



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 12:47 AM EST

PDB ID : 6X35
EMDB ID : EMD-22018
Title : Pig R615C RyR1 in complex with CaM, EGTA (class 1, open)
Authors : Woll, K.W.; Haji-Ghassemi, O.; Van Petegem, F.
Deposited on : 2020-05-21
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM Validation 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

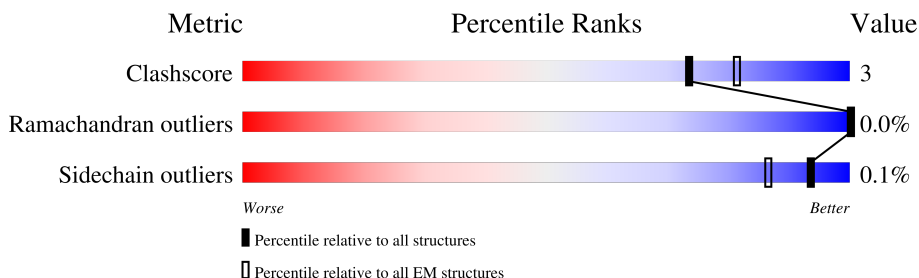
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	110	<div> <div>21%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	D	110	<div> <div>22%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	G	110	<div> <div>21%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	J	110	<div> <div>21%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
2	B	3801	<div> <div>34%</div> <div>92%</div> <div>8%</div> </div>
2	E	3801	<div> <div>34%</div> <div>92%</div> <div>8%</div> </div>
2	H	3801	<div> <div>34%</div> <div>92%</div> <div>8%</div> </div>
2	K	3801	<div> <div>34%</div> <div>92%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	148	<p>53% 87% 9%</p>
3	F	148	<p>53% 87% 9%</p>
3	I	148	<p>53% 87% 9%</p>
3	L	148	<p>53% 87% 9%</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 111888 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	106	Total	C	N	O	S	0	0
			740	472	128	137	3		
1	D	106	Total	C	N	O	S	0	0
			740	472	128	137	3		
1	G	106	Total	C	N	O	S	0	0
			740	472	128	137	3		
1	J	106	Total	C	N	O	S	0	0
			740	472	128	137	3		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P68106
A	-1	ASN	-	expression tag	UNP P68106
A	0	ALA	-	expression tag	UNP P68106
D	-2	SER	-	expression tag	UNP P68106
D	-1	ASN	-	expression tag	UNP P68106
D	0	ALA	-	expression tag	UNP P68106
G	-2	SER	-	expression tag	UNP P68106
G	-1	ASN	-	expression tag	UNP P68106
G	0	ALA	-	expression tag	UNP P68106
J	-2	SER	-	expression tag	UNP P68106
J	-1	ASN	-	expression tag	UNP P68106
J	0	ALA	-	expression tag	UNP P68106

- Molecule 2 is a protein called Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3801	Total	C	N	O	S	6	0
			26463	16948	4708	4641	166		
2	E	3801	Total	C	N	O	S	6	0
			26463	16948	4708	4641	166		
2	H	3801	Total	C	N	O	S	6	0
			26463	16948	4708	4641	166		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	3801	Total	C	N	O	S	6	0
			26463	16948	4708	4641	166		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	135	Total	C	N	O	S	0	0
			768	477	138	151	2		
3	F	135	Total	C	N	O	S	0	0
			768	477	138	151	2		
3	I	135	Total	C	N	O	S	0	0
			768	477	138	151	2		
3	L	135	Total	C	N	O	S	0	0
			768	477	138	151	2		

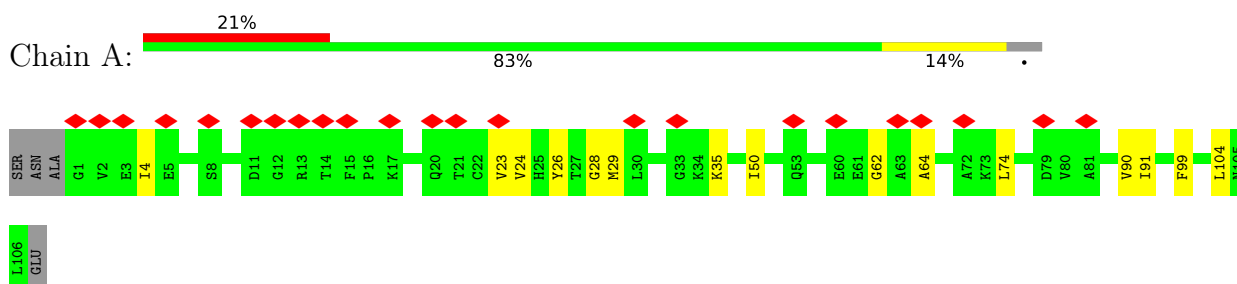
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	
4	H	1	Total	Zn	0
			1	1	
4	K	1	Total	Zn	0
			1	1	

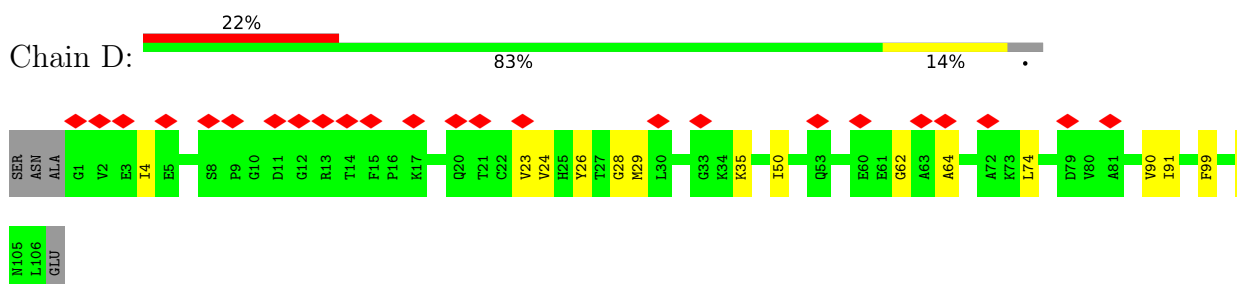
3 Residue-property plots [i](#)

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

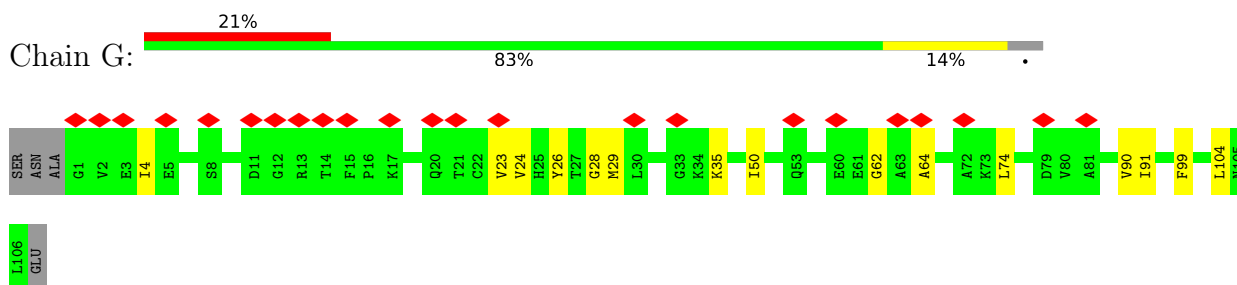
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



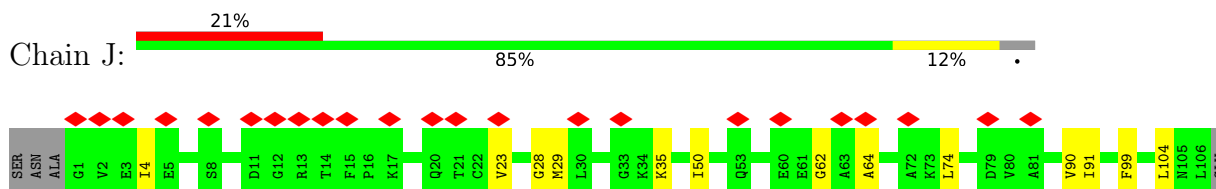
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



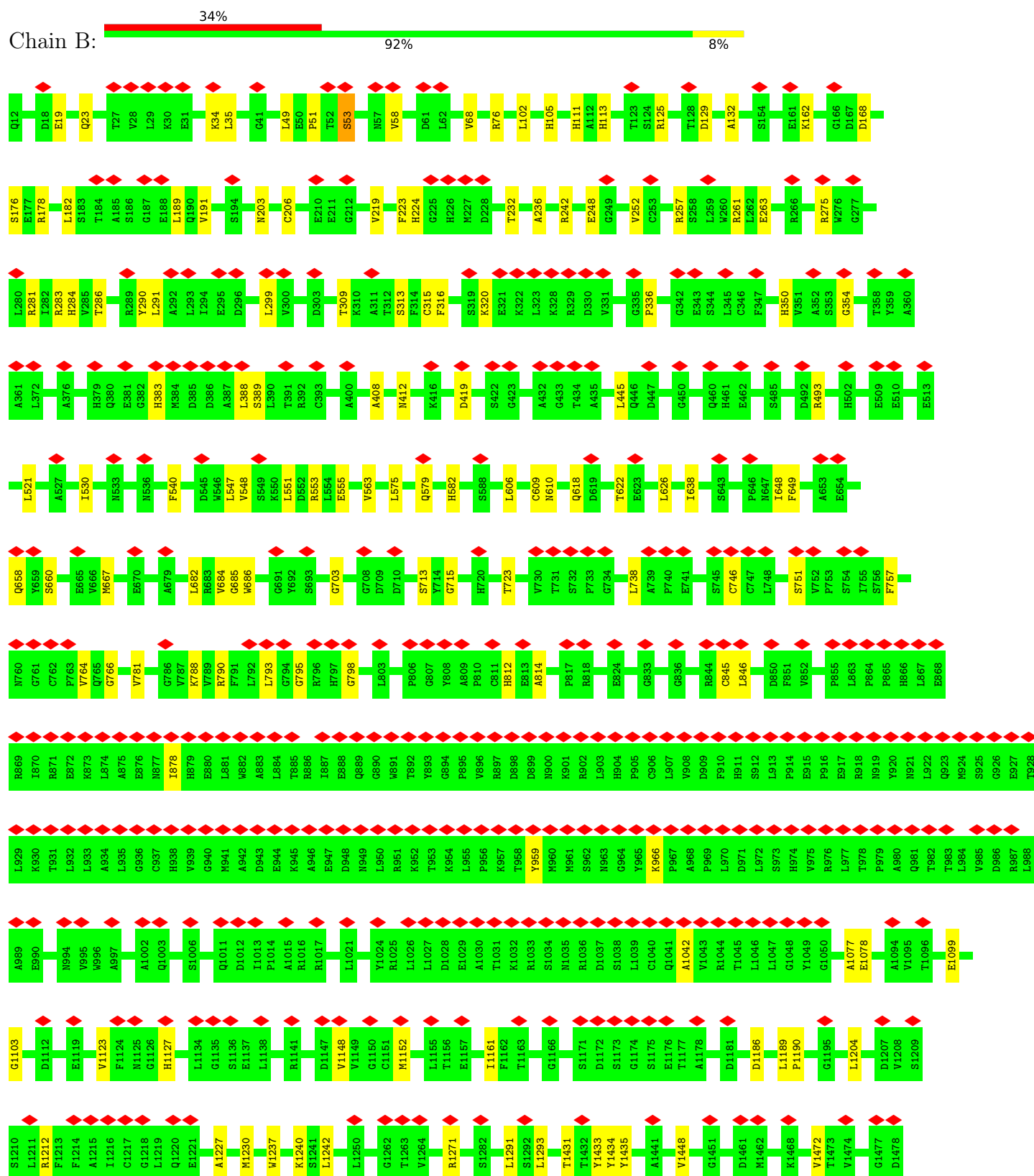
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



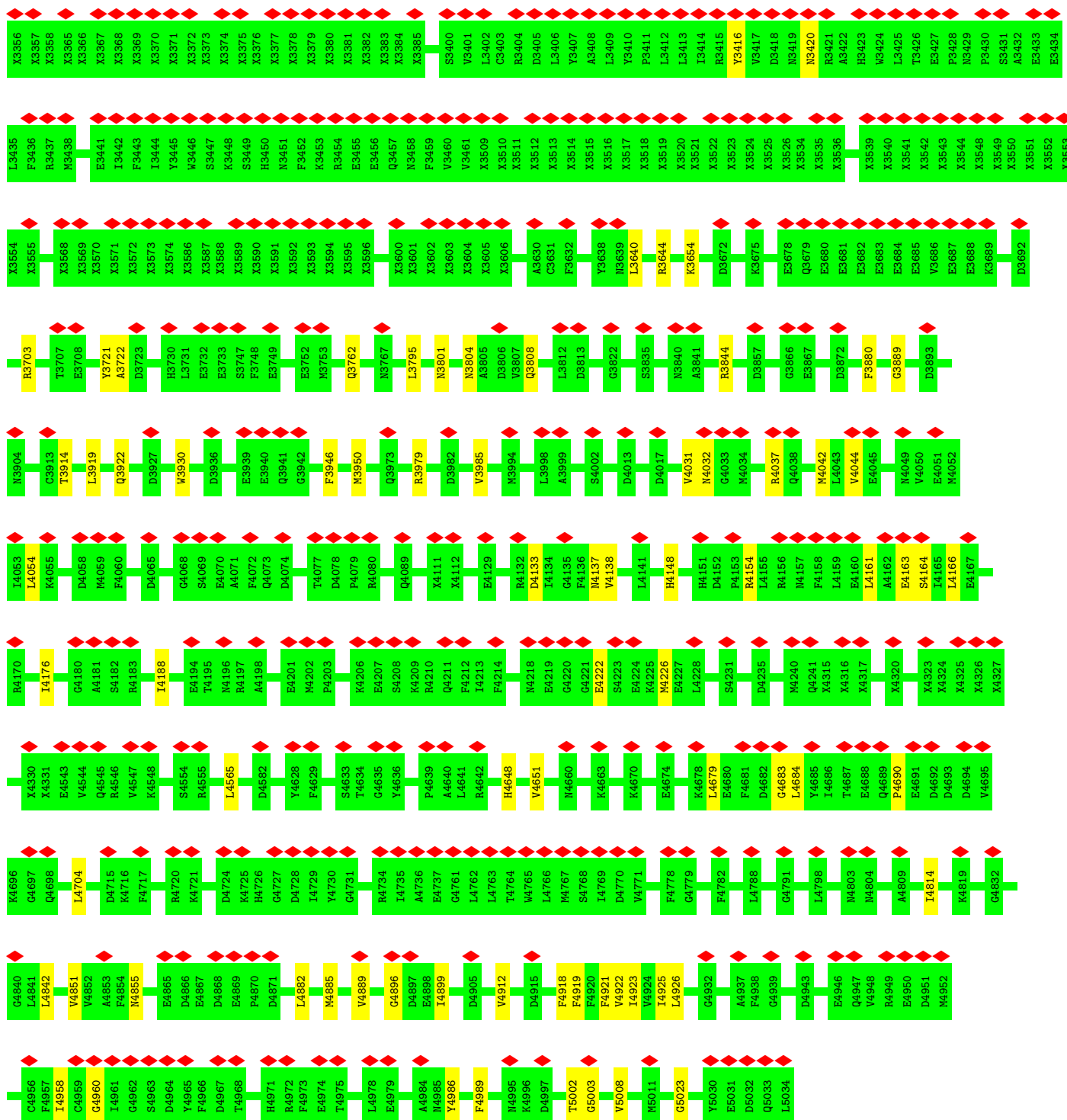
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 2: Ryanodine Receptor

