



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 10:12 AM JST

PDB ID : 5GKZ
EMDB ID : EMD-9519
Title : Structure of RyR1 in a closed state (C3 conformer)
Authors : Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-07
Resolution : 4.00 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

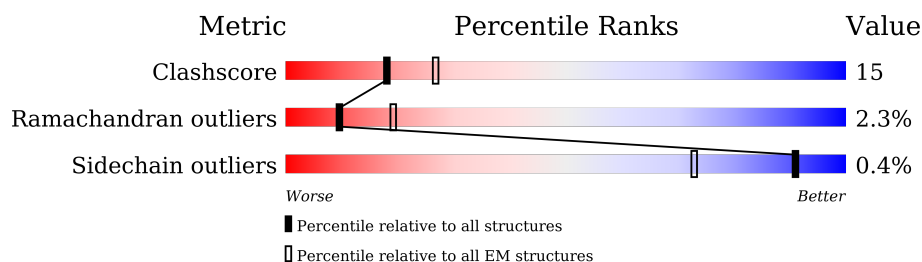
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




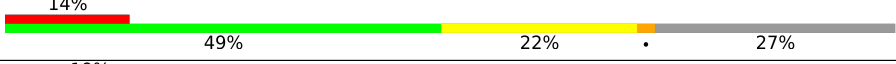


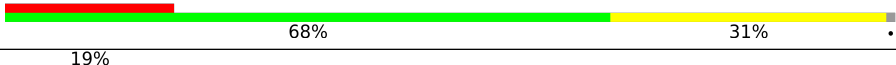

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5037	
1	C	5037	
1	E	5037	
1	G	5037	
2	B	108	
2	D	108	
2	F	108	
2	H	108	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 111000 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		
1	C	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		
1	E	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		
1	G	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		

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

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

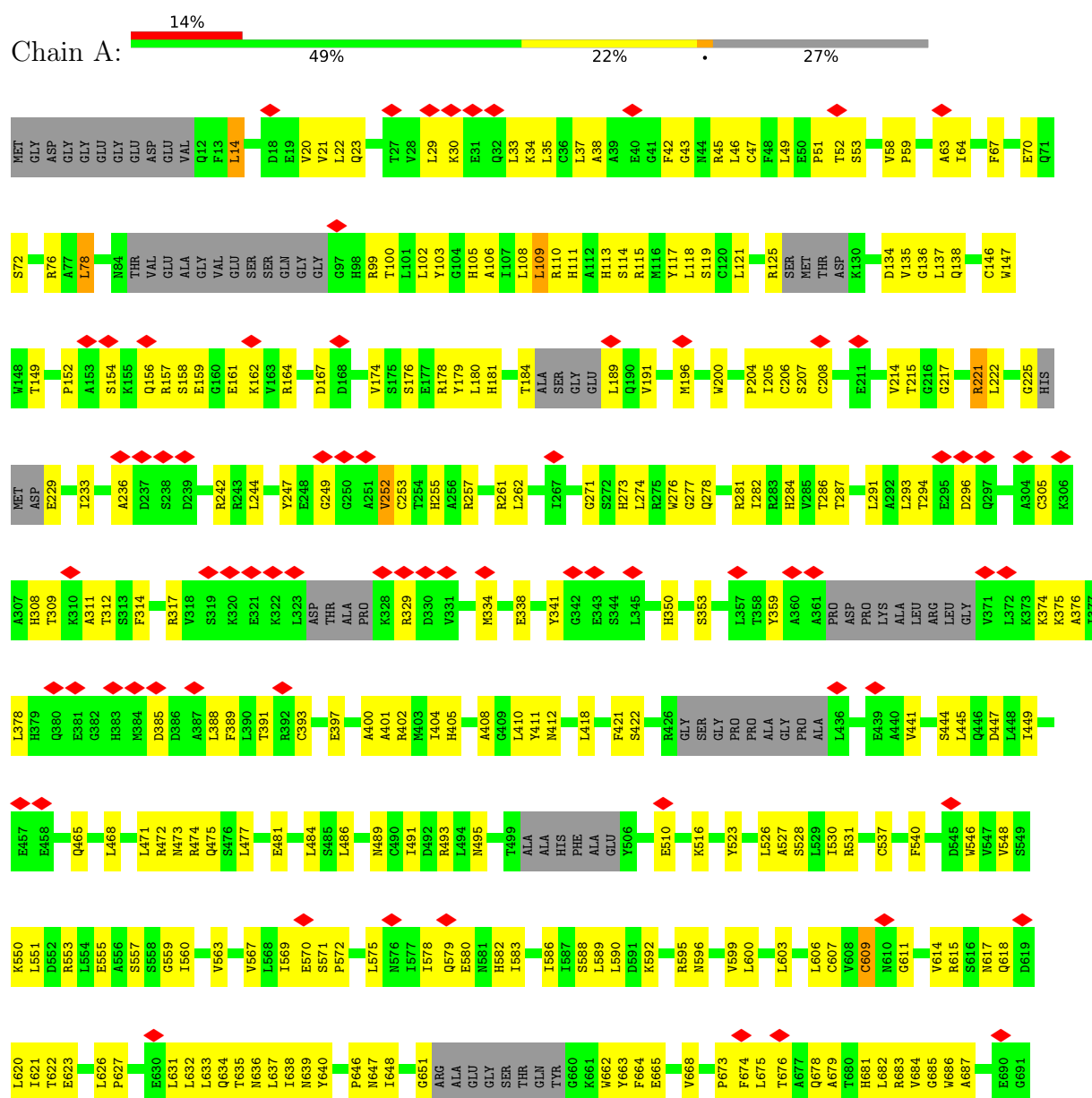
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

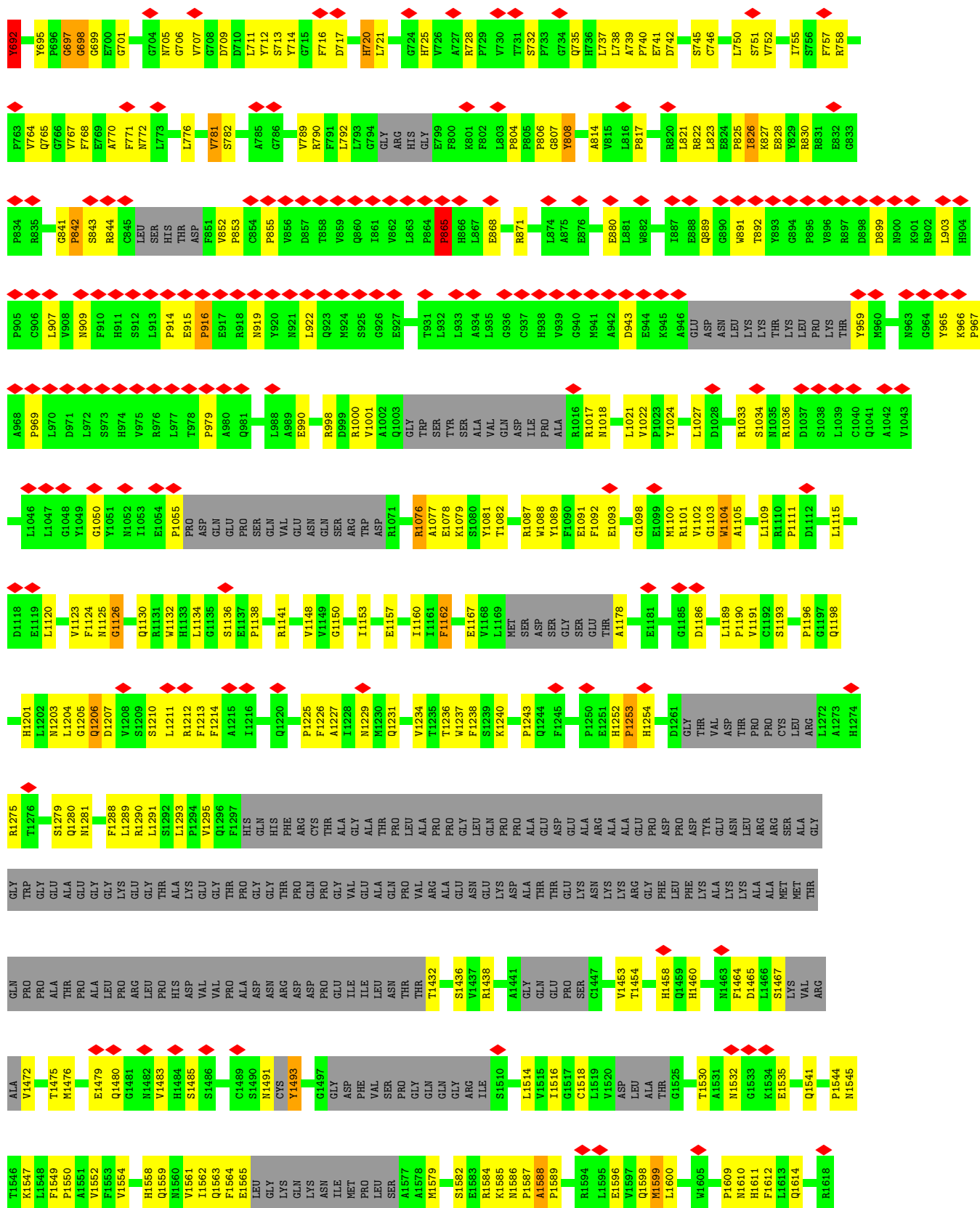
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

