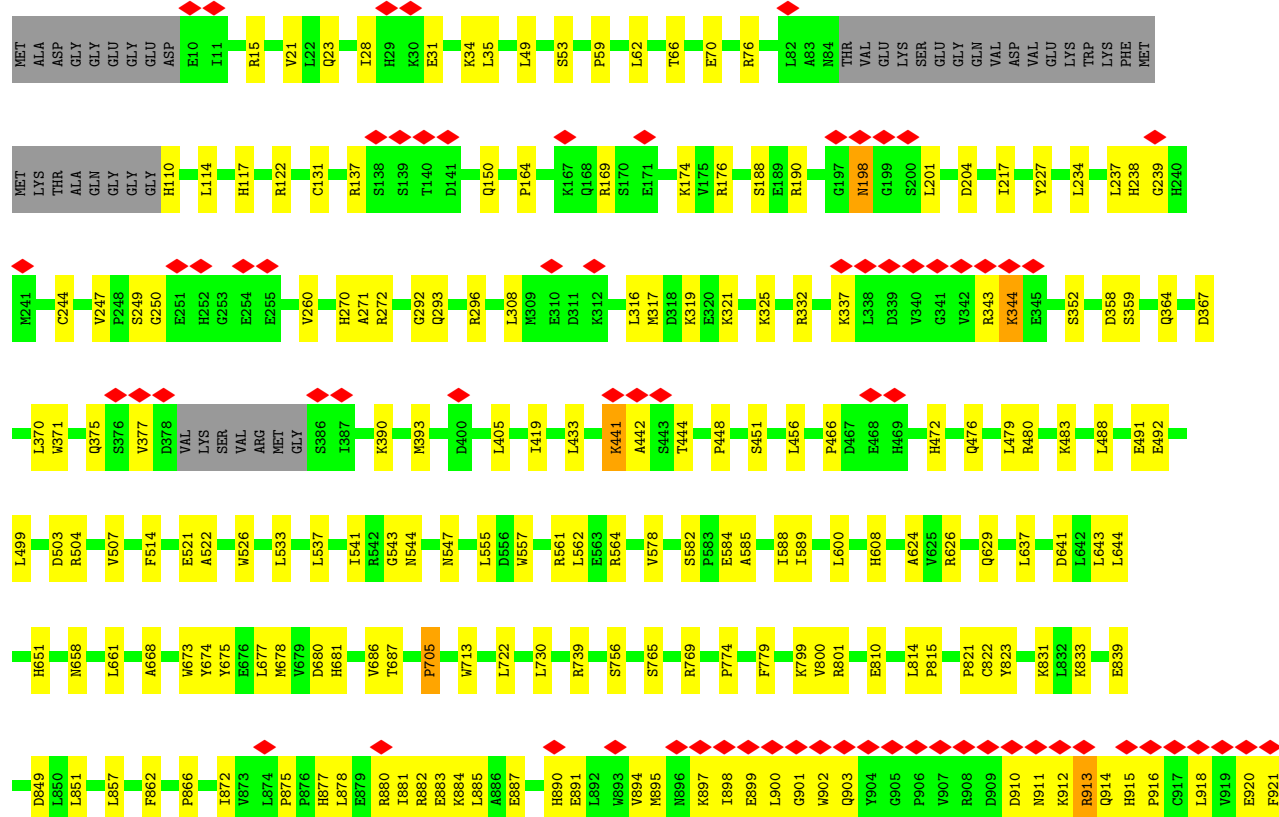


D3067	A996	I2917	W2852	W2785	L2711	G2693	Q2481	D2300	H2168	ARG	Q1949	GLU
L3068	S2997	E2918	A2853	G2786	L2717	N2629	F2482	F2301	M2172	GLY	A1950	SER
K3069	N2998	K2919	K2854	W2787	E2718	F2630	F2483	L2323	E2173	THR	L1951	ASP
K3070	K2999	K2920	K2855	K2788	Y2719	E2635	L2484	L2323	E2174	LEU	N1952	LEU
K3071	K3001	F2921	K2856	E2789	K2723	L2638	L2485	G2332	M2175	SER	M1953	GLU
K3072	E3002	Y2923	K2857	E2790	K2724	H2639	H2486	P2333	W2176	LEU	S1954	LYS
K3073	M3003	Y2924	M2858	T2792	Y2725	S2641	L2487	G2336	M2177	VAL	A1955	GLU
K3074	F2925	F2925	E2859	T2791	E2726	E2489	E2489	R2336	V2178	GLU	A1955	LEU
K3075	T3005	L2926	L2860	K2793	E2727	V2490	E2491	R2336	L2179	SER	A1956	SER
K3076	S3006	Q2927	E2861	E2794	H2727	G2491	F2492	P2364	G2180	VAL	L1957	VAL
Q3077	Q3077	Q2928	E2862	G2795	K2644	K2643	F2492	ASN	G2181	THR	T1958	ASP
G3078	L3007	L2929	K2863	D2796	K2730	L2644	F2645	SER	G2182	TYR	A1959	ASP
Q3079	C3009	Y2932	G2864	A2799	K2731	D2650	L2496	GLY	G2183	LEU	R1960	ALA
F3080	K3010	A2936	G2865	L2800	W2732	D2651	L2502	SER	E2184	LYS	K1961	LYS
F3081	L3011	H2937	G2866	L2801	E2733	L2652	L2502	GLY	S2184	LYS	T1962	LEU
HIS	G3012	H2937	G2866	L2801	M2734	S2653	L2507	SER	K2185	GLN	F1966	GLY
THR	V3013	Q2938	G2867	L2802	K2736	Q2654	L2520	THR	E2186	ALA	R1966	ALA
ARG	L3014	Y2939	H2868	ARG	K2736	Q2654	L2520	LEU	E2187	GLU	S1967	GLY
ASN	V3015	Y2939	H2868	THR	K2736	Q2654	L2520	ASP	M2192	LYS	P1968	GLU
R3016	R3016	F2943	F2869	ARG	K2736	Q2654	L2520	THR	Y2202	VAL	Q1972	GLU
D3025	D3025	D2944	L2870	ARG	K2736	Q2654	L2520	THR	I2206	GLU	L1976	LYS
A3026	A3026	D2944	L2870	ARG	K2736	Q2654	L2520	THR	M2214	ASP	L1977	GLY
T3027	T3027	G2946	Y2874	ILE	K2741	E2660	L2525	GLU	Y2220	SER	N1978	GLY
S3028	S3028	G2946	D2875	ASP	Y2743	F2662	E2539	GLU	L2222	ASP	F1979	LYS
L3029	L3029	S2947	T2876	GLN	Y2743	F2662	H2540	GLU	M2214	SER	D1982	ARG
V3030	V3030	S2947	L2877	THR	E2744	K2663	L2548	GLU	Y2220	ASP	K1983	ARG
N3031	N3031	G2948	T2878	SER	E2745	L2664	L2549	GLU	L2222	ASP	S1984	ARG
C3032	C3032	G2949	T2878	GLN	E2746	L2664	L2549	GLU	S2225	ASP	E1985	ARG
L3033	L3033	K2950	K2882	VAL	Y2747	P2667	H2550	GLU	P2232	ASP	K1986	ARG
H3034	H3034	K2950	K2882	VAL	Y2747	P2667	H2550	GLU	A2233	ASP	P1987	ARG
I3035	I3035	G2951	K2884	ASP	S2748	Q2674	Q2565	GLU	M2234	ASP	E1991	ARG
L3036	L3036	E2952	R2885	ALA	D2749	A2675	R2566	GLU	R2235	ASP	I1992	ARG
L3040	L3040	H2953	R2885	ALA	S2750	D2567	S2568	GLU	L2240	ASP	I1993	ARG
L3044	L3044	E2955	E2887	HIS	S2751	P2677	S2568	GLU	D2241	ASP	L1996	ARG
R3043	R3043	Y2956	K2888	GLN	K2752	E2682	E2570	GLU	L2240	ASP	H2000	ARG
V3044	V3044	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU	E2259	ASP	M2004	ARG
M3045	M3045	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU	P2260	ASP	E2010	ARG
M3046	M3046	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU	D2261	ASP	L2087	ARG
G3047	G3047	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU	K2264	ASP	R2090	ARG
G3048	G3048	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU	V2265	ASP	Q2091	ARG
G3049	G3049	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU	V2266	ASP	D2115	ARG
L3050	L3050	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU	C2277	ASP	L2119	ARG
E3051	E3051	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU	E2138	ASP	E2139	ARG
S3052	S3052	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU	M2279	ASP	L1936	ARG
V3053	V3053	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU	L2280	ASP	Q1937	ARG
K3054	K3054	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU	K2283	ASN	Y1947	ARG
L3057	L3057	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU	R2297	SER	M1948	ARG
R3058	R3058	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU		THR		
A3059	A3059	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU		ILE		
F3060	F3060	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
L3061	L3061	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
G3062	G3062	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
N3063	N3063	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
A3064	A3064	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
A3065	A3065	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
S3066	S3066	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
I3122	I3122	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
L3123	L3123	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
E3124	E3124	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
D3125	D3125	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
V3126	V3126	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
Q3127	Q3127	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
V3128	V3128	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
S3129	S3129	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
C3130	C3130	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
Y3131	Y3131	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
R3132	R3132	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				
I3133	I3133	Y2956	K2888	GLN	Y2753	S2683	E2570	GLU				





