



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:34 AM UTC

PDB ID : 6X33 / pdb_00006x33
EMDB ID : EMD-22016
Title : Wt pig RyR1 in complex with apoCaM, EGTA condition (class 3, 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

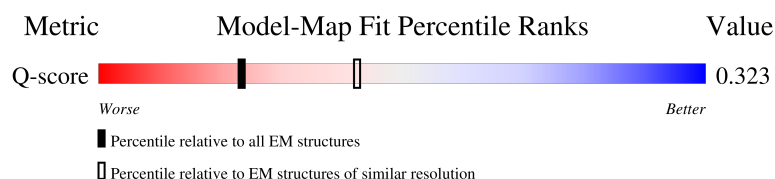
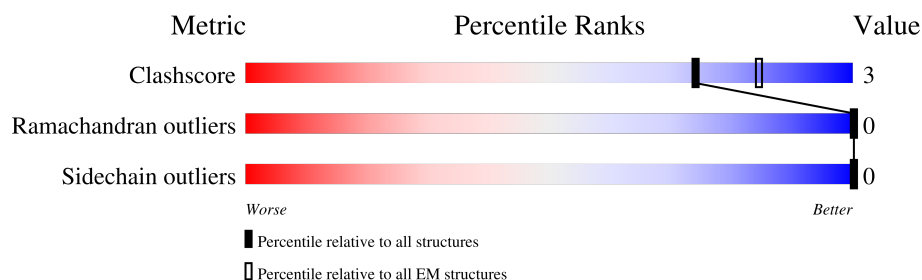
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



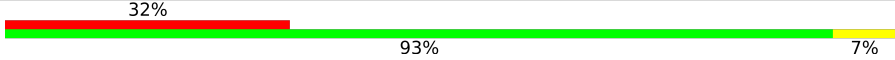
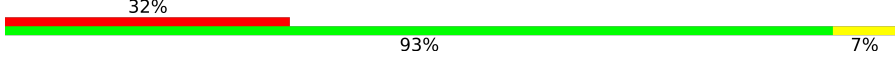
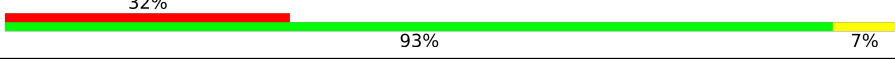
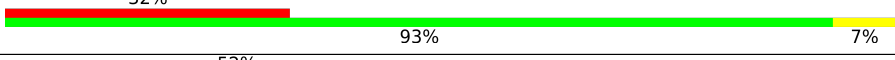
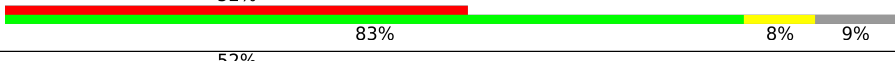
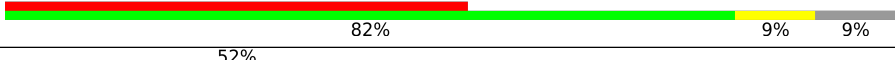
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	107	19% 89% 10%
1	D	107	19% 89% 10%
1	G	107	20% 89% 10%
1	J	107	19% 89% 10%

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Mol	Chain	Length	Quality of chain
2	B	3816	
2	E	3816	
2	H	3816	
2	K	3816	
3	C	148	
3	F	148	
3	I	148	
3	L	148	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 112372 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
			727	460	124	139	4		
1	D	106	Total	C	N	O	S	0	0
			727	460	124	139	4		
1	G	106	Total	C	N	O	S	0	0
			727	460	124	139	4		
1	J	106	Total	C	N	O	S	0	0
			727	460	124	139	4		

- Molecule 2 is a protein called Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3816	Total	C	N	O	S	6	0
			26597	17002	4711	4735	149		
2	E	3816	Total	C	N	O	S	6	0
			26597	17002	4711	4735	149		
2	H	3816	Total	C	N	O	S	6	0
			26597	17002	4711	4735	149		
2	K	3816	Total	C	N	O	S	6	0
			26597	17002	4711	4735	149		

- 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		

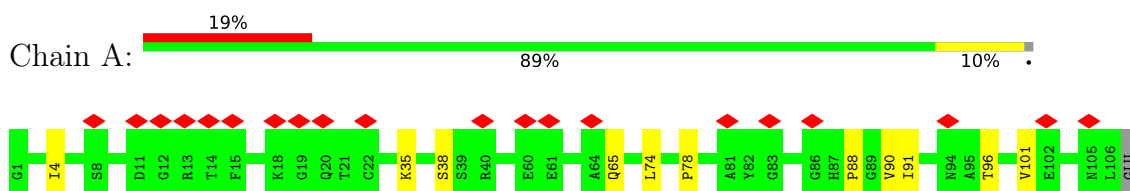
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

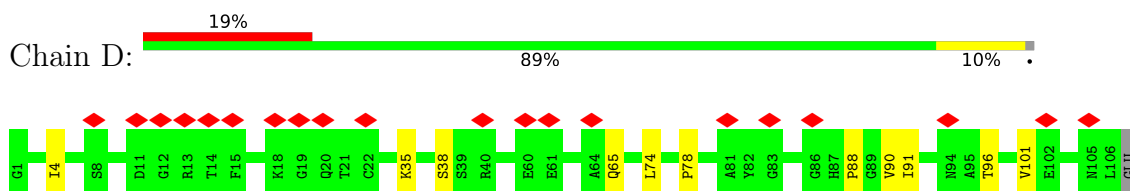
3 Residue-property plots

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.

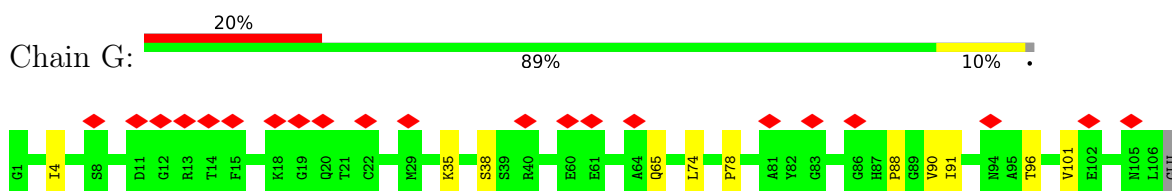
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



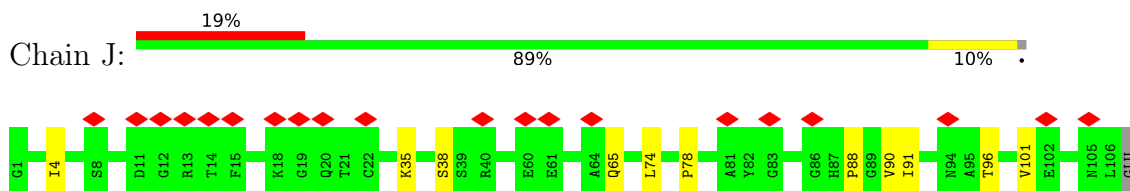
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



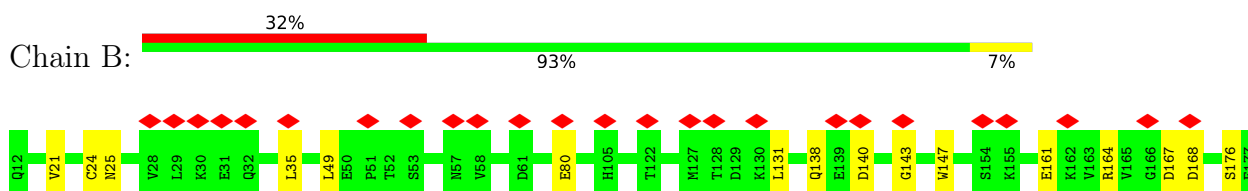
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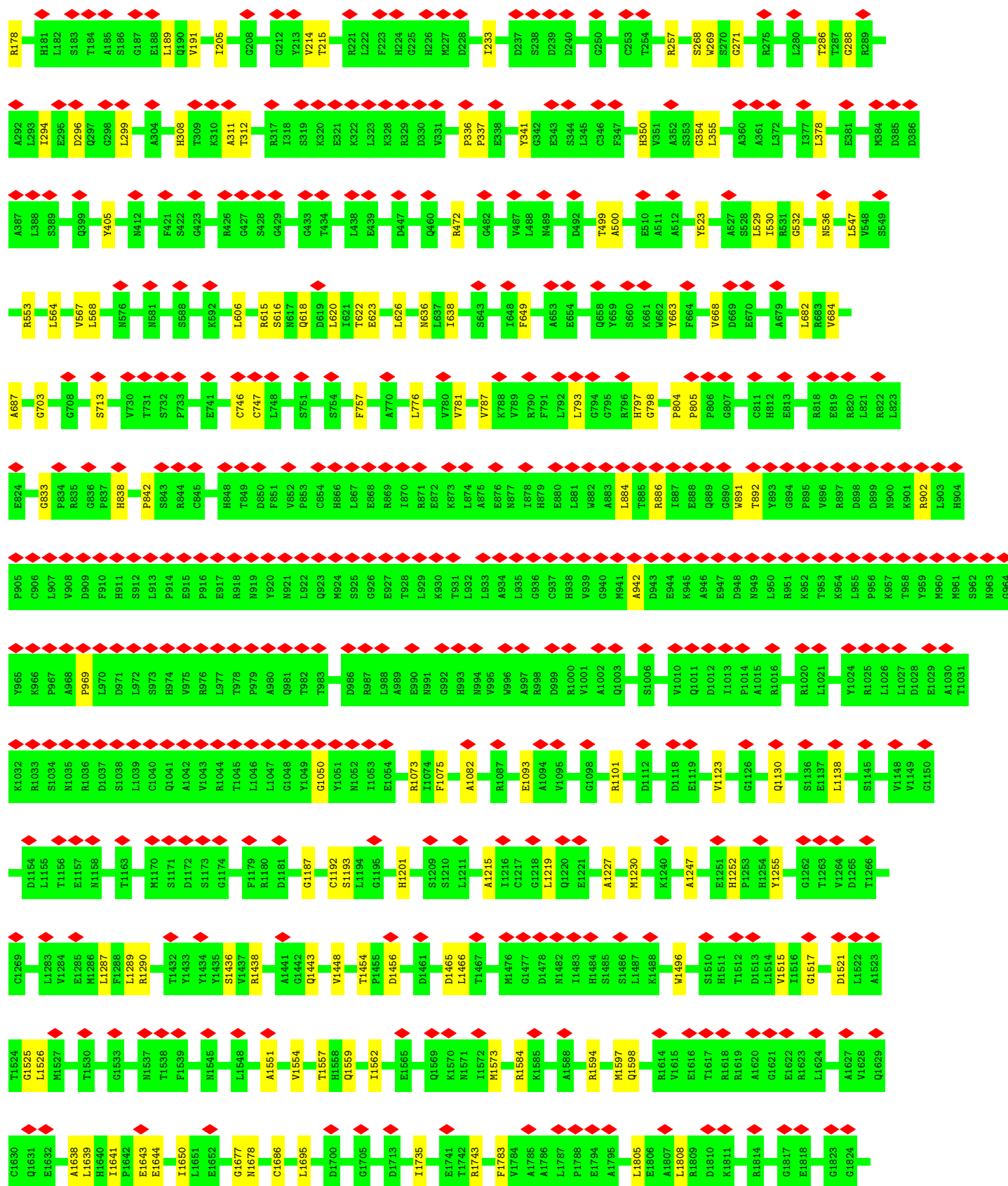