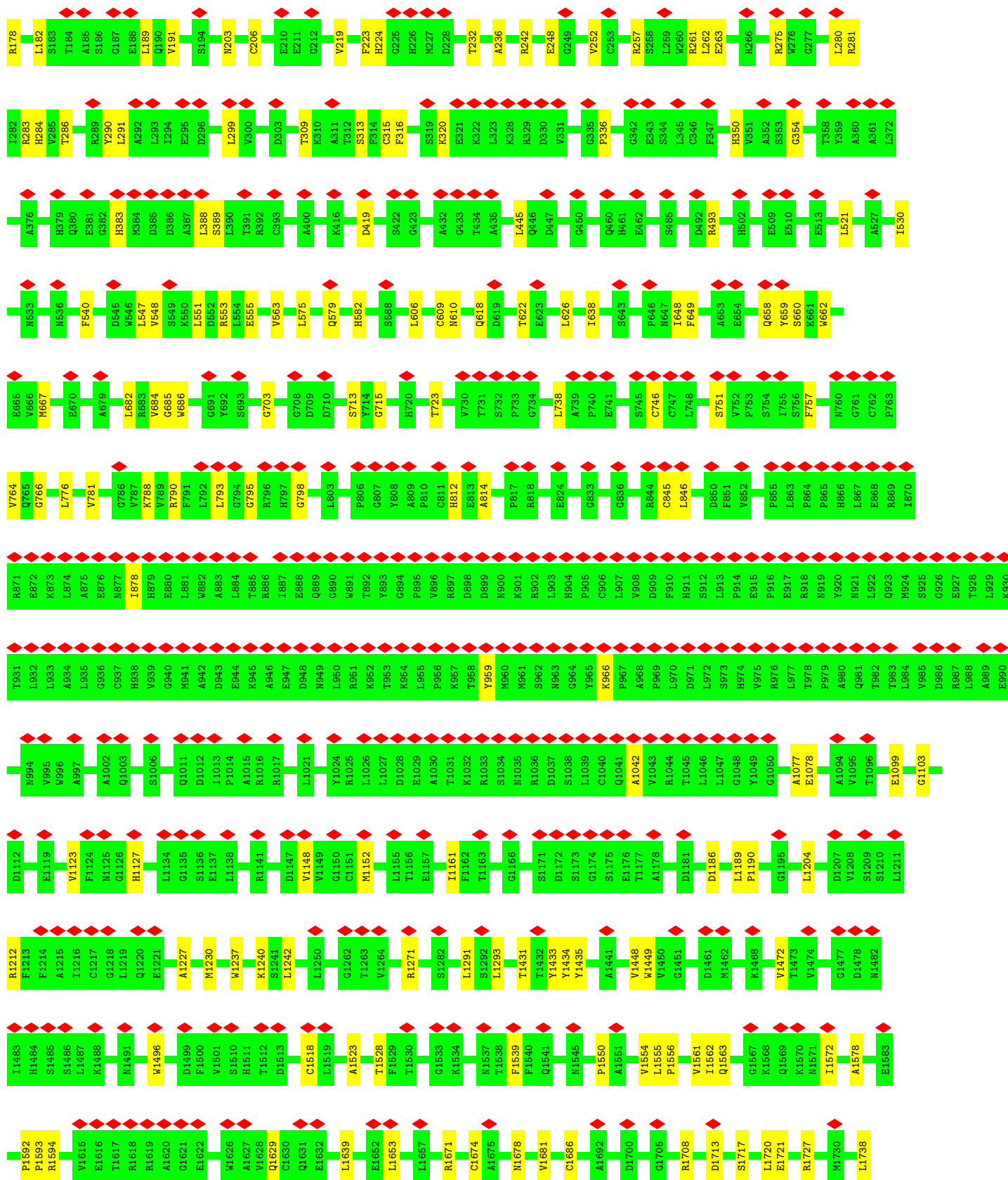


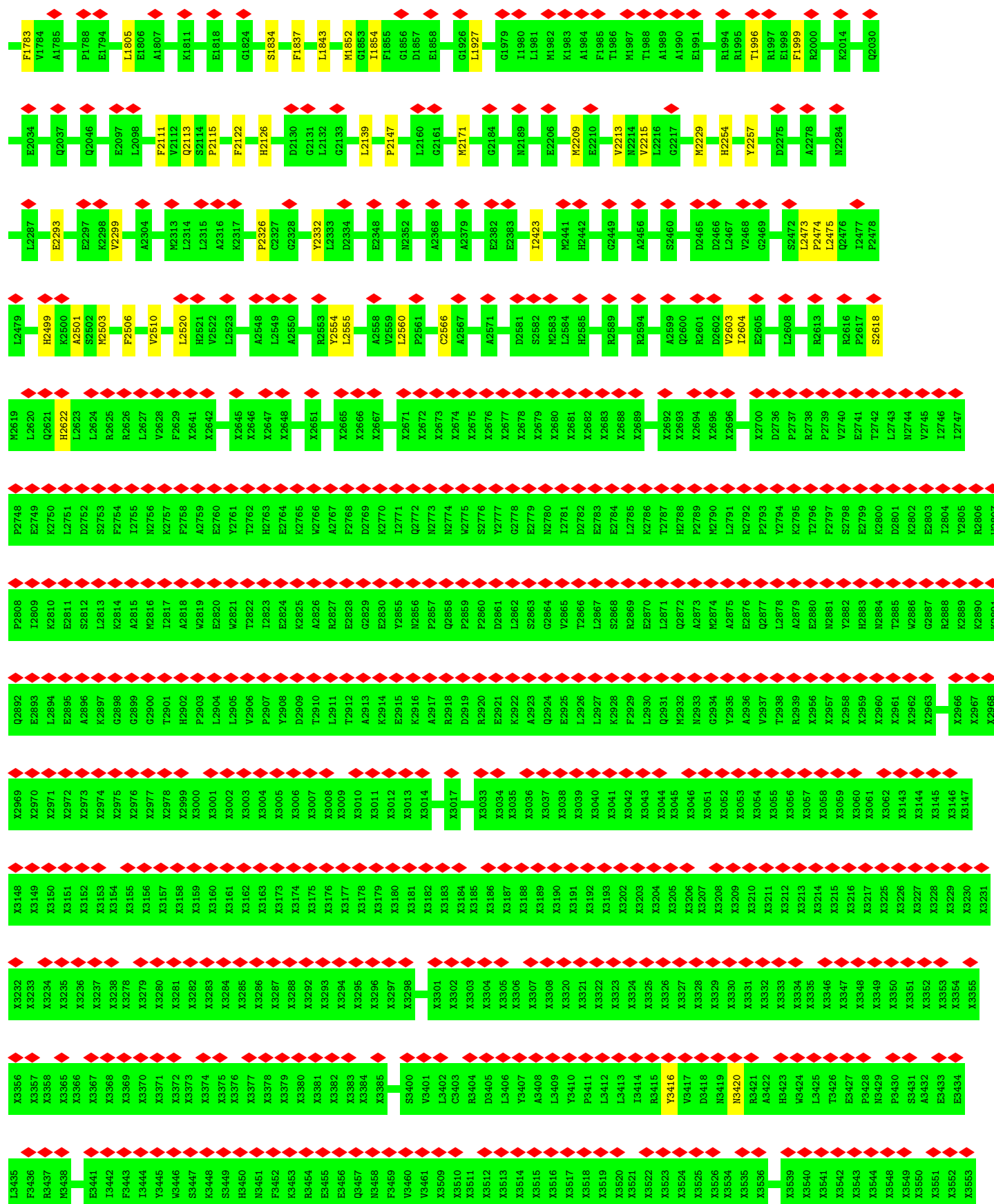


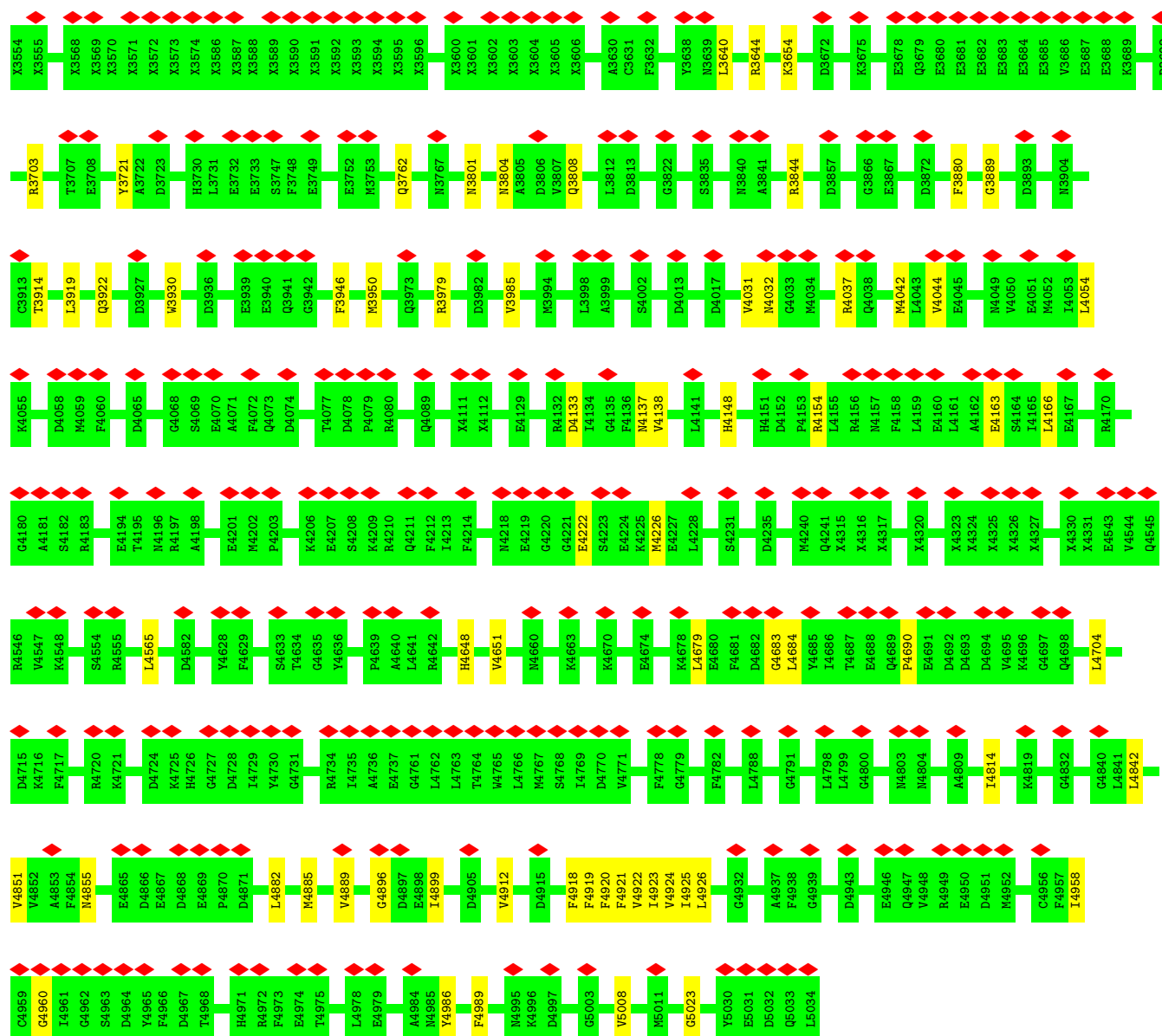


• Molecule 2: Ryanodine Receptor

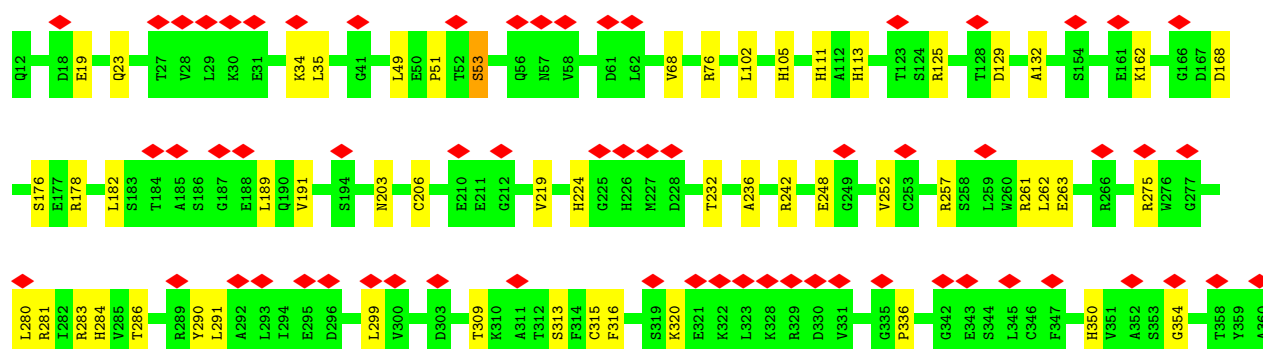
Chain E: 34% 92% 8%

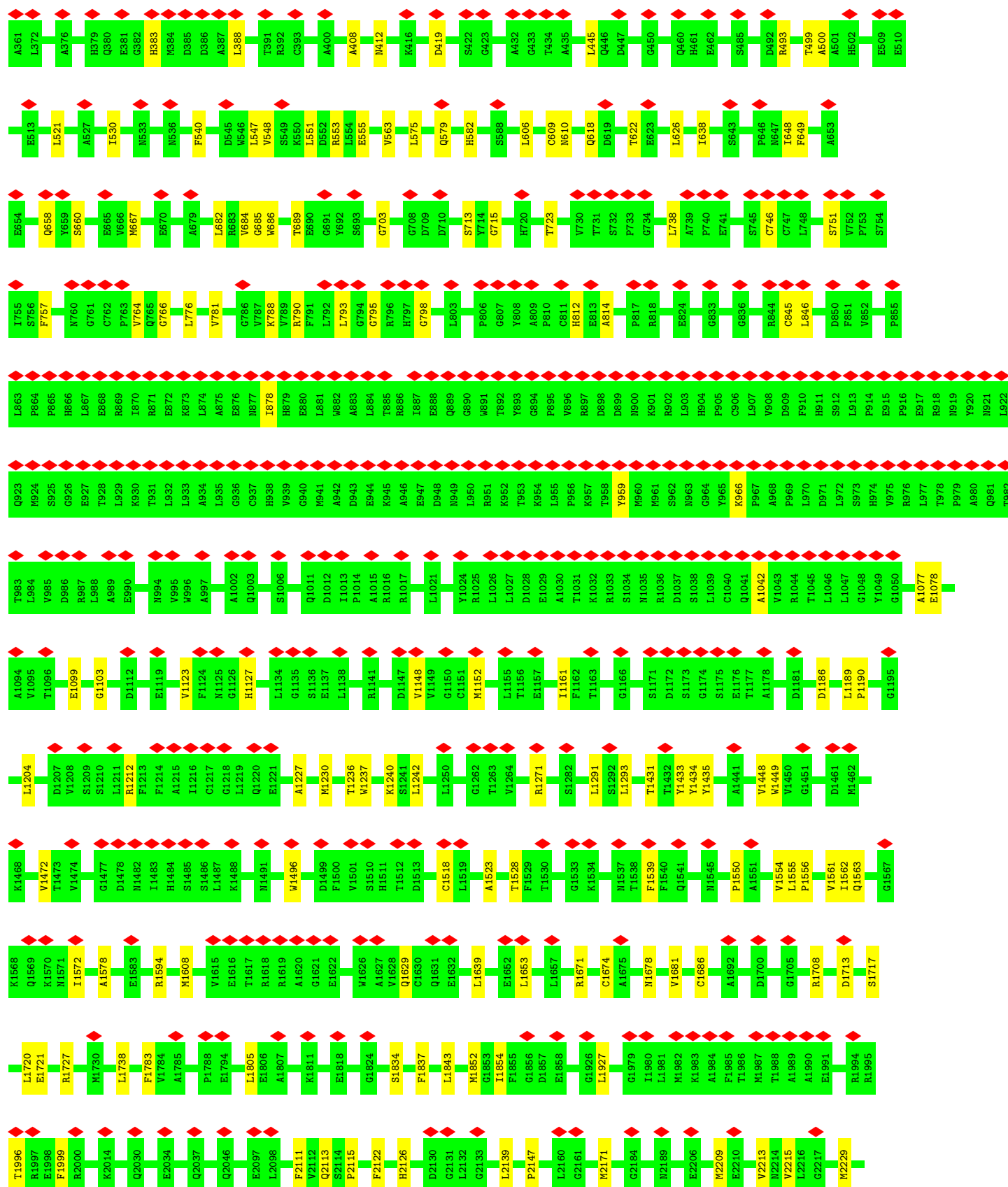


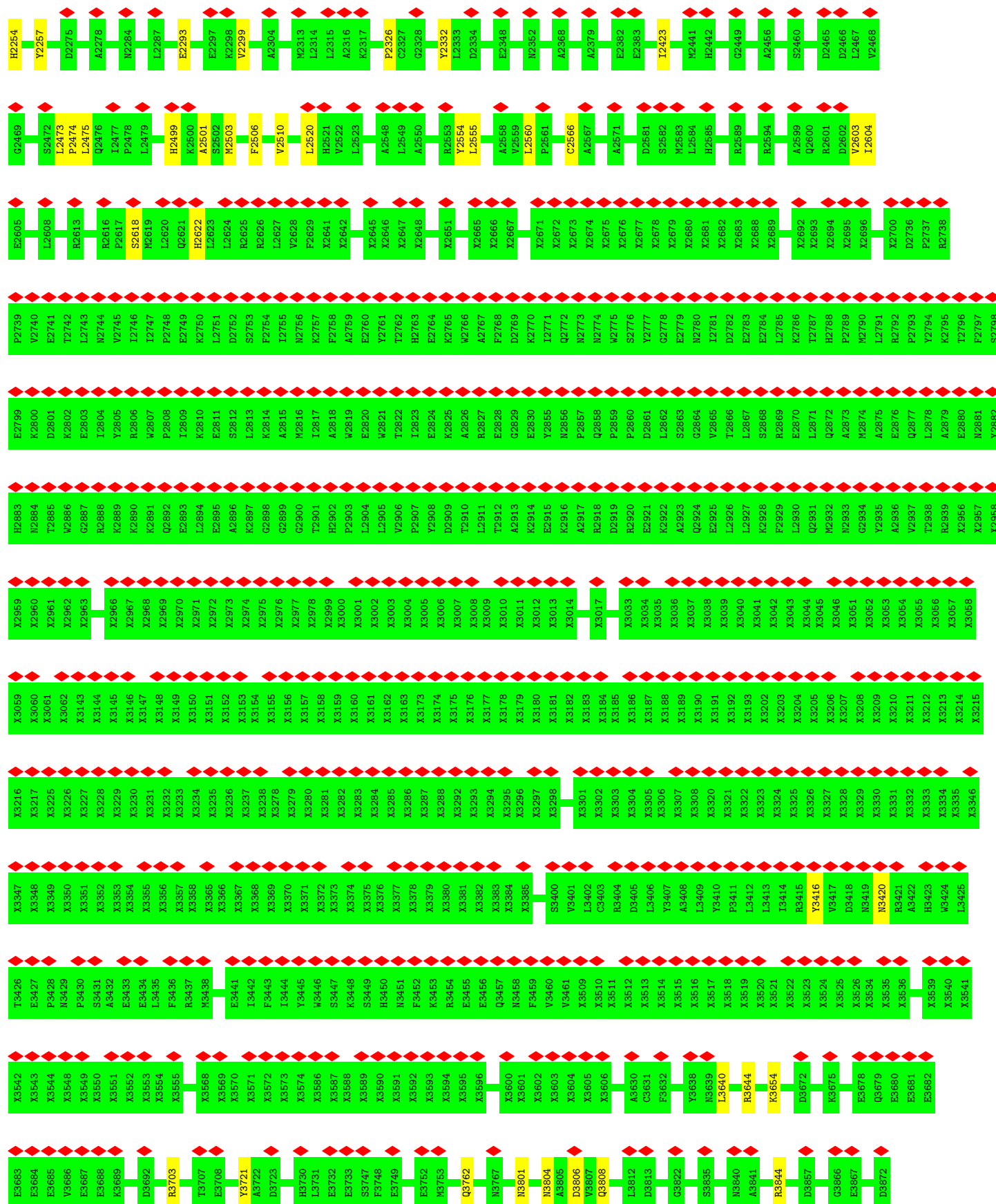


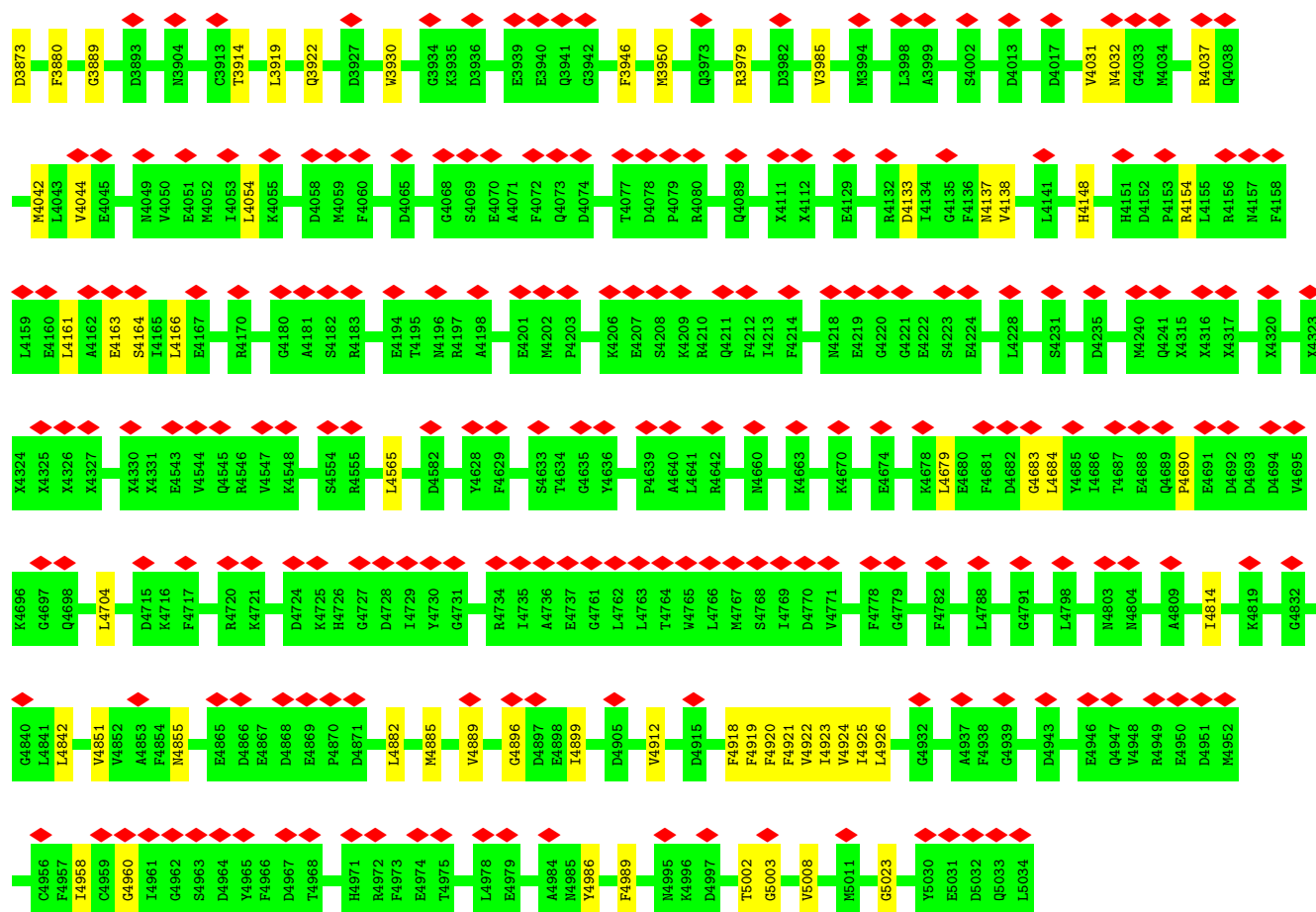


● Molecule 2: Ryanodine Receptor

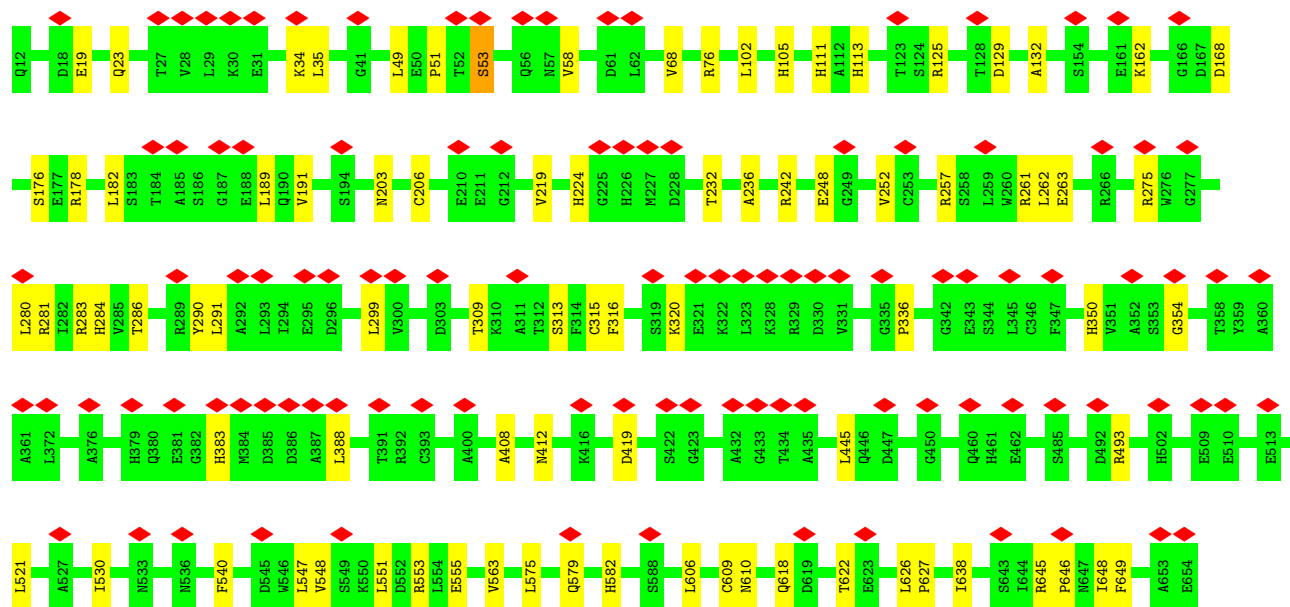


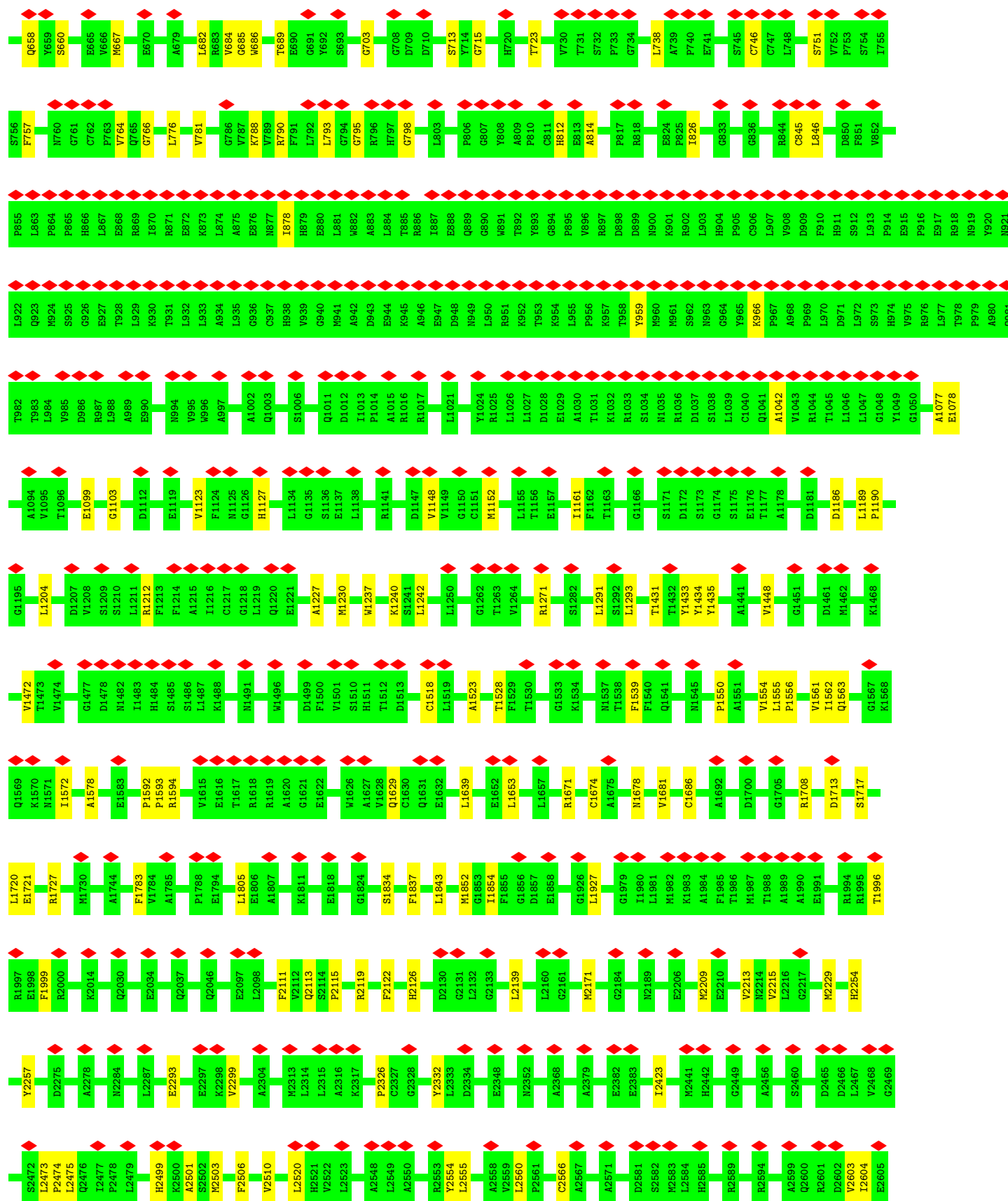




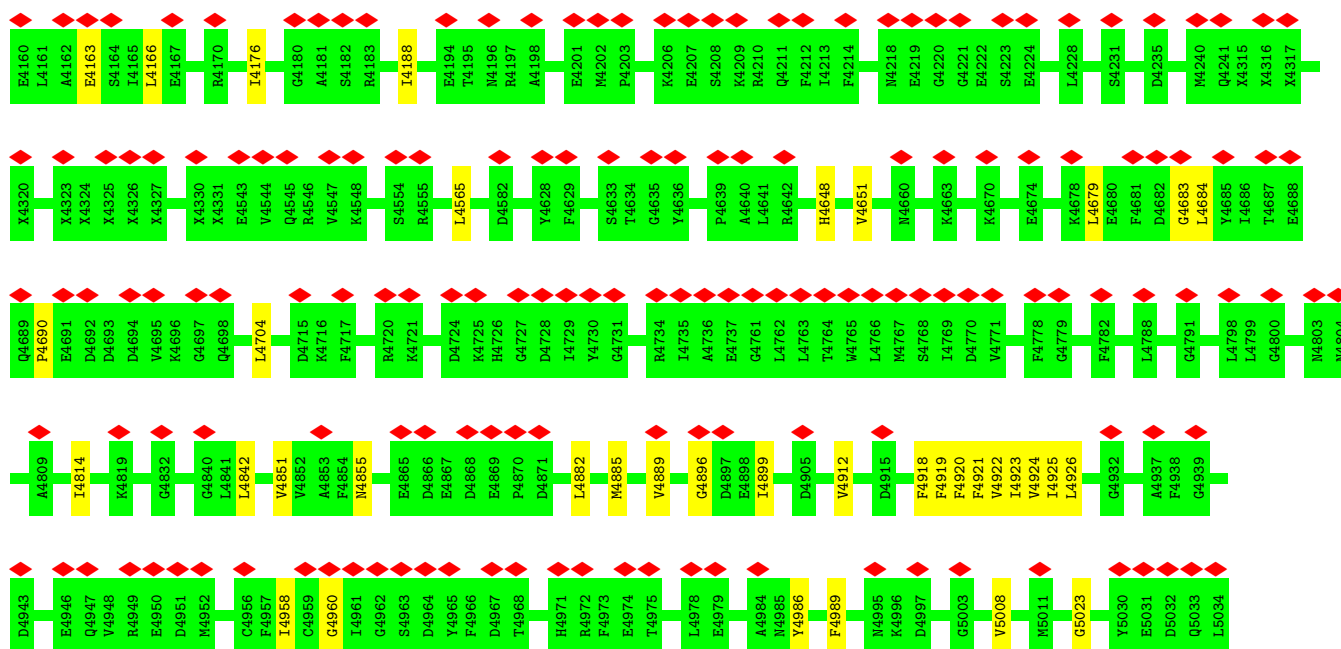


• Molecule 2: Ryanodine Receptor



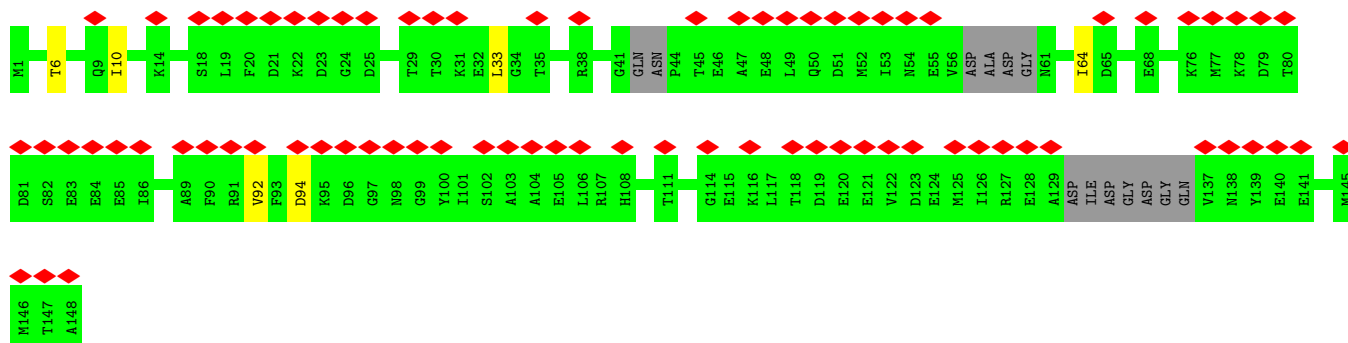


M4042	L4043	V4044	E4045	H4049	V4050	E4051	M4052	L4053	L4054	K4055	D4058	H4059	F4060	D4065	G4068	S4069	E4070	A4071	F4072	Q4073	D4074	F4077	D4078	P4079	R4080	Q4089	X4111	X4112	E4129	R4132	D4133	T4134	G4135	F4136	M4137	V4138	L4141	H4148	H4151	D4152	P4153	R4154	L4155	R4156	H4157	F4158	L4159												
V3869	M3870	D3872	F3880	G3889	N3904	C3913	T3914	L3919	Q3922	D3927	V3930	D3936	E3939	E3940	Q3941	G3942	F3946	M3950	Q3973	R3979	D3982	V3985	M3994	L3998	A3999	S4002	D4013	D4017	V4031	M4032	G4033	M4034	R4037	Q4038																									
E3684	E3685	V3686	E3687	E3688	K3689	D3692	R3703	T3707	E3708	D3715	Y3721	A3722	D3723	H3730	L3731	E3732	E3733	E3734	F3748	E3749	E3752	M3753	Q3762	N3767	N3801	M3804	A3805	D3806	V3807	Q3808	L3812	D3813	G3822	S3835	N3840	A3841	R3844	D3857	G3866	E3867	K3868																		
X3543	X3544	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3568	X3569	X3570	X3571	X3572	X3573	X3574	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3594	X3595	X3596	X3600	X3601	X3602	X3603	X3604	X3605	X3606	A3630	C3631	F3632	Y3638	N3639	L3640	R3644	K3654	D3672	K3675	E3678	Q3679	E3680	E3681	E3682	E3683									
X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	S3400	V3401	L3402	C3403	R3404	D3405	L3406	F3407	A3408	L3409	Y3410	P3411	L3412	L3413	L3414	R3415	Y3416	V3417	D3418	N3419	N3420	R3421	A3422	H3423	V3424	L3425	T3426	
X3217	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3237	X3238	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3346	X3347	
X3060	X3061	X3062	X3143	X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3151	X3152	X3153	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3183	X3184	X3185	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3202	X3203	X3204	X3205	X3206	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216