• Molecule 1: Ryanodine receptor 2

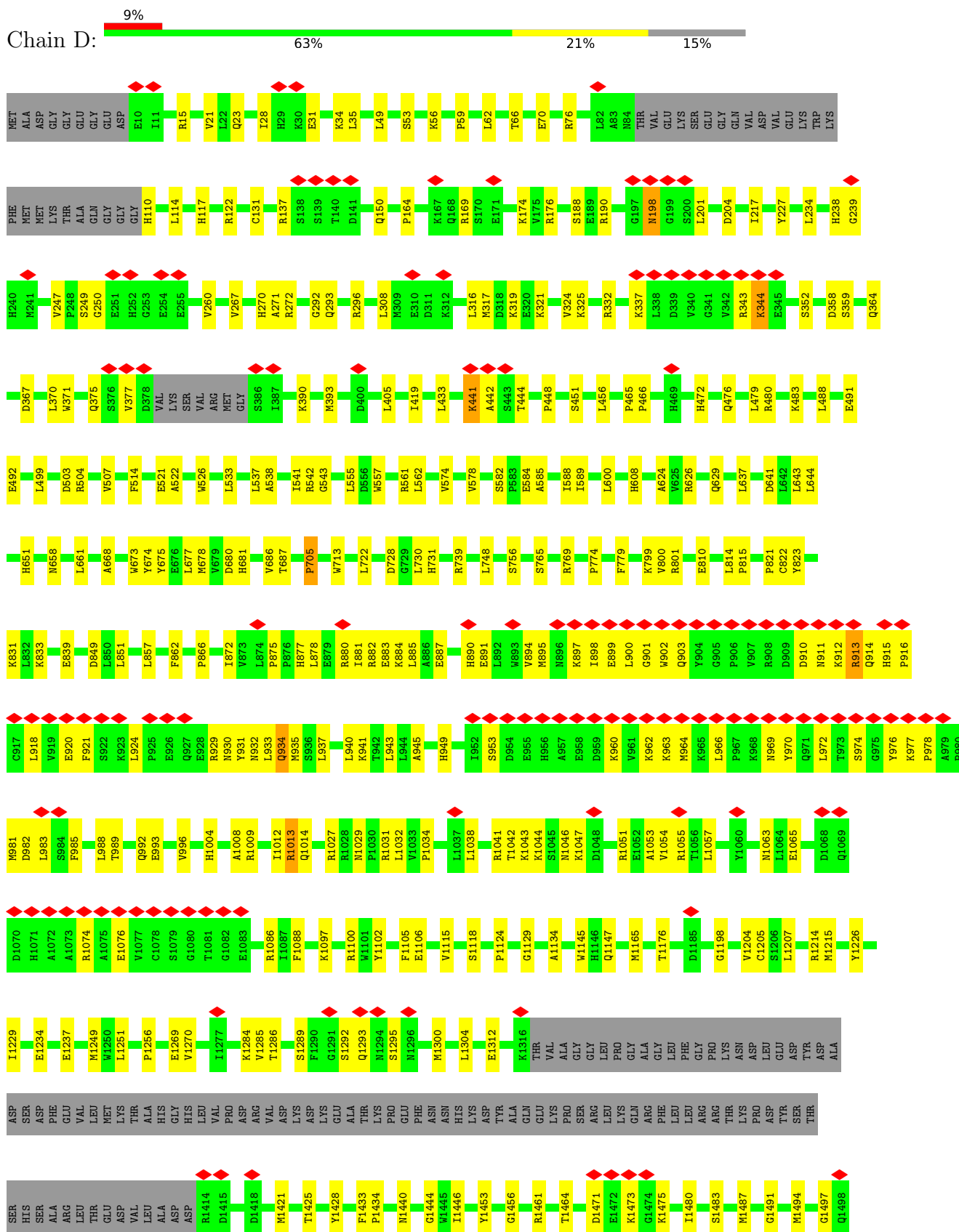




SER	GLU	LEU	L3277	G3278	N3207	V3126	A3959	A2986	F2907	R2835	R2772	G2899	R2456	S2457
MET	GLN	LYS	N3279	N3278	L3211	Q3127	F3060	S2987	K2908	D2836	W2773	N2700	S2457	
THR	PHE	GLU	S3128	S3129	L3211	S3128	D3062	R2988	D2909	L2837	P2774	F2701	K2465	
SER	ILE	ALA	C3130	C3131	N3063	C3130	N3063	P2989	L2910	M2840	K2776	Q2704	V2469	
LEU	THR	ARG	K3213	K3214	A3064	R3132	A3065	C2991	E2911	M2843	L2779	P2705	V2475	
ILE	THR	GLY	R3132	R3133	E3066	R3132	E3066	S2992	L2912	M2844	K2780	N2710		
VAL	LYS	ASP	L3133	L3134	S3067	L3133	S3067	S2992	L2913	A2845	L2781	I2711	Q2481	
ALA	LYS	SER	E3217	E3218	L3068	L3134	L3068	G2993	T2914	E2846	M2782	I2711	D2482	
LEU	HIS	SER	L3137	L3138	E3069	L3137	E3069	G2994	P2915				F2483	
LYS	ASN	ALA	V3138	A3139	K3070	V3138	K3070	H2995	S2916	W2852	V2785	L2717	L2484	
ARG	PHE	GLU	A3139						I2917	A2853	G2786	E2718	L2484	
LEU	LYS	LEU			N2998		N3072	K2999	L2918	K2854	W2787	Y2719	L2485	
LEU	ARG	LEU			E3073		N3074		K2919	K2855	L2788		L2486	
PRO	GLU	ILE	Y3147		L3075		N3074		F2920	K2856	L2789		L2487	
ILE	GLU	LEU			K3076		K3076		E2921	K2857	L2790		L2488	
GLY	ASN	ASP	R3150					E3002	F2922		K2723		L2489	
LEU	ASN	GLY	Q3151				Q3077	M3003	V3004	M2858	Y2724		V2490	
ASN	PHE	GLY	R3152				Q3078	T3005	Y2923	E2859	A2725		K2491	
ILE	VAL	THR	G3156				Q3079	S3006	S2924	L2860	R2791		F2492	
THR	THR	THR					F3080	L3007	F2925	E2861	L2792			
LEU	ALA	LEU						K3008	L2926	E2794	R2793			
ALA	GLN	ALA	L3159				T3081	C3009	Q2927	G2795	H2727			
PRO	ASN	ALA					HIS		D2928	D2796			L2496	
GLY	GLU	ARG	F3162				THR	K3010	L2929	K2731			L2502	
ASP	ILE	ASP					ARG	L3011		W2732			L2507	
LEU	ASN	LEU	A3163				ASN	G3012		S2733			L2520	
LEU	GLU	TYR	G3164				ASN	G3013		M2734			L2525	
ILE	MET	ALA	A3165				GLN	V3013		D2735			L2539	
ALA	PHE	PHE	F3166				PRO	L3014		K2736			H2540	
LEU	LEU	PRO					K3088	R3016					L2548	
ALA	ILE	LEU	V3168				G3089						H2550	
LYS	THR	LEU	A3169				V3090						Q2565	
ASN	ASP	ILE	F3170				T3091						R2566	
THR	THR	ILE	L3171				Q3092						D2567	
ARG	ARG	THR					L3093						S2568	
PHE	LYS	PHE	F3177				L3094						E2570	
VAL	SER	VAL	H3175				K3095						V2571	
LYS	LYS	ASP					Y3096						R2581	
MET	LYS	TYR	D3176				T3097						M2584	
ASP	ASN	ASN	K3177				L3101						L2589	
THR	LYS	ARG	N3179				M3104						R2590	
ALA	ALA	LYS					L3105						K2591	
VAL	VAL	TRP	Y3184				F3109						L2592	
SER	SER	LEU	K3187					R3043					V2593	
ASP	ASP	LYS	S3188				G3113	T3044					M2605	
ILE	ILE	PRO	S3189				Q3114	V3045					S2696	
ASN	ASN	ASN	R3190				H3115	M3046					Q2692	
PRO	PRO	PRO	E3191				Q3116	K3047					S2693	
ALA	ALA	ALA	R3192				Q3117	T3048					S2694	
GLU	GLU	GLU	A3193				G3118	G3049					S2695	
LEU	LEU	LEU	A3194				E3119	S3052					S2696	
PHE	PHE	PHE	L3197				D3120	V3053					S2697	
ARG	ARG	ARG	T3198				L3122	K3054					S2698	
LYS	LYS	LYS	N3200				L3123	L3057						
GLY	GLY	GLY	D3203				E3124	R3058						
ASP	ASP	VAL	V3204				D3125							
HIS	HIS	HIS												
			L3277	G3278	N3207	V3126	A3959	A2986	F2907	R2835	R2772	G2899	R2456	S2457
			N3279	N3278	L3211	S3128	F3060	S2987	K2908	D2836	W2773	N2700	S2457	
			S3128	S3129	L3211	S3128	D3062	R2988	D2909	L2837	P2774	F2701	K2465	
			C3130	C3131	N3063	C3130	N3063	P2989	L2910	M2840	K2776	Q2704	V2469	
			K3213	K3214	A3064	R3132	A3065	C2991	E2911	M2843	L2779	P2705	V2475	
			R3132	R3133	E3066	R3132	E3066	S2992	L2912	M2844	K2780	N2710		
			L3133	L3134	S3067	L3133	S3067	S2992	L2913	A2845	L2781	I2711	Q2481	
			E3217	E3218	L3068	L3134	L3068	G2993	T2914	E2846	M2782		D2482	
			L3137	L3138	E3069	L3137	E3069	G2994	P2915				F2483	
			V3138	A3139	K3070	V3138	K3070	H2995	S2916	W2852	V2785	L2717	L2484	
			A3139						I2917	A2853	G2786	E2718	L2485	
					N2998		N3072	K2999	L2918	K2854	W2787	Y2719	L2486	
			Y3147		L3075		N3074		K2919	K2855	L2788		L2487	
					K3076		K3076		E2920	K2856	L2789		L2488	
			R3150					E3002	F2922	K2857	L2790		L2489	
			Q3151				Q3077	M3003	V3004	M2858	Y2724		V2490	
			R3152				Q3078	T3005	Y2923	E2859	A2725		K2491	
			G3156				Q3079	S3006	S2924	L2860	R2791		F2492	
							F3080	L3007	F2925	E2861	L2792			
								K3008	L2926	E2794	R2793			
			L3159				T3081	C3009	Q2927	G2795	H2727		L2496	
							HIS		D2928	D2796			L2502	
			F3162				THR	K3010	L2929	K2731			L2507	
			A3163				ASN	G3012		S2733			L2520	
			G3164				ASN	G3013		M2734			L2525	
			A3165				GLN	V3013		D2735			L2539	
			F3166				PRO	L3014		K2736			H2540	
							K3088	R3016					L2548	
			V3168				G3089						H2550	
			A3169				V3090						Q2565	
			F3170				T3091						R2566	
			L3171				Q3092						D2567	
							L3093						S2568	
							L3094						E2570	
							K3095						V2571	
			H3175				Y3096						R2581	
			D3176				T3097						M2584	
			K3177				L3101						L2589	
			N3179				M3104						R2590	
							L3105						K2591	
			Y3184				F3109						L2592	
			K3187					R3043					V2593	
			S3188				G3113	T3044					M2605	
			S3189				Q3114	V3045					S2696	
			R3190				H3115	M3046					Q2692	
			E3191				Q3116	K3047					S2693	
			R3192				Q3117	T3048					S2694	
			A3193				G3118	G3049					S2695	
			A3194				E3119	S3052					S2696	
			L3197				D3120	V3053					S2697	
			T3198				L3122	K3054					S2698	
			N3200				L3123	L3057						
			D3203				E3124	R3058						
			V3204				D3125							
			L3277	G3278	N3207	V3126	A3959	A2986	F2907	R2835	R2772	G2899	R2456	S2457
			N3279	N3278	L3211	S3128	F3060	S2987	K2908	D2836	W2773	N2700	S2457	
			S3128	S3129	L3211	S3128	D3062	R2988	D2909	L2837	P2774	F2701	K2465	
			C3130	C3131	N3063	C3130	N3063	P2989	L2910	M2840	K2776	Q2704	V2469	
			K3213	K3214	A3064	R3132	A3065	C2991	E2911	M2843	L2779	P2705	V2475	
			R3132	R3133	E3066	R3132	E3066	S2992	L2912	M2844	K2780	N2710		
			L3133	L3134	S3067	L3133	S3067	S2992	L2913	A2845	L2781	I2711	Q2481	
			E3217	E3218	L3068	L3134	L3068	G2993	T2914	E2846	M2782		D2482	
			L3137	L3138	E3069	L3137	E3069	G2994	P2915				F2483	
			V3138	A3139	K3070	V3138	K3070	H2995	S2916	W2852	V2785	L2717	L2484	
			A3139						I2917	A2853	G2786	E2718	L2485	
					N2998		N3072	K2999	L2918	K2854	W2787	Y2719	L2486	
			Y3147		L3075		N3074		K2919	K2855	L2788		L2487	
					K3076		K3076		E2920	K2856	L2789		L2488	
			R3150					E3002	F2922	K2857	L2790		L2489	
			Q3151				Q3077							