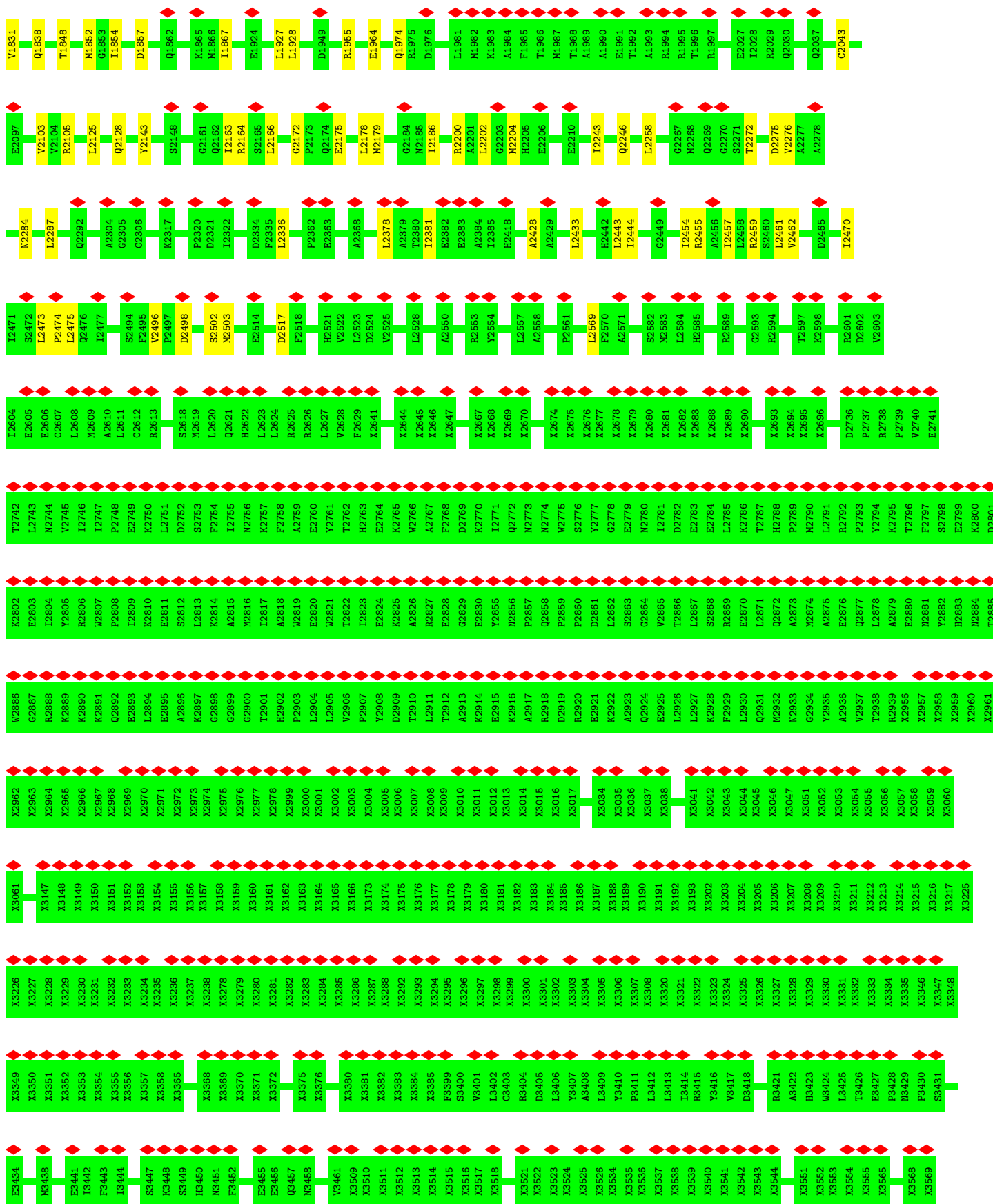
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

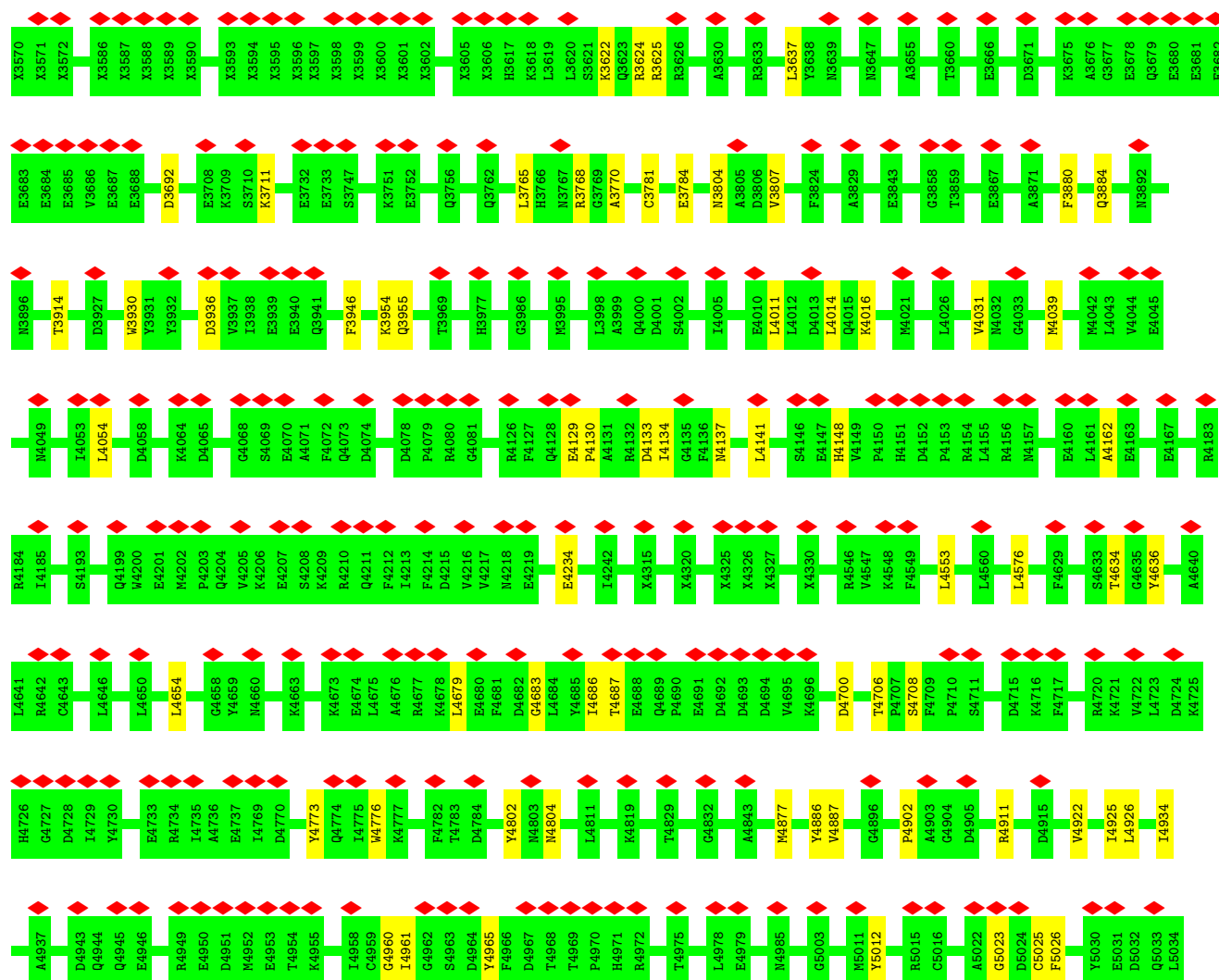


- Molecule 2: Ryanodine Receptor

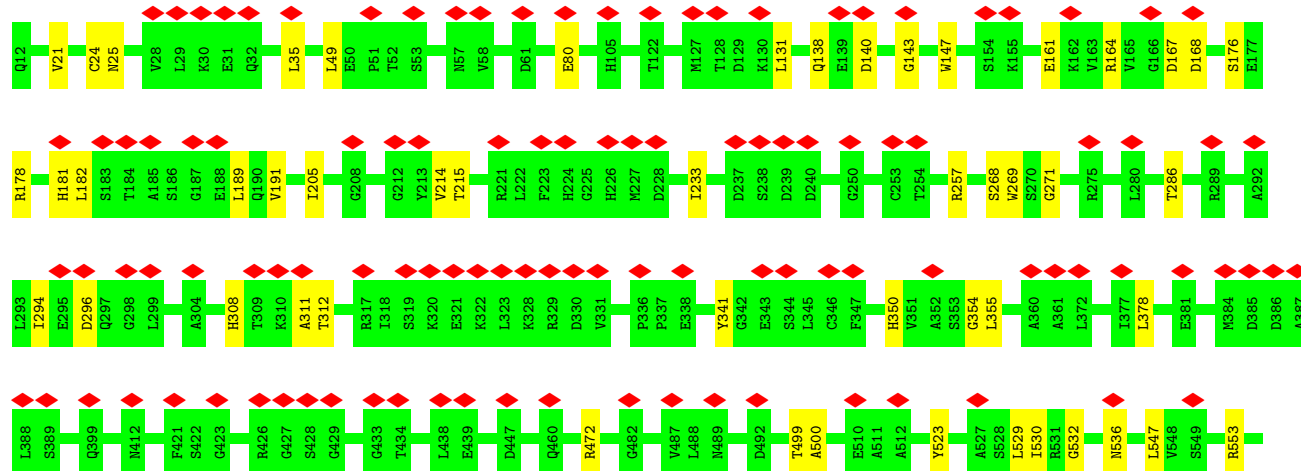
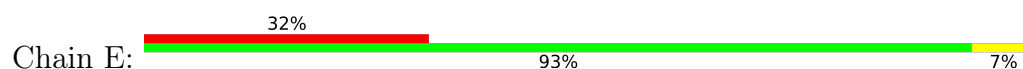