X2960	X2961	X2962	X2963	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2977	X2978	X2979	X2980	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3009	X3010	X3011	X3012	X3013	X3014	X3017	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3051	X3052	X3053	X3054	X3055	X3056	X3057	X3058	X3059		
N2884	T2885	W2886	Q2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	N2916	A2917	R2918	D2919	R2920	E2921	R2922	A2923	Q2924	E2925	L2926	L2927	Q2928	P2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	L2956	X2957	X2958	X2959
K2800	D2801	K2802	E2803	L2804	Y2805	K2806	W2807	P2808	E2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	Q2829	E2830	Y2855	N2856	P2857	Q2858	P2859	D2860	L2861	L2862	S2863	X2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	R2879	E2880	N2881	Y2882	H2883
V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	L2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	L2796	F2797	S2798	E2799	



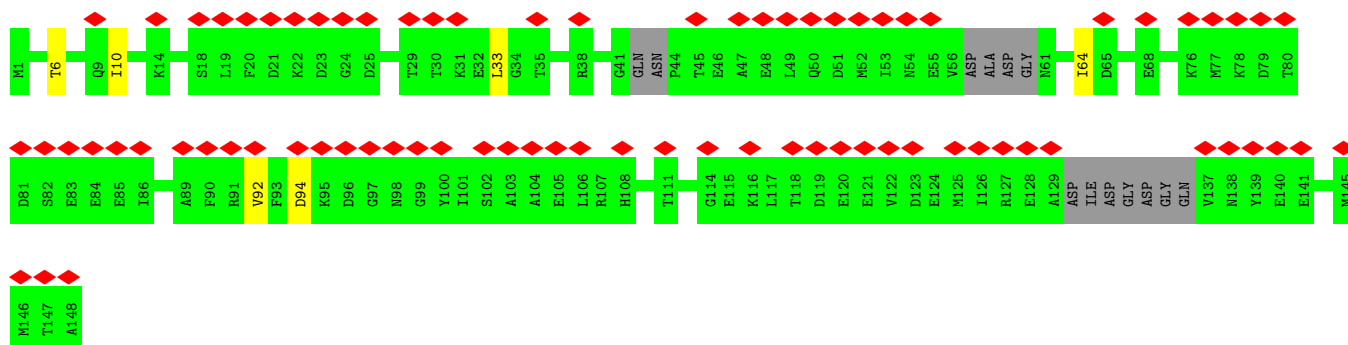
• Molecule 3: Calmodulin-1

Chain C: 53% 87% 9%

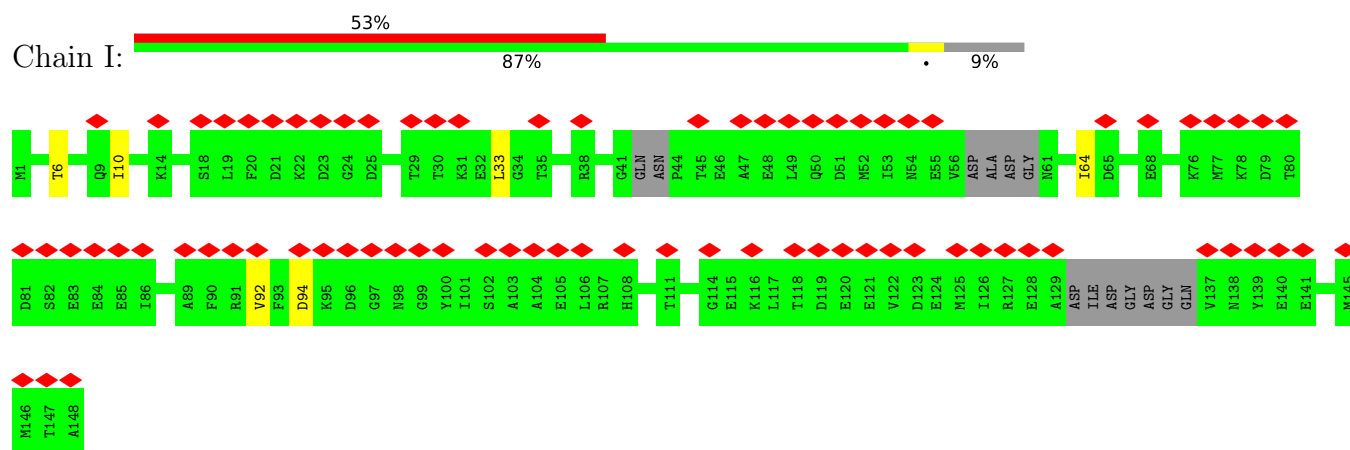


• Molecule 3: Calmodulin-1

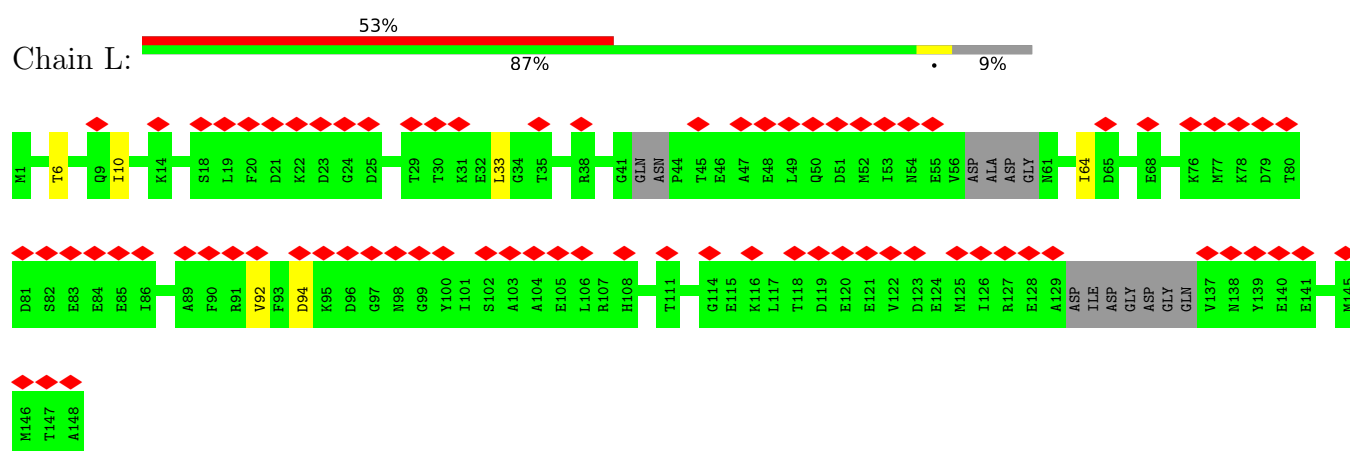
Chain F: 53% 87% 9%



• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25122	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.192	Depositor
Minimum map value	-0.147	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size (\AA)	523.2, 523.2, 523.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.09, 1.09, 1.09	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.25	0/756	0.42	0/1030
1	D	0.25	0/756	0.42	0/1030
1	G	0.25	0/756	0.42	0/1030
1	J	0.25	0/756	0.42	0/1030
2	B	0.24	0/25212	0.37	0/34385
2	E	0.23	0/25212	0.37	0/34385
2	H	0.23	0/25212	0.37	0/34385
2	K	0.24	0/25212	0.37	0/34385
3	C	0.24	0/772	0.36	0/1059
3	F	0.24	0/772	0.36	0/1059
3	I	0.24	0/772	0.36	0/1059
3	L	0.24	0/772	0.36	0/1059
All	All	0.24	0/106960	0.37	0/145896

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	740	0	689	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	740	0	689	8	0
1	G	740	0	689	8	0
1	J	740	0	689	7	0
2	B	26463	0	22978	161	0
2	E	26463	0	22978	161	0
2	H	26463	0	22978	165	0
2	K	26463	0	22978	165	0
3	C	768	0	486	4	0
3	F	768	0	486	4	0
3	I	768	0	486	4	0
3	L	768	0	486	4	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
All	All	111888	0	96612	687	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 3.