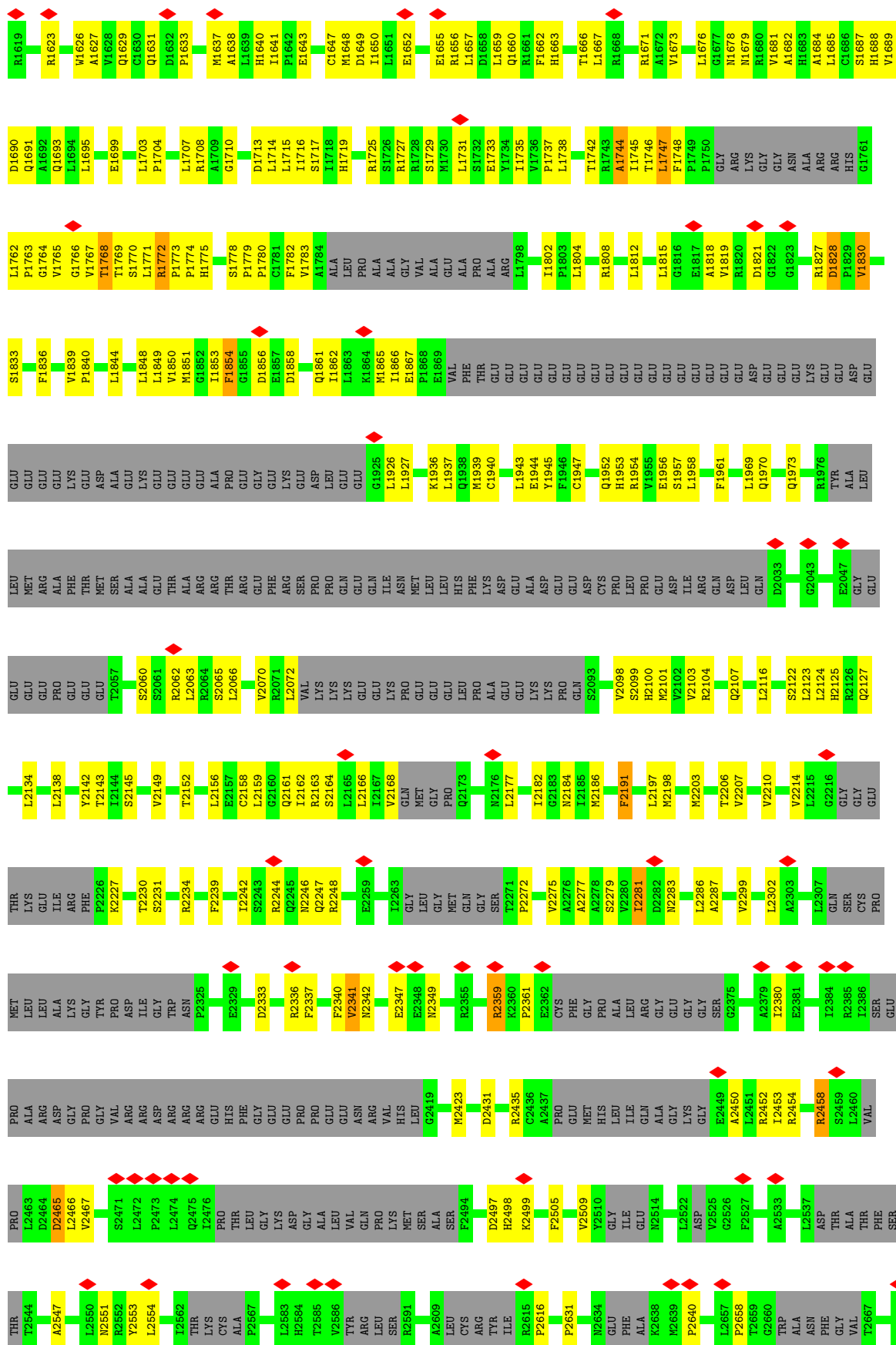
3 Residue-property plots

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

• Molecule 1: Ryanodine receptor 1

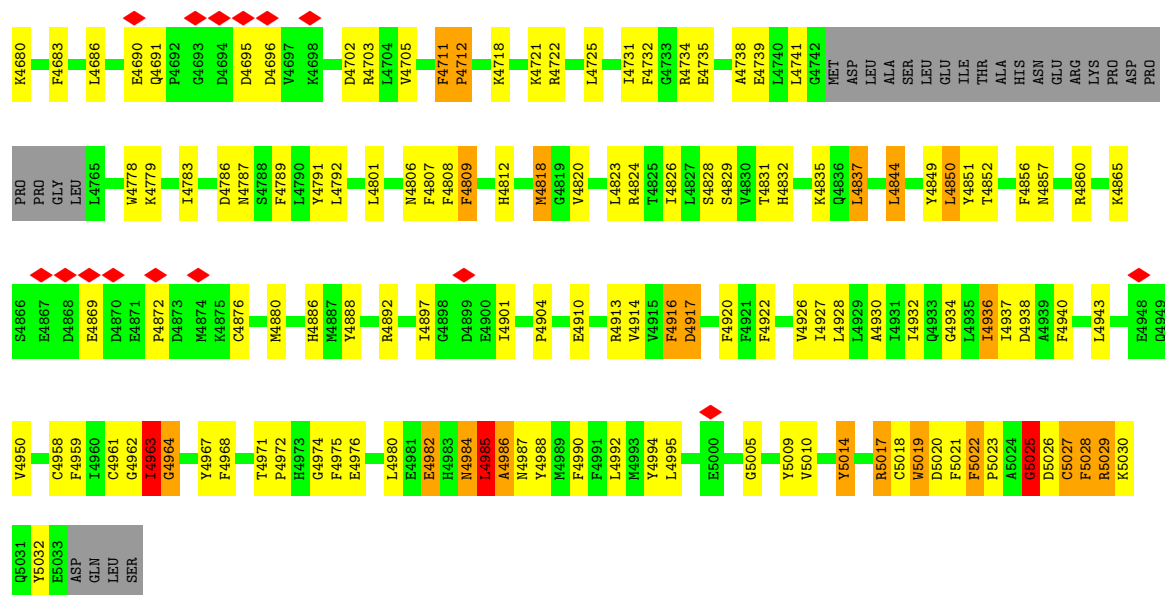




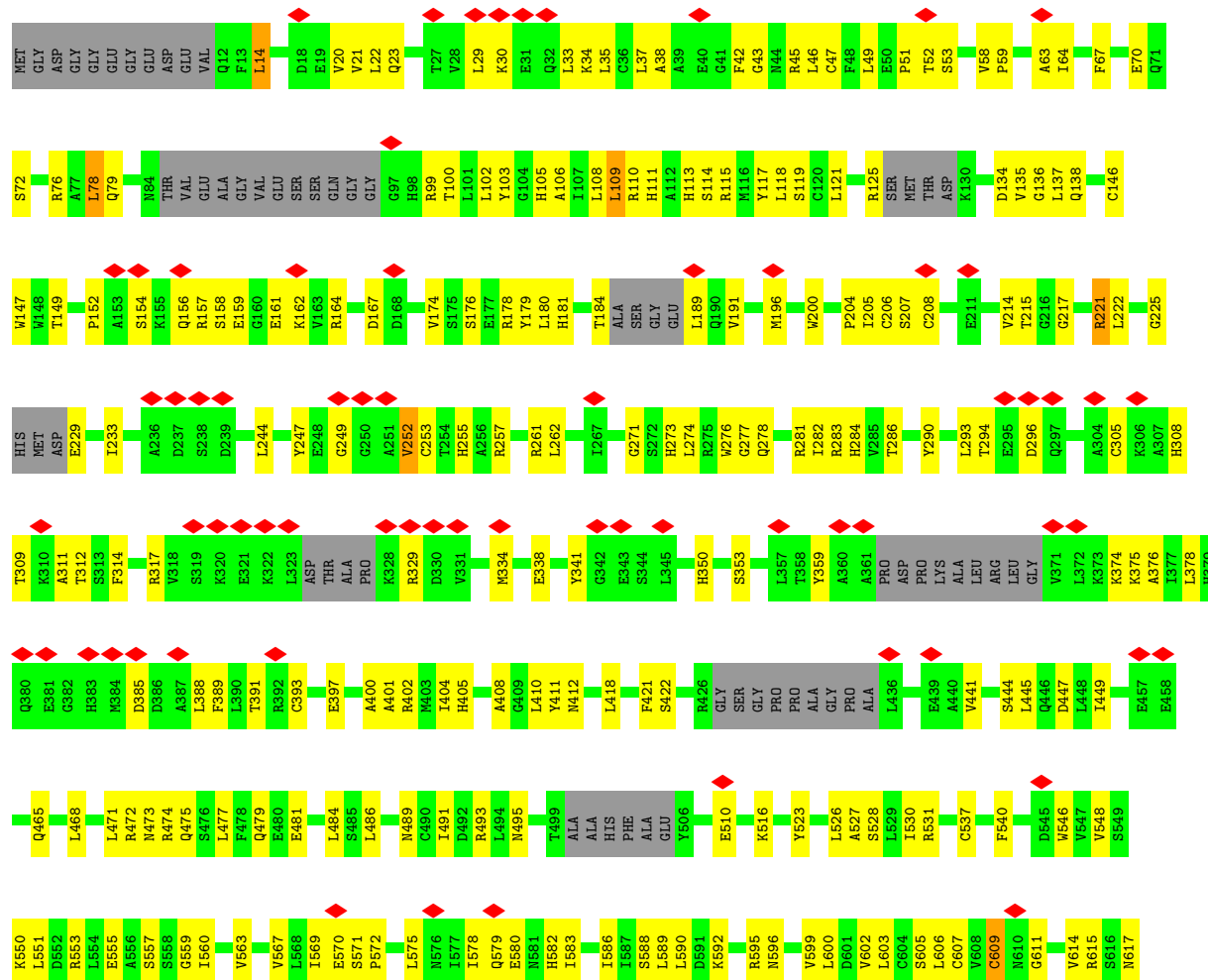








• Molecule 1: Ryanodine receptor 1

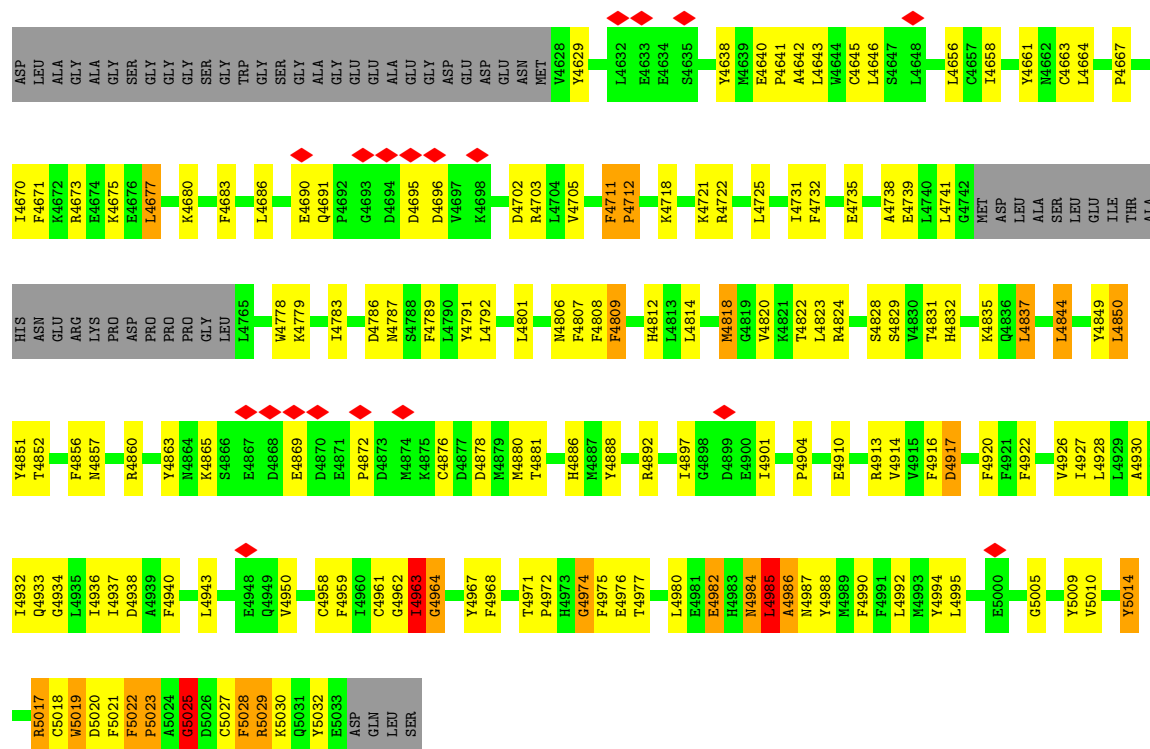




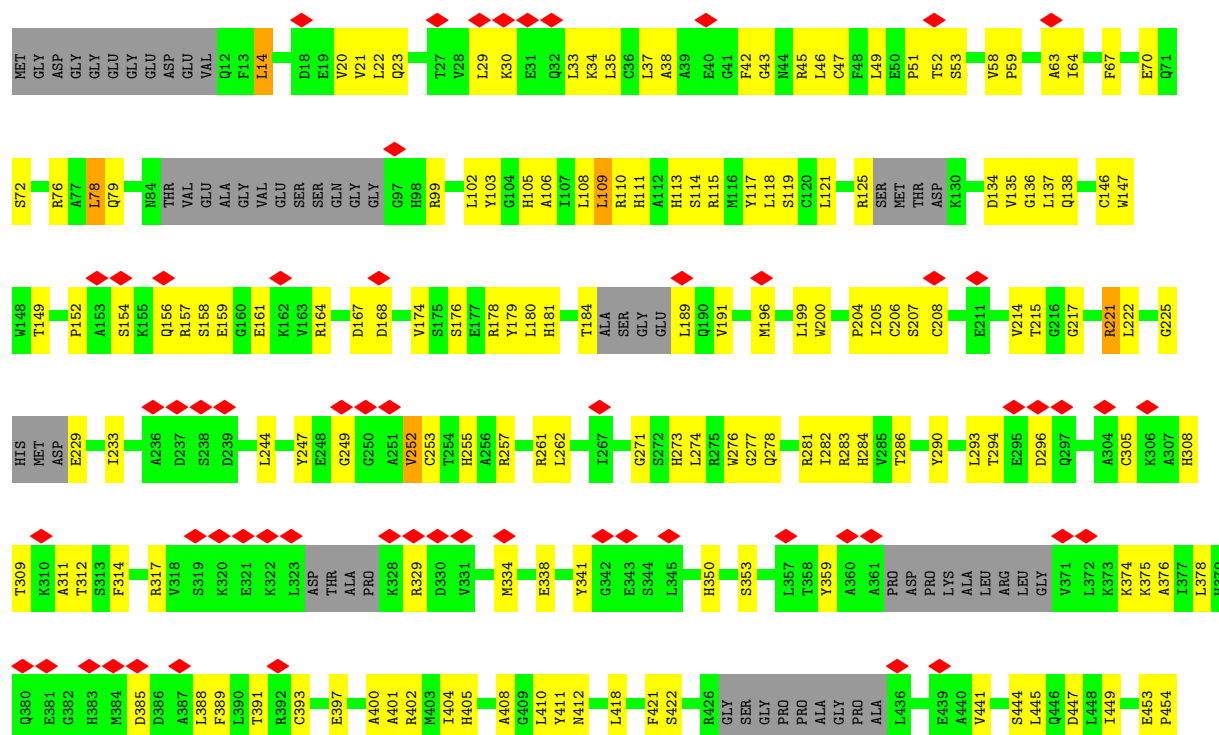


THR	ALA	THR	PHE	VAL	THR	T2544	A2547	L2550	N2551	Y2553	L2554	L2561	L2562	THR	LYS	CYS	ALA	L2567	L2583	H2584	T2585	V2586	TYR	ARG	LEU	SER	R2591	D2601	A2609	LEU	CYS	ARG	TYR	LEU	ILE	R2615	P2616	P2631	V2634	GLU	PHE	ALA	R2638	M2639	P2640	L2657	P2658	T2659	G2660	TRP										
ALA	ASN	PHE	GLY	VAL	T2667	F2679	L2682	L2686	ALA	HIS	LYS	Y2691	P2701	L2706	A2707	G2708	A2709	L2710	P2711	P2712	ASP	TYR	TRP	VAL	ASP	ALA	SER	R2591	D2601	A2609	LEU	CYS	ARG	TYR	LEU	ILE	R2615	P2616	P2631	V2634	GLU	PHE	ALA	R2638	M2639	P2640	L2657	P2658	T2659	G2660	TRP									
I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	T2754	L2755	N2756	K2757	A2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	A2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	N2775	S2776	Y2777	G2778	E2779	L2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	L2794	K2795	T2796	P2797	S2798	E2799	K2800	D2801	E2802	E2803	T2804	Y2805