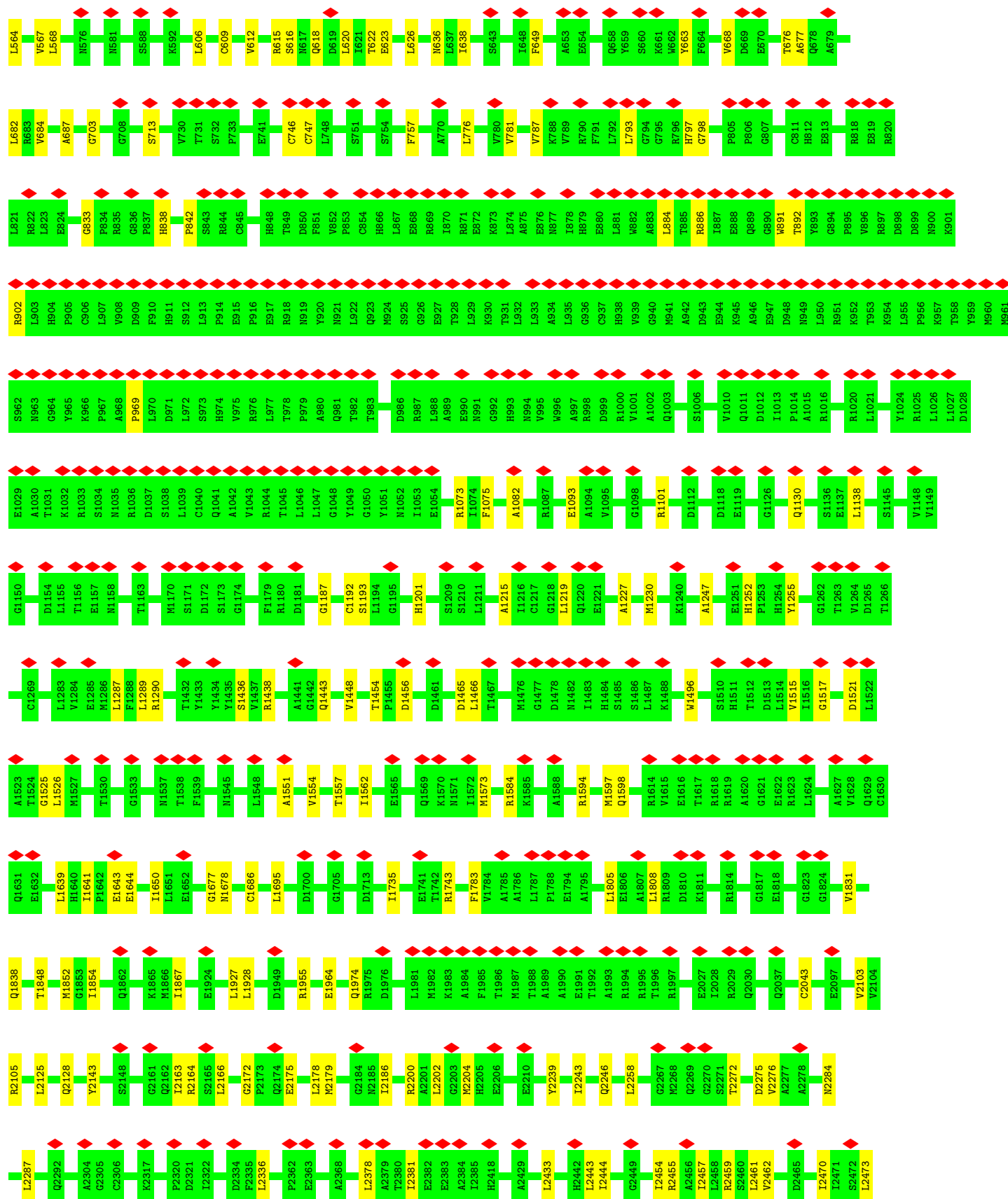


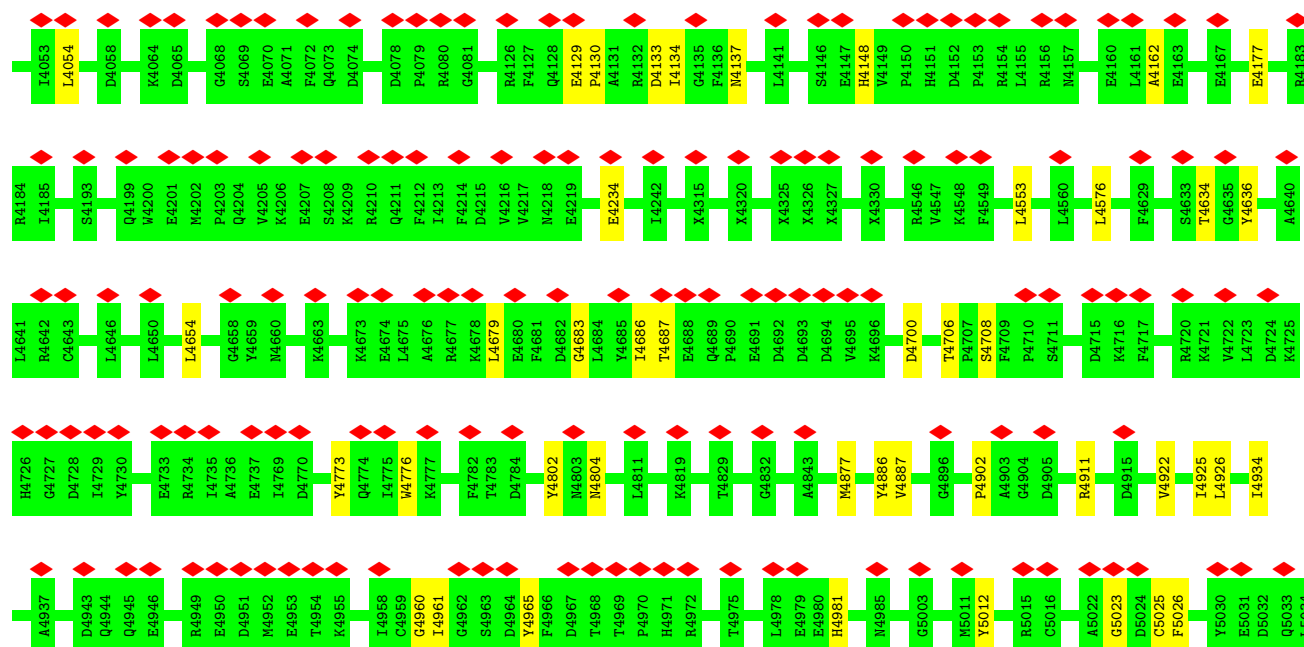




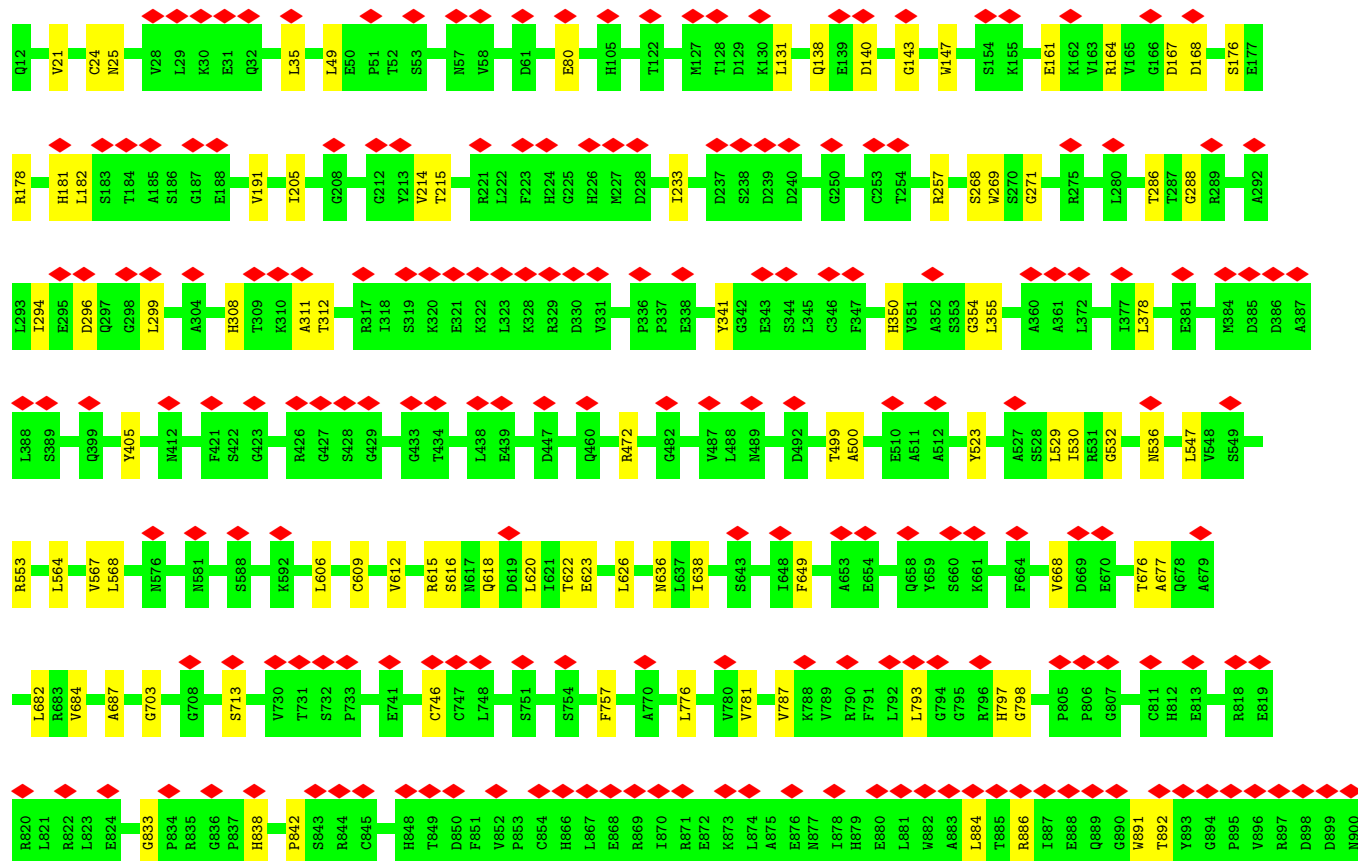
• Molecule 2: Ryanodine Receptor





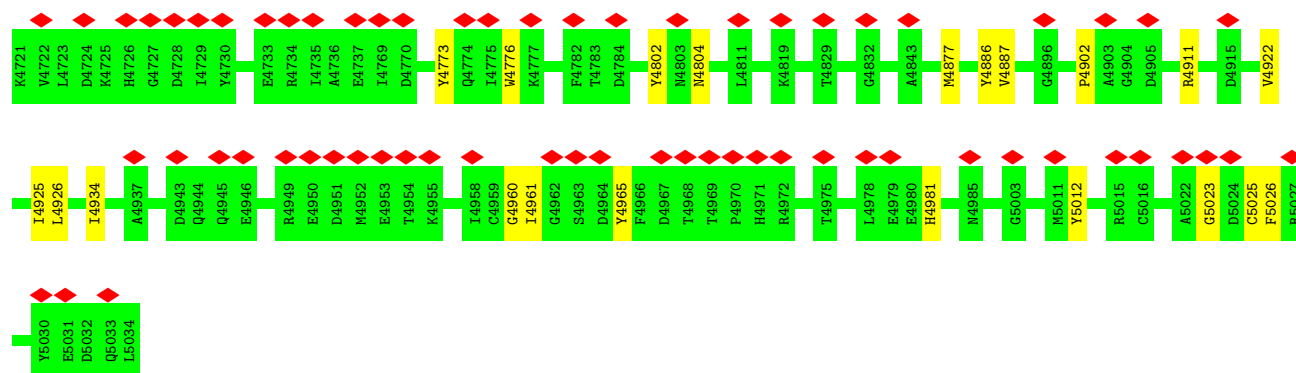


• Molecule 2: Ryanodine Receptor

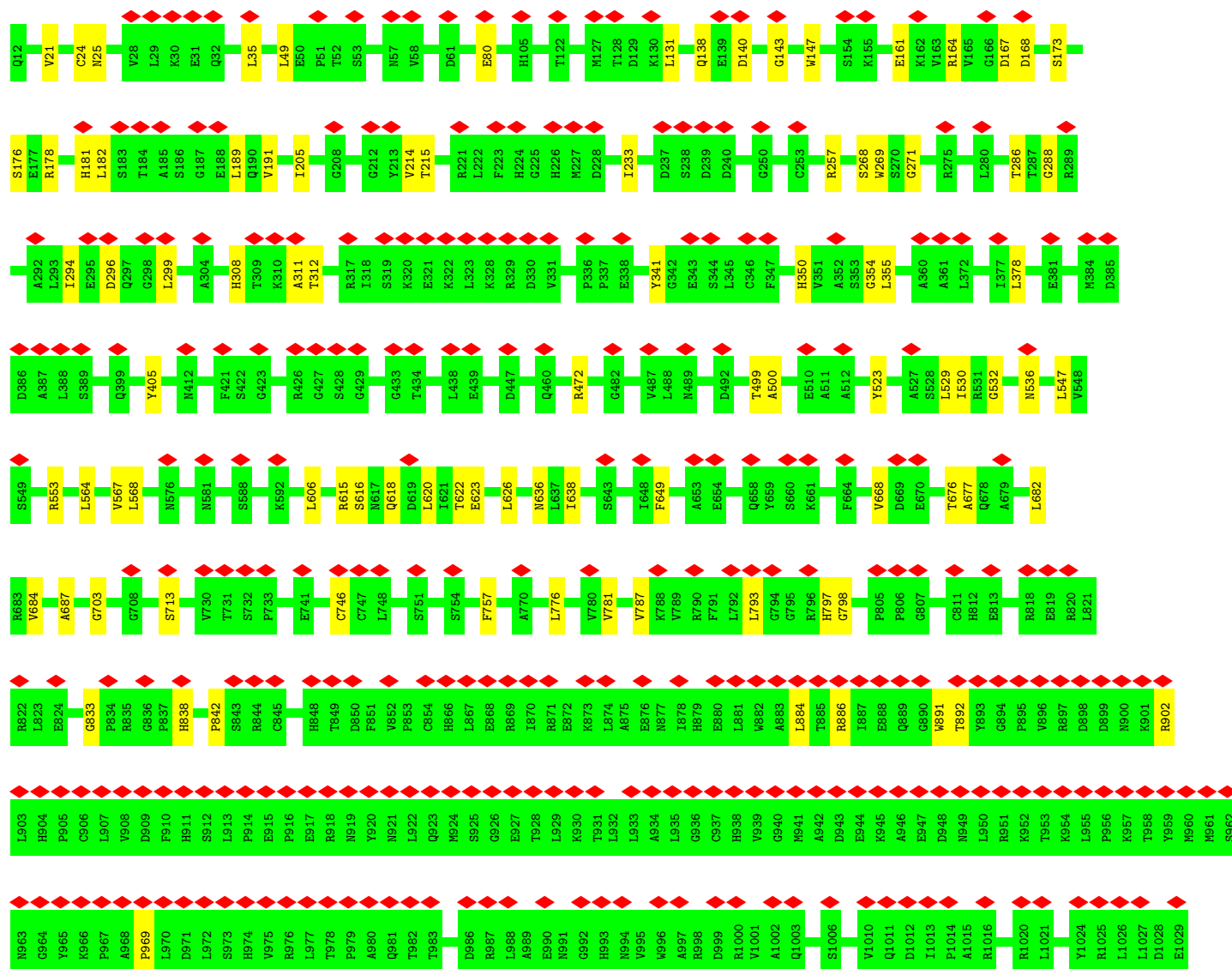


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T2938	R2939	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2977	X2978	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3009	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3034	X3035	X3036	X3037	X3038	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3051	X3052		
L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	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	K2916	A2917	D2918	D2919	R2920	E2921	P2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937
K2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	E2805	K2806	W2807	P2808	L2809	E2810	E2811	S2812	L2813	A2814	K2815	K2816	L2817	A2818	W2819	E2820	W2821	T2822	T2823	E2824	K2825	A2826	E2828	G2829	E2830	E2835	K2856	P2857	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	K2869	E2870	Q2872	A2873	K2874	A2875	E2876	Q2877			