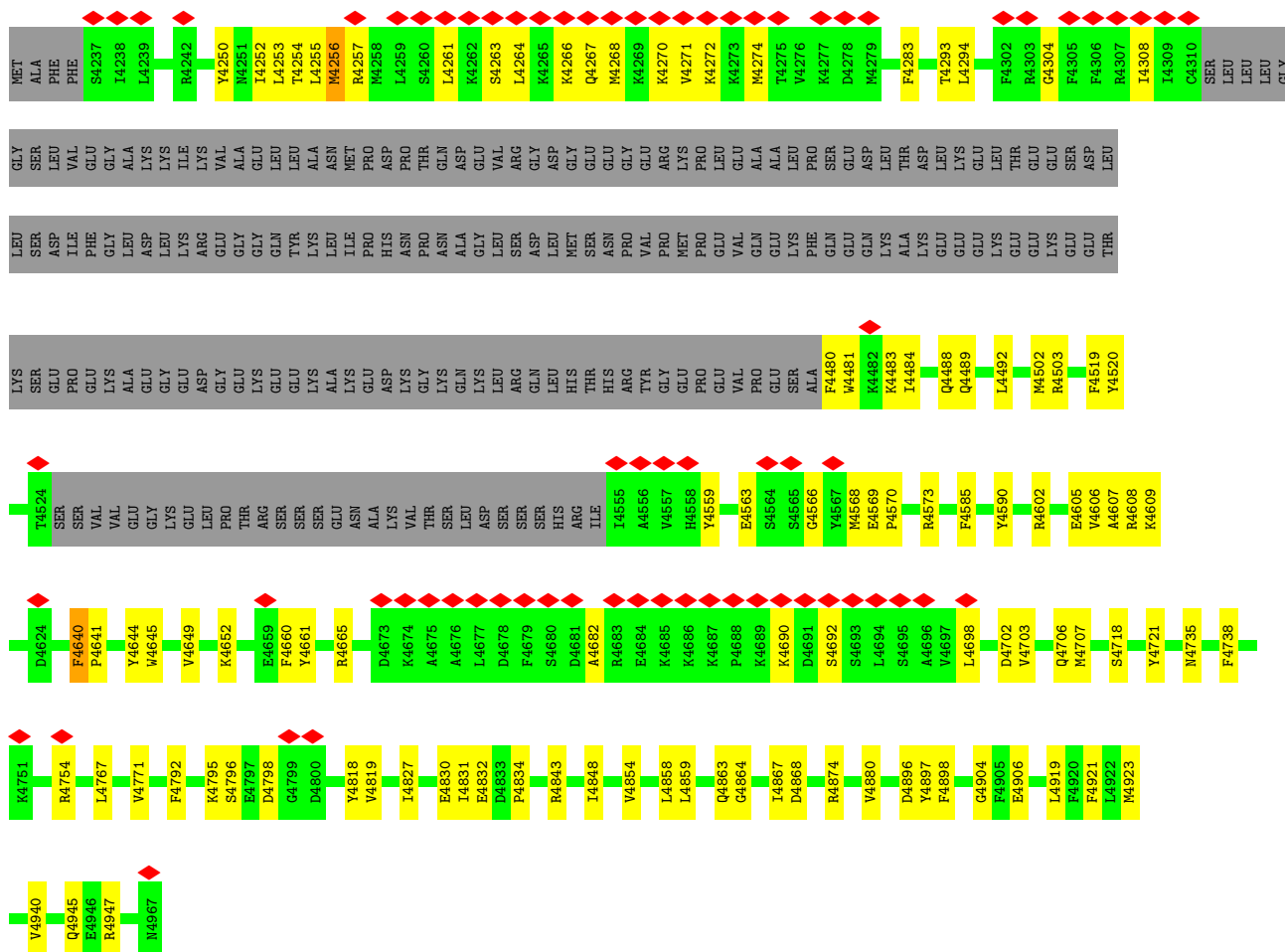


- Molecule 1: Ryanodine receptor 2



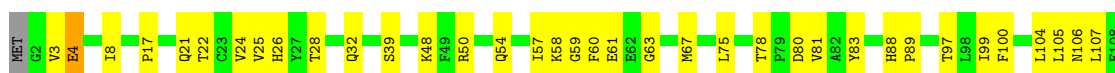
L2898	N2899	A2902	V2903	S2904	R2905	G2906	T2907	K2908	D2909	L2910	E2911	L2912	D2913	T2914	P2915	S2916	L2917	E2918	K2919	R2920	F2921	A2922	S2923	S2924	G2925	L2926	D2927	L2928	L2929	Y2932	A2936	H2937	D2938	Y2939	F2943	D2944	G2945	L2946	S2947	R2948	G2949	K2950	D2951	L2952	H2953	F2954	P2955	Y2956	T2960	V2966	V2967	L2968	P2969				
M2828	S2829	N2830	T2831	T2832	L2833	S2834	R2835	T2836	L2837	M2840	M2843	M2844	A2845	E2846	V2852	A2853	K2854	K2855	K2856	K2857	M2858	E2859	L2860	S2861	S2862	K2863	G2864	G2865	G2866	N2867	H2868	P2869	L2870	Y2874	D2875	T2876	L2877	T2878	E2881	K2882	A2883	K2884	D2885	R2886	E2887	K2888	A2889	Q2890	D2891	L2892	L2893	K2894	F2895				
E2765	K2766	E2767	K2768	E2769	L2770	Y2771	K2772	R2773	T2774	L2775	K2776	L2779	K2780	T2781	N2782	K2785	G2786	K2787	R2788	L2789	E2790	R2791	T2792	R2793	E2794	G2795	D2796	A2799	L2800	Y2801	M2802	ARG	THR	N2739	G2740	W2741	L2742	Y2743	G2744	E2745	L2746	Y2747	S2748	D2749	S2750	S2751	K2752	L2753	Q2754	P2755	L2756	M2757	K2758	P2759	L2762	L2763	S2764
M2584	L2589	R2590	R2591	L2592	V2593	M2605	P2606	C2617	V2618	K2619	Y2620	Y2621	C2622	W2627	G2628	N2629	F2630	E2635	L2638	H2639	L2640	S2641	R2642	K2643	L2644	F2645	D2650	A2651	L2652	S2653	Q2654	Q2659	F2662	K2663	L2664	P2667	G2674	L2675	L2676	P2677	E2682	S2683	Y2684	Y2685	M2688	M2689											
D2431	V2435	T2436	A2446	K2447	V2452	D2455	N2456	S2457	K2465	V2469	V2475	Q2481	D2482	F2483	L2484	H2486	L2487	L2488	E2489	G2491	F2492	L2496	L2502	L2507	L2520	L2525	E2539	H2540	L2548	L2549	H2550	Q2565	R2566	D2567	S2568	L2569	V2570	V2571	R2581																		
P2260	D2261	K2264	V2265	D2266	C2277	Q2278	L2280	K2283	G2295	E2296	R2297	D2300	F2301	L2323	G2332	P2333	R2336	P2364	ASN	GLY	SER	SER	SER	LYS	THR	LEU	ASP	THR	GLU	E2377	E2378	D2379	D2380	N2386	M2389	T2390	F2391	A2403	K2413	G2414	E2415	L2429	G2430														
L2087	R2090	Q2091	D2115	L2119	E2138	E2139	N2152	K2153	V2154	H2168	K2172	E2173	V2174	L2175	V2176	N2177	L2179	G2180	Q2181	G2182	E2183	S2184	K2185	E2186	L2187	K2192	Y2202	L2206	M2214	Y2220	L2221	L2222	S2225	P2232	K2233	K2234	R2235	L2240	D2241	L2255	E2259																
E2010	LEU	ASP	GLU	ASP	GLY	SER	LEU	LEU	ASP	GLY	ASN	SER	ASP	LEU	THR	ILE	ARG	GLY	ARG	ARG	LEU	LEU	SER	LEU	VAL	GLU	LYS	VAL	THR	TYR	ASN	LYS	GLY	LYS	GLN	ALA	GLU	PRO	VAL	GLU	SER	ASP	SER	K2053	K2054	S2055	S2056	Q2059	T2065	T2075	E2076	D2077	V2081	R2082			
C1914	V1918	R1919	I1922	V1926	D1930	D1931	F1932	L1936	Q1937	V1947	M1948	Q1949	A1950	L1951	M1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	K1960	K1961	T1962	F1965	R1966	S1967	P1968	Q1972	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	E1991	I1992	R1993	L1996	H2000	M2004												
I1833	F1834	D1838	L1839	I1842	S1849	E1853	A1854	ALA	THR	PRO	GLU	GLU	SER	GLY	THR	LEU	GLU	SER	VAL	ASP	ASP	ALA	LYS	GLN	GLY	GLY	GLY	GLY	GLU	GLU	ALA	LYS	GLY	GLY	LYS	ARG	P1889	K1890	L1894	Q1895	M1896	K1897	L1898	V1902	Q1911	Y1912	L1913										
I1689	R1699	Y1703	L1706	L1711	Y1714	R1718	L1719	N1722	M1729	E1732	T1733	K1734	S1735	I1736	N1743	K1744	K1745	L1748	T1751	G1752	S1754	T1755	R1758	M1761	F1768	E1774	P1783	L1784	D1785	K1788	Q1793	E1797	L1829	I1830	M1831	G1832																					
G1499	R1500	M1501	L1518	Y1531	A1542	Q1546	A1547	T1548	S1549	P1550	M1551	Q1554	Y1563	M1564	P1565	K1572	K1576	V1594	V1608	I1611	R1614	S1618	F1627	L1630	E1634	E1635	E1649	L1650	H1656	T1657	L1667	G1668	N1669	S1678	H1679	E1682	L1685																				

R4114	T3994	E3823	H3665	CYS	HIS	ARG	GLU	V3334	S3270	A3193	Q3116	T3048	R4115	L4116	G3824	Q3666	LEU	LEU	GLN	LEU	HIS	ASP	S3335	E3336	E3337	S3271	E3272	M3273	L3276	L3277	G3278	LYS	LEU	HIS	ASP	A3194	Q3117	T3049	R4117	Q3998	L3667	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
-------	-------	-------	-------	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



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

Chain E: 66% 32% ::



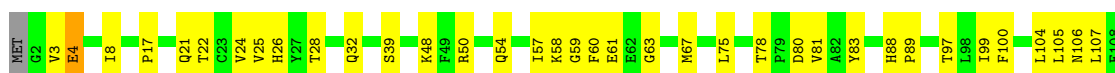
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 69% 30% ::



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

Chain G: 66% 32% ::



- 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	191898	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	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.628	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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

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	0.15	0/34511	0.44	7/46614 (0.0%)
1	B	0.15	0/34511	0.44	7/46614 (0.0%)
1	C	0.15	0/34511	0.44	7/46614 (0.0%)
1	D	0.15	0/34511	0.44	7/46614 (0.0%)
2	E	0.17	0/834	0.40	0/1123
2	F	0.17	0/834	0.40	0/1123
2	G	0.17	0/834	0.40	0/1123
2	H	0.17	0/834	0.40	0/1123
All	All	0.15	0/141380	0.44	28/190948 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	705	PRO	CA-C-N	6.74	132.09	121.17
1	A	705	PRO	C-N-CA	6.74	132.09	121.17
1	D	705	PRO	CA-C-N	6.71	132.05	121.17
1	D	705	PRO	C-N-CA	6.71	132.05	121.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	705	PRO	CA-C-N	6.71	132.03	121.17

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3227	ARG	Sidechain
1	A	3606	ALA	Peptide
1	A	4640	PHE	Peptide
1	B	3227	ARG	Sidechain
1	B	3606	ALA	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	33771	0	33455	795	0
1	B	33771	0	33455	785	0
1	C	33771	0	33455	791	0
1	D	33771	0	33455	789	0
2	E	818	0	821	25	0
2	F	818	0	821	22	0
2	G	818	0	821	23	0
2	H	818	0	821	25	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	0	0
4	B	62	0	24	0	0
4	C	62	0	24	0	0
4	D	62	0	24	0	0
All	All	138608	0	137200	3181	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 12.