R2806	V2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	L2819	E2820	N2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	Y2849	D2850	P2851	R2852	E2853	G2854	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	G2864	V2865			
T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	T2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	TRP	MET	ASP	ILE	SER	GLN	THR	Y2849	D2850	P2851	R2852	E2853	G2854	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	G2864	V2865			
L2926	L2927	K2928	F2929	L2930	Q2931	Q2932	N2933	G2934	Y2935	A2936	V2937	L2938	R2939	G2940	LYS	ASP	GLN	TYR	PHE	THR	SER	LYS	ILE	GLU	LYS	ARG	PHE	GLY	PHE	GLN	GLN	LEU	ARG	TRP	MET	ASP	ILE	SER	GLN	THR	Y2849	D2850	P2851	R2852	E2853	G2854	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	G2864	V2865				
VAL	GLU	LYS	SER	PRO	HIS	GLU	GLN	ILE	LYS	PHE	PHE	ALA	LYS	LEU	PRO	LEU	ILE	ASN	GLN	TYR	PHE	THR	ASN	HIS	LEU	Y3016	F3017	L3018	S3019	T3020	P3021	A3022	K3023	V3024	S3027	S3032	N3033	K3036	I3039	THR	SER	LEU	F3043	P3062	ALA	VAL	VAL	ASN	CYS	L3068										
H3069	I3070	L3071	S3074	P3085	E3086	I3087	A3090	GLY	LEU	ARG	SER	F3095	F3096	F3097	S3098	E3104	K3105	M3106	V3107	E3108	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	LYS	GLY	VAL	GLN	ASN	LEU	THR	T3132	L3137	P3138	Q3151	F3152	GLY	ASP	ASP	VAL	ILE	L3158										