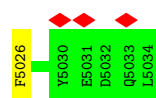


• Molecule 2: Ryanodine Receptor

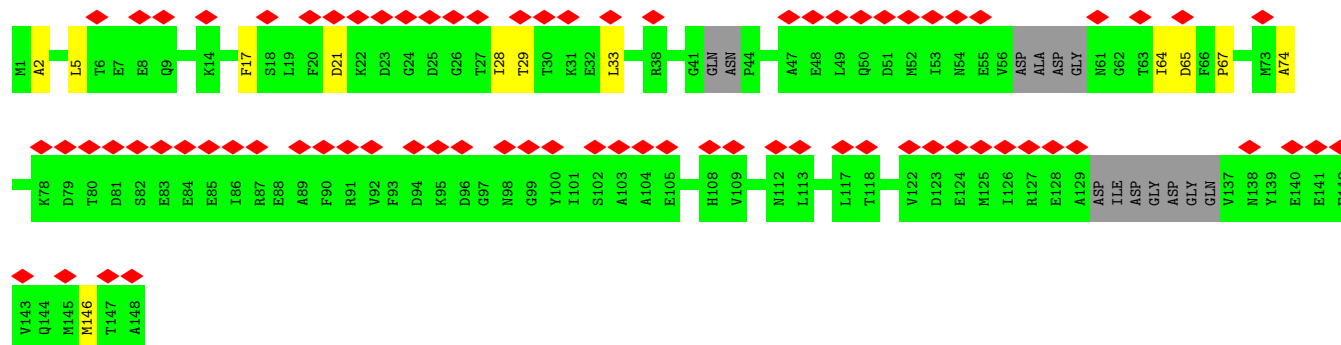
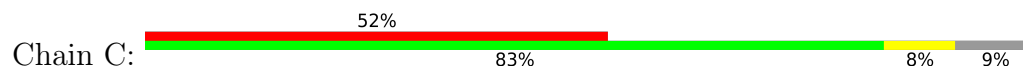




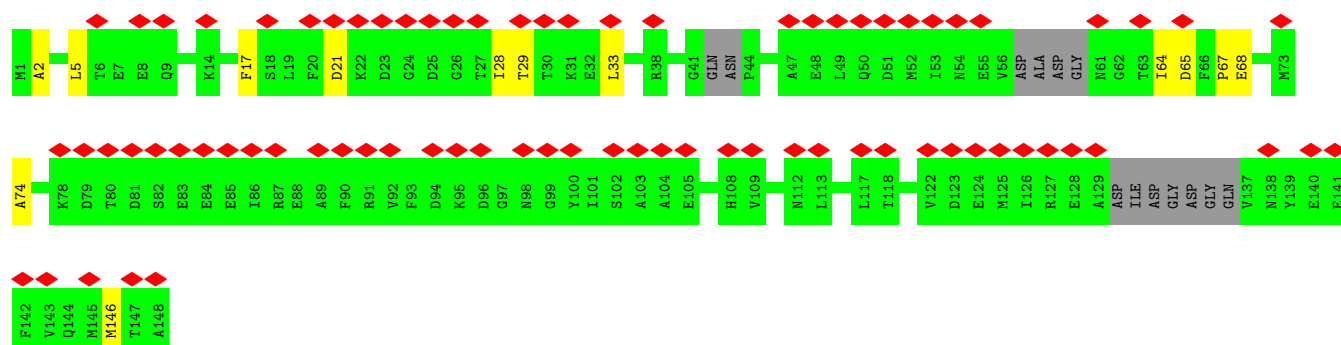
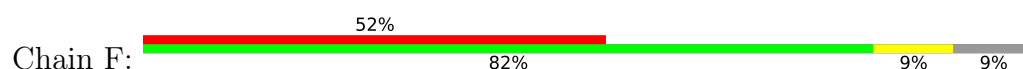
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L4926	V4722	G4635	E4177	N3992	E3680	X3568	P3430	X3336	X3216	X3058	X2959
L4934	L4723	Y4636	E4177	N3996	E3681	X3569	S3431	X3337	X3217	X3059	X2960
A4937	K4724	A4640	E4183	T3914	E3682	X3570	E3434	X3338	X3225	X3060	X2961
D4943	K4725	L4641	R4183	D3927	E3683	X3572	M3438	X3339	X3226	X3061	X2962
Q4945	H4726	R4642	R4184	Y3930	E3684	X3586	E3441	X3340	X3227		X2963
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	D4728	L4646	D4058	Y3932	V3686	X3588	F3443	X3342	X3229		X2965
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	Y4730	L4650	D4064	D3937	E3688	X3590	S3447	X3344	X3231		X2967
	E4733	L4654	D4065	V3937	D3692	X3593	K3448	X3345	X3232		X2968
	R4734	G4658	G4068	I3938	E3708	X3594	K3449	X3346	X3233		X2969
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	E4736	N4660	E4070	E3940	S3710	X3596	N3451	X3348	X3235		X2971
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	I4769		F4072	F3946	E3732	X3598	E3455	X3350	X3237		X2973
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	Y4773		D4074	Q3955	E3734	X3600	Q3457	X3352	X3239		X2975
	Q4774		D4075	T3969	E3735	X3601	N3458	X3353	X3240		X2976
	I4775		D4076	H3977	E3736	X3602	V3461	X3354	X3241		X2977
	W4776		D4077	G3986	E3737	X3605	X3509	X3355	X3242		X2978
	K4777		D4078	M3995	E3738	X3606	X3510	X3356	X3243		X2979
	F4782		D4079	M3995	E3739	X3607	X3511	X3357	X3244		X2980
	D4783		D4080	L3998	E3740	X3608	X3512	X3358	X3245		X2981
	D4784		D4081	A3999	E3741	X3609	X3513	X3359	X3246		X2982
	Y4802		R4126	I3999	E3742	X3610	X3514	X3360	X3247		X2983
	N4803		F4127	A3999	E3743	X3611	X3515	X3361	X3248		X2984
	N4804		Q4128	Q4000	E3744	X3612	X3516	X3362	X3249		X2985
	L4811		E4129	Q4000	E3745	X3613	X3517	X3363	X3250		X2986
	L4811		A4131	D4001	E3746	X3614	X3518	X3364	X3251		X2987
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	T4829		D4133	S4002	E3748	X3616	X3520	X3366	X3253		X2989
	G4832		I4134	L4005	E3749	X3617	X3521	X3367	X3254		X2990
	A4843		G4135	E4010	E3750	X3618	X3522	X3368	X3255		X2991
	M4877		F4136	L4011	E3751	X3619	X3523	X3369	X3256		X2992
	Y4886		N4137	L4012	E3752	X3620	X3524	X3370	X3257		X2993
	V4887		L4141	L4013	E3753	X3621	X3525	X3371	X3258		X2994
	G4896		S4146	L4014	E3754	X3622	X3526	X3372	X3259		X2995
	P4902		E4147	L4015	E3755	X3623	X3527	X3373	X3260		X2996
	A4903		Y4148	K4016	E3756	X3624	X3528	X3374	X3261		X2997
	Q4904		V4149	M4021	E3757	X3625	X3529	X3375	X3262		X2998
	D4905		P4150	L4026	E3758	X3626	X3530	X3376	X3263		X2999
	R4911		D4151	V4031	E3759	X3627	X3531	X3377	X3264		X3000
	D4915		R4152	W4032	E3760	X3628	X3532	X3378	X3265		X3001
			R4153	G4033	E3761	X3629	X3533	X3379	X3266		X3002
			R4154	M4039	E3762	X3630	X3534	X3380	X3267		X3003
			R4155		E3763	X3631	X3535	X3381	X3268		X3004
			R4156		E3764	X3632	X3536	X3382	X3269		X3005
			R4157		E3765	X3633	X3537	X3383	X3270		X3006
			E4160		E3766	X3634	X3538	X3384	X3271		X3007
			L4161		E3767	X3635	X3539	X3385	X3272		X3008
			A4162		E3768	X3636	X3540	X3386	X3273		X3009
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					E3770	X3638	X3542	X3388	X3275		X3011
					E3771	X3639	X3543	X3389	X3276		X3012
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					E3783	X3651	X3555	X3401	X3288		X3024
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					E3786	X3654	X3558	X3404	X3291		X3027
					E3787	X3655	X3559	X3405	X3292		X3028
					E3788	X3656	X3560	X3406	X3293		X3029
					E3789	X3657	X3561	X3407	X3294		X3030
					E3790	X3658	X3562	X3408	X3295		X3031
					E3791	X3659	X3563	X3409	X3296		X3032
					E3792	X3660	X3564	X3410	X3297		X3033
					E3793	X3661	X3565	X3411	X3298		X3034
					E3794	X3662	X3566	X3412	X3299		X3035
					E3795	X3663	X3567	X3413	X3300		X3036
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					E3806	X3674	X3578	X3424	X3311		X3047
					E3807	X3675	X3579	X3425	X3312		X3048
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					E3811	X3679	X3583	X3429	X3316		X3052
					E3812	X3680	X3584	X3430	X3317		X3053
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					E3814	X3682	X3586	X3432	X3319		X3055
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					E3818	X3686	X3590	X3436	X3323		X3059
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					E3820	X3688	X3592	X3438	X3325		X3061
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					E3824	X3692	X3596	X3442	X3329		X3065
					E3825	X3693	X3597	X3443	X3330		X3066
					E3826	X3694	X3598	X3444	X3331		X3067
					E3827	X3695	X3599	X3445	X3332		X3068
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					E3838	X3706	X3610	X3456	X3343		X3079
					E3839	X3707	X3611	X3457	X3344		X3080
					E3840	X3708	X3612	X3458	X3345		X3081
					E3841	X3709	X3613	X3459	X3346		X3082
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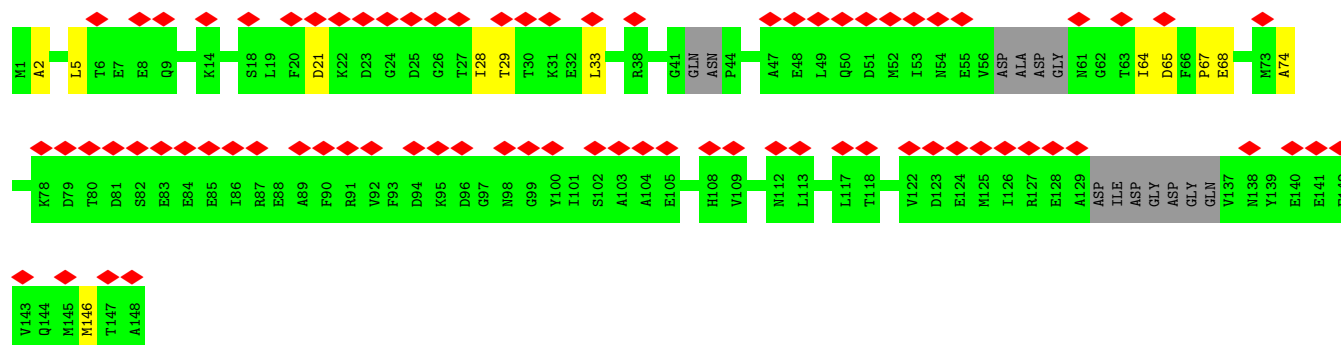
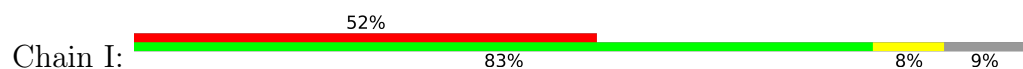
• Molecule 3: Calmodulin-1