All (687) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:579:GLN:H	2:H:582:HIS:HD2	1.39	0.70
2:K:4565:LEU:HG	2:K:4814:ILE:HD12	1.73	0.70
2:B:579:GLN:H	2:B:582:HIS:HD2	1.39	0.70
2:E:579:GLN:H	2:E:582:HIS:HD2	1.39	0.70
2:K:579:GLN:H	2:K:582:HIS:HD2	1.39	0.70
2:B:4565:LEU:HG	2:B:4814:ILE:HD12	1.73	0.69
2:H:4565:LEU:HG	2:H:4814:ILE:HD12	1.73	0.69
2:E:4565:LEU:HG	2:E:4814:ILE:HD12	1.73	0.68
2:K:34:LYS:H	2:K:53:SER:HB2	1.56	0.68
2:E:4842:LEU:HD13	2:E:4926:LEU:HG	1.78	0.65
2:B:4842:LEU:HD13	2:B:4926:LEU:HG	1.78	0.65
2:H:350:HIS:HB3	2:H:354:GLY:H	1.62	0.65
2:K:350:HIS:HB3	2:K:354:GLY:H	1.62	0.65
2:E:350:HIS:HB3	2:E:354:GLY:H	1.62	0.65
2:H:4842:LEU:HD13	2:H:4926:LEU:HG	1.78	0.64
2:K:4842:LEU:HD13	2:K:4926:LEU:HG	1.78	0.63
2:K:2560:LEU:HD23	2:K:2603:VAL:HG12	1.81	0.63
2:H:2560:LEU:HD23	2:H:2603:VAL:HG12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:HIS:HB3	2:B:354:GLY:H	1.62	0.63
2:B:2560:LEU:HD23	2:B:2603:VAL:HG12	1.81	0.62
2:K:622:THR:HG23	2:K:626:LEU:HD12	1.81	0.62
2:E:2560:LEU:HD23	2:E:2603:VAL:HG12	1.81	0.62
2:B:49:LEU:HD11	2:B:191:VAL:HG23	1.82	0.62
2:B:622:THR:HG23	2:B:626:LEU:HD12	1.81	0.61
2:E:622:THR:HG23	2:E:626:LEU:HD12	1.81	0.61
2:K:618:GLN:OE1	2:K:1678:ASN:ND2	2.32	0.61
2:K:1727:ARG:HD2	2:K:1852:MET:HA	1.83	0.60
2:B:1727:ARG:HD2	2:B:1852:MET:HA	1.83	0.60
2:E:1727:ARG:HD2	2:E:1852:MET:HA	1.83	0.60
2:H:622:THR:HG23	2:H:626:LEU:HD12	1.81	0.60
2:H:1727:ARG:HD2	2:H:1852:MET:HA	1.83	0.60
2:K:667:MET:SD	2:K:790:ARG:NH2	2.74	0.60
2:K:19:GLU:HG2	2:K:68:VAL:HG12	1.83	0.60
2:K:553:ARG:NH2	2:K:555:GLU:OE1	2.31	0.60
2:B:553:ARG:NH2	2:B:555:GLU:OE1	2.31	0.60
2:H:3762:GLN:OE1	2:H:3804:ASN:ND2	2.35	0.60
2:E:19:GLU:HG2	2:E:68:VAL:HG12	1.83	0.60
2:E:2139:LEU:HD23	2:E:3654:LYS:HB2	1.84	0.60
2:H:3416:TYR:O	2:H:3420:ASN:ND2	2.35	0.60
2:H:19:GLU:HG2	2:H:68:VAL:HG12	1.83	0.60
2:E:3416:TYR:O	2:E:3420:ASN:ND2	2.35	0.60
2:K:3416:TYR:O	2:K:3420:ASN:ND2	2.35	0.60
2:E:667:MET:SD	2:E:790:ARG:NH2	2.74	0.59
2:B:19:GLU:HG2	2:B:68:VAL:HG12	1.83	0.59
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.32	0.59
2:B:667:MET:SD	2:B:790:ARG:NH2	2.74	0.59
2:B:2139:LEU:HD23	2:B:3654:LYS:HB2	1.84	0.59
2:B:3416:TYR:O	2:B:3420:ASN:ND2	2.35	0.59
2:B:3762:GLN:OE1	2:B:3804:ASN:ND2	2.35	0.59
2:E:129:ASP:HB2	2:E:132:ALA:HB2	1.84	0.59
2:H:667:MET:SD	2:H:790:ARG:NH2	2.74	0.59
2:B:686:TRP:O	2:B:713:SER:OG	2.20	0.59
2:H:878:ILE:HD11	2:H:1042:ALA:HA	1.84	0.59
2:E:3762:GLN:OE1	2:E:3804:ASN:ND2	2.35	0.59
2:H:129:ASP:HB2	2:H:132:ALA:HB2	1.84	0.59
2:K:3762:GLN:OE1	2:K:3804:ASN:ND2	2.35	0.59
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.32	0.59
2:K:878:ILE:HD11	2:K:1042:ALA:HA	1.84	0.59
2:H:2139:LEU:HD23	2:H:3654:LYS:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2139:LEU:HD23	2:K:3654:LYS:HB2	1.84	0.59
2:K:1271:ARG:HA	2:K:1563:GLN:HG2	1.85	0.58
2:K:129:ASP:HB2	2:K:132:ALA:HB2	1.84	0.58
2:B:129:ASP:HB2	2:B:132:ALA:HB2	1.84	0.58
2:E:1271:ARG:HA	2:E:1563:GLN:HG2	1.85	0.58
2:K:176:SER:HB2	2:K:178:ARG:HH21	1.69	0.58
2:B:878:ILE:HD11	2:B:1042:ALA:HA	1.84	0.58
2:B:1271:ARG:HA	2:B:1563:GLN:HG2	1.85	0.58
2:E:878:ILE:HD11	2:E:1042:ALA:HA	1.84	0.58
2:H:1078:GLU:HG2	2:H:1237:TRP:HE1	1.69	0.58
2:H:2111:PHE:HD2	2:H:2113:GLN:HG2	1.69	0.58
2:B:1435:TYR:HB3	2:B:1518:CYS:HB2	1.86	0.58
2:E:1078:GLU:HG2	2:E:1237:TRP:HE1	1.69	0.58
2:H:176:SER:HB2	2:H:178:ARG:HH21	1.69	0.58
2:H:553:ARG:NH2	2:H:555:GLU:OE1	2.31	0.58
2:H:1271:ARG:HA	2:H:1563:GLN:HG2	1.85	0.58
2:B:4679:LEU:HD12	2:B:4683:GLY:HA2	1.86	0.57
2:B:2111:PHE:HD2	2:B:2113:GLN:HG2	1.69	0.57
2:K:4679:LEU:HD12	2:K:4683:GLY:HA2	1.86	0.57
2:B:648:ILE:HG23	2:B:814:ALA:HB3	1.87	0.57
2:E:291:LEU:HD12	2:E:299:LEU:HD22	1.87	0.57
2:E:1435:TYR:HB3	2:E:1518:CYS:HB2	1.86	0.57
2:H:648:ILE:HG23	2:H:814:ALA:HB3	1.87	0.57
1:A:62:GLY:HA3	1:A:74:LEU:HD22	1.87	0.57
2:B:1078:GLU:HG2	2:B:1237:TRP:HE1	1.69	0.57
2:E:176:SER:HB2	2:E:178:ARG:HH21	1.69	0.57
2:B:176:SER:HB2	2:B:178:ARG:HH21	1.69	0.57
2:H:618:GLN:OE1	2:H:1678:ASN:ND2	2.32	0.57
2:E:686:TRP:O	2:E:713:SER:OG	2.20	0.57
2:K:682:LEU:HB3	2:K:738:LEU:HD11	1.87	0.57
2:K:686:TRP:O	2:K:713:SER:OG	2.20	0.56
2:K:1078:GLU:HG2	2:K:1237:TRP:HE1	1.69	0.56
2:E:4679:LEU:HD12	2:E:4683:GLY:HA2	1.86	0.56
1:J:62:GLY:HA3	1:J:74:LEU:HD22	1.87	0.56
2:K:648:ILE:HG23	2:K:814:ALA:HB3	1.87	0.56
2:K:1435:TYR:HB3	2:K:1518:CYS:HB2	1.86	0.56
2:E:648:ILE:HG23	2:E:814:ALA:HB3	1.87	0.56
2:H:291:LEU:HD12	2:H:299:LEU:HD22	1.87	0.56
2:K:2111:PHE:HD2	2:K:2113:GLN:HG2	1.69	0.56
2:B:76:ARG:HB2	2:K:3930:TRP:HE3	1.71	0.56
2:B:682:LEU:HB3	2:B:738:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2111:PHE:HD2	2:E:2113:GLN:HG2	1.69	0.56
2:H:1435:TYR:HB3	2:H:1518:CYS:HB2	1.86	0.56
2:K:291:LEU:HD12	2:K:299:LEU:HD22	1.87	0.56
2:B:3930:TRP:HE3	2:E:76:ARG:HB2	1.71	0.56
2:E:553:ARG:NH2	2:E:555:GLU:OE1	2.31	0.56
2:H:4679:LEU:HD12	2:H:4683:GLY:HA2	1.86	0.56
1:D:62:GLY:HA3	1:D:74:LEU:HD22	1.87	0.56
2:H:682:LEU:HB3	2:H:738:LEU:HD11	1.87	0.56
2:E:682:LEU:HB3	2:E:738:LEU:HD11	1.87	0.56
2:E:3930:TRP:HE3	2:H:76:ARG:HB2	1.71	0.56
1:G:62:GLY:HA3	1:G:74:LEU:HD22	1.87	0.56
2:K:2171:MET:HG3	2:K:2215:VAL:HG12	1.88	0.56
2:E:275:ARG:HD3	2:E:336:PRO:HD2	1.89	0.56
2:B:291:LEU:HD12	2:B:299:LEU:HD22	1.87	0.55
2:H:2326:PRO:HG3	2:H:2423:ILE:HD13	1.89	0.55
2:E:845:CYS:SG	2:E:846:LEU:N	2.80	0.55
2:H:845:CYS:SG	2:H:846:LEU:N	2.80	0.55
2:H:2171:MET:HG3	2:H:2215:VAL:HG12	1.88	0.55
2:B:275:ARG:HD3	2:B:336:PRO:HD2	1.89	0.55
2:E:540:PHE:HE2	2:E:547:LEU:HD22	1.72	0.55
2:E:2326:PRO:HG3	2:E:2423:ILE:HD13	1.89	0.55
2:H:686:TRP:O	2:H:713:SER:OG	2.20	0.55
2:K:2326:PRO:HG3	2:K:2423:ILE:HD13	1.89	0.55
2:B:845:CYS:SG	2:B:846:LEU:N	2.80	0.55
2:B:2326:PRO:HG3	2:B:2423:ILE:HD13	1.89	0.55
2:H:540:PHE:HE2	2:H:547:LEU:HD22	1.72	0.55
2:H:3930:TRP:HE3	2:K:76:ARG:HB2	1.71	0.55
2:B:2171:MET:HG3	2:B:2215:VAL:HG12	1.88	0.55
2:E:2171:MET:HG3	2:E:2215:VAL:HG12	1.88	0.55
2:B:2122:PHE:O	2:B:3721:TYR:OH	2.26	0.54
2:K:275:ARG:HD3	2:K:336:PRO:HD2	1.89	0.54
2:K:723:THR:HG21	2:K:1472:VAL:HG11	1.89	0.54
2:H:1561:VAL:HG12	2:H:1562:ILE:HG12	1.90	0.54
2:K:845:CYS:SG	2:K:846:LEU:N	2.80	0.54
2:B:1561:VAL:HG12	2:B:1562:ILE:HG12	1.90	0.54
2:K:540:PHE:HE2	2:K:547:LEU:HD22	1.72	0.54
2:K:3762:GLN:NE2	2:K:3801:ASN:OD1	2.41	0.54
2:B:320:LYS:NZ	2:B:383:HIS:O	2.41	0.54
2:E:2115:PRO:HB3	2:E:3703:ARG:HH22	1.73	0.54
2:E:3762:GLN:NE2	2:E:3801:ASN:OD1	2.41	0.54
2:K:2115:PRO:HB3	2:K:3703:ARG:HH22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:540:PHE:HE2	2:B:547:LEU:HD22	1.72	0.54
2:B:3762:GLN:NE2	2:B:3801:ASN:OD1	2.41	0.54
2:E:1561:VAL:HG12	2:E:1562:ILE:HG12	1.90	0.54
2:E:4851:VAL:O	2:E:4855:ASN:ND2	2.31	0.54
2:E:723:THR:HG21	2:E:1472:VAL:HG11	1.89	0.54
2:K:1561:VAL:HG12	2:K:1562:ILE:HG12	1.90	0.54
2:B:2115:PRO:HB3	2:B:3703:ARG:HH22	1.73	0.54
2:E:2122:PHE:O	2:E:3721:TYR:OH	2.26	0.54
2:H:34:LYS:H	2:H:53:SER:HB2	1.70	0.54
2:H:2115:PRO:HB3	2:H:3703:ARG:HH22	1.73	0.54
2:H:3762:GLN:NE2	2:H:3801:ASN:OD1	2.41	0.54
2:H:4960:GLY:H	2:H:5023:GLY:HA2	1.73	0.54
2:H:2122:PHE:O	2:H:3721:TYR:OH	2.26	0.53
2:E:548:VAL:HA	2:E:551:LEU:HD13	1.90	0.53
2:H:723:THR:HG21	2:H:1472:VAL:HG11	1.89	0.53
2:K:3640:LEU:HD12	2:K:3644:ARG:HD3	1.90	0.53
2:E:3640:LEU:HD12	2:E:3644:ARG:HD3	1.90	0.53
2:K:548:VAL:HA	2:K:551:LEU:HD13	1.90	0.53
2:K:2122:PHE:O	2:K:3721:TYR:OH	2.26	0.53
2:B:3640:LEU:HD12	2:B:3644:ARG:HD3	1.90	0.53
2:H:3640:LEU:HD12	2:H:3644:ARG:HD3	1.90	0.53
2:H:4684:LEU:HD23	2:H:4704:LEU:HD11	1.91	0.53
2:H:275:ARG:HD3	2:H:336:PRO:HD2	1.89	0.53
2:E:1555:LEU:HD12	2:E:1556:PRO:HD2	1.91	0.53
2:K:1152:MET:HB2	2:K:1161:ILE:HB	1.91	0.53
2:K:4684:LEU:HD23	2:K:4704:LEU:HD11	1.91	0.53
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.91	0.53
2:B:23:GLN:NE2	2:B:203:ASN:OD1	2.42	0.53
2:B:1555:LEU:HD12	2:B:1556:PRO:HD2	1.91	0.53
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.91	0.53
2:E:4684:LEU:HD23	2:E:4704:LEU:HD11	1.91	0.53
2:B:723:THR:HG21	2:B:1472:VAL:HG11	1.89	0.53
2:B:746:CYS:HA	2:B:757:PHE:HA	1.92	0.53
2:K:746:CYS:HA	2:K:757:PHE:HA	1.92	0.53
2:K:4960:GLY:H	2:K:5023:GLY:HA2	1.73	0.53
2:B:548:VAL:HA	2:B:551:LEU:HD13	1.90	0.52
2:E:23:GLN:NE2	2:E:203:ASN:OD1	2.42	0.52
2:E:4960:GLY:H	2:E:5023:GLY:HA2	1.73	0.52
2:H:1152:MET:HB2	2:H:1161:ILE:HB	1.91	0.52
2:K:320:LYS:NZ	2:K:383:HIS:O	2.41	0.52
2:H:1674:CYS:HB3	2:H:1681:VAL:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4032:ASN:O	2:B:4037:ARG:NH1	2.42	0.52
2:H:548:VAL:HA	2:H:551:LEU:HD13	1.90	0.52
2:H:1555:LEU:HD12	2:H:1556:PRO:HD2	1.91	0.52
2:K:1674:CYS:HB3	2:K:1681:VAL:HB	1.91	0.52
2:B:2618:SER:O	2:B:2622:HIS:ND1	2.43	0.52
2:B:4684:LEU:HD23	2:B:4704:LEU:HD11	1.91	0.52
2:H:320:LYS:NZ	2:H:383:HIS:O	2.41	0.52
2:B:4960:GLY:H	2:B:5023:GLY:HA2	1.73	0.52
2:E:1674:CYS:HB3	2:E:1681:VAL:HB	1.91	0.52
2:B:2506:PHE:O	2:B:2510:VAL:HG22	2.11	0.51
2:E:746:CYS:HA	2:E:757:PHE:HA	1.92	0.51
2:H:23:GLN:NE2	2:H:203:ASN:OD1	2.42	0.51
2:H:746:CYS:HA	2:H:757:PHE:HA	1.92	0.51
2:E:320:LYS:NZ	2:E:383:HIS:O	2.41	0.51
2:K:23:GLN:NE2	2:K:203:ASN:OD1	2.42	0.51
2:K:638:ILE:HD13	2:K:703:GLY:HA2	1.92	0.51
2:H:4918:PHE:O	2:H:4922:VAL:HG22	2.10	0.51
2:E:2499:HIS:O	2:E:2503:MET:HG2	2.11	0.51
2:K:1555:LEU:HD12	2:K:1556:PRO:HD2	1.91	0.51
2:K:2618:SER:O	2:K:2622:HIS:ND1	2.43	0.51
2:B:638:ILE:HD13	2:B:703:GLY:HA2	1.92	0.51
2:E:2618:SER:O	2:E:2622:HIS:ND1	2.43	0.51
1:G:28:GLY:HA3	1:G:99:PHE:HA	1.92	0.51
2:H:2618:SER:O	2:H:2622:HIS:ND1	2.43	0.51
2:B:4918:PHE:O	2:B:4922:VAL:HG22	2.10	0.51
2:H:638:ILE:HD13	2:H:703:GLY:HA2	1.92	0.51
2:E:638:ILE:HD13	2:E:703:GLY:HA2	1.92	0.51
2:H:2499:HIS:O	2:H:2503:MET:HG2	2.11	0.51
2:E:2506:PHE:O	2:E:2510:VAL:HG22	2.11	0.51
2:E:1708:ARG:NH2	2:E:1837:PHE:O	2.44	0.51
2:H:4922:VAL:O	2:H:4926:LEU:HB2	2.11	0.51
1:A:28:GLY:HA3	1:A:99:PHE:HA	1.92	0.51
2:K:609:CYS:SG	2:K:610:ASN:N	2.84	0.51
2:B:1674:CYS:HB3	2:B:1681:VAL:HB	1.91	0.50
2:H:283:ARG:NH1	2:H:290:TYR:OH	2.44	0.50
2:K:49:LEU:HD11	2:K:191:VAL:HG23	1.93	0.50
2:K:2506:PHE:O	2:K:2510:VAL:HG22	2.11	0.50
2:B:283:ARG:NH1	2:B:290:TYR:OH	2.44	0.50
2:B:609:CYS:SG	2:B:610:ASN:N	2.84	0.50
2:E:283:ARG:NH1	2:E:290:TYR:OH	2.44	0.50
2:K:4922:VAL:O	2:K:4926:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1708:ARG:NH2	2:H:1837:PHE:O	2.44	0.50
2:K:2499:HIS:O	2:K:2503:MET:HG2	2.11	0.50
2:E:4922:VAL:O	2:E:4926:LEU:HB2	2.11	0.50
2:H:609:CYS:SG	2:H:610:ASN:N	2.84	0.50
2:K:4918:PHE:O	2:K:4922:VAL:HG22	2.10	0.50
2:B:1717:SER:HA	2:B:1721:GLU:HB2	1.93	0.50
2:H:2506:PHE:O	2:H:2510:VAL:HG22	2.11	0.50
2:B:2499:HIS:O	2:B:2503:MET:HG2	2.11	0.50
2:E:49:LEU:HD11	2:E:191:VAL:HG23	1.93	0.50
2:K:1708:ARG:NH2	2:K:1837:PHE:O	2.44	0.50
2:K:1717:SER:HA	2:K:1721:GLU:HB2	1.93	0.50
2:B:1708:ARG:NH2	2:B:1837:PHE:O	2.44	0.50
1:D:28:GLY:HA3	1:D:99:PHE:HA	1.92	0.50
2:E:4918:PHE:O	2:E:4922:VAL:HG22	2.10	0.50
2:K:4032:ASN:O	2:K:4037:ARG:NH1	2.42	0.50
2:E:4133:ASP:O	2:E:4137:ASN:ND2	2.38	0.50
2:H:49:LEU:HD11	2:H:191:VAL:HG23	1.93	0.50
2:H:236:ALA:O	2:H:242:ARG:NH2	2.45	0.50
2:K:236:ALA:O	2:K:242:ARG:NH2	2.45	0.50
2:B:788:LYS:HG3	2:B:1629:GLN:HG2	1.93	0.50
2:B:4922:VAL:O	2:B:4926:LEU:HB2	2.11	0.50
2:E:609:CYS:SG	2:E:610:ASN:N	2.84	0.50
2:E:4989:PHE:HE2	2:E:5008:VAL:HG11	1.77	0.50
2:K:283:ARG:NH1	2:K:290:TYR:OH	2.44	0.50
2:K:4989:PHE:HE2	2:K:5008:VAL:HG11	1.77	0.50
1:J:28:GLY:HA3	1:J:99:PHE:HA	1.92	0.49
2:B:19:GLU:HB2	2:B:206:CYS:H	1.78	0.49
2:E:236:ALA:O	2:E:242:ARG:NH2	2.45	0.49
2:E:1717:SER:HA	2:E:1721:GLU:HB2	1.93	0.49
2:K:1434:TYR:HB2	2:K:1572:ILE:HD11	1.94	0.49
2:B:236:ALA:O	2:B:242:ARG:NH2	2.45	0.49
2:B:408:ALA:O	2:B:412:ASN:ND2	2.36	0.49
2:B:1434:TYR:HB2	2:B:1572:ILE:HD11	1.94	0.49
2:B:4989:PHE:HE2	2:B:5008:VAL:HG11	1.77	0.49
2:H:795:GLY:N	2:H:798:GLY:O	2.37	0.49
2:H:1639:LEU:HD12	2:H:1653:LEU:HD13	1.93	0.49
3:I:33:LEU:HD22	3:I:64:ILE:HG12	1.94	0.49
2:K:445:LEU:HD23	2:K:521:LEU:HB3	1.94	0.49
2:B:315:CYS:SG	2:B:316:PHE:N	2.86	0.49
3:F:33:LEU:HD22	3:F:64:ILE:HG12	1.94	0.49
2:H:419:ASP:OD1	2:H:493:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:315:CYS:SG	2:K:316:PHE:N	2.86	0.49
2:B:1639:LEU:HD12	2:B:1653:LEU:HD13	1.93	0.49
2:B:4958:ILE:HG12	2:B:4986:TYR:HE2	1.78	0.49
2:E:315:CYS:SG	2:E:316:PHE:N	2.86	0.49
2:E:419:ASP:OD1	2:E:493:ARG:NH1	2.45	0.49
2:E:3919:LEU:HD11	2:E:3979:ARG:HB2	1.95	0.49
2:E:4958:ILE:HG12	2:E:4986:TYR:HE2	1.78	0.49
2:H:102:LEU:HB2	2:H:105:HIS:CD2	2.48	0.49
2:H:445:LEU:HD23	2:H:521:LEU:HB3	1.94	0.49
2:H:1717:SER:HA	2:H:1721:GLU:HB2	1.93	0.49
2:K:19:GLU:HB2	2:K:206:CYS:H	1.78	0.49
2:K:102:LEU:HB2	2:K:105:HIS:CD2	2.48	0.49
2:K:3919:LEU:HD11	2:K:3979:ARG:HB2	1.95	0.49
3:L:33:LEU:HD13	3:L:64:ILE:HG21	1.95	0.49
2:B:419:ASP:OD1	2:B:493:ARG:NH1	2.45	0.49
2:E:2555:LEU:HD21	2:E:2560:LEU:HD13	1.95	0.49
2:E:4032:ASN:O	2:E:4037:ARG:NH1	2.42	0.49
2:E:445:LEU:HD23	2:E:521:LEU:HB3	1.94	0.49
2:E:788:LYS:HG3	2:E:1629:GLN:HG2	1.93	0.49
3:F:33:LEU:HD13	3:F:64:ILE:HG21	1.95	0.49
2:H:219:VAL:HG22	2:H:261:ARG:HB2	1.95	0.49
2:H:315:CYS:SG	2:H:316:PHE:N	2.86	0.49
2:H:788:LYS:HG3	2:H:1629:GLN:HG2	1.93	0.49
2:K:788:LYS:HG3	2:K:1629:GLN:HG2	1.93	0.49
2:K:2555:LEU:HD21	2:K:2560:LEU:HD13	1.95	0.49
3:C:33:LEU:HD13	3:C:64:ILE:HG21	1.95	0.49
2:B:3919:LEU:HD11	2:B:3979:ARG:HB2	1.95	0.48
2:E:1639:LEU:HD12	2:E:1653:LEU:HD13	1.93	0.48
2:B:102:LEU:HB2	2:B:105:HIS:CD2	2.48	0.48
2:H:4989:PHE:HE2	2:H:5008:VAL:HG11	1.77	0.48
2:K:419:ASP:OD1	2:K:493:ARG:NH1	2.45	0.48
2:K:1639:LEU:HD12	2:K:1653:LEU:HD13	1.93	0.48
2:K:2473:LEU:HD12	2:K:2474:PRO:HD2	1.96	0.48
2:B:219:VAL:HG22	2:B:261:ARG:HB2	1.95	0.48
2:E:102:LEU:HB2	2:E:105:HIS:HD2	1.78	0.48
2:H:4032:ASN:O	2:H:4037:ARG:NH1	2.42	0.48
2:H:4044:VAL:HG11	2:H:4154:ARG:HD2	1.95	0.48
3:I:33:LEU:HD13	3:I:64:ILE:HG21	1.95	0.48
2:E:19:GLU:HB2	2:E:206:CYS:H	1.78	0.48
2:E:102:LEU:HB2	2:E:105:HIS:CD2	2.48	0.48
2:H:4958:ILE:HG12	2:H:4986:TYR:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:219:VAL:HG22	2:K:261:ARG:HB2	1.95	0.48
2:K:4044:VAL:HG11	2:K:4154:ARG:HD2	1.95	0.48
2:K:4054:LEU:HD21	2:K:4138:VAL:HG11	1.96	0.48
3:L:33:LEU:HD22	3:L:64:ILE:HG12	1.94	0.48
2:B:1528:THR:HG22	2:B:1539:PHE:HB3	1.96	0.48
2:B:2473:LEU:HD12	2:B:2474:PRO:HD2	1.96	0.48
2:E:2473:LEU:HD12	2:E:2474:PRO:HD2	1.96	0.48
2:H:19:GLU:HB2	2:H:206:CYS:H	1.78	0.48
2:H:3919:LEU:HD11	2:H:3979:ARG:HB2	1.95	0.48
2:B:4054:LEU:HD21	2:B:4138:VAL:HG11	1.96	0.48
3:C:33:LEU:HD22	3:C:64:ILE:HG12	1.94	0.48
2:E:3919:LEU:O	2:E:3922:GLN:HG3	2.14	0.48
2:H:168:ASP:OD1	2:H:168:ASP:N	2.46	0.48
2:K:3919:LEU:O	2:K:3922:GLN:HG3	2.14	0.48
2:B:168:ASP:OD1	2:B:168:ASP:N	2.46	0.48
2:K:4958:ILE:HG12	2:K:4986:TYR:HE2	1.78	0.48
2:E:1434:TYR:HB2	2:E:1572:ILE:HD11	1.94	0.48
2:H:2473:LEU:HD12	2:H:2474:PRO:HD2	1.96	0.48
2:H:1843:LEU:HD11	2:H:1927:LEU:HD21	1.96	0.48
2:K:1843:LEU:HD11	2:K:1927:LEU:HD21	1.96	0.48
2:B:248:GLU:OE2	2:B:257:ARG:NH1	2.47	0.48
2:B:1077:ALA:H	2:B:1189:LEU:HD12	1.79	0.48
2:E:1528:THR:HG22	2:E:1539:PHE:HB3	1.96	0.48
2:H:248:GLU:OE2	2:H:257:ARG:NH1	2.47	0.48
2:H:575:LEU:HG	2:H:606:LEU:HD12	1.95	0.48
2:H:1236:THR:OG1	2:H:1608:MET:SD	2.68	0.48
2:E:219:VAL:HG22	2:E:261:ARG:HB2	1.95	0.47
2:E:1099:GLU:HA	2:E:1127:HIS:HB2	1.96	0.47
2:H:102:LEU:HB2	2:H:105:HIS:HD2	1.78	0.47
2:H:1434:TYR:HB2	2:H:1572:ILE:HD11	1.94	0.47
2:H:2555:LEU:HD21	2:H:2560:LEU:HD13	1.95	0.47
2:H:3919:LEU:O	2:H:3922:GLN:HG3	2.14	0.47
2:H:4054:LEU:HD21	2:H:4138:VAL:HG11	1.96	0.47
2:K:795:GLY:N	2:K:798:GLY:O	2.37	0.47
2:B:445:LEU:HD23	2:B:521:LEU:HB3	1.94	0.47
2:E:575:LEU:HG	2:E:606:LEU:HD12	1.95	0.47
2:E:4044:VAL:HG11	2:E:4154:ARG:HD2	1.95	0.47
2:B:2555:LEU:HD21	2:B:2560:LEU:HD13	1.95	0.47
2:H:1099:GLU:HA	2:H:1127:HIS:HB2	1.96	0.47
2:H:2501:ALA:HB2	2:H:2554:TYR:HD1	1.80	0.47
2:K:1077:ALA:H	2:K:1189:LEU:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3880:PHE:HE1	2:H:3914:THR:HG23	1.80	0.47
1:J:4:ILE:HD11	1:J:62:GLY:HA2	1.96	0.47
3:F:92:VAL:O	3:F:94:ASP:N	2.47	0.47
3:I:92:VAL:O	3:I:94:ASP:N	2.47	0.47
2:B:102:LEU:HB2	2:B:105:HIS:HD2	1.78	0.47
2:B:685:GLY:HA3	2:B:715:GLY:HA2	1.96	0.47
2:B:3919:LEU:O	2:B:3922:GLN:HG3	2.14	0.47
2:B:4031:VAL:HG12	2:B:4148:HIS:HA	1.97	0.47
2:B:4044:VAL:HG11	2:B:4154:ARG:HD2	1.95	0.47
2:E:1293:LEU:HD11	2:E:1594:ARG:HD3	1.96	0.47
2:K:4031:VAL:HG12	2:K:4148:HIS:HA	1.97	0.47
2:B:1293:LEU:HD11	2:B:1594:ARG:HD3	1.96	0.47
2:B:2501:ALA:HB2	2:B:2554:TYR:HD1	1.80	0.47
2:E:1077:ALA:H	2:E:1189:LEU:HD12	1.79	0.47
2:E:3880:PHE:HE1	2:E:3914:THR:HG23	1.80	0.47
2:H:35:LEU:HD11	2:H:189:LEU:HD13	1.97	0.47
2:H:1293:LEU:HD11	2:H:1594:ARG:HD3	1.96	0.47