D3159	V3163	C3164	C3165	Y3166	R3167	S3171	I3172	L3175	T3178	LYS	ASN	THR	TYR	V3183	E3184	K3185	L3186	R3187	P3188	A3189	L3190	A3195	R3196	A3199	A3200	MET	PRO	VAL	A3204	F3205	P3208	E3212	Y3213	N3214	S3217	VAL	TYR	THR	THR	LYS	SER	PRO	ARG	GLU	ARG	ILE	GLY	LEU												
PRO	ASN	SER	VAL	GLU	MET	CYS	PRO	ASP	ILE	VAL	LEU	ASP	ARG	LEU	MET	ALA	GLU	GLY	ALA	GLU	SER	GLY	ALA	ARG	TYR	THR	GLU	MET	PRO	HIS	VAL	ILE	ILE	T3273	L3274	P3275	M3276	L3277	C3278	S3279	Y3280	L3281	P3282	R3283	R3287	G3288	P3289	E3290	ALA	PRO	PRO	P3294								
A3295	L3296	P3297	A3298	P3301	P3302	P3303	C3304	N3313	SER	LEU	LEU	G3317	N3318	L3319	L3320	R3321	D3330	E3331	A3339	VAL	PHE	ALA	GLN	PRO	ILE	V3346	P3351	L3354	H3355	S3356	H3357	F3358	I3359	P3360	T3361	T3362	G3363	ARG	LEU	ARG	K3367	K3371	Q3378	E3386	G3390	E3391	L3392	L3393	V3394											
R3395	D3396	E3397	PHE	SER	VAL	LEU	C3402	R3403	D3404	L3405	Y3406	P3410	L3411	L3412	I3413	N3418	N3419	R3420	A3421	H3422	V3423	L3424	THR	GLU	P3427	N3428	A3431	E3432	F3435	M3437	V3438	E3455	GLN	N3457	V3460	N3465	S3468	F3469	L3470	THR	ALA	ASP	SER	LYS	SER	LYS	M3478	G3482												
S3486	S3489	D3490	D3491	GLU	ARG	THR	L3494	K3495	K3496	K3497	S3504	VAL	GLN	THR	SER	LEU	ILE	ALA	T3513	K3516	M3517	L3518	P3519	K3524	C3525	A3526	P3527	THR	ASP	GLN	ASP	LEU	ILE	MET	LEU	ALA	K3537	T3538	A3541	L3542	K3543	D3544	THR	ASP	GLU	GLU	V3549	P3550	Q3554	H3558	P3567									





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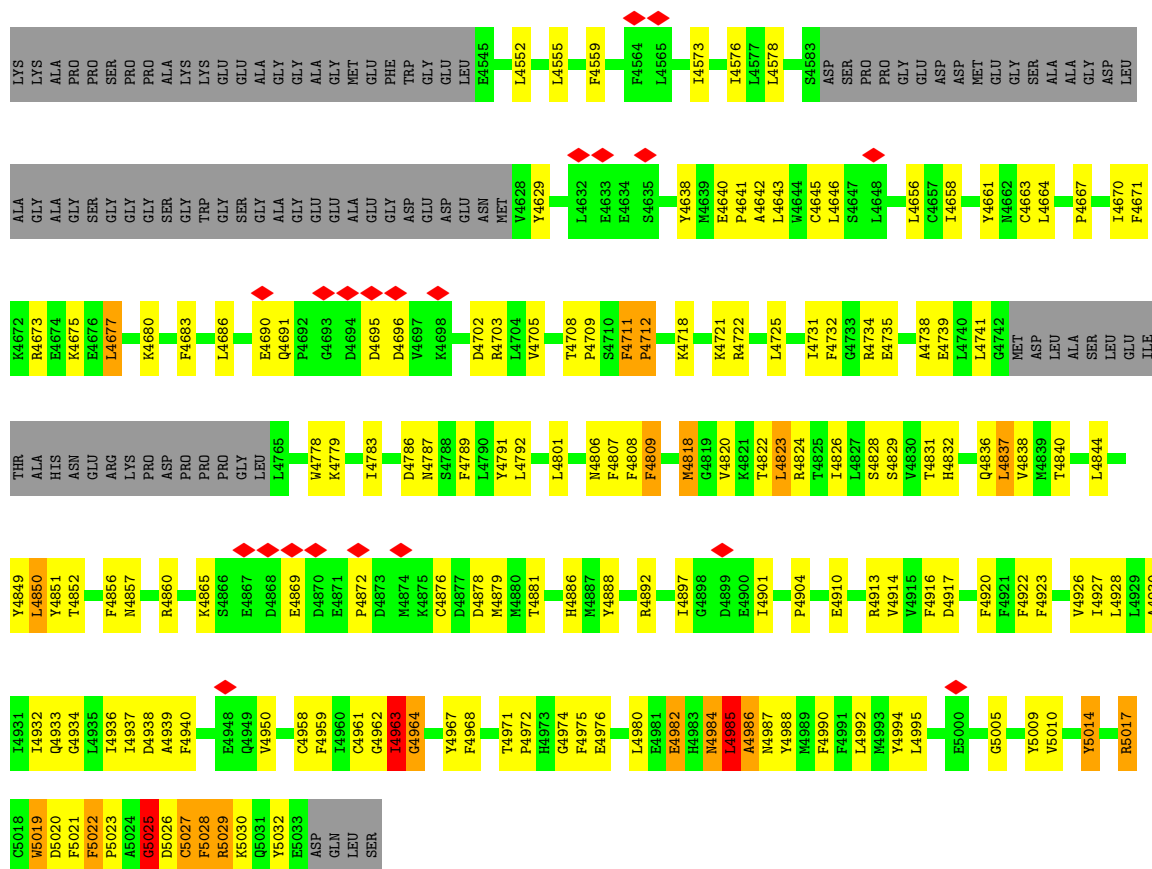