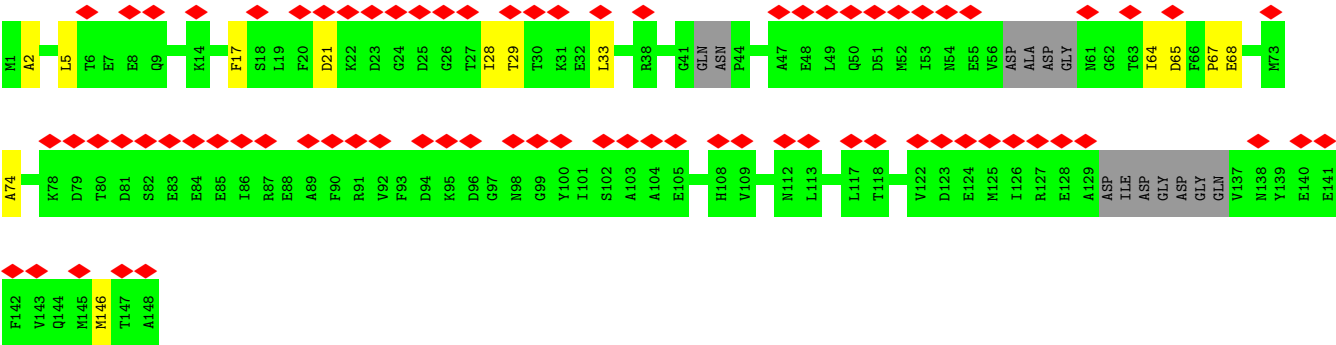
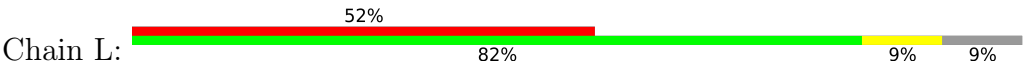
• Molecule 3: Calmodulin-1



• 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	0.173	Depositor
Minimum map value	-0.136	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	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	0.09	0/743	0.25	0/1014
1	D	0.09	0/743	0.25	0/1014
1	G	0.09	0/743	0.25	0/1014
1	J	0.09	0/743	0.25	0/1014
2	B	0.07	0/25353	0.21	0/34606
2	E	0.07	0/25353	0.21	0/34606
2	H	0.07	0/25353	0.21	0/34606
2	K	0.07	0/25353	0.21	0/34606
3	C	0.08	0/772	0.22	0/1059
3	F	0.08	0/772	0.22	0/1059
3	I	0.08	0/772	0.22	0/1059
3	L	0.08	0/772	0.22	0/1059
All	All	0.07	0/107472	0.22	0/146716