The worst 5 of 3181 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:2736:LYS:NZ	1:A:2757:MET:SD	2.38	0.97
1:D:2736:LYS:NZ	1:D:2757:MET:SD	2.38	0.97
1:C:2736:LYS:NZ	1:C:2757:MET:SD	2.38	0.97
1:B:2736:LYS:NZ	1:B:2757:MET:SD	2.38	0.96
1:A:901:GLY:HA3	1:A:913:ARG:HH22	1.36	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3550/4358 (82%)	3532 (100%)	18 (0%)	81	89
1	B	3708/4358 (85%)	3689 (100%)	19 (0%)	81	89
1	C	3708/4358 (85%)	3689 (100%)	19 (0%)	81	89
1	D	3708/4358 (85%)	3689 (100%)	19 (0%)	81	89
2	E	88/89 (99%)	87 (99%)	1 (1%)	65	82
2	F	88/89 (99%)	87 (99%)	1 (1%)	65	82
2	G	88/89 (99%)	87 (99%)	1 (1%)	65	82
2	H	88/89 (99%)	87 (99%)	1 (1%)	65	82
All	All	15026/17788 (84%)	14947 (100%)	79 (0%)	78	89

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3972	MET
1	D	2925	PHE
1	C	4754	ARG
1	D	1013	ARG
1	D	3215	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3770	ASN
1	D	2937	HIS
1	C	903	GLN
1	D	2830	ASN
1	D	4251	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 12 ligands modelled in this entry, 4 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
4	ATP	A	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	D	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	A	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	D	5003	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	B	5003	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	B	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	C	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	C	5002	-	32,33,33	0.27	0	48,52,52	0.30	0

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
4	ATP	A	5002	-	-	6/22/38/38	0/3/3/3
4	ATP	D	5002	-	-	6/22/38/38	0/3/3/3
4	ATP	A	5003	-	-	7/22/38/38	0/3/3/3
4	ATP	D	5003	-	-	7/22/38/38	0/3/3/3
4	ATP	B	5003	-	-	7/22/38/38	0/3/3/3
4	ATP	B	5002	-	-	6/22/38/38	0/3/3/3
4	ATP	C	5003	-	-	7/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

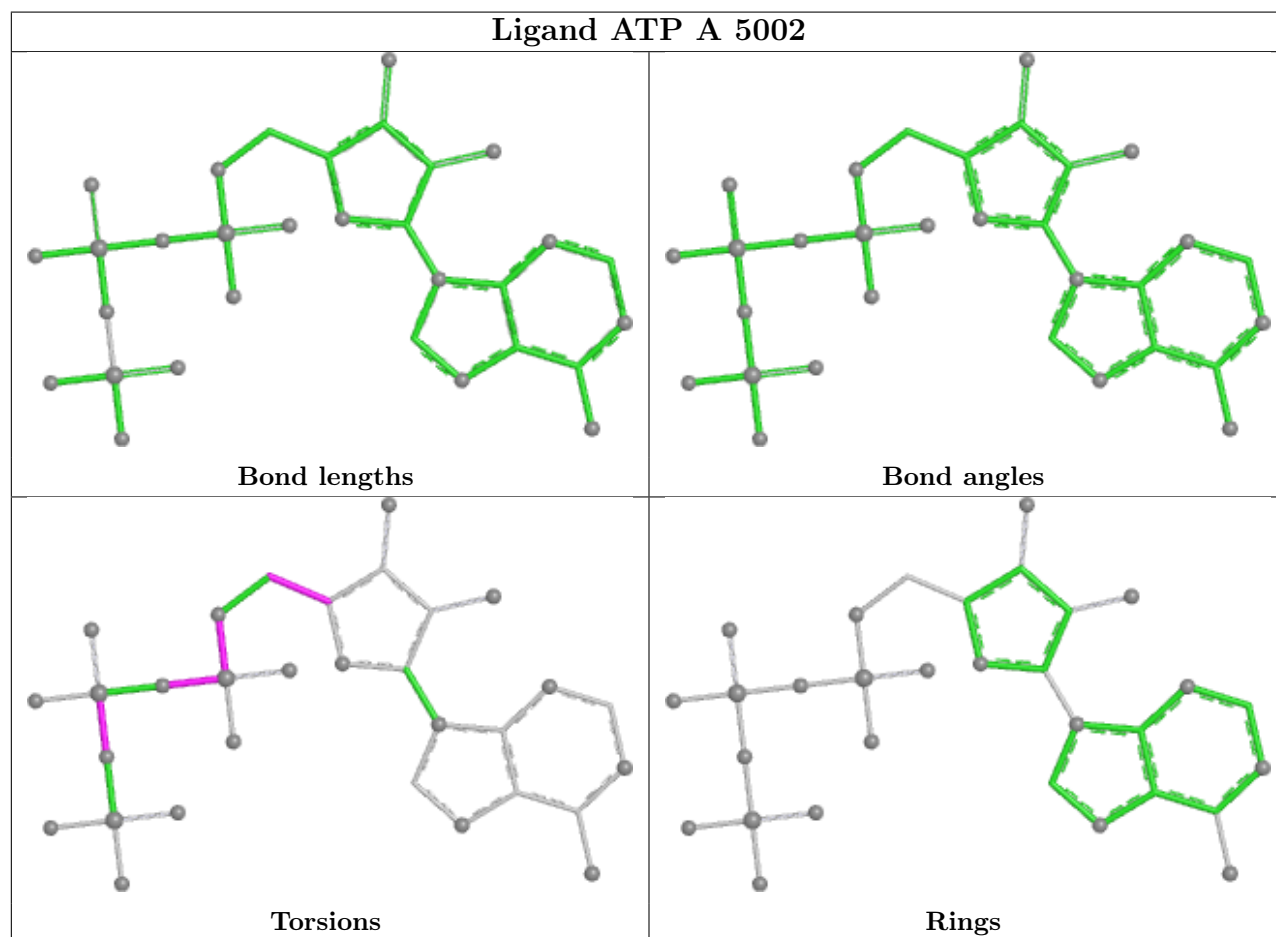
5 of 52 torsion outliers are listed below:

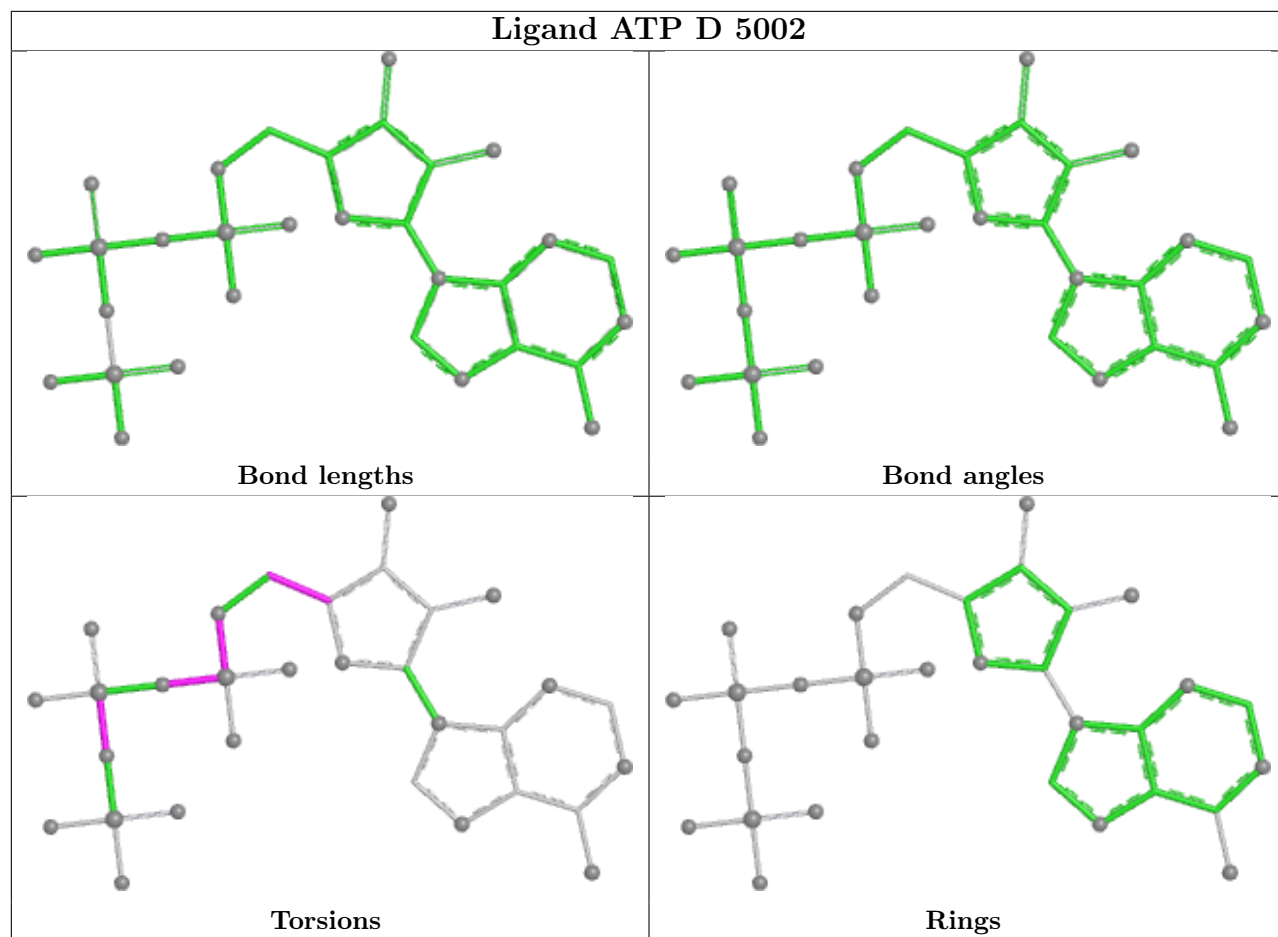
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	PB-O3B-PG-O3G
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A

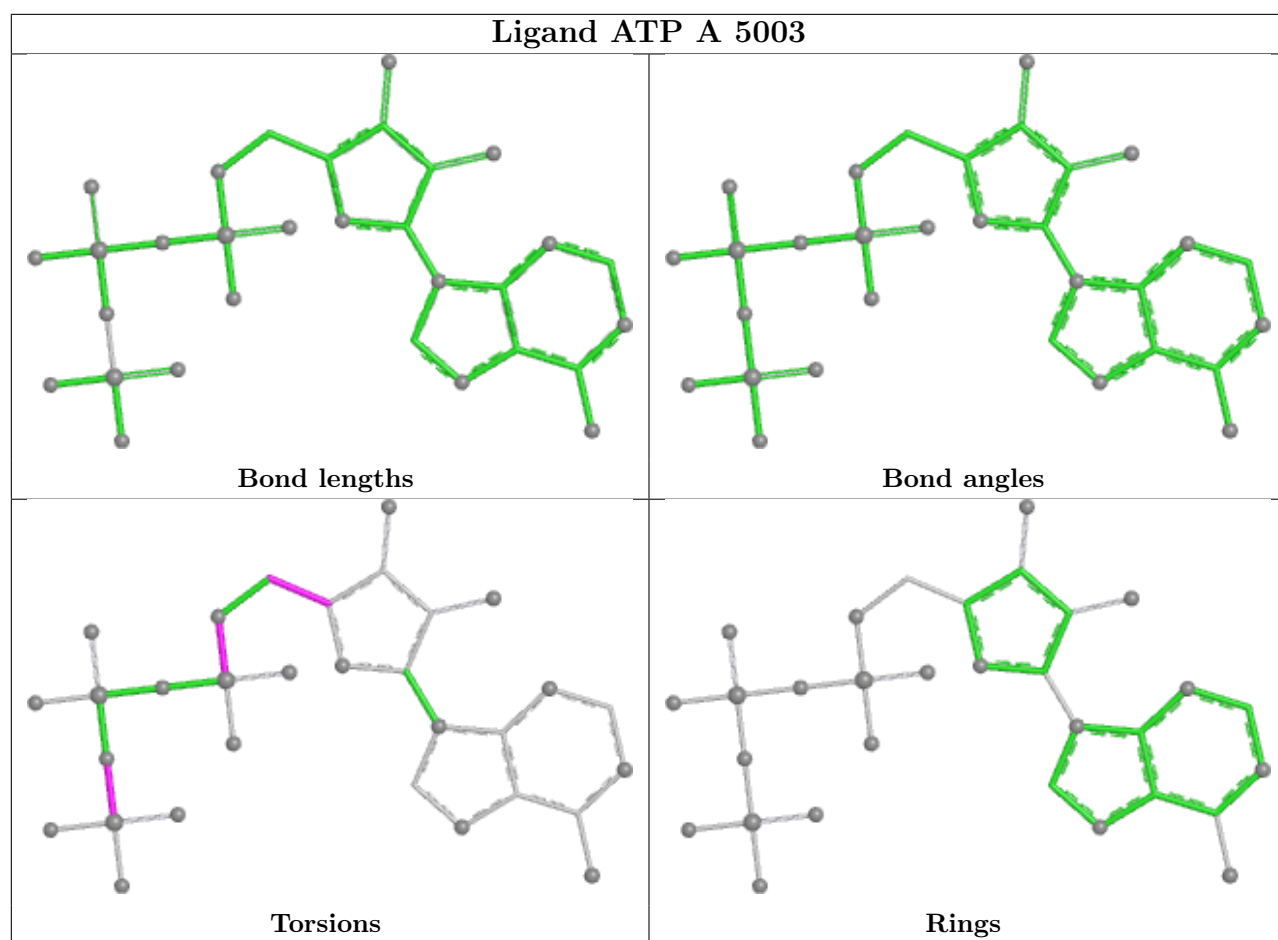
There are no ring outliers.