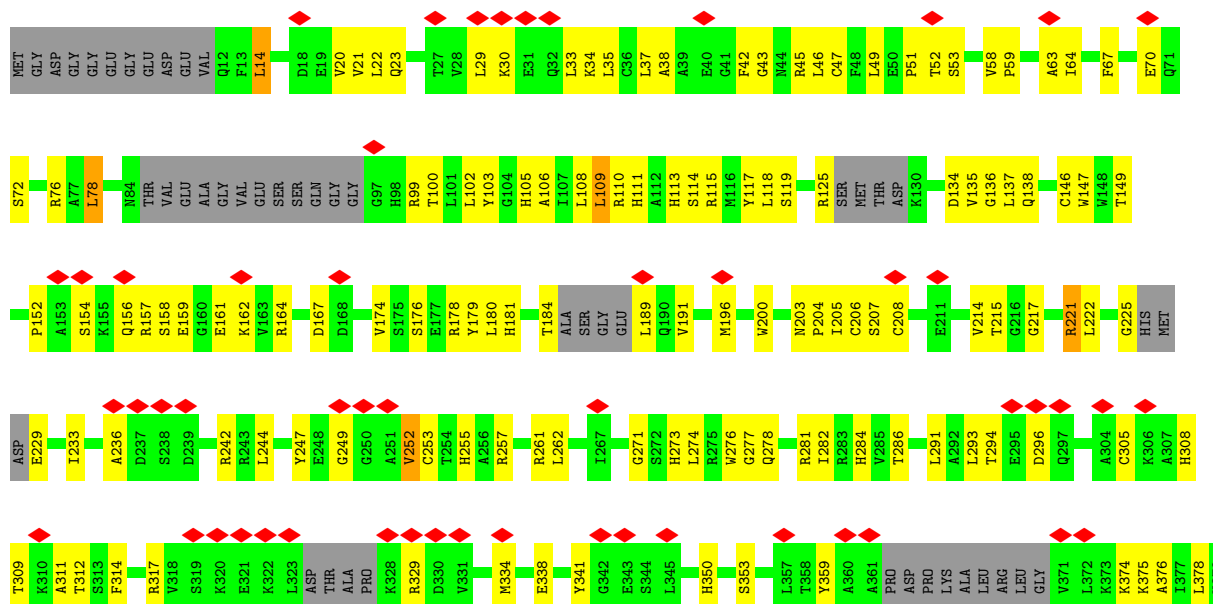








Molecule 1: Ryanodine receptor 1

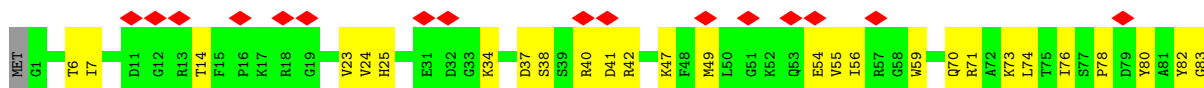


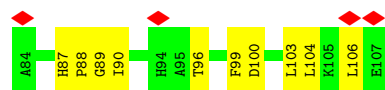




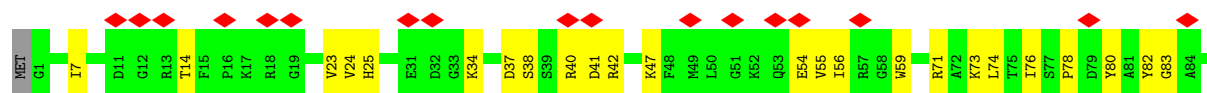
P3275	M3276	L3277	C3278	S3279	Y3280	L3281	R3283	W3284	R3287	G3288	P3289	E3290	ALA	PRO	PRO	P3294	A3295	L3296	P3297	P3301	P3302	P3303	C3304	N3313	SER	LEU	LEU	G3317	N3318	L3319	L3320	R3321	D3330	E3331	R3337	L3338	A3339	VAL	PHE	ALA	GLN	PRO	ILE	W3346	P3351	E3352	L3353	L3354	H3355	S3356	H3357	F3358																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
N3214	S3217	VAL	THR	THR	THR	LYS	SER	PRO	ARG	GLU	ARG	ALA	ALA	ILE	LEU	GLY	LEU	LEU	ASN	ASN	VAL	VAL	CYS	PRO	ASP	ASP	ASP	PRO	PRO	ASN	VAL	GLY	GLY	GLY	THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR



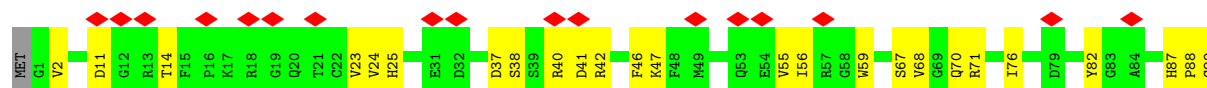




- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.428	Depositor
Minimum map value	-0.192	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.98	87/27385 (0.3%)	0.88	108/37104 (0.3%)
1	C	0.98	89/27385 (0.3%)	0.88	114/37104 (0.3%)
1	E	0.98	87/27385 (0.3%)	0.88	108/37104 (0.3%)
1	G	0.99	94/27385 (0.3%)	0.88	112/37104 (0.3%)
2	B	0.63	0/851	0.63	0/1146
2	D	0.63	0/851	0.63	0/1146
2	F	0.63	0/851	0.63	0/1146
2	H	0.63	0/851	0.62	0/1146
All	All	0.98	357/112944 (0.3%)	0.88	442/153000 (0.3%)

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	20
1	C	0	20
1	E	0	20
1	G	0	20
All	All	0	80

The worst 5 of 357 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4988	TYR	CG-CD2	-20.55	1.12	1.39
1	E	4988	TYR	CG-CD2	-19.42	1.14	1.39
1	C	4988	TYR	CG-CD2	-19.41	1.14	1.39
1	A	4988	TYR	CG-CD2	-19.37	1.14	1.39
1	G	4988	TYR	CE1-CZ	-17.94	1.15	1.38

The worst 5 of 442 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	5029	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	E	5029	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	E	4988	TYR	CB-CG-CD1	10.56	127.34	121.00
1	A	4988	TYR	CB-CG-CD1	10.55	127.33	121.00
1	C	4988	TYR	CB-CG-CD1	10.53	127.32	121.00

There are no chirality outliers.

5 of 80 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1464	PHE	Mainchain,Peptide
1	A	1465	ASP	Peptide
1	A	697	GLY	Mainchain,Peptide
1	A	807	GLY	Mainchain,Peptide
1	A	841	GLY	Mainchain,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	26917	0	24461	801	0
1	C	26917	0	24461	789	0
1	E	26917	0	24461	787	0
1	G	26917	0	24461	770	0
2	B	832	0	831	34	0
2	D	832	0	831	35	0
2	F	832	0	831	33	0
2	H	832	0	831	28	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
All	All	111000	0	101168	3132	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 15.

The worst 5 of 3132 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:G:1782:PHE:O	2:H:82:TYR:OH	1.75	1.03
1:A:1782:PHE:O	2:B:82:TYR:OH	1.76	1.03
1:A:4888:TYR:CD1	1:G:4914:VAL:HG23	1.95	1.02
1:C:1782:PHE:O	2:D:82:TYR:OH	1.78	1.01
1:E:1782:PHE:O	2:F:82:TYR:OH	1.77	1.00

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	3496/5037 (69%)	3185 (91%)	227 (6%)	84 (2%)	6	36
1	C	3496/5037 (69%)	3185 (91%)	228 (6%)	83 (2%)	6	36
1	E	3496/5037 (69%)	3187 (91%)	226 (6%)	83 (2%)	6	36
1	G	3496/5037 (69%)	3192 (91%)	217 (6%)	87 (2%)	5	35
2	B	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	D	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
All	All	14404/20580 (70%)	13130 (91%)	937 (6%)	337 (2%)	9	37

5 of 337 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	701	GLY
1	A	915	GLU
1	A	916	PRO

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Mol	Chain	Res	Type
1	A	969	PRO
1	A	1589	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2503/4276 (58%)	2493 (100%)	10 (0%)	91	94
1	C	2502/4276 (58%)	2492 (100%)	10 (0%)	91	94
1	E	2500/4276 (58%)	2491 (100%)	9 (0%)	91	94
1	G	2501/4276 (58%)	2489 (100%)	12 (0%)	88	93
2	B	89/90 (99%)	88 (99%)	1 (1%)	73	85
2	D	89/90 (99%)	88 (99%)	1 (1%)	73	85
2	F	89/90 (99%)	88 (99%)	1 (1%)	73	85
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	10362/17464 (59%)	10318 (100%)	44 (0%)	91	94

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1055	PRO
1	G	916	PRO
1	E	4850	LEU
1	G	806	PRO
1	G	1001	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 208 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	582	HIS
1	E	3906	GLN
1	G	4223	ASN

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Mol	Chain	Res	Type
1	E	765	GLN
1	E	1678	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

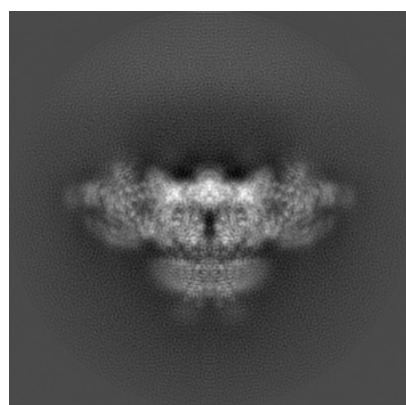
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9519. These allow visual inspection of the internal detail of the map and identification of artifacts.