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	727	0	651	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	727	0	651	8	0
1	G	727	0	651	8	0
1	J	727	0	651	8	0
2	B	26597	0	22867	162	0
2	E	26597	0	22867	157	0
2	H	26597	0	22867	160	0
2	K	26597	0	22867	164	0
3	C	768	0	486	8	0
3	F	768	0	486	9	0
3	I	768	0	486	8	0
3	L	768	0	486	9	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	112372	0	96016	674	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 (674) 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:E:886:ARG:HB2	2:E:891:TRP:HB2	1.73	0.71
2:B:886:ARG:HB2	2:B:891:TRP:HB2	1.73	0.71
2:H:886:ARG:HB2	2:H:891:TRP:HB2	1.73	0.71
2:K:886:ARG:HB2	2:K:891:TRP:HB2	1.73	0.71
2:E:4706:THR:HG21	2:E:4773:TYR:HB2	1.74	0.70
2:K:173:SER:HG	2:K:178:ARG:H	1.40	0.70
2:H:4706:THR:HG21	2:H:4773:TYR:HB2	1.74	0.69
2:K:1101:ARG:HB2	2:K:1193:SER:HB2	1.74	0.69
2:H:1101:ARG:HB2	2:H:1193:SER:HB2	1.74	0.69
2:K:4706:THR:HG21	2:K:4773:TYR:HB2	1.74	0.69
2:B:4706:THR:HG21	2:B:4773:TYR:HB2	1.74	0.69
2:B:1101:ARG:HB2	2:B:1193:SER:HB2	1.74	0.68
2:B:1082:ALA:HB1	2:B:1187:GLY:HA3	1.76	0.68
2:E:1082:ALA:HB1	2:E:1187:GLY:HA3	1.76	0.68
2:E:1101:ARG:HB2	2:E:1193:SER:HB2	1.74	0.67
2:H:1082:ALA:HB1	2:H:1187:GLY:HA3	1.76	0.67
2:K:1082:ALA:HB1	2:K:1187:GLY:HA3	1.76	0.66
2:E:3781:CYS:HB2	2:E:3784:GLU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3781:CYS:HB2	2:B:3784:GLU:HB3	1.78	0.65
2:K:4960:GLY:HA3	2:K:5023:GLY:H	1.61	0.65
2:K:3781:CYS:HB2	2:K:3784:GLU:HB3	1.78	0.65
2:E:4960:GLY:HA3	2:E:5023:GLY:H	1.61	0.65
2:H:4960:GLY:HA3	2:H:5023:GLY:H	1.61	0.65
2:B:4960:GLY:HA3	2:B:5023:GLY:H	1.61	0.65
2:E:4902:PRO:HB3	2:E:4911:ARG:HG2	1.79	0.64
2:H:3781:CYS:HB2	2:H:3784:GLU:HB3	1.78	0.64
2:K:4902:PRO:HB3	2:K:4911:ARG:HG2	1.79	0.64
2:B:4902:PRO:HB3	2:B:4911:ARG:HG2	1.79	0.64
2:B:833:GLY:HA3	2:B:838:HIS:HD2	1.63	0.64
2:E:833:GLY:HA3	2:E:838:HIS:HD2	1.63	0.63
2:H:4902:PRO:HB3	2:H:4911:ARG:HG2	1.79	0.63
2:K:833:GLY:HA3	2:K:838:HIS:HD2	1.63	0.63
2:H:833:GLY:HA3	2:H:838:HIS:HD2	1.63	0.62
2:K:294:ILE:HG23	2:K:296:ASP:H	1.67	0.60
2:B:294:ILE:HG23	2:B:296:ASP:H	1.67	0.60
2:E:176:SER:HB2	2:E:178:ARG:HH21	1.67	0.60
2:E:2496:VAL:HG12	2:E:2498:ASP:H	1.67	0.60
2:H:2496:VAL:HG12	2:H:2498:ASP:H	1.67	0.60
2:E:294:ILE:HG23	2:E:296:ASP:H	1.67	0.60
2:B:176:SER:HB2	2:B:178:ARG:HH21	1.67	0.60
2:H:294:ILE:HG23	2:H:296:ASP:H	1.67	0.59
2:K:2496:VAL:HG12	2:K:2498:ASP:H	1.67	0.59
2:E:793:LEU:HD12	2:E:797:HIS:HB2	1.84	0.59
2:H:793:LEU:HD12	2:H:797:HIS:HB2	1.84	0.59
2:H:176:SER:HB2	2:H:178:ARG:HH21	1.67	0.59
2:K:176:SER:HB2	2:K:178:ARG:HH21	1.67	0.59
2:B:793:LEU:HD12	2:B:797:HIS:HB2	1.84	0.58
2:B:1974:GLN:HG2	2:B:3637:LEU:HB3	1.86	0.58
2:B:2496:VAL:HG12	2:B:2498:ASP:H	1.67	0.58
2:E:1974:GLN:HG2	2:E:3637:LEU:HB3	1.86	0.58
2:E:3946:PHE:HE2	2:E:4011:LEU:HD21	1.69	0.58
2:K:523:TYR:OH	2:K:553:ARG:NH1	2.37	0.58
2:B:3946:PHE:HE2	2:B:4011:LEU:HD21	1.69	0.57
2:H:523:TYR:OH	2:H:553:ARG:NH1	2.37	0.57
2:K:793:LEU:HD12	2:K:797:HIS:HB2	1.84	0.57
2:B:523:TYR:OH	2:B:553:ARG:NH1	2.37	0.57
2:E:523:TYR:OH	2:E:553:ARG:NH1	2.37	0.57
2:B:568:LEU:HD13	2:B:606:LEU:HD21	1.87	0.57
2:H:568:LEU:HD13	2:H:606:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:3765:LEU:HB3	2:K:3770:ALA:HB3	1.86	0.57
2:K:1521:ASP:HB3	2:K:1525:GLY:HA3	1.87	0.57
2:B:1521:ASP:HB3	2:B:1525:GLY:HA3	1.87	0.57
2:E:568:LEU:HD13	2:E:606:LEU:HD21	1.87	0.57
2:H:3946:PHE:HE2	2:H:4011:LEU:HD21	1.69	0.57
2:B:24:CYS:SG	2:B:25:ASN:N	2.78	0.57
2:B:4922:VAL:HA	2:B:4926:LEU:HB3	1.87	0.57
2:H:1521:ASP:HB3	2:H:1525:GLY:HA3	1.87	0.57
2:B:4934:ILE:HG21	2:E:4925:ILE:HG23	1.87	0.56
2:H:3765:LEU:HB3	2:H:3770:ALA:HB3	1.86	0.56
2:K:568:LEU:HD13	2:K:606:LEU:HD21	1.87	0.56
2:K:3946:PHE:HE2	2:K:4011:LEU:HD21	1.69	0.56
2:E:4934:ILE:HG21	2:H:4925:ILE:HG23	1.87	0.56
2:H:1974:GLN:HG2	2:H:3637:LEU:HB3	1.86	0.56
2:K:24:CYS:SG	2:K:25:ASN:N	2.78	0.56
2:K:2470:ILE:HG21	2:K:2503:MET:HG3	1.88	0.56
2:K:4922:VAL:HA	2:K:4926:LEU:HB3	1.87	0.56
1:D:88:PRO:HB3	2:E:623:GLU:HG2	1.88	0.56
2:E:24:CYS:SG	2:E:25:ASN:N	2.78	0.56
2:K:1974:GLN:HG2	2:K:3637:LEU:HB3	1.86	0.56
2:E:2164:ARG:NH2	2:E:2202:LEU:O	2.39	0.56
2:H:4922:VAL:HA	2:H:4926:LEU:HB3	1.87	0.56
2:E:4922:VAL:HA	2:E:4926:LEU:HB3	1.87	0.56
2:K:3692:ASP:OD2	2:K:3768:ARG:NH2	2.39	0.56
2:B:2164:ARG:NH2	2:B:2202:LEU:O	2.39	0.56
2:E:233:ILE:O	2:E:257:ARG:NH1	2.39	0.56
1:A:88:PRO:HB3	2:B:623:GLU:HG2	1.88	0.56
1:G:88:PRO:HB3	2:H:623:GLU:HG2	1.88	0.56
2:H:3692:ASP:OD2	2:H:3768:ARG:NH2	2.39	0.56
2:K:2164:ARG:NH2	2:K:2202:LEU:O	2.39	0.56
2:B:2470:ILE:HG21	2:B:2503:MET:HG3	1.88	0.56
2:E:2470:ILE:HG21	2:E:2503:MET:HG3	1.88	0.56
2:H:233:ILE:O	2:H:257:ARG:NH1	2.39	0.56
2:H:4576:LEU:HA	2:K:4877:MET:HG2	1.88	0.56
2:K:233:ILE:O	2:K:257:ARG:NH1	2.39	0.56
2:H:2470:ILE:HG21	2:H:2503:MET:HG3	1.88	0.56
2:B:3765:LEU:HB3	2:B:3770:ALA:HB3	1.86	0.56
2:B:4877:MET:HG2	2:K:4576:LEU:HA	1.88	0.56
2:E:3692:ASP:OD2	2:E:3768:ARG:NH2	2.39	0.56
2:H:4934:ILE:HG21	2:K:4925:ILE:HG23	1.87	0.56
2:E:1215:ALA:HA	2:E:1219:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3765:LEU:HB3	2:E:3770:ALA:HB3	1.86	0.55
2:H:24:CYS:SG	2:H:25:ASN:N	2.78	0.55
2:B:233:ILE:O	2:B:257:ARG:NH1	2.39	0.55
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.39	0.55
2:E:1521:ASP:HB3	2:E:1525:GLY:HA3	1.87	0.55
2:K:618:GLN:OE1	2:K:1678:ASN:ND2	2.39	0.55
2:K:1215:ALA:HA	2:K:1219:LEU:HB2	1.88	0.55
2:B:1215:ALA:HA	2:B:1219:LEU:HB2	1.88	0.55
2:H:1215:ALA:HA	2:H:1219:LEU:HB2	1.88	0.55
2:K:4706:THR:HG22	2:K:4708:SER:H	1.71	0.55
2:B:3692:ASP:OD2	2:B:3768:ARG:NH2	2.39	0.55
2:B:4925:ILE:HG23	2:K:4934:ILE:HG21	1.87	0.55
2:H:2164:ARG:NH2	2:H:2202:LEU:O	2.39	0.55
2:B:4961:ILE:HD11	2:B:4965:TYR:HB2	1.89	0.55
2:E:2443:LEU:HD12	2:E:2444:ILE:HG13	1.89	0.55
2:K:4961:ILE:HD11	2:K:4965:TYR:HB2	1.89	0.55
2:B:842:PRO:HD3	2:B:1073:ARG:HG2	1.89	0.55
2:E:4961:ILE:HD11	2:E:4965:TYR:HB2	1.89	0.54
2:E:5025:CYS:SG	2:E:5026:PHE:N	2.80	0.54
2:H:618:GLN:OE1	2:H:1678:ASN:ND2	2.39	0.54
1:J:88:PRO:HB3	2:K:623:GLU:HG2	1.88	0.54
2:K:842:PRO:HD3	2:K:1073:ARG:HG2	1.89	0.54
2:B:1928:LEU:O	2:B:2105:ARG:NH2	2.41	0.54
2:B:4576:LEU:HA	2:E:4877:MET:HG2	1.88	0.54
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.39	0.54
2:B:4706:THR:HG22	2:B:4708:SER:H	1.71	0.54
2:E:842:PRO:HD3	2:E:1073:ARG:HG2	1.89	0.54
2:E:4706:THR:HG22	2:E:4708:SER:H	1.71	0.54
2:H:1928:LEU:O	2:H:2105:ARG:NH2	2.41	0.54
2:H:4961:ILE:HD11	2:H:4965:TYR:HB2	1.89	0.54
2:K:1928:LEU:O	2:K:2105:ARG:NH2	2.41	0.54
2:E:4576:LEU:HA	2:H:4877:MET:HG2	1.88	0.54
2:B:2443:LEU:HD12	2:B:2444:ILE:HG13	1.89	0.54
2:B:5025:CYS:SG	2:B:5026:PHE:N	2.80	0.54
2:H:4706:THR:HG22	2:H:4708:SER:H	1.71	0.54
2:K:5025:CYS:SG	2:K:5026:PHE:N	2.80	0.54
2:E:793:LEU:H	2:E:798:GLY:HA3	1.73	0.53
2:H:5025:CYS:SG	2:H:5026:PHE:N	2.80	0.53
2:B:3711:LYS:NZ	2:B:3784:GLU:OE2	2.39	0.53
2:E:1928:LEU:O	2:E:2105:ARG:NH2	2.41	0.53
2:H:622:THR:HG23	2:H:626:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:842:PRO:HD3	2:H:1073:ARG:HG2	1.89	0.53
1:J:74:LEU:HD22	1:J:101:VAL:HG21	1.91	0.53
2:B:793:LEU:H	2:B:798:GLY:HA3	1.73	0.53
1:G:74:LEU:HD22	1:G:101:VAL:HG21	1.91	0.53
2:K:2443:LEU:HD12	2:K:2444:ILE:HG13	1.89	0.53
2:K:472:ARG:NH1	2:K:532:GLY:O	2.42	0.53
2:K:547:LEU:HD22	2:K:564:LEU:HD13	1.91	0.53
2:E:622:THR:HG23	2:E:626:LEU:HD22	1.90	0.53
2:H:638:ILE:HD13	2:H:703:GLY:HA2	1.91	0.53
3:L:29:THR:O	3:L:33:LEU:N	2.40	0.53
2:B:472:ARG:NH1	2:B:532:GLY:O	2.42	0.52
2:B:547:LEU:HD22	2:B:564:LEU:HD13	1.91	0.52
2:B:2336:LEU:HB2	2:B:2433:LEU:HD11	1.91	0.52
2:H:1466:LEU:HD23	2:H:1496:TRP:HE3	1.74	0.52
2:K:1466:LEU:HD23	2:K:1496:TRP:HE3	1.74	0.52
1:A:74:LEU:HD22	1:A:101:VAL:HG21	1.91	0.52
2:E:638:ILE:HD13	2:E:703:GLY:HA2	1.91	0.52
2:H:472:ARG:NH1	2:H:532:GLY:O	2.42	0.52
2:K:1955:ARG:NH1	2:K:2043:CYS:SG	2.82	0.52
2:B:1436:SER:HA	2:B:1517:GLY:HA2	1.92	0.52
1:D:35:LYS:HD3	1:D:38:SER:HB2	1.91	0.52
2:H:793:LEU:H	2:H:798:GLY:HA3	1.73	0.52
2:K:793:LEU:H	2:K:798:GLY:HA3	1.73	0.52
2:K:1594:ARG:NH1	2:K:1643:GLU:OE2	2.42	0.52
1:A:35:LYS:HD3	1:A:38:SER:HB2	1.91	0.52
2:B:622:THR:HG23	2:B:626:LEU:HD22	1.90	0.52
2:B:1594:ARG:NH1	2:B:1643:GLU:OE2	2.42	0.52