2:K:248:GLU:OE2	2:K:257:ARG:NH1	2.47	0.47
2:K:530:ILE:HG21	2:K:563:VAL:HG23	1.97	0.47
2:K:2501:ALA:HB2	2:K:2554:TYR:HD1	1.80	0.47
2:K:3880:PHE:HE1	2:K:3914:THR:HG23	1.80	0.47
2:B:1843:LEU:HD11	2:B:1927:LEU:HD21	1.96	0.47
2:H:685:GLY:HA3	2:H:715:GLY:HA2	1.96	0.47
2:K:102:LEU:HB2	2:K:105:HIS:HD2	1.78	0.47
2:K:685:GLY:HA3	2:K:715:GLY:HA2	1.96	0.47
2:B:224:HIS:HA	2:B:388:LEU:HA	1.97	0.47
2:B:575:LEU:HG	2:B:606:LEU:HD12	1.95	0.47
2:E:248:GLU:OE2	2:E:257:ARG:NH1	2.47	0.47
2:B:3880:PHE:HE1	2:B:3914:THR:HG23	1.80	0.47
2:E:224:HIS:HA	2:E:388:LEU:HA	1.97	0.47
2:E:4054:LEU:HD21	2:E:4138:VAL:HG11	1.96	0.47
2:K:1528:THR:HG22	2:K:1539:PHE:HB3	1.96	0.47
2:B:795:GLY:N	2:B:798:GLY:O	2.37	0.46
2:H:4133:ASP:O	2:H:4137:ASN:ND2	2.38	0.46
2:K:575:LEU:HG	2:K:606:LEU:HD12	1.95	0.46
2:E:1671:ARG:NH1	2:E:1713:ASP:OD2	2.44	0.46
2:H:649:PHE:O	2:H:658:GLN:NE2	2.47	0.46
2:H:1528:THR:HG22	2:H:1539:PHE:HB3	1.96	0.46
2:H:1671:ARG:NH1	2:H:1713:ASP:OD2	2.44	0.46
1:A:4:ILE:HD11	1:A:62:GLY:HA2	1.96	0.46
1:D:4:ILE:HD11	1:D:62:GLY:HA2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:649:PHE:O	2:E:658:GLN:NE2	2.47	0.46
2:E:685:GLY:HA3	2:E:715:GLY:HA2	1.96	0.46
2:E:1843:LEU:HD11	2:E:1927:LEU:HD21	1.96	0.46
2:E:4919:PHE:CD2	2:E:4923:ILE:HD12	2.51	0.46
2:H:1996:THR:HA	2:H:1999:PHE:HD2	1.81	0.46
2:K:309:THR:O	2:K:313:SER:OG	2.31	0.46
2:E:35:LEU:HD11	2:E:189:LEU:HD13	1.97	0.46
2:E:795:GLY:N	2:E:798:GLY:O	2.37	0.46
2:E:2209:MET:SD	2:E:2254:HIS:ND1	2.89	0.46
2:E:2501:ALA:HB2	2:E:2554:TYR:HD1	1.80	0.46
2:H:1077:ALA:H	2:H:1189:LEU:HD12	1.79	0.46
2:K:224:HIS:HA	2:K:388:LEU:HA	1.97	0.46
2:K:1099:GLU:HA	2:K:1127:HIS:HB2	1.96	0.46
2:B:1099:GLU:HA	2:B:1127:HIS:HB2	1.96	0.46
2:H:530:ILE:HG21	2:H:563:VAL:HG23	1.97	0.46
2:K:35:LEU:HD11	2:K:189:LEU:HD13	1.97	0.46
2:K:649:PHE:O	2:K:658:GLN:NE2	2.47	0.46
2:E:575:LEU:HD22	2:E:609:CYS:HB2	1.98	0.46
2:H:309:THR:O	2:H:313:SER:OG	2.31	0.46
2:H:2209:MET:SD	2:H:2254:HIS:ND1	2.89	0.46
2:K:1996:THR:HA	2:K:1999:PHE:HD2	1.81	0.46
2:K:2560:LEU:HD21	2:K:2604:ILE:HA	1.97	0.46
2:B:2209:MET:SD	2:B:2254:HIS:ND1	2.89	0.46
2:B:4919:PHE:CD2	2:B:4923:ILE:HD12	2.51	0.46
2:B:579:GLN:H	2:B:582:HIS:CD2	2.28	0.46
2:E:309:THR:O	2:E:313:SER:OG	2.31	0.46
2:H:4031:VAL:HG12	2:H:4148:HIS:HA	1.97	0.46
2:K:1293:LEU:HD11	2:K:1594:ARG:HD3	1.96	0.46
2:K:4885:MET:O	2:K:4889:VAL:HG22	2.16	0.46
2:E:4031:VAL:HG12	2:E:4148:HIS:HA	1.97	0.46
2:H:2560:LEU:HD21	2:H:2604:ILE:HA	1.97	0.46
2:H:4919:PHE:CD2	2:H:4923:ILE:HD12	2.51	0.46
2:E:2475:LEU:HD23	2:E:2475:LEU:H	1.81	0.46
1:G:4:ILE:HD11	1:G:62:GLY:HA2	1.96	0.46
2:H:224:HIS:HA	2:H:388:LEU:HA	1.97	0.46
2:B:35:LEU:HD11	2:B:189:LEU:HD13	1.97	0.45
2:B:4133:ASP:O	2:B:4137:ASN:ND2	2.38	0.45
2:B:4885:MET:O	2:B:4889:VAL:HG22	2.16	0.45
2:E:2560:LEU:HD21	2:E:2604:ILE:HA	1.97	0.45
2:H:575:LEU:HD22	2:H:609:CYS:HB2	1.98	0.45
2:H:2299:VAL:HG13	2:H:2332:TYR:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2299:VAL:HG13	2:K:2332:TYR:HD2	1.81	0.45
2:B:309:THR:O	2:B:313:SER:OG	2.31	0.45
2:B:2560:LEU:HD21	2:B:2604:ILE:HA	1.97	0.45
2:K:2209:MET:SD	2:K:2254:HIS:ND1	2.89	0.45
2:K:2215:VAL:HG11	2:K:2229:MET:HE1	1.97	0.45
2:K:4919:PHE:CD2	2:K:4923:ILE:HD12	2.51	0.45
2:B:2475:LEU:HD23	2:B:2475:LEU:H	1.81	0.45
2:E:530:ILE:HG21	2:E:563:VAL:HG23	1.97	0.45
2:E:1448:VAL:HG22	2:E:1554:VAL:HG23	1.98	0.45
2:E:1720:LEU:HB2	2:E:1852:MET:SD	2.56	0.45
2:E:1996:THR:HA	2:E:1999:PHE:HD2	1.81	0.45
2:E:4921:PHE:HA	2:E:4925:ILE:HD13	1.98	0.45
2:K:4133:ASP:O	2:K:4137:ASN:ND2	2.38	0.45
2:K:4851:VAL:O	2:K:4855:ASN:ND2	2.31	0.45
2:B:575:LEU:HD22	2:B:609:CYS:HB2	1.98	0.45
2:B:649:PHE:O	2:B:658:GLN:NE2	2.47	0.45
2:B:1720:LEU:HB2	2:B:1852:MET:SD	2.56	0.45
2:B:2299:VAL:HG13	2:B:2332:TYR:HD2	1.81	0.45
2:K:2475:LEU:H	2:K:2475:LEU:HD23	1.81	0.45
1:A:90:VAL:HG23	1:A:91:ILE:HG12	1.99	0.45
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.97	0.45
3:C:92:VAL:O	3:C:94:ASP:N	2.47	0.45
1:D:90:VAL:HG23	1:D:91:ILE:HG12	1.99	0.45
2:E:4882:LEU:HD11	2:H:4912:VAL:HG11	1.98	0.45
2:H:1448:VAL:HG22	2:H:1554:VAL:HG23	1.98	0.45
2:K:575:LEU:HD22	2:K:609:CYS:HB2	1.98	0.45
2:B:4912:VAL:HG11	2:K:4882:LEU:HD11	1.98	0.45
1:D:50:ILE:HD11	1:D:64:ALA:HB2	1.98	0.45
2:E:2299:VAL:HG13	2:E:2332:TYR:HD2	1.81	0.45
2:H:284:HIS:NE2	2:H:286:THR:OG1	2.50	0.45
2:H:2475:LEU:H	2:H:2475:LEU:HD23	1.81	0.45
2:H:4922:VAL:HA	2:H:4926:LEU:HD23	1.99	0.45
1:A:50:ILE:HD11	1:A:64:ALA:HB2	1.98	0.45
2:E:284:HIS:NE2	2:E:286:THR:OG1	2.50	0.45
2:H:1720:LEU:HB2	2:H:1852:MET:SD	2.56	0.45
2:H:4885:MET:O	2:H:4889:VAL:HG22	2.16	0.45
2:K:4922:VAL:HA	2:K:4926:LEU:HD23	1.99	0.45
2:B:3985:VAL:HG23	2:B:4042:MET:HG2	1.99	0.45
2:E:4885:MET:O	2:E:4889:VAL:HG22	2.16	0.45
1:G:50:ILE:HD11	1:G:64:ALA:HB2	1.98	0.45
2:K:1720:LEU:HB2	2:K:1852:MET:SD	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:ILE:HG21	2:B:563:VAL:HG23	1.97	0.45
2:E:3985:VAL:HG23	2:E:4042:MET:HG2	1.99	0.45
2:E:4922:VAL:HA	2:E:4926:LEU:HD23	1.99	0.45
2:K:168:ASP:OD1	2:K:168:ASP:N	2.46	0.45
2:K:3985:VAL:HG23	2:K:4042:MET:HG2	1.99	0.45
2:K:4921:PHE:HA	2:K:4925:ILE:HD13	1.98	0.45
2:B:1996:THR:HA	2:B:1999:PHE:HD2	1.81	0.44
2:H:4882:LEU:HD11	2:K:4912:VAL:HG11	1.98	0.44
2:K:1671:ARG:NH1	2:K:1713:ASP:OD2	2.44	0.44
2:B:4921:PHE:HA	2:B:4925:ILE:HD13	1.98	0.44
2:H:4921:PHE:HA	2:H:4925:ILE:HD13	1.98	0.44
2:K:4163:GLU:HA	2:K:4166:LEU:HB3	2.00	0.44
2:B:284:HIS:NE2	2:B:286:THR:OG1	2.50	0.44
2:H:3985:VAL:HG23	2:H:4042:MET:HG2	1.99	0.44
2:K:1448:VAL:HG22	2:K:1554:VAL:HG23	1.98	0.44
2:E:3979:ARG:HE	2:H:162:LYS:NZ	2.16	0.44
1:J:50:ILE:HD11	1:J:64:ALA:HB2	1.98	0.44
2:B:1448:VAL:HG22	2:B:1554:VAL:HG23	1.98	0.44
2:B:4882:LEU:HD11	2:E:4912:VAL:HG11	1.98	0.44
2:E:168:ASP:N	2:E:168:ASP:OD1	2.46	0.44
1:G:90:VAL:HG23	1:G:91:ILE:HG12	1.99	0.44
1:J:90:VAL:HG23	1:J:91:ILE:HG12	1.99	0.44
2:B:3979:ARG:HE	2:E:162:LYS:NZ	2.16	0.44
2:H:4851:VAL:O	2:H:4855:ASN:ND2	2.31	0.44
2:B:4684:LEU:HD11	2:B:4690:PRO:HB3	2.00	0.44
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	2.00	0.44
2:H:4163:GLU:HA	2:H:4166:LEU:HB3	2.00	0.44
2:K:4684:LEU:HD11	2:K:4690:PRO:HB3	2.00	0.44
2:B:162:LYS:NZ	2:K:3979:ARG:HE	2.16	0.43
2:B:2215:VAL:HG11	2:B:2229:MET:HE1	1.99	0.43
2:B:4922:VAL:HA	2:B:4926:LEU:HD23	1.99	0.43
2:H:1103:GLY:HA3	2:H:1123:VAL:HA	2.00	0.43
2:H:764:VAL:HG13	2:H:766:GLY:H	1.84	0.43
2:H:35:LEU:HD13	2:H:49:LEU:HD13	2.00	0.43
2:H:3979:ARG:HE	2:K:162:LYS:NZ	2.16	0.43
2:K:408:ALA:O	2:K:412:ASN:ND2	2.36	0.43
2:B:4163:GLU:HA	2:B:4166:LEU:HB3	2.00	0.43
2:K:35:LEU:HD13	2:K:49:LEU:HD13	2.00	0.43
2:K:540:PHE:HZ	2:K:547:LEU:HD13	1.84	0.43
2:K:2293:GLU:OE2	2:K:3844:ARG:NH2	2.52	0.43
2:H:1186:ASP:N	2:H:1186:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2213:VAL:HG22	2:H:2257:TYR:CZ	2.54	0.43
2:K:2213:VAL:HG22	2:K:2257:TYR:CZ	2.54	0.43
1:D:29:MET:HG3	1:D:35:LYS:HA	2.01	0.43
2:H:959:TYR:HA	2:H:966:LYS:HA	2.01	0.43
2:H:2215:VAL:HG11	2:H:2229:MET:HE1	2.00	0.43
2:K:1186:ASP:OD1	2:K:1186:ASP:N	2.52	0.43
2:K:284:HIS:NE2	2:K:286:THR:OG1	2.50	0.43
3:L:92:VAL:O	3:L:94:ASP:N	2.47	0.43
1:A:29:MET:HG3	1:A:35:LYS:HA	2.01	0.43
2:B:232:THR:HB	2:B:252:VAL:HG23	2.00	0.43
2:B:1671:ARG:NH1	2:B:1713:ASP:OD2	2.44	0.43
2:B:2213:VAL:HG22	2:B:2257:TYR:CZ	2.54	0.43
3:C:6:THR:O	3:C:10:ILE:HG12	2.19	0.43
2:E:232:THR:HB	2:E:252:VAL:HG23	2.00	0.43
2:E:2213:VAL:HG22	2:E:2257:TYR:CZ	2.54	0.43
2:E:4684:LEU:HD11	2:E:4690:PRO:HB3	2.00	0.43
2:H:540:PHE:HZ	2:H:547:LEU:HD13	1.84	0.43
2:K:3808:GLN:HE22	2:K:3889:GLY:H	1.67	0.43
2:E:684:VAL:HG22	2:E:781:VAL:HG13	2.01	0.43
3:F:6:THR:O	3:F:10:ILE:HG12	2.19	0.43
3:I:6:THR:O	3:I:10:ILE:HG12	2.19	0.43
2:K:764:VAL:HG13	2:K:766:GLY:H	1.84	0.43
2:H:3808:GLN:HE22	2:H:3889:GLY:H	1.67	0.43
2:K:1431:THR:HG21	2:K:1523:ALA:HB2	2.01	0.43
2:B:1227:ALA:HB1	2:B:1230:MET:HB2	2.01	0.42
2:B:2293:GLU:OE2	2:B:3844:ARG:NH2	2.52	0.42
2:B:3808:GLN:HE22	2:B:3889:GLY:H	1.67	0.42
2:E:764:VAL:HG13	2:E:766:GLY:H	1.84	0.42
2:E:1227:ALA:HB1	2:E:1230:MET:HB2	2.01	0.42
2:H:1227:ALA:HB1	2:H:1230:MET:HB2	2.01	0.42
2:H:4684:LEU:HD11	2:H:4690:PRO:HB3	2.00	0.42
2:K:793:LEU:HB3	2:K:812:HIS:HB3	2.01	0.42
2:E:1431:THR:HG21	2:E:1523:ALA:HB2	2.01	0.42
2:E:1834:SER:HB3	2:E:1837:PHE:HD2	1.84	0.42
2:E:4163:GLU:HA	2:E:4166:LEU:HB3	2.00	0.42
2:H:1431:THR:HG21	2:H:1523:ALA:HB2	2.01	0.42
2:H:4161:LEU:O	2:H:4164:SER:OG	2.27	0.42
2:B:4896:GLY:HA2	2:B:4899:ILE:HG22	2.02	0.42
2:H:2293:GLU:OE2	2:H:3844:ARG:NH2	2.52	0.42
2:H:4896:GLY:HA2	2:H:4899:ILE:HG22	2.02	0.42
2:K:959:TYR:HA	2:K:966:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1103:GLY:HA3	2:K:1123:VAL:HA	2.00	0.42
2:K:1227:ALA:HB1	2:K:1230:MET:HB2	2.01	0.42
2:B:1431:THR:HG21	2:B:1523:ALA:HB2	2.01	0.42
2:E:793:LEU:HB3	2:E:812:HIS:HB3	2.01	0.42
2:H:1291:LEU:HB2	2:H:1550:PRO:HG2	2.01	0.42
3:L:6:THR:O	3:L:10:ILE:HG12	2.19	0.42
2:H:1190:PRO:HG2	2:H:1204:LEU:HD11	2.02	0.42
2:K:1190:PRO:HG2	2:K:1204:LEU:HD11	2.02	0.42
2:K:1291:LEU:HB2	2:K:1550:PRO:HG2	2.01	0.42
2:K:4896:GLY:HA2	2:K:4899:ILE:HG22	2.02	0.42
2:B:684:VAL:HG22	2:B:781:VAL:HG13	2.01	0.42
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	2.00	0.42
2:E:659:TYR:O	2:E:662:TRP:NE1	2.52	0.42
2:E:1291:LEU:HB2	2:E:1550:PRO:HG2	2.01	0.42
2:E:1433:TYR:CZ	2:E:1578:ALA:HB2	2.55	0.42
2:E:3808:GLN:HE22	2:E:3889:GLY:H	1.67	0.42
2:E:4896:GLY:HA2	2:E:4899:ILE:HG22	2.02	0.42
1:G:29:MET:HG3	1:G:35:LYS:HA	2.01	0.42
2:H:232:THR:HB	2:H:252:VAL:HG23	2.00	0.42
2:K:1592:PRO:HA	2:K:1593:PRO:HD3	1.95	0.42
2:K:1834:SER:HB3	2:K:1837:PHE:HD2	1.84	0.42
2:K:2126:HIS:HB2	2:K:3721:TYR:HE1	1.85	0.42
2:B:1433:TYR:CZ	2:B:1578:ALA:HB2	2.55	0.42
2:B:1834:SER:HB3	2:B:1837:PHE:HD2	1.84	0.42
2:B:2520:LEU:HD11	2:B:2566:CYS:SG	2.60	0.42
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.00	0.42
2:E:223:PHE:O	2:E:389:SER:N	2.50	0.42
1:J:29:MET:HG3	1:J:35:LYS:HA	2.01	0.42
2:K:1240:LYS:HG2	2:K:1242:LEU:H	1.85	0.42
2:K:2119:ARG:NH1	2:K:3715:ASP:OD2	2.45	0.42
2:K:2520:LEU:HD11	2:K:2566:CYS:SG	2.60	0.42
2:B:764:VAL:HG13	2:B:766:GLY:H	1.84	0.42
2:B:1291:LEU:HB2	2:B:1550:PRO:HG2	2.01	0.42
2:E:1190:PRO:HG2	2:E:1204:LEU:HD11	2.02	0.42
2:E:2293:GLU:OE2	2:E:3844:ARG:NH2	2.52	0.42
2:H:1834:SER:HB3	2:H:1837:PHE:HD2	1.84	0.42
2:K:1433:TYR:CZ	2:K:1578:ALA:HB2	2.55	0.42
2:B:1186:ASP:OD1	2:B:1186:ASP:N	2.52	0.42
2:E:2126:HIS:HB2	2:E:3721:TYR:HE1	1.85	0.42
2:H:2520:LEU:HD11	2:H:2566:CYS:SG	2.60	0.42
2:H:684:VAL:HG22	2:H:781:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:684:VAL:HG22	2:K:781:VAL:HG13	2.01	0.42
2:B:34:LYS:H	2:B:53:SER:HB3	1.84	0.41
2:B:540:PHE:HZ	2:B:547:LEU:HD13	1.84	0.41
2:B:959:TYR:HA	2:B:966:LYS:HA	2.01	0.41
2:B:3946:PHE:O	2:B:3950:MET:HG2	2.20	0.41
2:E:263:GLU:HG2	2:E:281:ARG:HB3	2.02	0.41
2:E:540:PHE:HZ	2:E:547:LEU:HD13	1.84	0.41
2:E:1240:LYS:HG2	2:E:1242:LEU:H	1.85	0.41
2:H:2126:HIS:HB2	2:H:3721:TYR:HE1	1.85	0.41
2:B:1148:VAL:HG21	2:B:1212:ARG:HD2	2.02	0.41
2:H:793:LEU:HB3	2:H:812:HIS:HB3	2.01	0.41
2:E:660:SER:HB2	2:E:751:SER:H	1.86	0.41
2:E:2520:LEU:HD11	2:E:2566:CYS:SG	2.60	0.41
2:B:1240:LYS:HG2	2:B:1242:LEU:H	1.85	0.41
2:B:4851:VAL:O	2:B:4855:ASN:ND2	2.31	0.41
2:K:1148:VAL:HG21	2:K:1212:ARG:HD2	2.02	0.41
2:B:263:GLU:HG2	2:B:281:ARG:HB3	2.02	0.41
2:B:793:LEU:HB3	2:B:812:HIS:HB3	2.01	0.41
2:H:263:GLU:HG2	2:H:281:ARG:HB3	2.02	0.41
2:H:660:SER:HB2	2:H:751:SER:H	1.86	0.41
2:K:49:LEU:HD23	2:K:49:LEU:HA	1.94	0.41
2:K:232:THR:HB	2:K:252:VAL:HG23	2.00	0.41
2:B:111:HIS:CE1	2:B:113:HIS:HB3	2.56	0.41
2:B:660:SER:HB2	2:B:751:SER:H	1.86	0.41
2:B:1190:PRO:HG2	2:B:1204:LEU:HD11	2.02	0.41
2:B:2126:HIS:HB2	2:B:3721:TYR:HE1	1.85	0.41
2:E:182:LEU:HG	2:E:191:VAL:HG22	2.02	0.41
2:E:959:TYR:HA	2:E:966:LYS:HA	2.01	0.41
2:K:111:HIS:CE1	2:K:113:HIS:HB3	2.56	0.41
2:K:1686:CYS:HB3	2:K:1783:PHE:HZ	1.86	0.41
1:A:24:VAL:HG12	1:A:26:TYR:HD2	1.86	0.41
2:B:182:LEU:HG	2:B:191:VAL:HG22	2.02	0.41
1:D:23:VAL:HB	1:D:104:LEU:HB2	2.03	0.41
1:D:24:VAL:HG12	1:D:26:TYR:HD2	1.86	0.41
2:H:1433:TYR:CZ	2:H:1578:ALA:HB2	2.55	0.41
2:K:660:SER:HB2	2:K:751:SER:H	1.86	0.41
2:E:1186:ASP:OD1	2:E:1186:ASP:N	2.52	0.41
2:E:1592:PRO:HA	2:E:1593:PRO:HD3	1.95	0.41
2:E:3946:PHE:O	2:E:3950:MET:HG2	2.20	0.41
2:K:689:THR:HG22	2:K:776:LEU:H	1.86	0.41
1:A:23:VAL:HB	1:A:104:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4222:GLU:O	2:E:4226:MET:HG2	2.21	0.41
2:H:689:THR:HG22	2:H:776:LEU:H	1.86	0.41
2:H:1240:LYS:HG2	2:H:1242:LEU:H	1.85	0.41
2:H:3946:PHE:O	2:H:3950:MET:HG2	2.20	0.41
2:K:182:LEU:HG	2:K:191:VAL:HG22	2.02	0.41
2:K:645:ARG:HA	2:K:646:PRO:HD3	1.95	0.41
2:K:1805:LEU:HD13	2:K:1854:ILE:HD12	2.03	0.41
2:B:1686:CYS:HB3	2:B:1783:PHE:HZ	1.86	0.41
2:B:4648:HIS:HA	2:B:4651:VAL:HG22	2.03	0.41
2:E:1738:LEU:HB2	2:E:2147:PRO:HD3	2.03	0.41
2:H:1805:LEU:HD13	2:H:1854:ILE:HD12	2.03	0.41
2:K:3946:PHE:O	2:K:3950:MET:HG2	2.20	0.41
2:B:4222:GLU:O	2:B:4226:MET:HG2	2.21	0.40
2:E:111:HIS:CE1	2:E:113:HIS:HB3	2.56	0.40
2:E:262:LEU:HB3	2:E:280:LEU:HD23	2.04	0.40
2:E:649:PHE:HB3	2:E:776:LEU:HD13	2.03	0.40
2:E:2215:VAL:HG11	2:E:2229:MET:HE1	2.03	0.40
1:G:23:VAL:HB	1:G:104:LEU:HB2	2.03	0.40
2:H:408:ALA:O	2:H:412:ASN:ND2	2.36	0.40
2:H:3873:ASP:OD1	2:H:3873:ASP:N	2.53	0.40
2:H:4920:PHE:O	2:H:4924:VAL:HB	2.21	0.40
1:J:23:VAL:HB	1:J:104:LEU:HB2	2.03	0.40
2:K:262:LEU:HB3	2:K:280:LEU:HD23	2.04	0.40
2:K:4648:HIS:HA	2:K:4651:VAL:HG22	2.03	0.40
2:K:4920:PHE:O	2:K:4924:VAL:HB	2.21	0.40
2:B:4161:LEU:O	2:B:4164:SER:OG	2.27	0.40
2:B:5002:THR:OG1	2:B:5003:GLY:N	2.55	0.40
2:B:3722:ALA:HB1	2:B:3795:LEU:HB2	2.04	0.40
2:E:1805:LEU:HD13	2:E:1854:ILE:HD12	2.03	0.40
2:E:4648:HIS:HA	2:E:4651:VAL:HG22	2.03	0.40
2:E:4920:PHE:O	2:E:4924:VAL:HB	2.21	0.40
2:H:499:THR:OG1	2:H:500:ALA:N	2.54	0.40
2:H:1738:LEU:HB2	2:H:2147:PRO:HD3	2.03	0.40
2:H:5002:THR:OG1	2:H:5003:GLY:N	2.55	0.40
2:K:263:GLU:HG2	2:K:281:ARG:HB3	2.02	0.40
2:B:1805:LEU:HD13	2:B:1854:ILE:HD12	2.03	0.40
2:E:1148:VAL:HG21	2:E:1212:ARG:HD2	2.02	0.40
2:E:1686:CYS:HB3	2:E:1783:PHE:HZ	1.86	0.40
1:G:24:VAL:HG12	1:G:26:TYR:HD2	1.86	0.40
2:H:1449:TRP:HE1	2:H:1496:TRP:HD1	1.69	0.40
2:K:622:THR:O	2:K:627:PRO:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:3869:VAL:HG12	2:K:3870:MET:HG3	2.04	0.40
2:K:4176:ILE:HD11	2:K:4188:ILE:HB	2.04	0.40
2:B:223:PHE:O	2:B:389:SER:N	2.50	0.40
2:B:4176:ILE:HD11	2:B:4188:ILE:HB	2.04	0.40
2:E:1449:TRP:HE1	2:E:1496:TRP:HD1	1.69	0.40
2:H:111:HIS:CE1	2:H:113:HIS:HB3	2.56	0.40
2:H:182:LEU:HG	2:H:191:VAL:HG22	2.02	0.40
2:H:262:LEU:HB3	2:H:280:LEU:HD23	2.04	0.40
2:H:649:PHE:HB3	2:H:776:LEU:HD13	2.03	0.40
2:H:1148:VAL:HG21	2:H:1212:ARG:HD2	2.02	0.40
2:H:1686:CYS:HB3	2:H:1783:PHE:HZ	1.86	0.40
2:H:3806:ASP:N	2:H:3806:ASP:OD1	2.53	0.40
2:K:645:ARG:HG2	2:K:826:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	104/110 (94%)	95 (91%)	9 (9%)	0	100	100
1	D	104/110 (94%)	95 (91%)	9 (9%)	0	100	100
1	G	104/110 (94%)	95 (91%)	9 (9%)	0	100	100
1	J	104/110 (94%)	95 (91%)	9 (9%)	0	100	100
2	B	3380/3801 (89%)	3327 (98%)	52 (2%)	1 (0%)	100	100
2	E	3380/3801 (89%)	3327 (98%)	53 (2%)	0	100	100
2	H	3380/3801 (89%)	3327 (98%)	52 (2%)	1 (0%)	100	100
2	K	3380/3801 (89%)	3327 (98%)	52 (2%)	1 (0%)	100	100
3	C	127/148 (86%)	122 (96%)	5 (4%)	0	100	100
3	F	127/148 (86%)	122 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	127/148 (86%)	122 (96%)	5 (4%)	0	100	100
3	L	127/148 (86%)	122 (96%)	5 (4%)	0	100	100
All	All	14444/16236 (89%)	14176 (98%)	265 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	51	PRO
2	B	51	PRO
2	K	51	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	69/90 (77%)	69 (100%)	0	100	100
1	D	69/90 (77%)	69 (100%)	0	100	100
1	G	69/90 (77%)	69 (100%)	0	100	100
1	J	69/90 (77%)	69 (100%)	0	100	100
2	B	2218/3020 (73%)	2215 (100%)	3 (0%)	93	97
2	E	2218/3020 (73%)	2216 (100%)	2 (0%)	93	97
2	H	2218/3020 (73%)	2216 (100%)	2 (0%)	93	97
2	K	2218/3020 (73%)	2215 (100%)	3 (0%)	93	97
3	C	29/126 (23%)	29 (100%)	0	100	100
3	F	29/126 (23%)	29 (100%)	0	100	100
3	I	29/126 (23%)	29 (100%)	0	100	100
3	L	29/126 (23%)	29 (100%)	0	100	100
All	All	9264/12944 (72%)	9254 (100%)	10 (0%)	93	97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	53	SER
2	B	58	VAL
2	B	125	ARG
2	E	53	SER
2	E	125	ARG
2	H	53	SER
2	H	125	ARG
2	K	53	SER
2	K	58	VAL
2	K	125	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	23	GLN
2	B	203	ASN
2	B	3420	ASN
2	B	3804	ASN
2	E	23	GLN
2	E	203	ASN
2	E	3420	ASN
2	E	3804	ASN
2	H	23	GLN
2	H	203	ASN
2	H	3420	ASN
2	H	3804	ASN
2	K	23	GLN
2	K	203	ASN
2	K	3420	ASN
2	K	3804	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	57
2	E	57
2	H	57
2	K	57