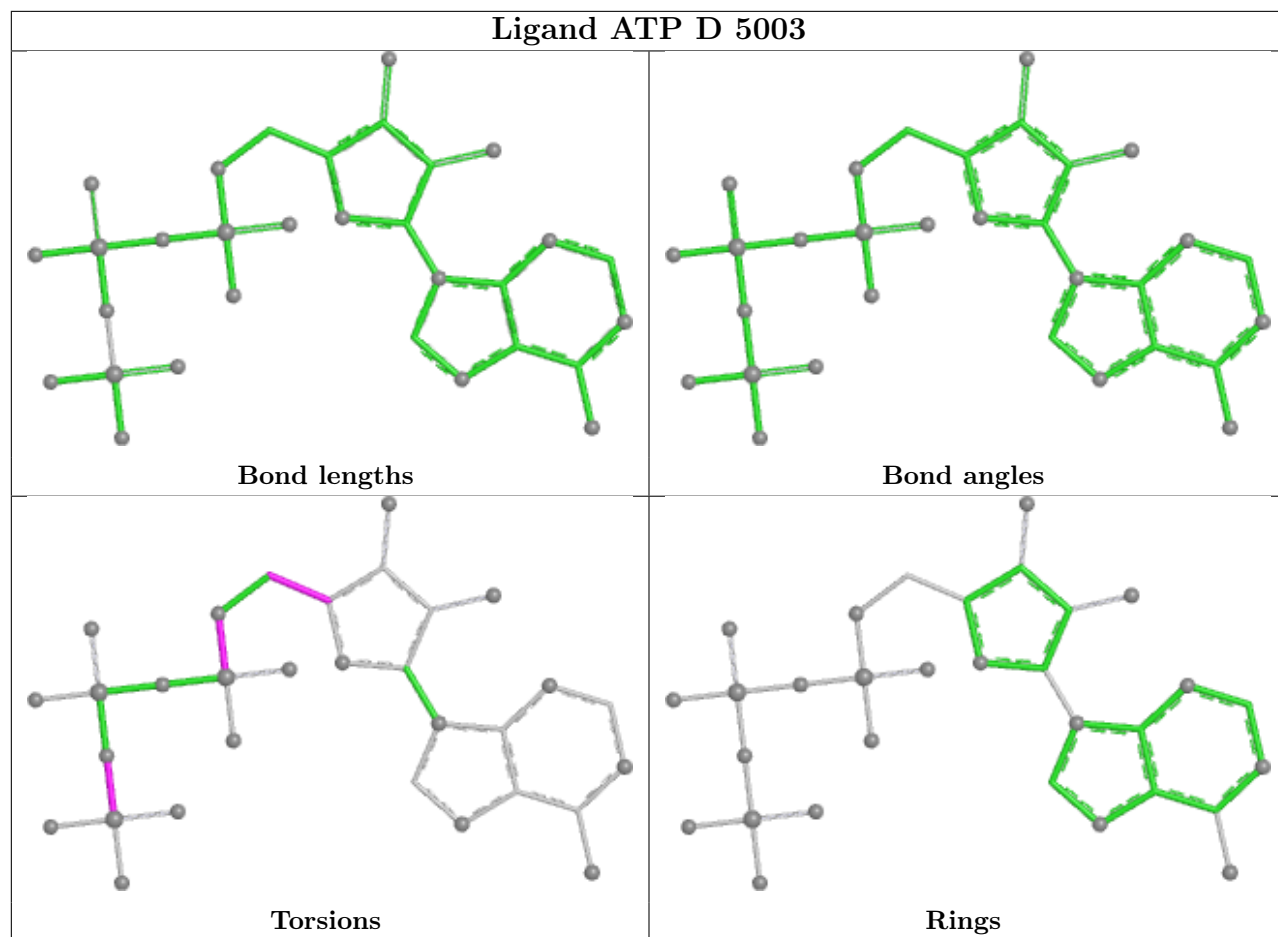
No monomer is involved in short contacts.

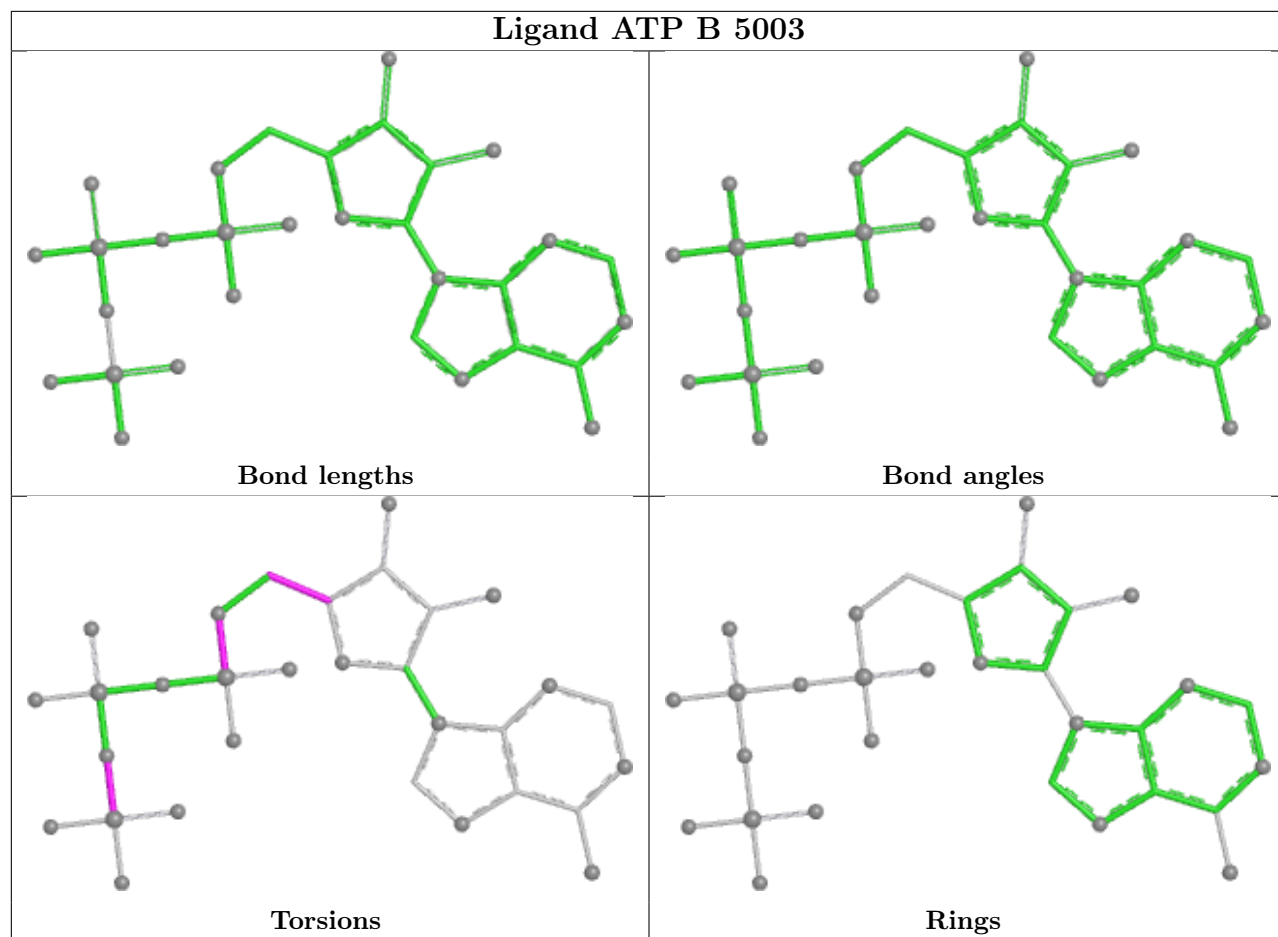
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