1:D:74:LEU:HD22	1:D:101:VAL:HG21	1.91	0.52
2:H:2336:LEU:HB2	2:H:2433:LEU:HD11	1.91	0.52
2:H:4133:ASP:O	2:H:4137:ASN:ND2	2.41	0.52
2:B:4054:LEU:HD13	2:B:4162:ALA:HB2	1.92	0.52
2:E:1955:ARG:NH1	2:E:2043:CYS:SG	2.82	0.52
2:H:1594:ARG:NH1	2:H:1643:GLU:OE2	2.42	0.52
2:H:1955:ARG:NH1	2:H:2043:CYS:SG	2.82	0.52
2:B:1955:ARG:NH1	2:B:2043:CYS:SG	2.82	0.52
2:E:1594:ARG:NH1	2:E:1643:GLU:OE2	2.42	0.52
2:H:2443:LEU:HD12	2:H:2444:ILE:HG13	1.89	0.52
2:K:2166:LEU:HG	2:K:2178:LEU:HD22	1.92	0.52
2:B:168:ASP:OD1	2:B:168:ASP:N	2.43	0.52
2:E:4054:LEU:HD13	2:E:4162:ALA:HB2	1.92	0.52
2:H:4054:LEU:HD13	2:H:4162:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1436:SER:HA	2:K:1517:GLY:HA2	1.92	0.52
2:K:622:THR:HG23	2:K:626:LEU:HD22	1.90	0.52
2:E:472:ARG:NH1	2:E:532:GLY:O	2.42	0.52
2:E:547:LEU:HD22	2:E:564:LEU:HD13	1.91	0.52
2:H:547:LEU:HD22	2:H:564:LEU:HD13	1.91	0.52
2:B:638:ILE:HD13	2:B:703:GLY:HA2	1.91	0.52
2:B:4133:ASP:O	2:B:4137:ASN:ND2	2.41	0.52
2:E:2336:LEU:HB2	2:E:2433:LEU:HD11	1.91	0.52
1:J:35:LYS:HD3	1:J:38:SER:HB2	1.91	0.51
2:B:1466:LEU:HD23	2:B:1496:TRP:HE3	1.74	0.51
2:E:1466:LEU:HD23	2:E:1496:TRP:HE3	1.74	0.51
2:H:1436:SER:HA	2:H:1517:GLY:HA2	1.92	0.51
2:K:4133:ASP:O	2:K:4137:ASN:ND2	2.41	0.51
2:H:2166:LEU:HG	2:H:2178:LEU:HD22	1.92	0.51
2:K:2336:LEU:HB2	2:K:2433:LEU:HD11	1.91	0.51
1:G:35:LYS:HD3	1:G:38:SER:HB2	1.91	0.51
3:I:29:THR:O	3:I:33:LEU:N	2.40	0.51
2:K:168:ASP:OD1	2:K:168:ASP:N	2.43	0.51
2:K:3711:LYS:NZ	2:K:3784:GLU:OE2	2.39	0.51
2:E:4177:GLU:CB	2:E:4981:HIS:HE1	2.23	0.51
2:K:638:ILE:HD13	2:K:703:GLY:HA2	1.91	0.51
3:F:29:THR:O	3:F:33:LEU:N	2.40	0.51
2:B:2166:LEU:HG	2:B:2178:LEU:HD22	1.92	0.51
2:H:4177:GLU:CB	2:H:4981:HIS:HE1	2.24	0.51
2:E:1438:ARG:HG2	2:E:1515:VAL:HG12	1.93	0.51
2:K:1289:LEU:HD12	2:K:1562:ILE:HD11	1.93	0.51
2:K:4054:LEU:HD13	2:K:4162:ALA:HB2	1.92	0.51
2:E:4133:ASP:O	2:E:4137:ASN:ND2	2.41	0.51
2:K:1438:ARG:HG2	2:K:1515:VAL:HG12	1.93	0.51
2:B:1289:LEU:HD12	2:B:1562:ILE:HD11	1.93	0.50
2:H:168:ASP:OD1	2:H:168:ASP:N	2.43	0.50
2:B:1597:MET:SD	2:B:1597:MET:N	2.85	0.50
2:E:1436:SER:HA	2:E:1517:GLY:HA2	1.92	0.50
2:E:3711:LYS:NZ	2:E:3784:GLU:OE2	2.39	0.50
3:C:29:THR:O	3:C:33:LEU:N	2.40	0.50
2:E:1831:VAL:HB	2:E:1838:GLN:HG3	1.94	0.50
2:H:1438:ARG:HG2	2:H:1515:VAL:HG12	1.93	0.50
2:K:1597:MET:SD	2:K:1597:MET:N	2.85	0.50
2:B:308:HIS:CD2	2:B:311:ALA:H	2.30	0.50
2:B:2473:LEU:HD12	2:B:2474:PRO:HD2	1.94	0.50
2:E:308:HIS:CD2	2:E:311:ALA:H	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1831:VAL:HB	2:H:1838:GLN:HG3	1.94	0.50
2:K:308:HIS:CD2	2:K:311:ALA:H	2.30	0.50
2:B:1438:ARG:HG2	2:B:1515:VAL:HG12	1.93	0.50
2:E:2166:LEU:HG	2:E:2178:LEU:HD22	1.92	0.50
2:H:268:SER:HG	2:H:269:TRP:CD1	2.30	0.50
2:H:1597:MET:SD	2:H:1597:MET:N	2.85	0.50
2:K:3884:GLN:OE1	2:K:3955:GLN:NE2	2.45	0.50
2:B:268:SER:HG	2:B:269:TRP:CD1	2.29	0.50
2:E:161:GLU:OE2	2:E:164:ARG:NH2	2.45	0.50
2:E:268:SER:HG	2:E:269:TRP:CD1	2.30	0.50
2:E:2473:LEU:HD12	2:E:2474:PRO:HD2	1.94	0.50
2:H:308:HIS:CD2	2:H:311:ALA:H	2.30	0.50
2:H:2200:ARG:NH2	2:H:2246:GLN:OE1	2.45	0.50
2:K:1831:VAL:HB	2:K:1838:GLN:HG3	1.94	0.50
2:K:4679:LEU:HD12	2:K:4683:GLY:HA2	1.94	0.50
2:B:3884:GLN:OE1	2:B:3955:GLN:NE2	2.45	0.50
2:E:1597:MET:SD	2:E:1597:MET:N	2.85	0.50
2:H:1289:LEU:HD12	2:H:1562:ILE:HD11	1.93	0.50
2:H:4679:LEU:HD12	2:H:4683:GLY:HA2	1.94	0.50
2:B:1743:ARG:NH1	2:B:1964:GLU:OE2	2.44	0.50
2:K:161:GLU:OE2	2:K:164:ARG:NH2	2.45	0.50
2:H:4686:ILE:HG22	2:H:4687:THR:HG23	1.94	0.49
2:E:1289:LEU:HD12	2:E:1562:ILE:HD11	1.93	0.49
2:H:3884:GLN:OE1	2:H:3955:GLN:NE2	2.45	0.49
2:K:2200:ARG:NH2	2:K:2246:GLN:OE1	2.45	0.49
2:K:4686:ILE:HG22	2:K:4687:THR:HG23	1.94	0.49
2:E:3884:GLN:OE1	2:E:3955:GLN:NE2	2.45	0.49
2:B:1735:ILE:HG22	2:B:2143:TYR:HB3	1.95	0.49
2:B:1831:VAL:HB	2:B:1838:GLN:HG3	1.94	0.49
2:K:268:SER:HG	2:K:269:TRP:CD1	2.30	0.49
2:K:1695:LEU:HD11	2:K:1808:LEU:HD11	1.95	0.49
2:E:2200:ARG:NH2	2:E:2246:GLN:OE1	2.45	0.49
1:G:90:VAL:HG23	1:G:91:ILE:HG12	1.95	0.49
2:H:1695:LEU:HD11	2:H:1808:LEU:HD11	1.95	0.49
2:H:2473:LEU:HD12	2:H:2474:PRO:HD2	1.94	0.49
2:B:161:GLU:OE2	2:B:164:ARG:NH2	2.45	0.49
2:B:1290:ARG:HG3	2:B:1551:ALA:HB2	1.95	0.49
2:E:1695:LEU:HD11	2:E:1808:LEU:HD11	1.95	0.49
2:H:1743:ARG:NH1	2:H:1964:GLU:OE2	2.44	0.49
2:B:4679:LEU:HD12	2:B:4683:GLY:HA2	1.94	0.49
2:E:4679:LEU:HD12	2:E:4683:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:649:PHE:HB3	2:H:776:LEU:HD13	1.95	0.49
1:A:90:VAL:HG23	1:A:91:ILE:HG12	1.95	0.48
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.95	0.48
2:K:2473:LEU:HD12	2:K:2474:PRO:HD2	1.94	0.48
2:B:1075:PHE:HB2	2:B:1192:CYS:HB3	1.95	0.48
2:E:2517:ASP:HA	2:E:2569:LEU:HD21	1.95	0.48
2:K:649:PHE:HB3	2:K:776:LEU:HD13	1.95	0.48
2:K:1290:ARG:HG3	2:K:1551:ALA:HB2	1.95	0.48
2:K:1735:ILE:HG22	2:K:2143:TYR:HB3	1.95	0.48
2:K:2163:ILE:HD11	2:K:2179:MET:HG3	1.95	0.48
2:B:2200:ARG:NH2	2:B:2246:GLN:OE1	2.45	0.48
2:E:350:HIS:HB3	2:E:354:GLY:H	1.79	0.48
2:E:1075:PHE:HB2	2:E:1192:CYS:HB3	1.95	0.48
2:E:1735:ILE:HG22	2:E:2143:TYR:HB3	1.95	0.48
2:H:2517:ASP:HA	2:H:2569:LEU:HD21	1.95	0.48
2:B:1093:GLU:HB3	2:B:1201:HIS:HB3	1.95	0.48
2:B:1695:LEU:HD11	2:B:1808:LEU:HD11	1.95	0.48
2:B:2103:VAL:HG11	2:B:2125:LEU:HD13	1.95	0.48
2:B:4686:ILE:HG22	2:B:4687:THR:HG23	1.94	0.48
2:E:4686:ILE:HG22	2:E:4687:THR:HG23	1.94	0.48
2:H:3711:LYS:NZ	2:H:3784:GLU:OE2	2.39	0.48
2:B:4802:TYR:CE2	2:B:4804:ASN:HB2	2.49	0.48
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.95	0.48
2:H:884:LEU:HD11	2:H:969:PRO:HA	1.95	0.48
2:B:2163:ILE:HD11	2:B:2179:MET:HG3	1.95	0.48
1:D:90:VAL:HG23	1:D:91:ILE:HG12	1.95	0.48
2:H:1735:ILE:HG22	2:H:2143:TYR:HB3	1.95	0.48
2:K:4802:TYR:CE2	2:K:4804:ASN:HB2	2.49	0.48
2:B:4234:GLU:OE2	2:B:5012:TYR:OH	2.30	0.48
2:E:2163:ILE:HD11	2:E:2179:MET:HG3	1.95	0.48
2:H:1093:GLU:HB3	2:H:1201:HIS:HB3	1.95	0.48
2:H:2103:VAL:HG11	2:H:2125:LEU:HD13	1.95	0.48
2:B:530:ILE:HG21	2:B:567:VAL:HG12	1.96	0.48
1:D:4:ILE:HD13	1:D:65:GLN:HG2	1.96	0.48
2:K:2517:ASP:HA	2:K:2569:LEU:HD21	1.95	0.48
1:D:78:PRO:HG3	1:D:96:THR:HA	1.96	0.48
2:H:350:HIS:HB3	2:H:354:GLY:H	1.79	0.48
2:K:350:HIS:HB3	2:K:354:GLY:H	1.79	0.48
2:K:530:ILE:HG21	2:K:567:VAL:HG12	1.96	0.48
1:A:78:PRO:HG3	1:A:96:THR:HA	1.96	0.47
2:E:1454:THR:HG22	2:E:1456:ASP:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:GLU:OE2	2:H:164:ARG:NH2	2.45	0.47
2:H:1290:ARG:HG3	2:H:1551:ALA:HB2	1.95	0.47
1:J:90:VAL:HG23	1:J:91:ILE:HG12	1.95	0.47
2:B:1643:GLU:HG3	2:B:1644:GLU:HG3	1.96	0.47
2:K:1454:THR:HG22	2:K:1456:ASP:H	1.79	0.47
2:K:3880:PHE:HE1	2:K:3914:THR:HG23	1.79	0.47
2:B:2517:ASP:HA	2:B:2569:LEU:HD21	1.95	0.47
2:E:168:ASP:N	2:E:168:ASP:OD1	2.43	0.47
2:E:2103:VAL:HG11	2:E:2125:LEU:HD13	1.95	0.47
2:K:2103:VAL:HG11	2:K:2125:LEU:HD13	1.95	0.47
2:B:350:HIS:HB3	2:B:354:GLY:H	1.79	0.47
2:B:1454:THR:HG22	2:B:1456:ASP:H	1.79	0.47
2:B:4886:TYR:HD2	2:B:4887:VAL:HG13	1.80	0.47
2:E:3880:PHE:HE1	2:E:3914:THR:HG23	1.79	0.47
2:H:530:ILE:HG21	2:H:567:VAL:HG12	1.96	0.47
1:J:78:PRO:HG3	1:J:96:THR:HA	1.96	0.47
2:B:884:LEU:HD11	2:B:969:PRO:HA	1.95	0.47
2:E:1290:ARG:HG3	2:E:1551:ALA:HB2	1.95	0.47
2:H:676:THR:OG1	2:H:677:ALA:N	2.46	0.47
2:H:3880:PHE:HE1	2:H:3914:THR:HG23	1.79	0.47
2:K:884:LEU:HD11	2:K:969:PRO:HA	1.95	0.47
1:A:4:ILE:HD13	1:A:65:GLN:HG2	1.96	0.47
2:B:3880:PHE:HE1	2:B:3914:THR:HG23	1.79	0.47
2:K:676:THR:OG1	2:K:677:ALA:N	2.46	0.47
2:E:530:ILE:HG21	2:E:567:VAL:HG12	1.96	0.47
2:E:676:THR:OG1	2:E:677:ALA:N	2.46	0.47
2:E:884:LEU:HD11	2:E:969:PRO:HA	1.95	0.47
2:E:1093:GLU:HB3	2:E:1201:HIS:HB3	1.95	0.47
1:G:78:PRO:HG3	1:G:96:THR:HA	1.96	0.47
2:H:2163:ILE:HD11	2:H:2179:MET:HG3	1.95	0.47
2:H:4802:TYR:CE2	2:H:4804:ASN:HB2	2.49	0.47
2:K:1075:PHE:HB2	2:K:1192:CYS:HB3	1.95	0.47
2:K:1093:GLU:HB3	2:K:1201:HIS:HB3	1.95	0.47
2:K:1643:GLU:HG3	2:K:1644:GLU:HG3	1.96	0.47
2:K:4234:GLU:OE2	2:K:5012:TYR:OH	2.30	0.47
2:K:4886:TYR:HD2	2:K:4887:VAL:HG13	1.80	0.47
2:E:746:CYS:HA	2:E:757:PHE:HA	1.97	0.47
2:E:2454:ILE:HA	2:E:2457:ILE:HD12	1.96	0.47
2:H:616:SER:O	2:H:620:LEU:HD13	2.15	0.47
2:H:1075:PHE:HB2	2:H:1192:CYS:HB3	1.95	0.47