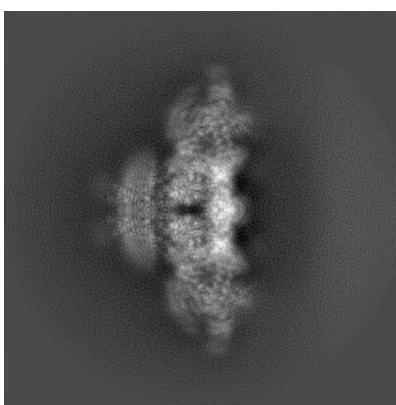
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

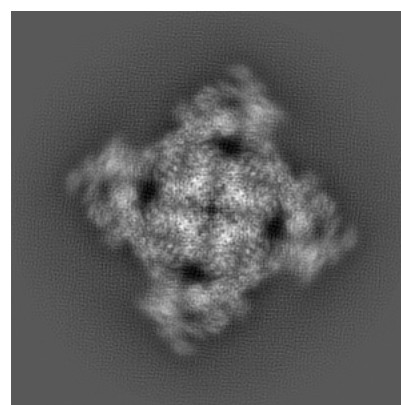
6.1.1 Primary map



X



Y

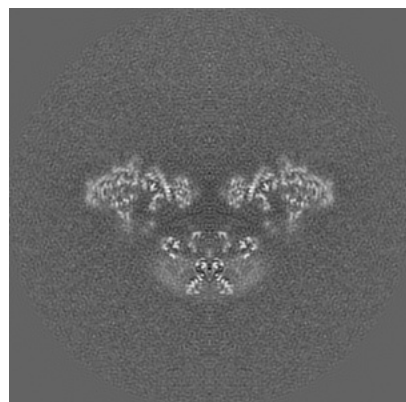


Z

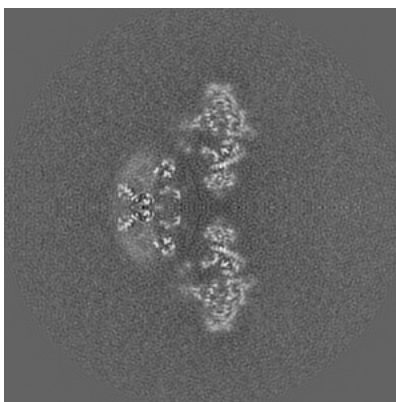
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

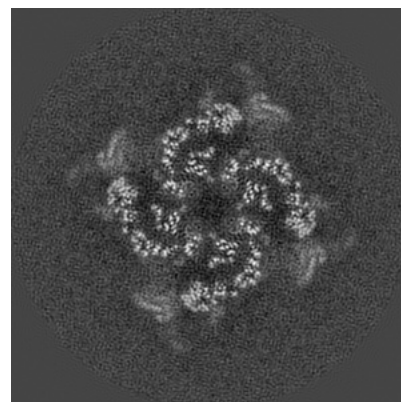
6.2.1 Primary map



X Index: 180



Y Index: 180

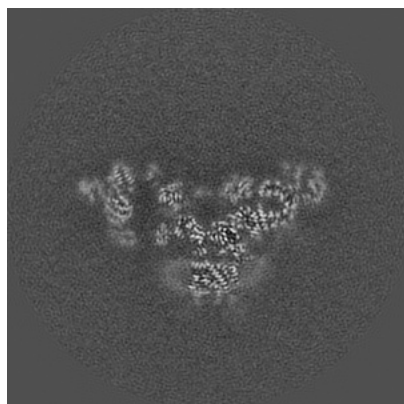


Z Index: 180

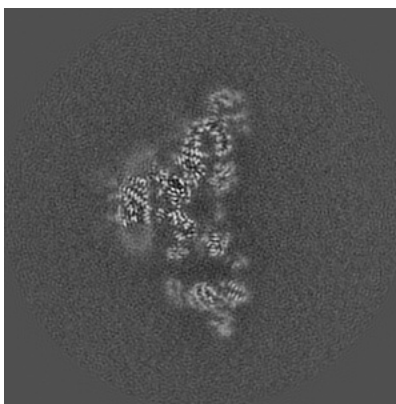
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

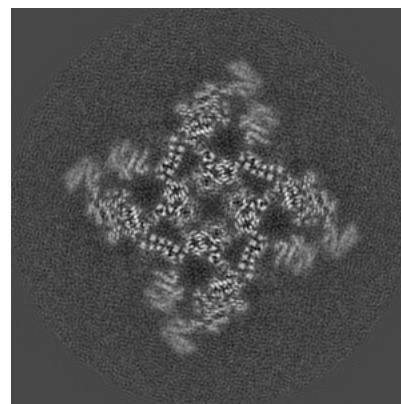
6.3.1 Primary map



X Index: 169



Y Index: 191

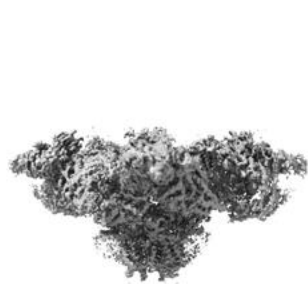


Z Index: 190

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

6.4 Orthogonal surface views [i](#)

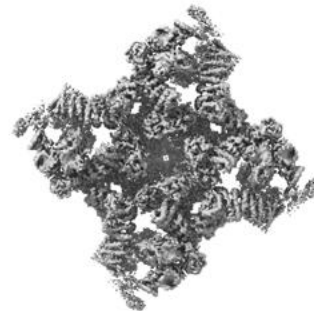
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