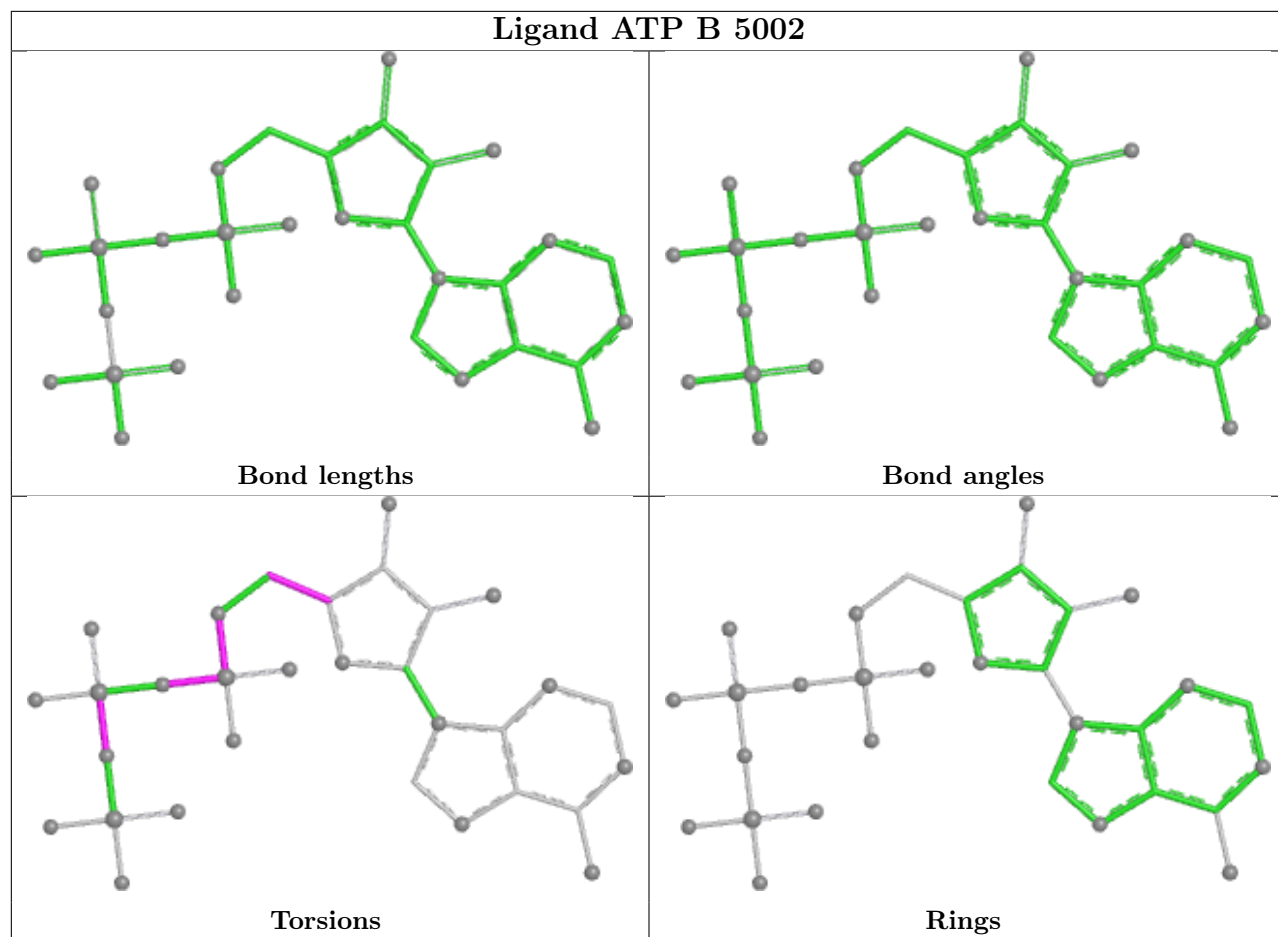


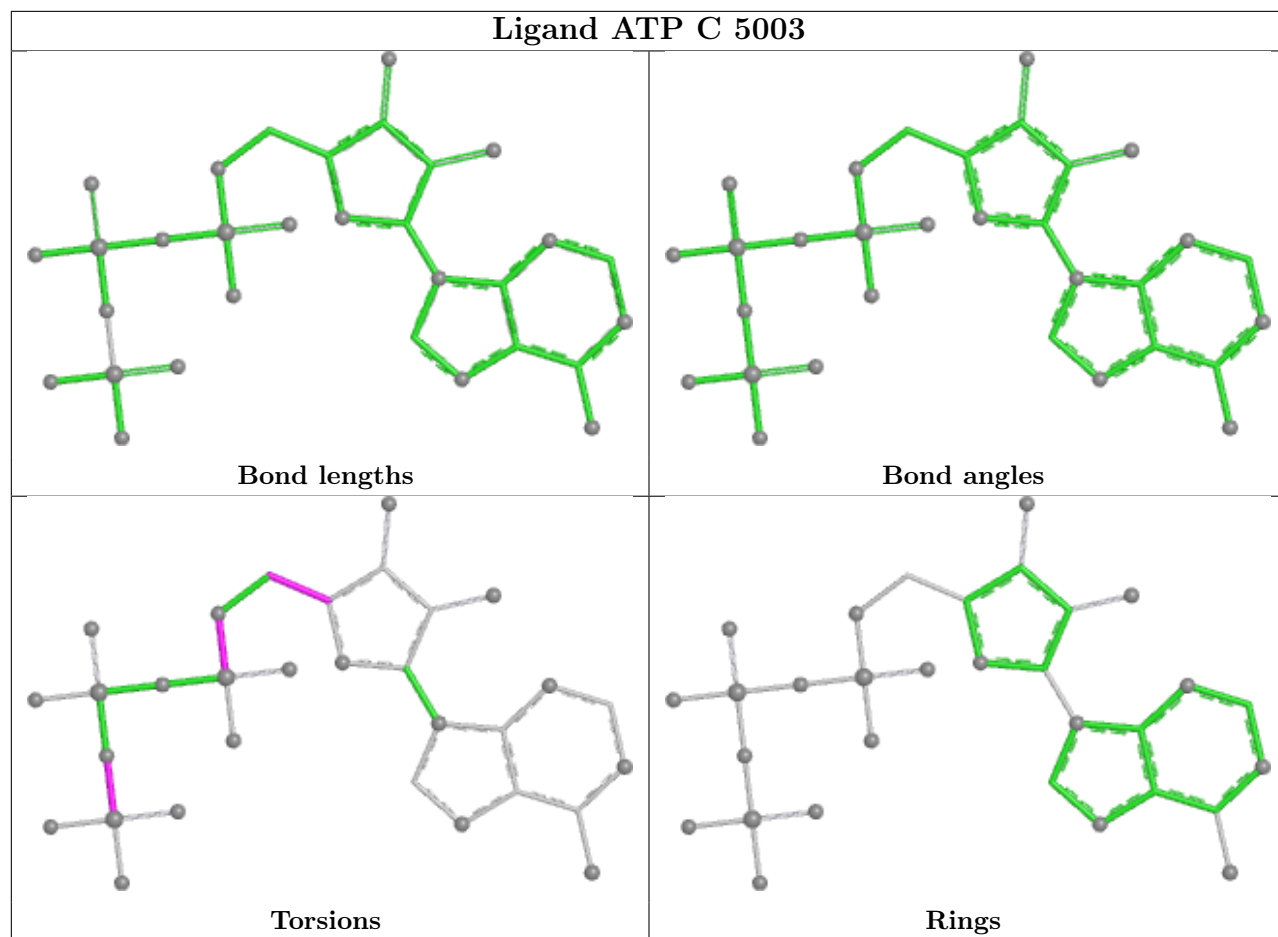


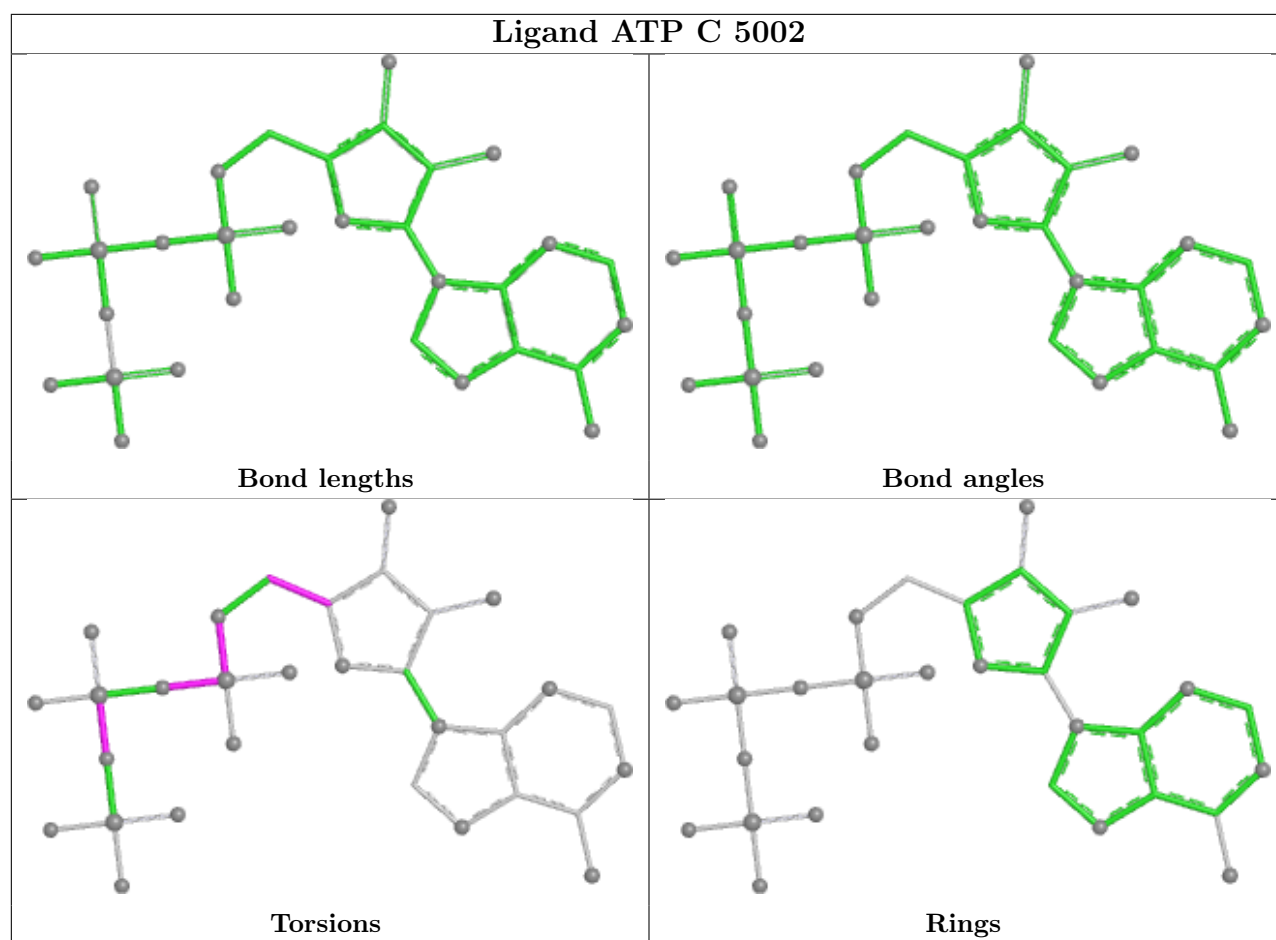












5.7 Other polymers [i](#)

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-42458. These allow visual inspection of the internal detail of the map and identification of artifacts.

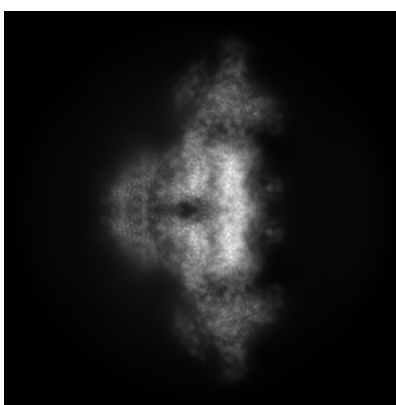
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

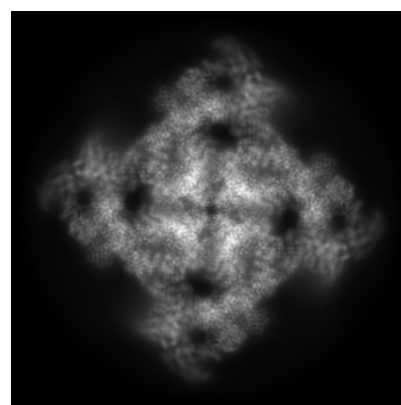
6.1.1 Primary map



X



Y

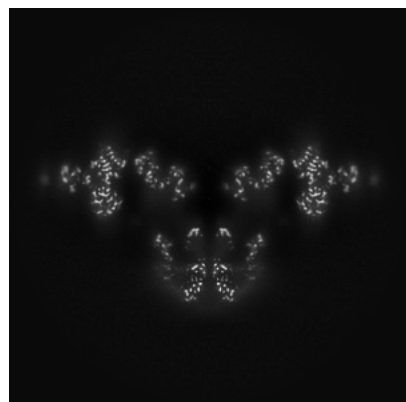


Z

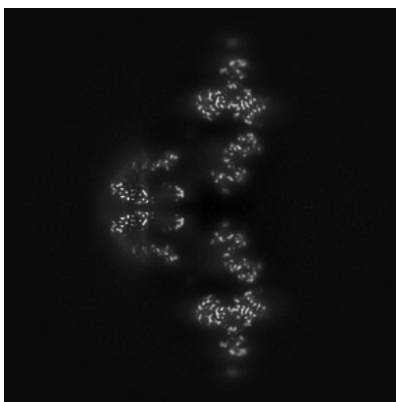
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

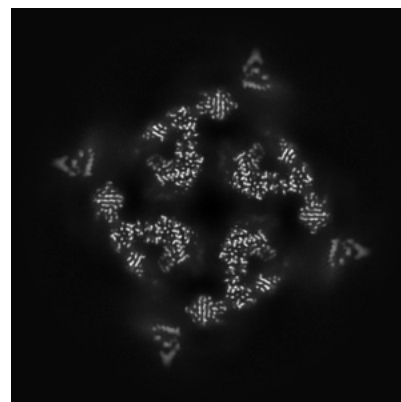
6.2.1 Primary map



X Index: 256



Y Index: 256

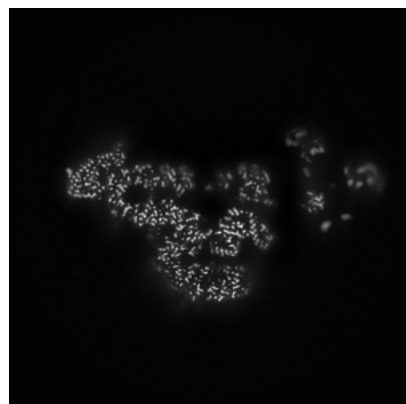


Z Index: 256

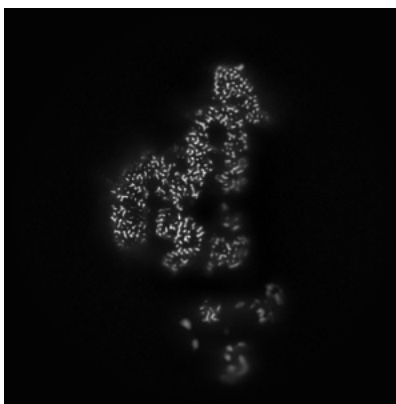
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