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4331:UNK	C	4543:GLU	N	51.63
1	E	4331:UNK	C	4543:GLU	N	51.63
1	H	4331:UNK	C	4543:GLU	N	51.63
1	K	4331:UNK	C	4543:GLU	N	51.63
1	B	1050:GLY	C	1071:ARG	N	45.66
1	E	1050:GLY	C	1071:ARG	N	45.66
1	H	1050:GLY	C	1071:ARG	N	45.66
1	K	1050:GLY	C	1071:ARG	N	45.66
1	B	3606:UNK	C	3625:ARG	N	34.72

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3606:UNK	C	3625:ARG	N	34.72
1	H	3606:UNK	C	3625:ARG	N	34.72
1	K	3606:UNK	C	3625:ARG	N	34.72
1	B	4737:GLU	C	4761:GLY	N	33.88
1	E	4737:GLU	C	4761:GLY	N	33.88
1	H	4737:GLU	C	4761:GLY	N	33.88
1	K	4737:GLU	C	4761:GLY	N	33.88
1	B	4241:GLN	C	4315:UNK	N	28.24
1	E	4241:GLN	C	4315:UNK	N	28.24
1	H	4241:GLN	C	4315:UNK	N	28.24
1	K	4241:GLN	C	4315:UNK	N	28.24
1	B	2700:UNK	C	2736:ASP	N	27.93
1	E	2700:UNK	C	2736:ASP	N	27.93
1	H	2700:UNK	C	2736:ASP	N	27.93
1	K	2700:UNK	C	2736:ASP	N	27.93
1	B	2939:ARG	C	2956:UNK	N	25.14
1	E	2939:ARG	C	2956:UNK	N	25.14
1	H	2939:ARG	C	2956:UNK	N	25.14
1	K	2939:ARG	C	2956:UNK	N	25.14
1	B	3555:UNK	C	3565:UNK	N	24.53
1	E	3555:UNK	C	3565:UNK	N	24.53
1	H	3555:UNK	C	3565:UNK	N	24.53
1	K	3555:UNK	C	3565:UNK	N	24.53
1	B	2830:GLU	C	2855:TYR	N	23.95
1	E	2830:GLU	C	2855:TYR	N	23.95
1	H	2830:GLU	C	2855:TYR	N	23.95
1	K	2830:GLU	C	2855:TYR	N	23.95
1	B	84:ASN	C	97:GLY	N	22.11
1	E	84:ASN	C	97:GLY	N	22.11
1	H	84:ASN	C	97:GLY	N	22.11
1	K	84:ASN	C	97:GLY	N	22.11
1	B	1299:GLN	C	1428:LEU	N	21.21
1	E	1299:GLN	C	1428:LEU	N	21.21
1	H	1299:GLN	C	1428:LEU	N	21.21
1	K	1299:GLN	C	1428:LEU	N	21.21
1	B	855:PRO	C	863:LEU	N	21.03
1	E	855:PRO	C	863:LEU	N	21.03
1	H	855:PRO	C	863:LEU	N	21.03
1	K	855:PRO	C	863:LEU	N	21.03
1	B	3574:UNK	C	3586:UNK	N	20.43
1	E	3574:UNK	C	3586:UNK	N	20.43
1	H	3574:UNK	C	3586:UNK	N	20.43