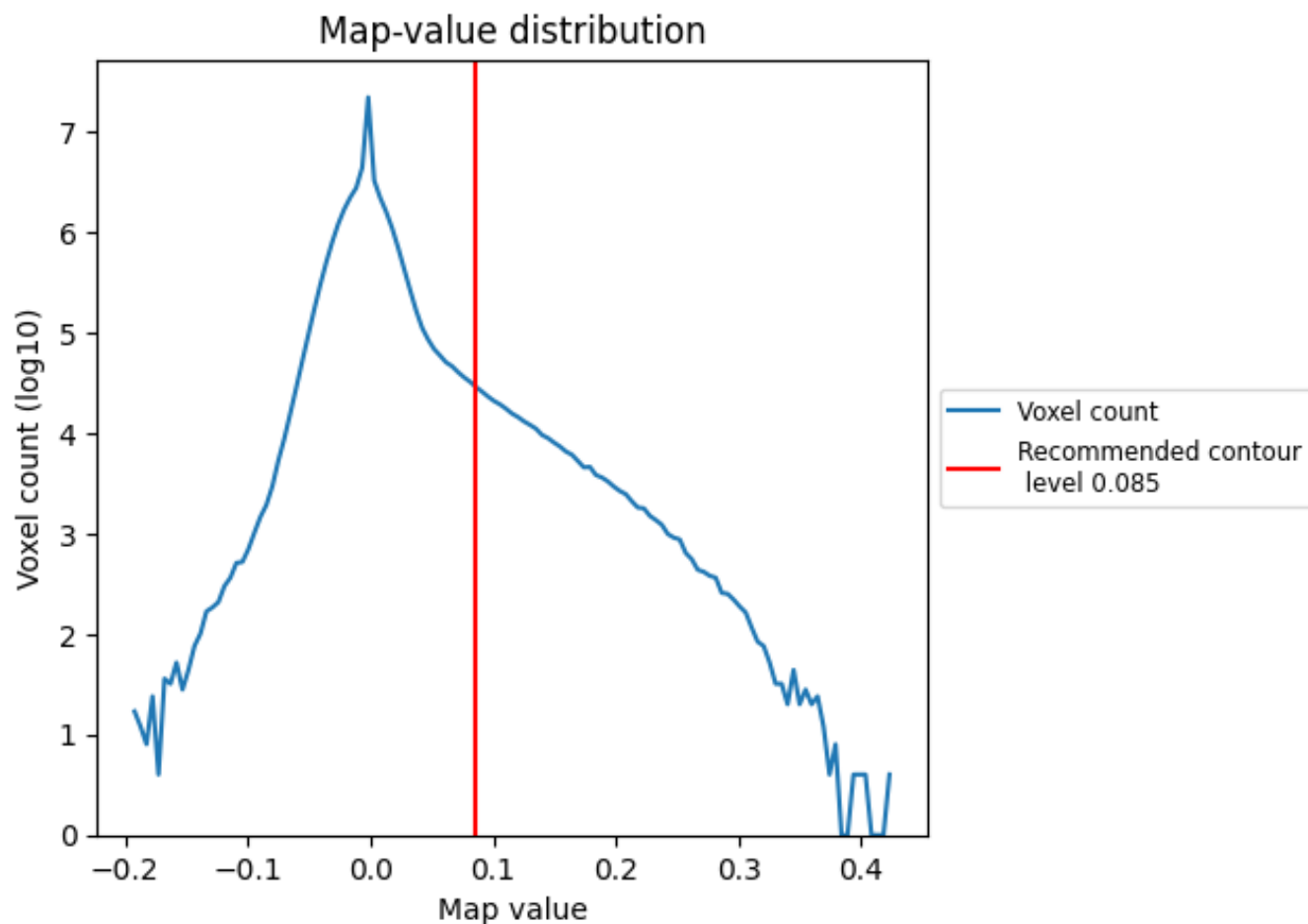
6.5 Mask visualisation

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

7 Map analysis [i](#)

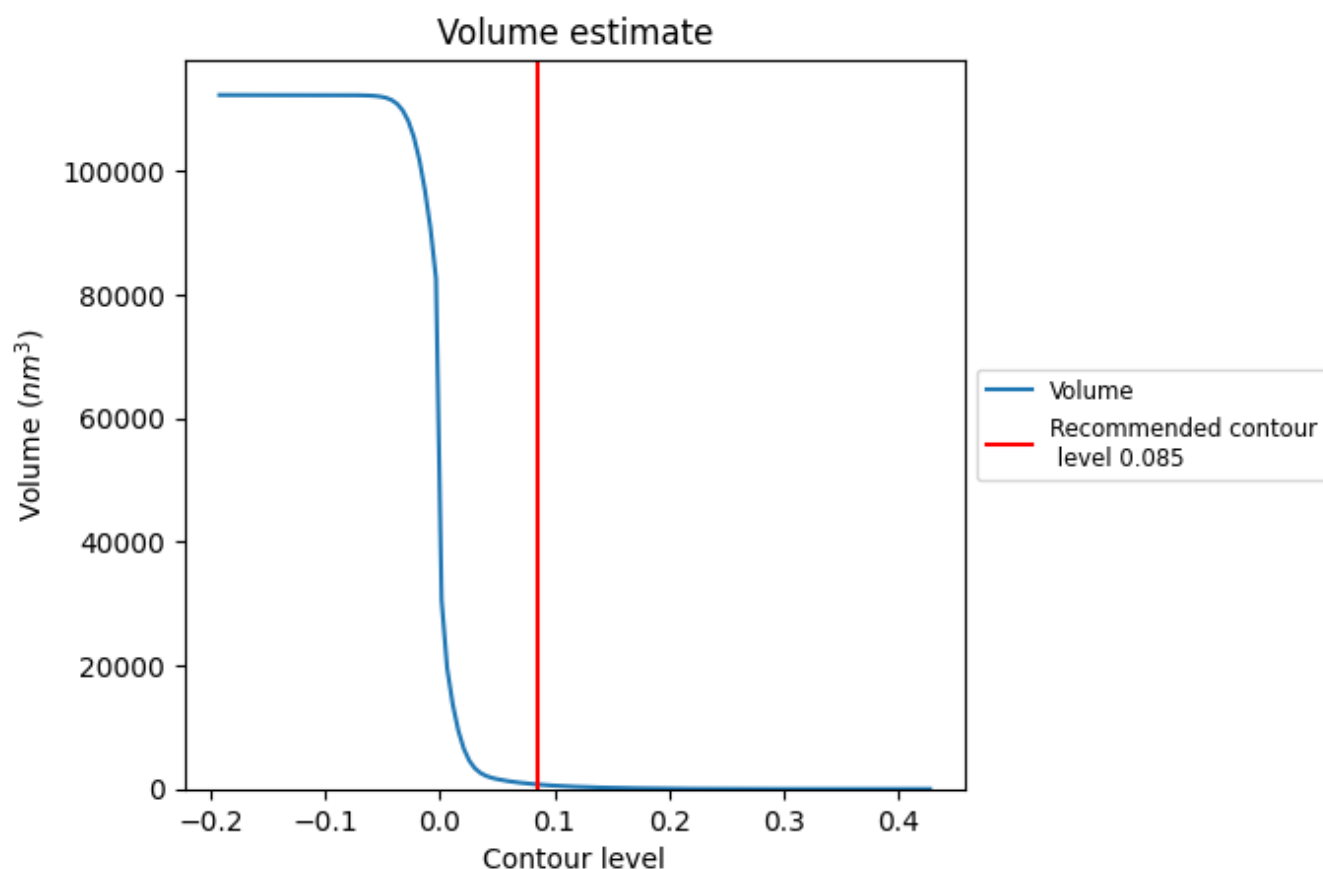
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

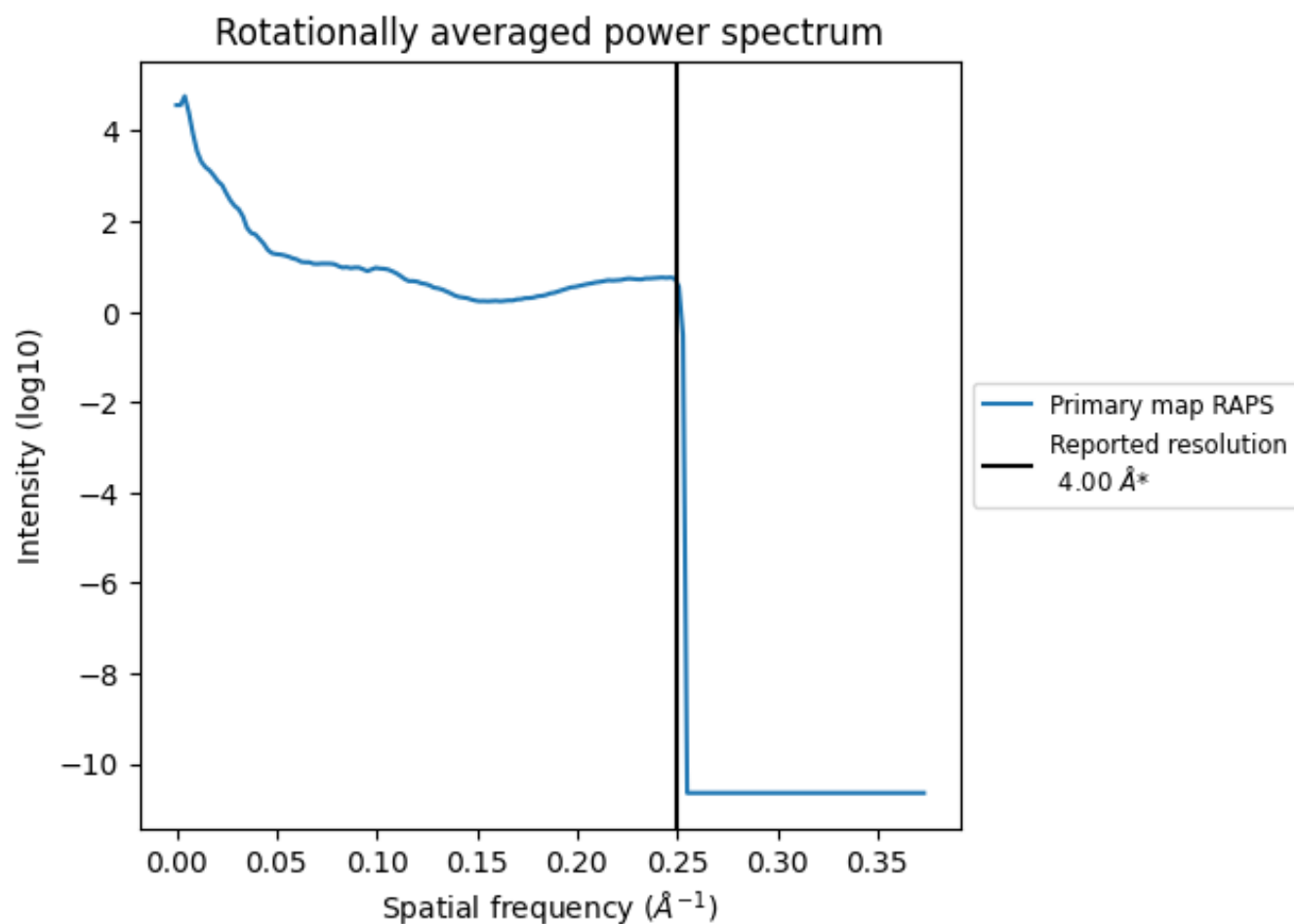
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 734 nm³; this corresponds to an approximate mass of 663 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 0.250 \AA^{-1}

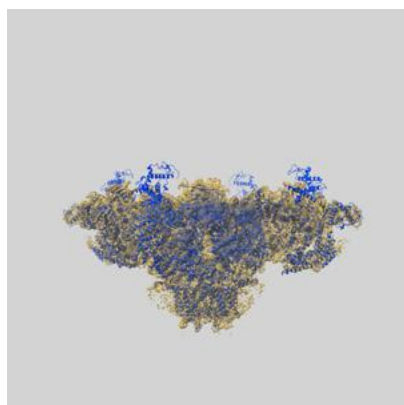
8 Fourier-Shell correlation

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

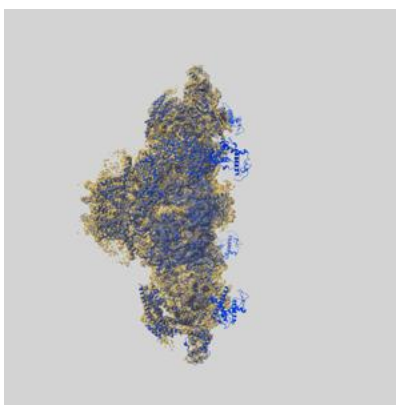
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9519 and PDB model 5GKZ. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