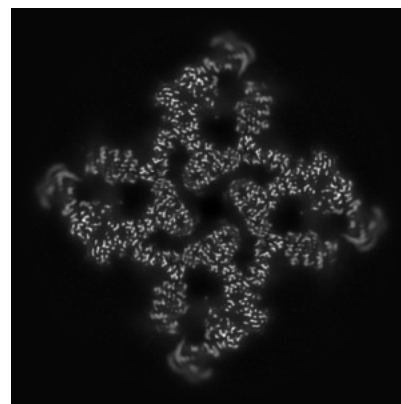
6.3.1 Primary map



X Index: 279



Y Index: 279

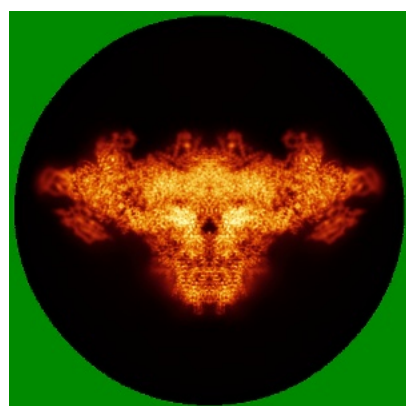


Z Index: 290

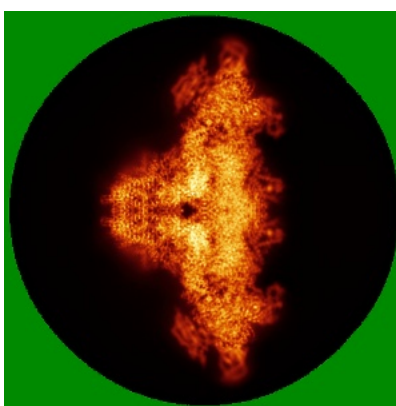
The images above show the largest variance slices of the map in three orthogonal directions.

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

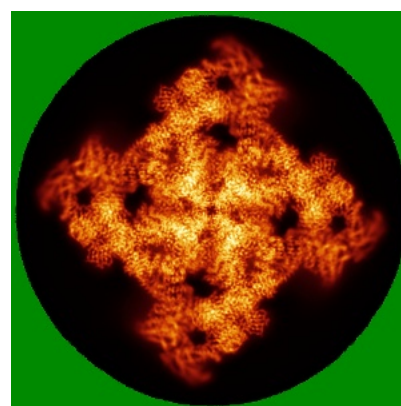
6.4.1 Primary map



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

This section was not generated.

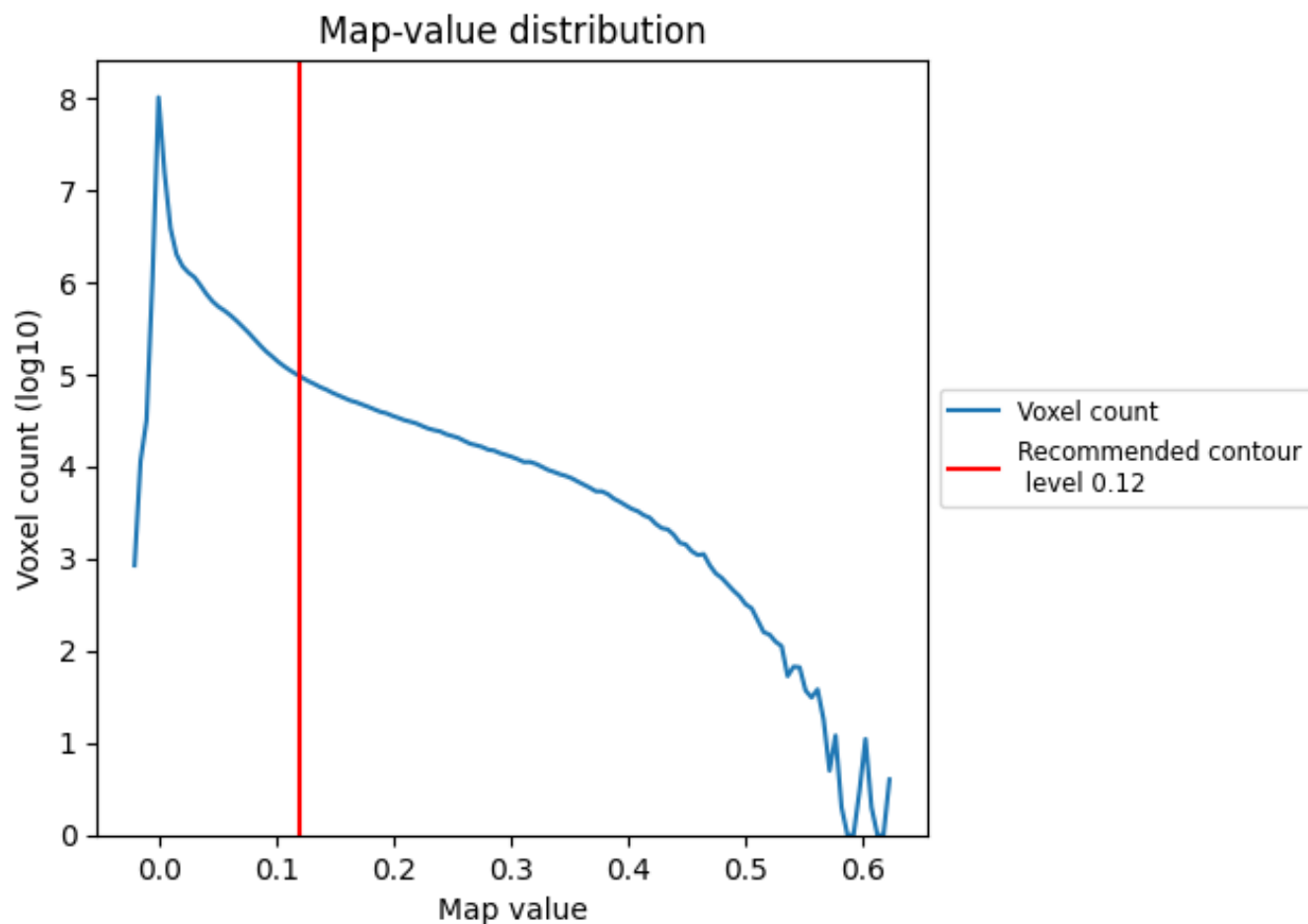
6.6 Mask visualisation

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

7 Map analysis [i](#)

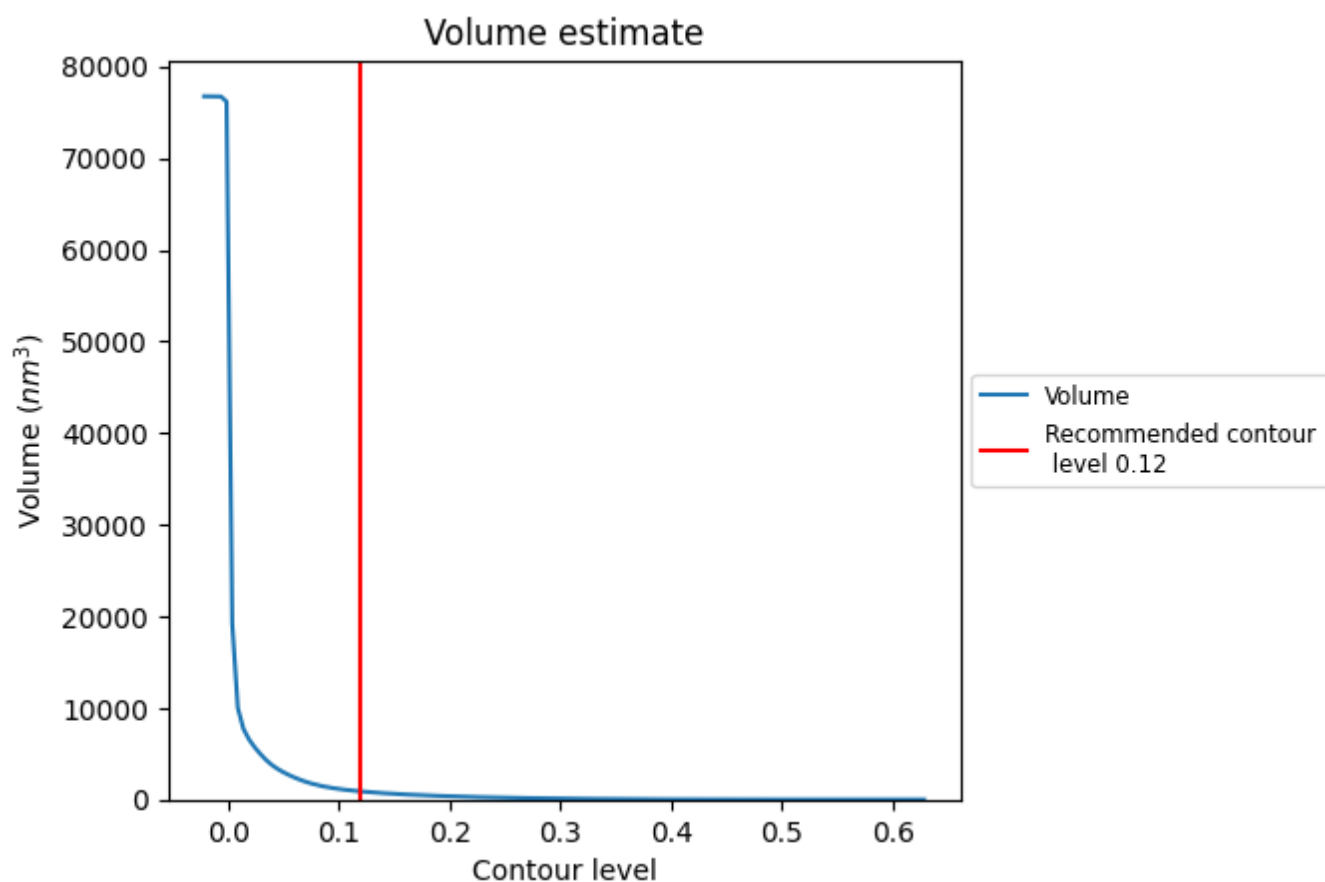
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