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	3574:UNK	C	3586:UNK	N	20.43
1	B	2527:PHE	C	2546:GLU	N	19.89
1	E	2527:PHE	C	2546:GLU	N	19.89
1	H	2527:PHE	C	2546:GLU	N	19.89
1	K	2527:PHE	C	2546:GLU	N	19.89
1	B	3733:GLU	C	3747:SER	N	18.58
1	E	3733:GLU	C	3747:SER	N	18.58
1	H	3733:GLU	C	3747:SER	N	18.58
1	K	3733:GLU	C	3747:SER	N	18.58
1	B	3238:UNK	C	3278:UNK	N	18.53
1	E	3238:UNK	C	3278:UNK	N	18.53
1	H	3238:UNK	C	3278:UNK	N	18.53
1	K	3238:UNK	C	3278:UNK	N	18.53
1	B	2046:GLN	C	2092:LEU	N	18.27
1	E	2046:GLN	C	2092:LEU	N	18.27
1	H	2046:GLN	C	2092:LEU	N	18.27
1	K	2046:GLN	C	2092:LEU	N	18.27
1	B	2653:UNK	C	2664:UNK	N	17.22
1	E	2653:UNK	C	2664:UNK	N	17.22
1	H	2653:UNK	C	2664:UNK	N	17.22
1	K	2653:UNK	C	2664:UNK	N	17.22
1	B	3193:UNK	C	3202:UNK	N	16.78
1	E	3193:UNK	C	3202:UNK	N	16.78
1	H	3193:UNK	C	3202:UNK	N	16.78
1	K	3193:UNK	C	3202:UNK	N	16.78
1	B	3062:UNK	C	3143:UNK	N	16.52
1	E	3062:UNK	C	3143:UNK	N	16.52
1	H	3062:UNK	C	3143:UNK	N	16.52
1	K	3062:UNK	C	3143:UNK	N	16.52
1	B	3358:UNK	C	3365:UNK	N	16.06
1	E	3358:UNK	C	3365:UNK	N	16.06
1	H	3358:UNK	C	3365:UNK	N	16.06
1	K	3358:UNK	C	3365:UNK	N	16.06
1	B	2978:UNK	C	2999:UNK	N	16.04
1	E	2978:UNK	C	2999:UNK	N	16.04
1	H	2978:UNK	C	2999:UNK	N	16.04
1	K	2978:UNK	C	2999:UNK	N	16.04
1	B	1871:VAL	C	1924:GLU	N	14.64
1	E	1871:VAL	C	1924:GLU	N	14.64
1	H	1871:VAL	C	1924:GLU	N	14.64
1	K	1871:VAL	C	1924:GLU	N	14.64
1	B	4090:LYS	C	4109:UNK	N	14.47

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4090:LYS	C	4109:UNK	N	14.47
1	H	4090:LYS	C	4109:UNK	N	14.47
1	K	4090:LYS	C	4109:UNK	N	14.47
1	B	2263:GLY	C	2271:SER	N	13.98
1	E	2263:GLY	C	2271:SER	N	13.98
1	H	2263:GLY	C	2271:SER	N	13.98
1	K	2263:GLY	C	2271:SER	N	13.98
1	B	3385:UNK	C	3398:GLU	N	13.77
1	E	3385:UNK	C	3398:GLU	N	13.77
1	H	3385:UNK	C	3398:GLU	N	13.77
1	K	3385:UNK	C	3398:GLU	N	13.77
1	B	3018:UNK	C	3032:UNK	N	13.76
1	E	3018:UNK	C	3032:UNK	N	13.76
1	H	3018:UNK	C	3032:UNK	N	13.76
1	K	3018:UNK	C	3032:UNK	N	13.76
1	B	3308:UNK	C	3320:UNK	N	13.41
1	E	3308:UNK	C	3320:UNK	N	13.41
1	H	3308:UNK	C	3320:UNK	N	13.41
1	K	3308:UNK	C	3320:UNK	N	13.41
1	B	2479:LEU	C	2491:MET	N	13.28
1	E	2479:LEU	C	2491:MET	N	13.28
1	H	2479:LEU	C	2491:MET	N	13.28
1	K	2479:LEU	C	2491:MET	N	13.28
1	B	323:LEU	C	328:LYS	N	13.18
1	E	323:LEU	C	328:LYS	N	13.18
1	H	323:LEU	C	328:LYS	N	13.18
1	K	323:LEU	C	328:LYS	N	13.18
1	B	3046:UNK	C	3051:UNK	N	12.16
1	E	3046:UNK	C	3051:UNK	N	12.16
1	H	3046:UNK	C	3051:UNK	N	12.16
1	K	3046:UNK	C	3051:UNK	N	12.16
1	B	2629:PHE	C	2641:UNK	N	12.13
1	E	2629:PHE	C	2641:UNK	N	12.13
1	H	2629:PHE	C	2641:UNK	N	12.13
1	K	2629:PHE	C	2641:UNK	N	12.13
1	B	3335:UNK	C	3346:UNK	N	12.09
1	E	3335:UNK	C	3346:UNK	N	12.09
1	H	3335:UNK	C	3346:UNK	N	12.09
1	K	3335:UNK	C	3346:UNK	N	12.09
1	B	4585:PRO	C	4626:VAL	N	11.83
1	E	4585:PRO	C	4626:VAL	N	11.83
1	H	4585:PRO	C	4626:VAL	N	11.83

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	4585:PRO	C	4626:VAL	N	11.83
1	B	1501:VAL	C	1510:SER	N	11.80
1	B	2014:LYS	C	2023:PRO	N	11.80
1	E	1501:VAL	C	1510:SER	N	11.80
1	E	2014:LYS	C	2023:PRO	N	11.80
1	H	1501:VAL	C	1510:SER	N	11.80
1	H	2014:LYS	C	2023:PRO	N	11.80
1	K	1501:VAL	C	1510:SER	N	11.80
1	K	2014:LYS	C	2023:PRO	N	11.80
1	B	3526:UNK	C	3534:UNK	N	11.73
1	E	3526:UNK	C	3534:UNK	N	11.73
1	H	3526:UNK	C	3534:UNK	N	11.73
1	K	3526:UNK	C	3534:UNK	N	11.73
1	B	2571:ALA	C	2579:MET	N	11.69
1	E	2571:ALA	C	2579:MET	N	11.69
1	H	2571:ALA	C	2579:MET	N	11.69
1	K	2571:ALA	C	2579:MET	N	11.69
1	B	3461:VAL	C	3509:UNK	N	11.61
1	E	3461:VAL	C	3509:UNK	N	11.61
1	H	3461:VAL	C	3509:UNK	N	11.61
1	K	3461:VAL	C	3509:UNK	N	11.61
1	B	3217:UNK	C	3225:UNK	N	11.48
1	E	3217:UNK	C	3225:UNK	N	11.48
1	H	3217:UNK	C	3225:UNK	N	11.48
1	K	3217:UNK	C	3225:UNK	N	11.48
1	B	361:ALA	C	372:LEU	N	10.68
1	E	361:ALA	C	372:LEU	N	10.68
1	H	361:ALA	C	372:LEU	N	10.68
1	K	361:ALA	C	372:LEU	N	10.68
1	B	1788:PRO	C	1794:GLU	N	10.05
1	E	1788:PRO	C	1794:GLU	N	10.05
1	H	1788:PRO	C	1794:GLU	N	10.05
1	K	1788:PRO	C	1794:GLU	N	10.05
1	B	2370:ARG	C	2377:LEU	N	9.95
1	E	2370:ARG	C	2377:LEU	N	9.95
1	H	2370:ARG	C	2377:LEU	N	9.95
1	K	2370:ARG	C	2377:LEU	N	9.95
1	B	4114:UNK	C	4121:GLU	N	9.86
1	E	4114:UNK	C	4121:GLU	N	9.86
1	H	4114:UNK	C	4121:GLU	N	9.86
1	K	4114:UNK	C	4121:GLU	N	9.86
1	B	1750:PRO	C	1760:ARG	N	9.68

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	1750:PRO	C	1760:ARG	N	9.68
1	H	1750:PRO	C	1760:ARG	N	9.68
1	K	1750:PRO	C	1760:ARG	N	9.68
1	B	2683:UNK	C	2688:UNK	N	9.52
1	E	2683:UNK	C	2688:UNK	N	9.52
1	H	2683:UNK	C	2688:UNK	N	9.52
1	K	2683:UNK	C	2688:UNK	N	9.52
1	B	3163:UNK	C	3173:UNK	N	9.25
1	E	3163:UNK	C	3173:UNK	N	9.25
1	H	3163:UNK	C	3173:UNK	N	9.25
1	K	3163:UNK	C	3173:UNK	N	9.25
1	B	3861:ILE	C	3866:GLY	N	9.14
1	E	3861:ILE	C	3866:GLY	N	9.14
1	H	3861:ILE	C	3866:GLY	N	9.14
1	K	3861:ILE	C	3866:GLY	N	9.14
1	B	2385:ILE	C	2420:GLY	N	9.11
1	E	2385:ILE	C	2420:GLY	N	9.11
1	H	2385:ILE	C	2420:GLY	N	9.11
1	K	2385:ILE	C	2420:GLY	N	9.11
1	B	2514:GLU	C	2518:PHE	N	9.08
1	E	2514:GLU	C	2518:PHE	N	9.08
1	H	2514:GLU	C	2518:PHE	N	9.08
1	K	2514:GLU	C	2518:PHE	N	9.08
1	B	3288:UNK	C	3292:UNK	N	8.98
1	E	3288:UNK	C	3292:UNK	N	8.98
1	H	3288:UNK	C	3292:UNK	N	8.98
1	K	3288:UNK	C	3292:UNK	N	8.98
1	B	3544:UNK	C	3548:UNK	N	8.67
1	E	3544:UNK	C	3548:UNK	N	8.67
1	H	3544:UNK	C	3548:UNK	N	8.67
1	K	3544:UNK	C	3548:UNK	N	8.67
1	B	2217:GLY	C	2225:ARG	N	8.25
1	E	2217:GLY	C	2225:ARG	N	8.25
1	H	2217:GLY	C	2225:ARG	N	8.25
1	K	2217:GLY	C	2225:ARG	N	8.25
1	B	236:ALA	C	240:ASP	N	6.67
1	E	236:ALA	C	240:ASP	N	6.67
1	H	236:ALA	C	240:ASP	N	6.67
1	K	236:ALA	C	240:ASP	N	6.67
1	B	1478:ASP	C	1482:ASN	N	6.29
1	E	1478:ASP	C	1482:ASN	N	6.29
1	H	1478:ASP	C	1482:ASN	N	6.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	1478:ASP	C	1482:ASN	N	6.29
1	B	426:ARG	C	431:PRO	N	5.81
1	E	426:ARG	C	431:PRO	N	5.81
1	H	426:ARG	C	431:PRO	N	5.81
1	K	426:ARG	C	431:PRO	N	5.81
1	B	1275:ARG	C	1282:SER	N	5.36
1	E	1275:ARG	C	1282:SER	N	5.36
1	H	1275:ARG	C	1282:SER	N	5.36
1	K	1275:ARG	C	1282:SER	N	5.36

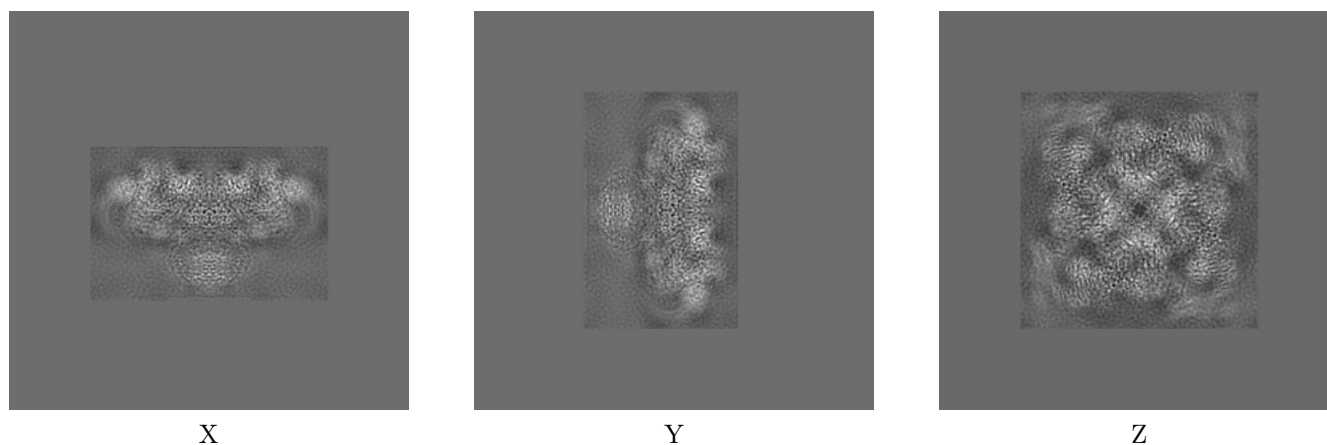
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22018. 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](#)

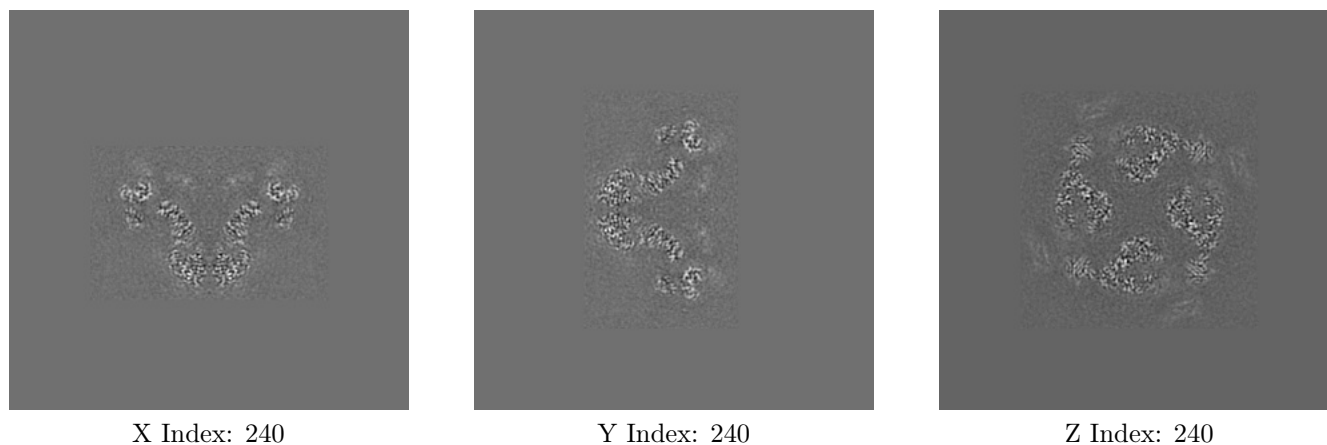
6.1.1 Primary map



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

6.2 Central slices [i](#)

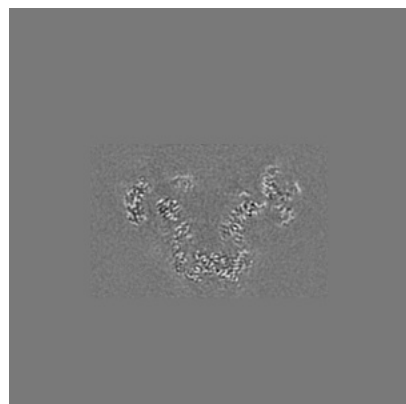
6.2.1 Primary map



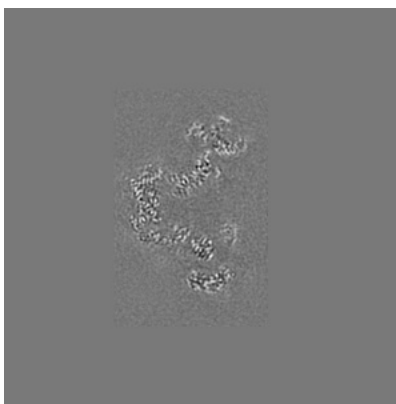
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

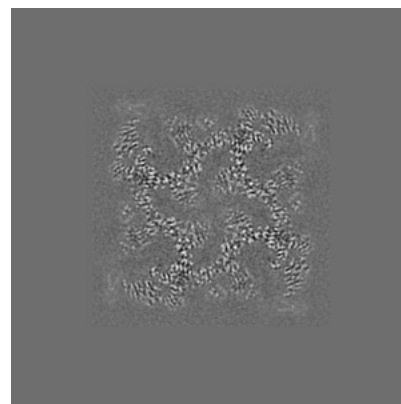
6.3.1 Primary map



X Index: 233



Y Index: 247



Z Index: 268

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

6.4 Orthogonal surface views [i](#)

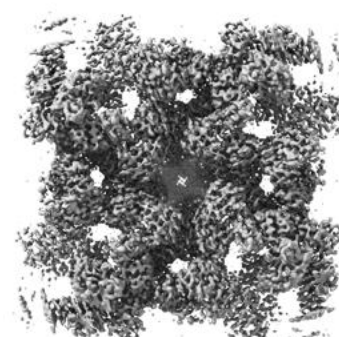
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