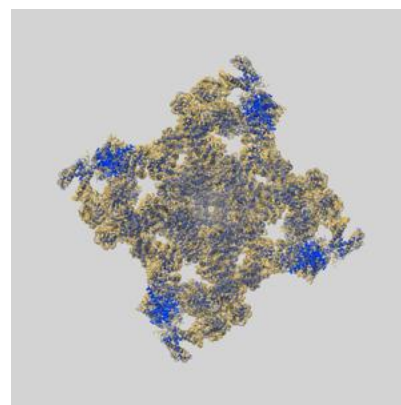
9.1 Map-model overlay [i](#)



X



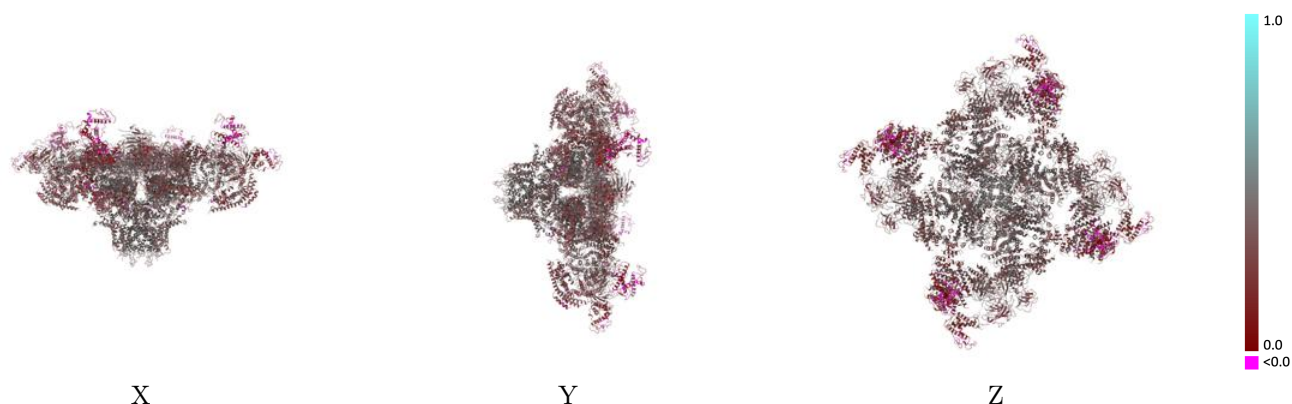
Y



Z

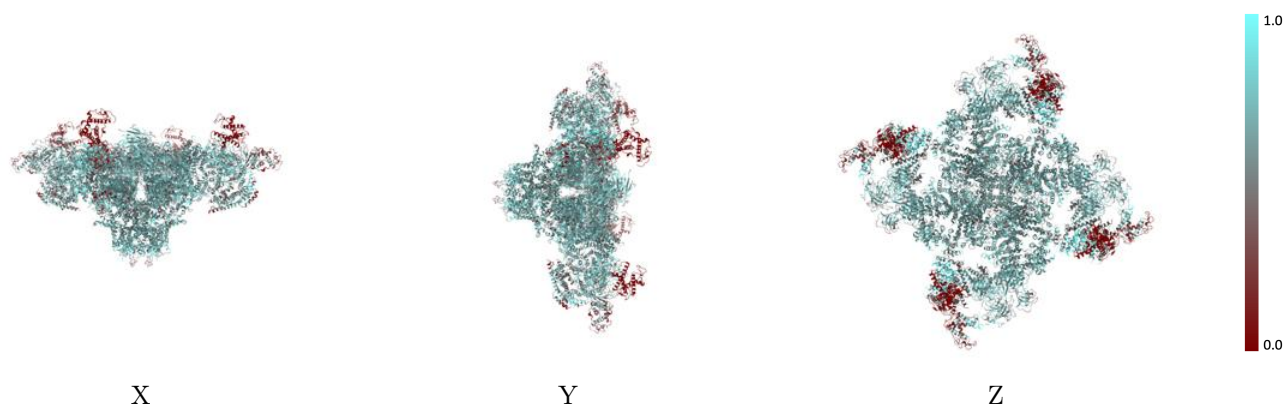
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



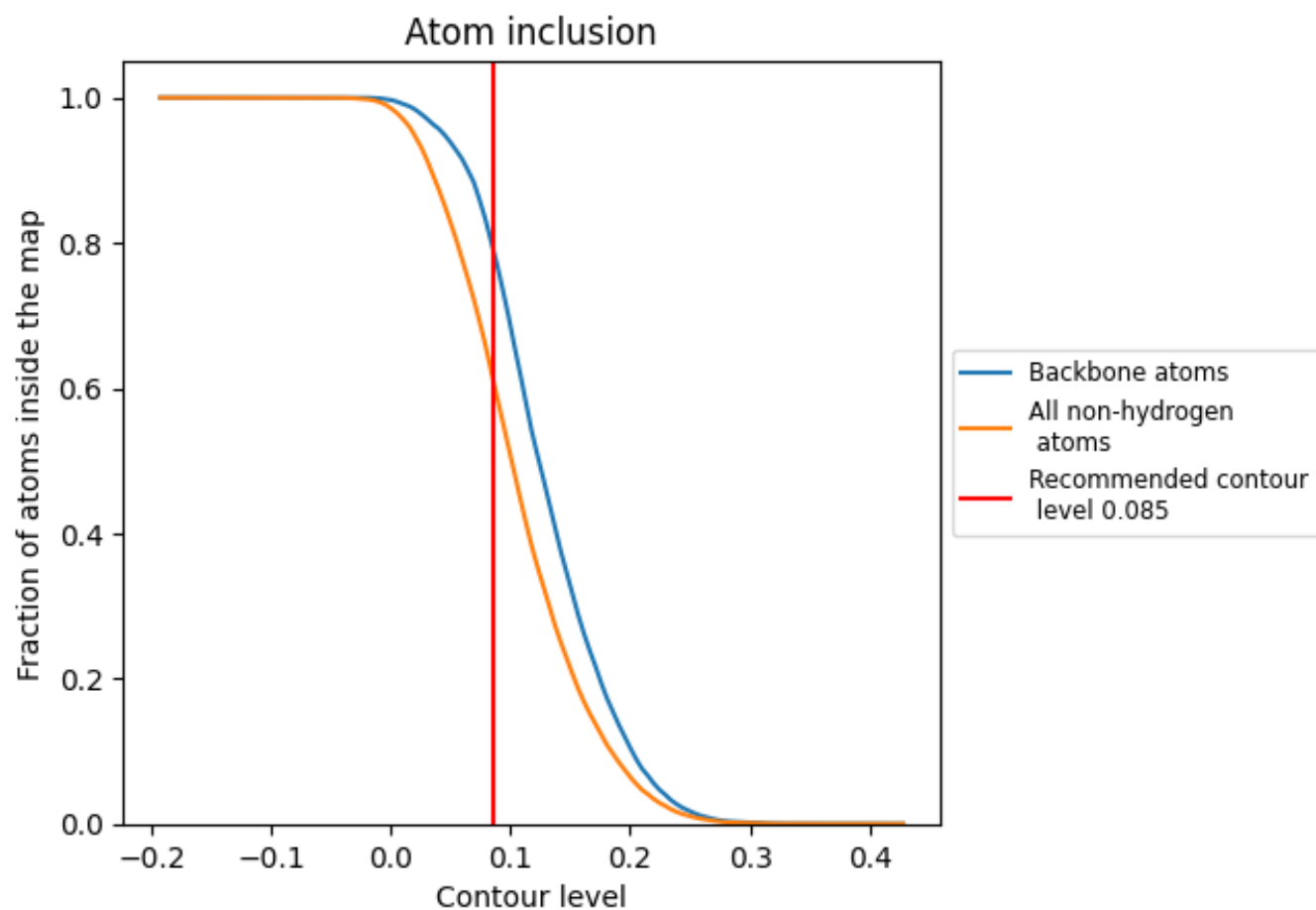
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.085).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6153	<div></div> 0.3370
A	<div></div> 0.6164	<div></div> 0.3370
B	<div></div> 0.5723	<div></div> 0.3390
C	<div></div> 0.6168	<div></div> 0.3360
D	<div></div> 0.5699	<div></div> 0.3370
E	<div></div> 0.6165	<div></div> 0.3360
F	<div></div> 0.5699	<div></div> 0.3360
G	<div></div> 0.6168	<div></div> 0.3400
H	<div></div> 0.5711	<div></div> 0.3380

1.0

0.0

<0.0