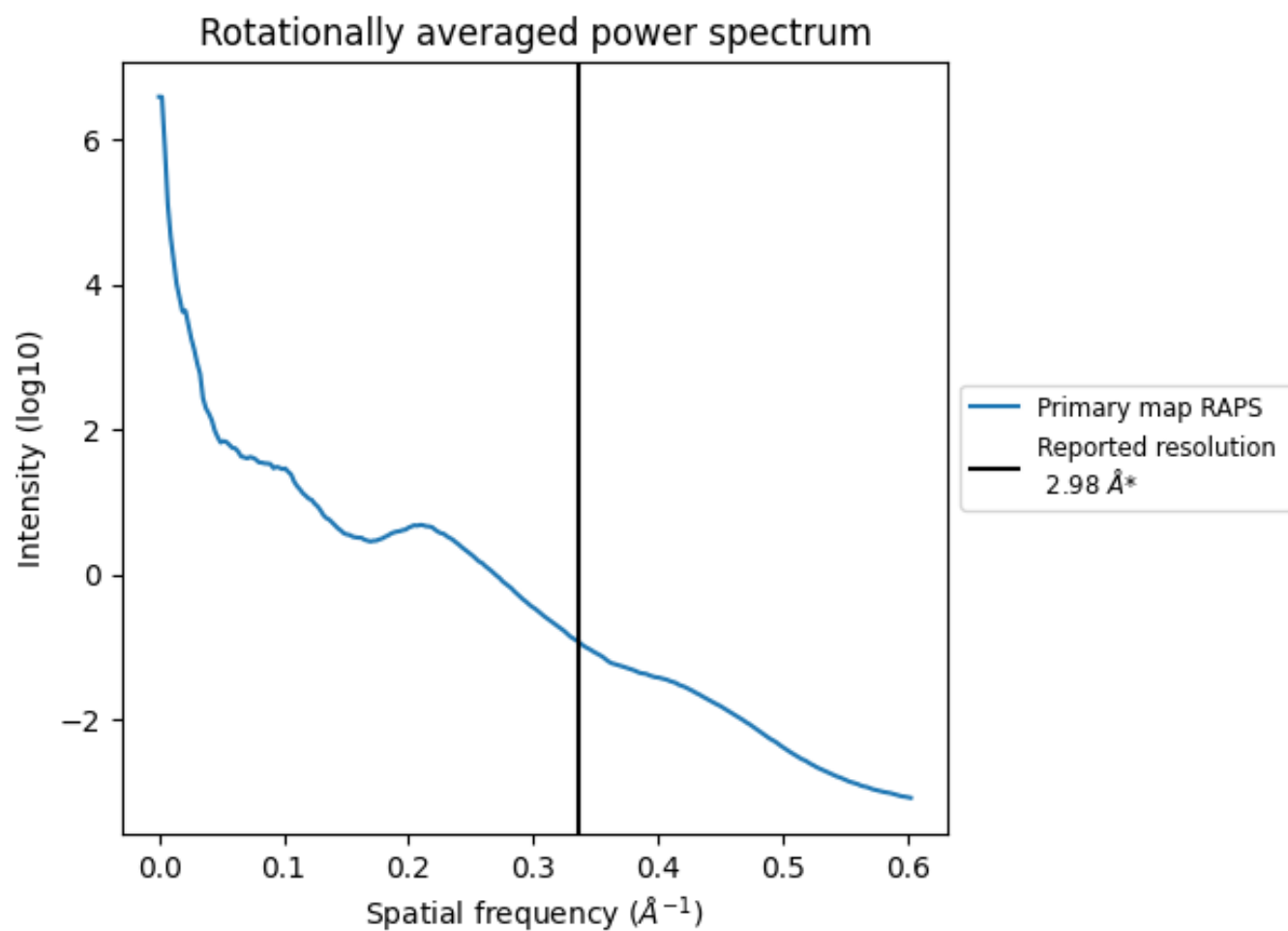
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 891 nm³; this corresponds to an approximate mass of 805 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 0.336 Å⁻¹

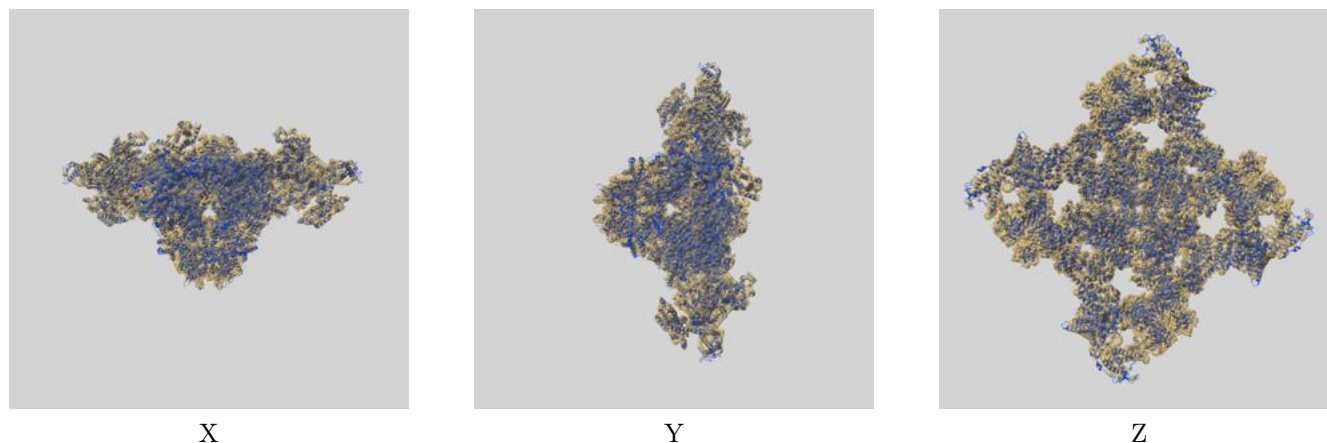
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

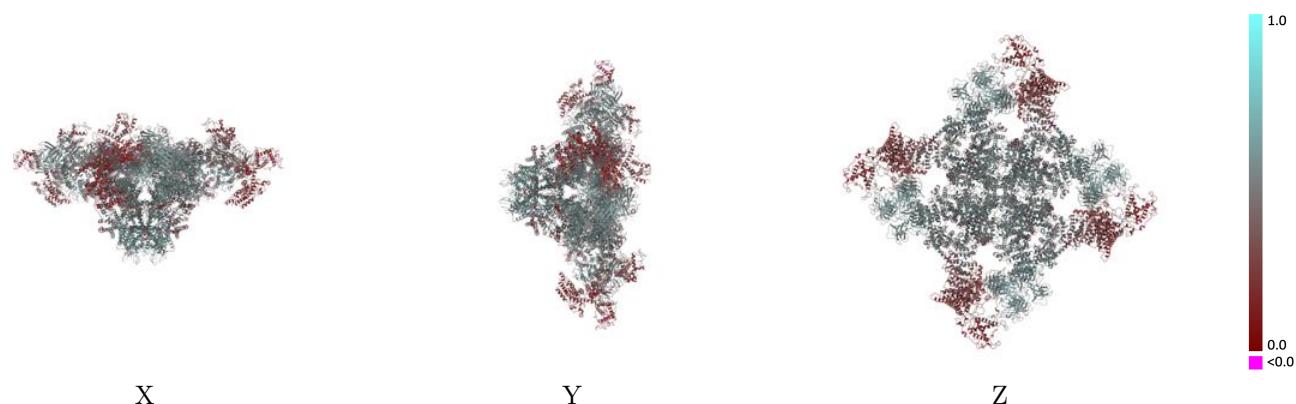
This section contains information regarding the fit between EMDB map EMD-42458 and PDB model 8UQ2. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



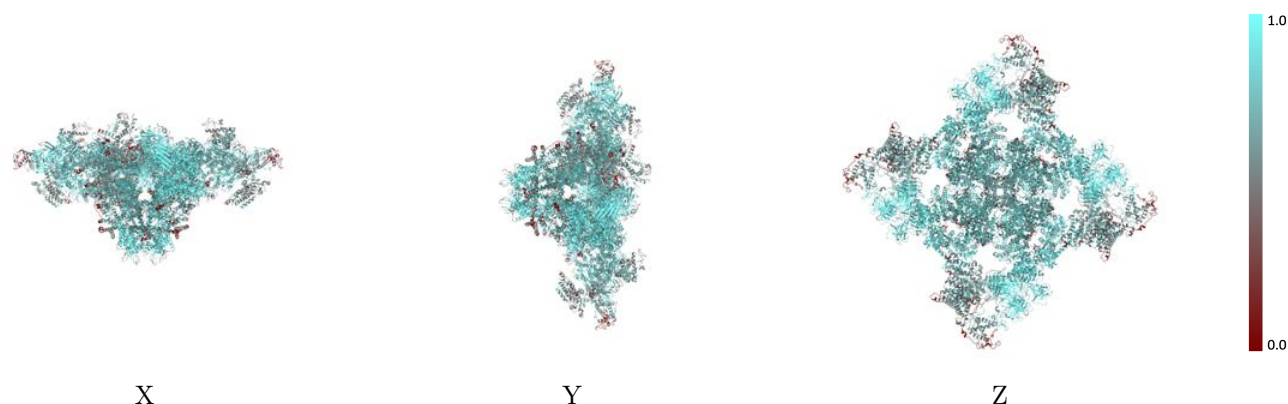
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



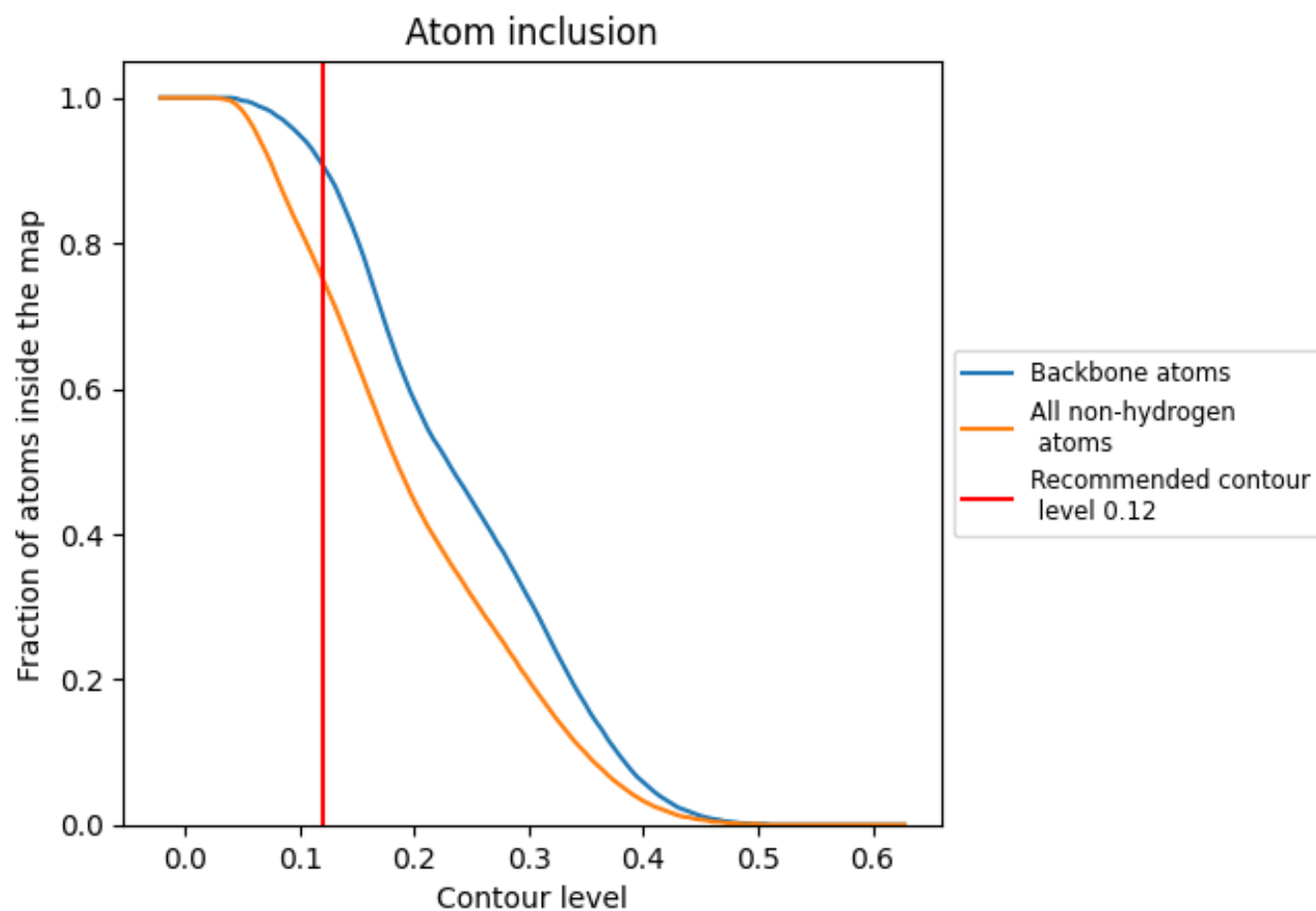
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 75% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.4430
A	0.7490	0.4400
B	0.7480	0.4410
C	0.7480	0.4410
D	0.7490	0.4410
E	0.8710	0.5380
F	0.8730	0.5370
G	0.8730	0.5370
H	0.8730	0.5370

1.0

0.0

<0.0