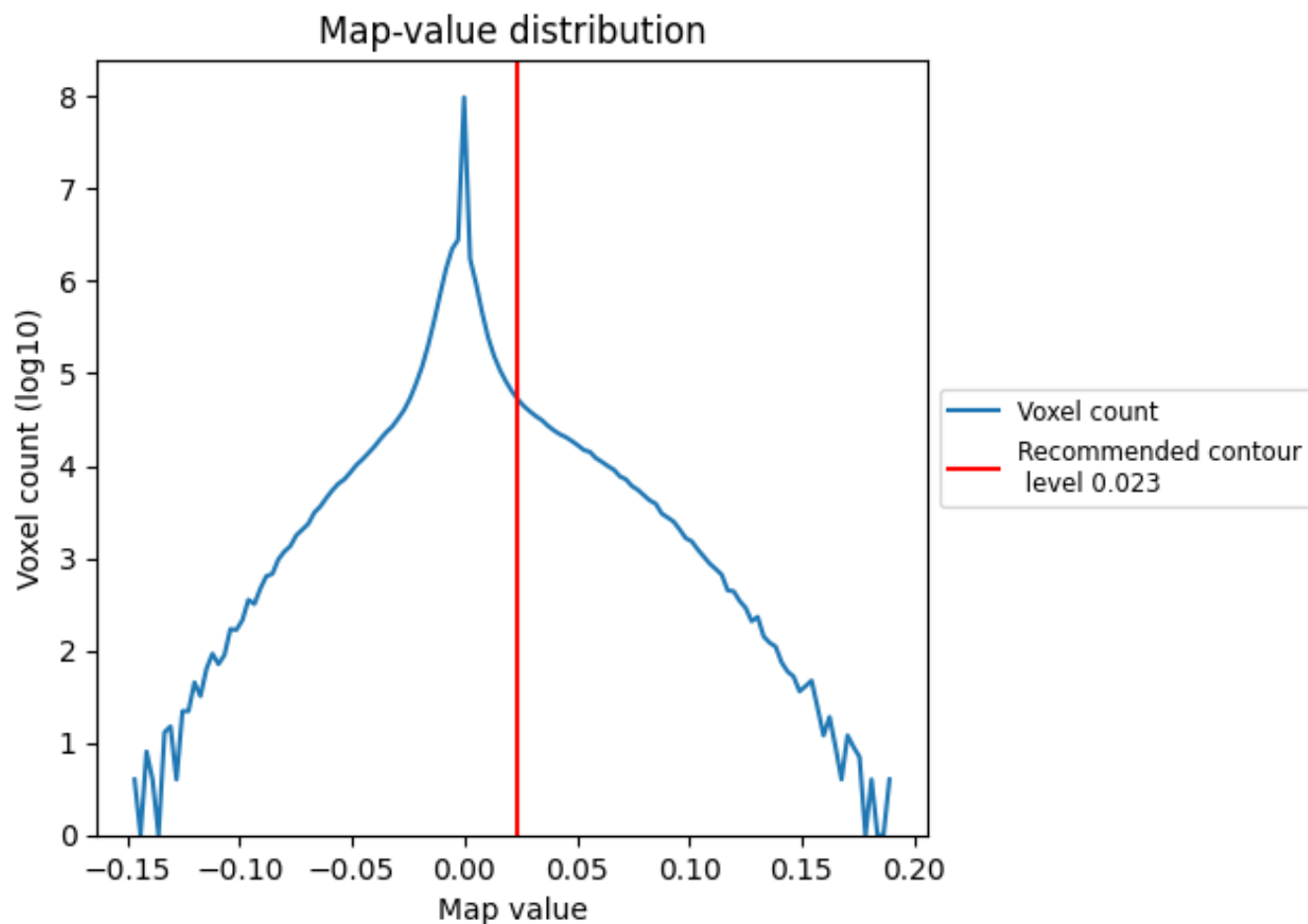
6.5 Mask visualisation

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

7 Map analysis [i](#)

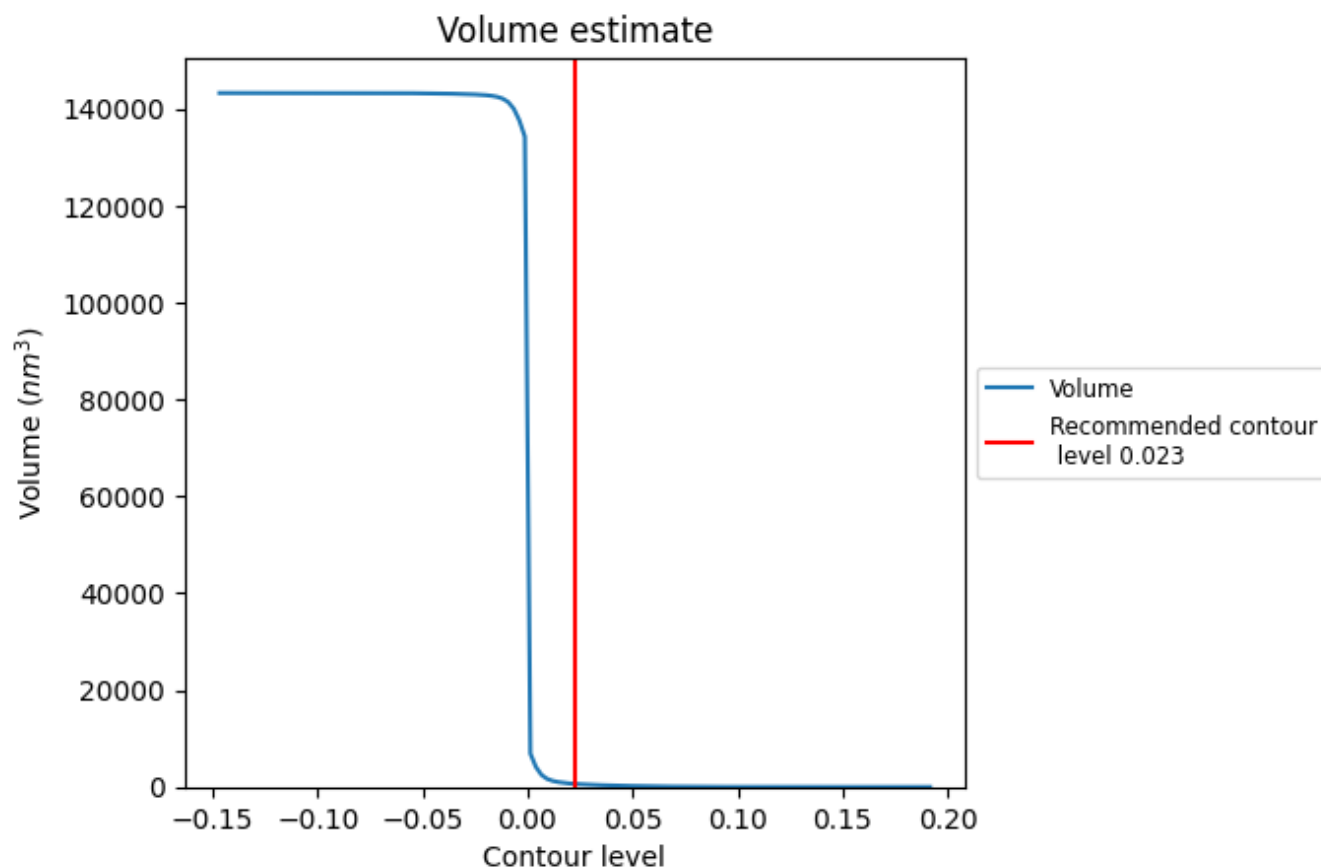
This section contains the results of statistical analysis of the map.

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.

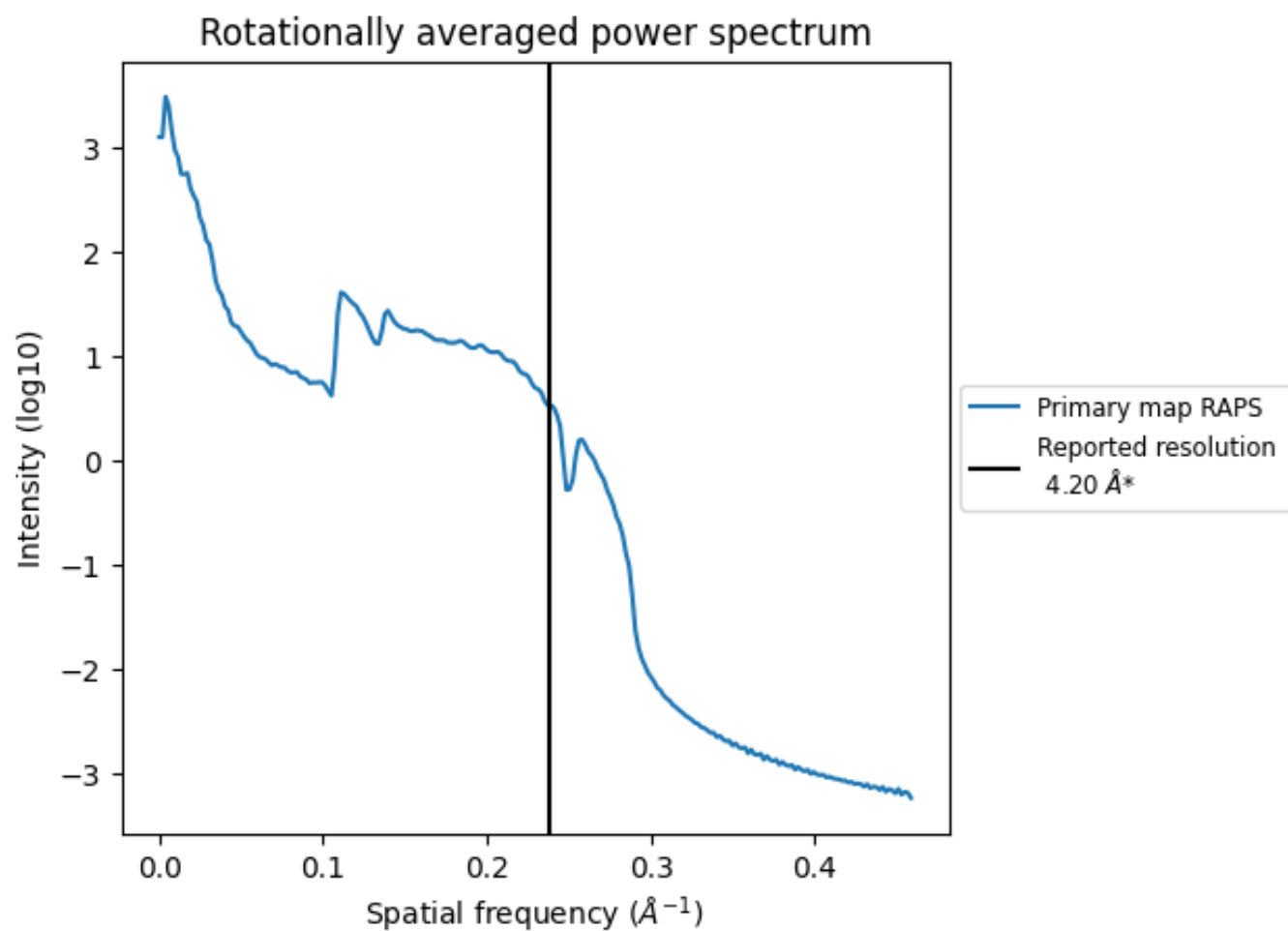
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 622 nm^3 ; this corresponds to an approximate mass of 562 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 0.238 Å⁻¹

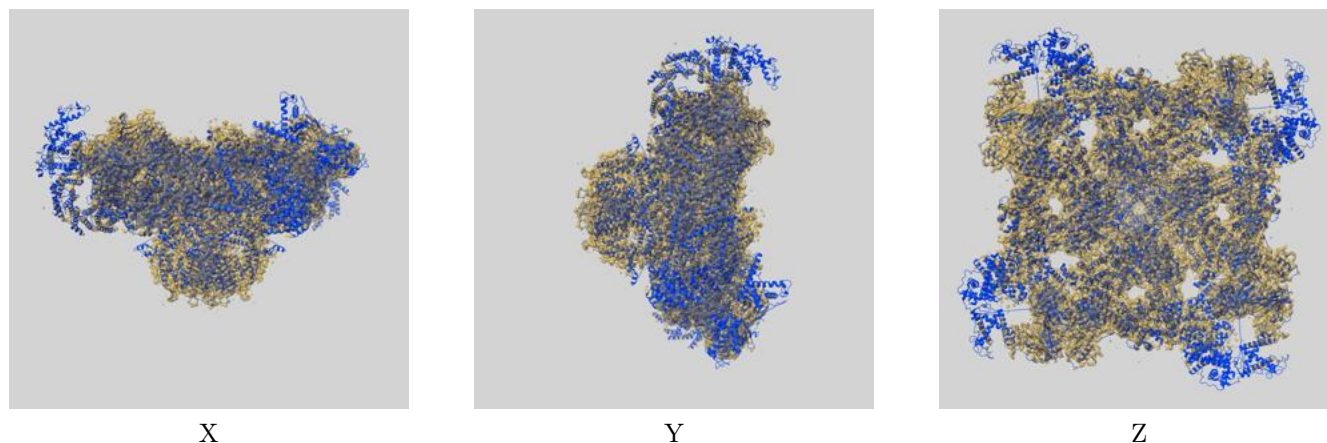
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

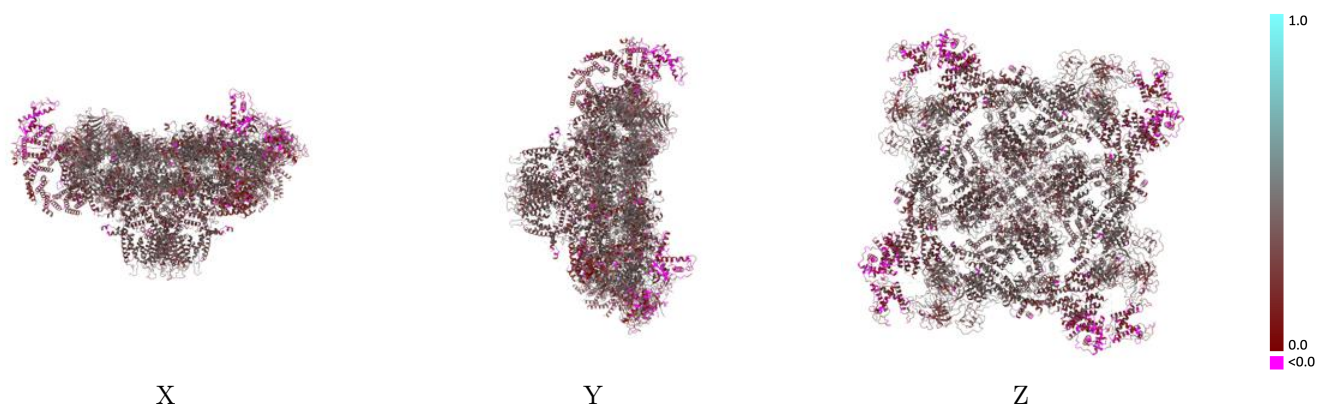
This section contains information regarding the fit between EMDB map EMD-22018 and PDB model 6X35. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



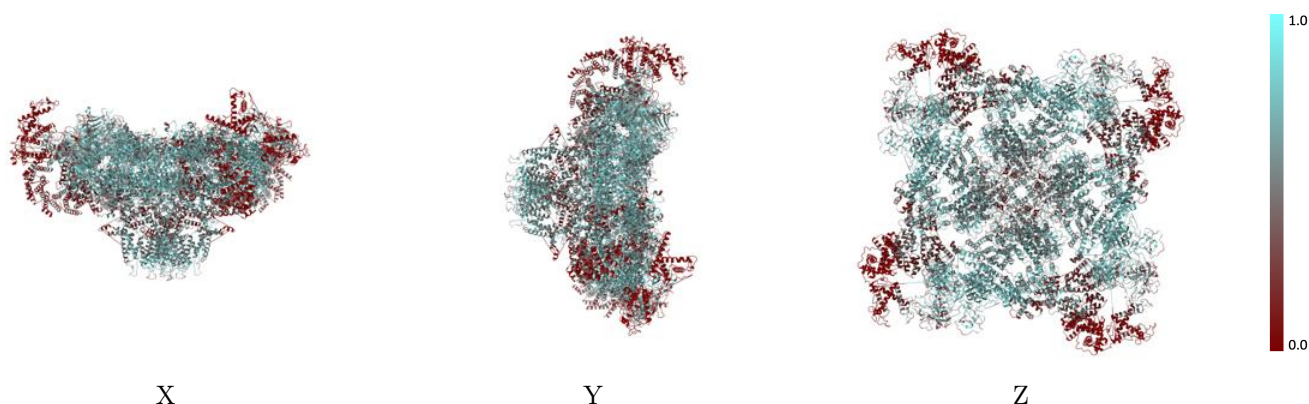
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



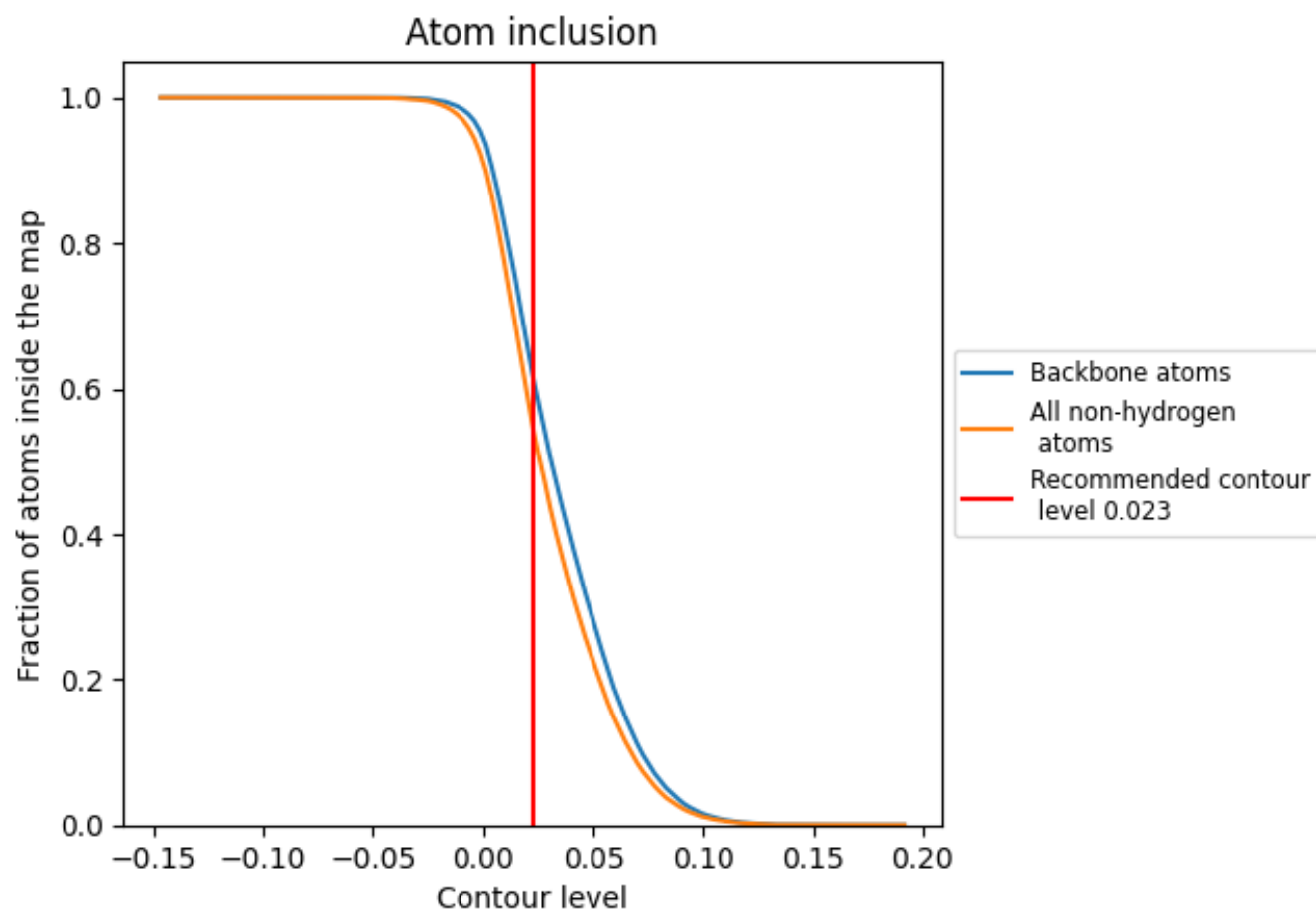
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 54% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.5408</div>	<div><div></div>0.3310</div>
A	<div><div></div>0.5926</div>	<div><div></div>0.3570</div>
B	<div><div></div>0.5440</div>	<div><div></div>0.3310</div>
C	<div><div></div>0.3760</div>	<div><div></div>0.2830</div>
D	<div><div></div>0.5899</div>	<div><div></div>0.3560</div>
E	<div><div></div>0.5445</div>	<div><div></div>0.3310</div>
F	<div><div></div>0.3760</div>	<div><div></div>0.2810</div>
G	<div><div></div>0.5913</div>	<div><div></div>0.3590</div>
H	<div><div></div>0.5443</div>	<div><div></div>0.3320</div>
I	<div><div></div>0.3747</div>	<div><div></div>0.2790</div>
J	<div><div></div>0.5913</div>	<div><div></div>0.3570</div>
K	<div><div></div>0.5442</div>	<div><div></div>0.3320</div>
L	<div><div></div>0.3760</div>	<div><div></div>0.2820</div>

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