2:H:4886:TYR:HD2	2:H:4887:VAL:HG13	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4802:TYR:CE2	2:E:4804:ASN:HB2	2.49	0.47
2:K:616:SER:O	2:K:620:LEU:HD13	2.15	0.47
2:K:2454:ILE:HA	2:K:2457:ILE:HD12	1.96	0.47
2:H:1454:THR:HG22	2:H:1456:ASP:H	1.79	0.47
2:H:2454:ILE:HA	2:H:2457:ILE:HD12	1.96	0.47
2:B:529:LEU:O	2:B:536:ASN:ND2	2.48	0.46
2:E:1643:GLU:HG3	2:E:1644:GLU:HG3	1.96	0.46
2:H:1443:GLN:HA	2:H:1557:THR:HG21	1.97	0.46
1:J:4:ILE:HD13	1:J:65:GLN:HG2	1.96	0.46
2:E:1641:ILE:HG22	2:E:1643:GLU:HG2	1.98	0.46
2:H:529:LEU:O	2:H:536:ASN:ND2	2.48	0.46
1:J:74:LEU:HD13	1:J:101:VAL:HB	1.97	0.46
2:K:1743:ARG:NH1	2:K:1964:GLU:OE2	2.44	0.46
2:E:616:SER:O	2:E:620:LEU:HD13	2.15	0.46
2:E:1130:GLN:HG3	2:E:1138:LEU:HA	1.98	0.46
2:E:2461:LEU:HD12	2:E:2462:VAL:HG23	1.97	0.46
2:E:4886:TYR:HD2	2:E:4887:VAL:HG13	1.80	0.46
2:B:746:CYS:HA	2:B:757:PHE:HA	1.97	0.46
2:H:1641:ILE:HG22	2:H:1643:GLU:HG2	1.98	0.46
2:K:529:LEU:O	2:K:536:ASN:ND2	2.48	0.46
2:B:616:SER:O	2:B:620:LEU:HD13	2.15	0.46
2:B:2128:GLN:HE21	2:B:2128:GLN:HA	1.80	0.46
2:B:2461:LEU:HD12	2:B:2462:VAL:HG23	1.97	0.46
2:E:892:THR:N	2:E:902:ARG:O	2.48	0.46
2:H:1643:GLU:HG3	2:H:1644:GLU:HG3	1.96	0.46
2:H:2461:LEU:HD12	2:H:2462:VAL:HG23	1.97	0.46
2:B:215:THR:OG1	2:B:271:GLY:O	2.34	0.46
1:G:4:ILE:HD13	1:G:65:GLN:HG2	1.96	0.46
2:K:1130:GLN:HG3	2:K:1138:LEU:HA	1.98	0.46
2:B:1443:GLN:HA	2:B:1557:THR:HG21	1.97	0.46
2:E:529:LEU:O	2:E:536:ASN:ND2	2.48	0.46
2:K:746:CYS:HA	2:K:757:PHE:HA	1.97	0.46
2:B:2454:ILE:HA	2:B:2457:ILE:HD12	1.96	0.46
1:D:74:LEU:HD13	1:D:101:VAL:HB	1.97	0.46
2:E:2128:GLN:HE21	2:E:2128:GLN:HA	1.80	0.46
2:E:3804:ASN:HB2	2:E:3807:VAL:HG12	1.98	0.46
2:E:4234:GLU:OE2	2:E:5012:TYR:OH	2.30	0.46
2:E:4553:LEU:HD11	2:E:4654:LEU:HD23	1.98	0.46
2:B:1641:ILE:HG22	2:B:1643:GLU:HG2	1.98	0.46
2:E:2475:LEU:HD23	2:E:2475:LEU:H	1.81	0.46
2:H:2475:LEU:H	2:H:2475:LEU:HD23	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1252:HIS:CE1	2:K:1255:TYR:HD2	2.34	0.46
3:C:65:ASP:OD2	3:C:67:PRO:HD2	2.17	0.45
2:E:215:THR:OG1	2:E:271:GLY:O	2.34	0.45
2:E:1743:ARG:NH1	2:E:1964:GLU:OE2	2.44	0.45
2:K:215:THR:OG1	2:K:271:GLY:O	2.34	0.45
2:K:4177:GLU:CB	2:K:4981:HIS:HE1	2.30	0.45
2:B:3804:ASN:HB2	2:B:3807:VAL:HG12	1.98	0.45
2:K:668:VAL:HG11	2:K:682:LEU:HD21	1.99	0.45
2:K:2475:LEU:H	2:K:2475:LEU:HD23	1.81	0.45
2:B:668:VAL:HG11	2:B:682:LEU:HD21	1.99	0.45
2:B:892:THR:N	2:B:902:ARG:O	2.48	0.45
2:B:1130:GLN:HG3	2:B:1138:LEU:HA	1.98	0.45
2:B:2381:ILE:HD13	2:B:2470:ILE:HG13	1.99	0.45
2:E:2381:ILE:HD13	2:E:2470:ILE:HG13	1.99	0.45
2:H:2239:TYR:OH	3:I:68:GLU:OE2	2.33	0.45
2:K:2461:LEU:HD12	2:K:2462:VAL:HG23	1.97	0.45
2:B:1573:MET:HE1	2:B:1584:ARG:HD3	1.99	0.45
2:E:1443:GLN:HA	2:E:1557:THR:HG21	1.97	0.45
1:G:74:LEU:HD13	1:G:101:VAL:HB	1.97	0.45
2:H:892:THR:N	2:H:902:ARG:O	2.48	0.45
2:K:1443:GLN:HA	2:K:1557:THR:HG21	1.97	0.45
2:E:499:THR:HG22	2:E:500:ALA:H	1.81	0.45
2:E:2378:LEU:HD12	2:E:2381:ILE:HD11	1.98	0.45
2:H:1130:GLN:HG3	2:H:1138:LEU:HA	1.98	0.45
2:K:1641:ILE:HG22	2:K:1643:GLU:HG2	1.98	0.45
1:A:74:LEU:HD13	1:A:101:VAL:HB	1.97	0.45
3:F:65:ASP:OD2	3:F:67:PRO:HD2	2.17	0.45
2:H:2128:GLN:HA	2:H:2128:GLN:HE21	1.80	0.45
3:I:65:ASP:OD2	3:I:67:PRO:HD2	2.17	0.45
2:K:1805:LEU:HD13	2:K:1854:ILE:HD12	1.99	0.45
2:H:215:THR:OG1	2:H:271:GLY:O	2.34	0.45
2:H:3622:LYS:C	2:H:3624:ARG:H	2.25	0.45
2:K:2128:GLN:HE21	2:K:2128:GLN:HA	1.80	0.45
2:K:2239:TYR:OH	3:L:68:GLU:OE2	2.33	0.45
2:B:1805:LEU:HD13	2:B:1854:ILE:HD12	1.99	0.45
2:H:668:VAL:HG11	2:H:682:LEU:HD21	1.99	0.45
2:B:2284:ASN:ND2	2:B:2287:LEU:HD13	2.32	0.45
2:E:1805:LEU:HD13	2:E:1854:ILE:HD12	1.99	0.45
2:H:167:ASP:OD1	2:H:167:ASP:N	2.50	0.45
2:H:257:ARG:HA	2:H:286:THR:HG21	1.99	0.45
2:H:2378:LEU:HD12	2:H:2381:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:167:ASP:N	2:K:167:ASP:OD1	2.50	0.45
2:K:257:ARG:HA	2:K:286:THR:HG21	1.99	0.45
3:L:65:ASP:OD2	3:L:67:PRO:HD2	2.17	0.45
2:B:2475:LEU:HD23	2:B:2475:LEU:H	1.81	0.45
2:E:668:VAL:HG11	2:E:682:LEU:HD21	1.99	0.45
2:E:1573:MET:HE1	2:E:1584:ARG:HD3	1.99	0.45
2:H:2284:ASN:ND2	2:H:2287:LEU:HD13	2.32	0.45
2:H:3954:LYS:HA	2:H:4014:LEU:HD13	1.99	0.45
2:K:3804:ASN:HB2	2:K:3807:VAL:HG12	1.98	0.45
2:B:2378:LEU:HD12	2:B:2381:ILE:HD11	1.98	0.44
2:B:4553:LEU:HD11	2:B:4654:LEU:HD23	1.98	0.44
2:H:499:THR:HG22	2:H:500:ALA:H	1.81	0.44
2:H:4234:GLU:OE2	2:H:5012:TYR:OH	2.30	0.44
2:B:1252:HIS:CE1	2:B:1255:TYR:HD2	2.34	0.44
2:E:1252:HIS:CE1	2:E:1255:TYR:HD2	2.34	0.44
2:H:1805:LEU:HD13	2:H:1854:ILE:HD12	1.99	0.44
2:H:4553:LEU:HD11	2:H:4654:LEU:HD23	1.98	0.44
2:K:1639:LEU:HD21	2:K:1650:ILE:HD13	1.99	0.44
2:K:2381:ILE:HD13	2:K:2470:ILE:HG13	1.99	0.44
2:K:3622:LYS:C	2:K:3624:ARG:H	2.25	0.44
2:H:746:CYS:HA	2:H:757:PHE:HA	1.97	0.44
2:K:1573:MET:HE1	2:K:1584:ARG:HD3	1.99	0.44
2:B:499:THR:HG22	2:B:500:ALA:H	1.81	0.44
2:H:1252:HIS:CE1	2:H:1255:TYR:HD2	2.34	0.44
2:H:2381:ILE:HD13	2:H:2470:ILE:HG13	1.99	0.44
2:K:4553:LEU:HD11	2:K:4654:LEU:HD23	1.98	0.44
2:B:3622:LYS:C	2:B:3624:ARG:H	2.25	0.44
2:E:167:ASP:OD1	2:E:167:ASP:N	2.50	0.44
2:E:2284:ASN:ND2	2:E:2287:LEU:HD13	2.32	0.44
2:H:138:GLN:HG2	2:H:140:ASP:H	1.83	0.44
2:H:1287:LEU:HD13	2:H:1289:LEU:HG	1.99	0.44
2:K:138:GLN:HG2	2:K:140:ASP:H	1.83	0.44
2:K:355:LEU:HB3	2:K:378:LEU:HB3	2.00	0.44
2:K:2284:ASN:ND2	2:K:2287:LEU:HD13	2.32	0.44
2:K:2378:LEU:HD12	2:K:2381:ILE:HD11	1.98	0.44
2:B:355:LEU:HB3	2:B:378:LEU:HB3	2.00	0.44
2:B:1287:LEU:HD13	2:B:1289:LEU:HG	1.99	0.44
2:E:3954:LYS:HA	2:E:4014:LEU:HD13	1.99	0.44
2:H:2172:GLY:H	2:H:2175:GLU:HB2	1.83	0.44
2:B:3954:LYS:HA	2:B:4014:LEU:HD13	1.99	0.44
2:E:214:VAL:HG22	2:E:341:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:21:ASP:HB2	3:I:28:ILE:HD11	2.00	0.44
2:K:892:THR:N	2:K:902:ARG:O	2.48	0.44
2:K:2172:GLY:H	2:K:2175:GLU:HB2	1.83	0.44
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.00	0.44
2:B:308:HIS:H	2:B:312:THR:HG21	1.83	0.44
2:E:2239:TYR:OH	3:F:68:GLU:OE2	2.33	0.44
2:E:2272:THR:HG23	2:E:2275:ASP:H	1.83	0.44
2:H:214:VAL:HG22	2:H:341:TYR:CZ	2.53	0.44
2:H:1573:MET:HE1	2:H:1584:ARG:HD3	1.99	0.44
2:H:1639:LEU:HD21	2:H:1650:ILE:HD13	1.99	0.44
2:K:1227:ALA:HB1	2:K:1230:MET:HB2	2.00	0.44
2:B:682:LEU:HD13	2:B:787:VAL:HG11	1.99	0.43
2:B:2172:GLY:H	2:B:2175:GLU:HB2	1.83	0.43
2:B:2457:ILE:HG23	2:E:131:LEU:HD23	2.00	0.43
2:E:3622:LYS:C	2:E:3624:ARG:H	2.25	0.43
2:H:308:HIS:H	2:H:312:THR:HG21	1.83	0.43
2:H:1227:ALA:HB1	2:H:1230:MET:HB2	2.00	0.43
2:K:2272:THR:HG23	2:K:2275:ASP:H	1.83	0.43
2:B:138:GLN:HG2	2:B:140:ASP:H	1.83	0.43
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.00	0.43
2:E:682:LEU:HD13	2:E:787:VAL:HG11	1.99	0.43
2:K:499:THR:HG22	2:K:500:ALA:H	1.81	0.43
2:K:1287:LEU:HD13	2:K:1289:LEU:HG	1.99	0.43
2:B:257:ARG:HA	2:B:286:THR:HG21	1.99	0.43
2:E:257:ARG:HA	2:E:286:THR:HG21	1.99	0.43
2:E:1227:ALA:HB1	2:E:1230:MET:HB2	2.00	0.43
2:E:1287:LEU:HD13	2:E:1289:LEU:HG	1.99	0.43
3:F:21:ASP:HB2	3:F:28:ILE:HD11	2.00	0.43
2:H:35:LEU:HD13	2:H:49:LEU:HD13	2.00	0.43
2:E:2172:GLY:H	2:E:2175:GLU:HB2	1.83	0.43
2:H:355:LEU:HB3	2:H:378:LEU:HB3	2.00	0.43
2:H:3804:ASN:HB2	2:H:3807:VAL:HG12	1.98	0.43
2:K:214:VAL:HG22	2:K:341:TYR:CZ	2.53	0.43
2:K:308:HIS:H	2:K:312:THR:HG21	1.83	0.43
2:H:615:ARG:NH2	2:H:1677:GLY:O	2.52	0.43
2:H:1448:VAL:HG22	2:H:1554:VAL:HG23	2.01	0.43
2:H:2457:ILE:HG23	2:K:131:LEU:HD23	2.00	0.43
2:K:3954:LYS:HA	2:K:4014:LEU:HD13	1.99	0.43
2:B:615:ARG:NH2	2:B:1677:GLY:O	2.52	0.43
2:B:1639:LEU:HD21	2:B:1650:ILE:HD13	1.99	0.43
2:E:1639:LEU:HD21	2:E:1650:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2186:ILE:HD13	2:E:2204:MET:HE2	2.01	0.43
2:K:35:LEU:HD13	2:K:49:LEU:HD13	2.00	0.43
2:B:1227:ALA:HB1	2:B:1230:MET:HB2	2.00	0.43
2:B:2428:ALA:O	2:B:2502:SER:OG	2.36	0.43
2:B:214:VAL:HG22	2:B:341:TYR:CZ	2.53	0.43
2:B:804:PRO:HA	2:B:805:PRO:HD3	1.96	0.43
2:B:2272:THR:HG23	2:B:2275:ASP:H	1.83	0.43
2:E:138:GLN:HG2	2:E:140:ASP:H	1.83	0.43
2:E:615:ARG:NH2	2:E:1677:GLY:O	2.52	0.43
2:E:1448:VAL:HG22	2:E:1554:VAL:HG23	2.01	0.43
2:E:2457:ILE:HG23	2:H:131:LEU:HD23	2.00	0.43
2:H:2272:THR:HG23	2:H:2275:ASP:H	1.83	0.43
2:K:21:VAL:HB	2:K:205:ILE:HD11	2.01	0.43
2:H:1848:THR:HG22	2:H:1852:MET:HE1	2.00	0.43
2:B:1867:ILE:HG22	2:B:1927:LEU:HD23	2.01	0.43
2:E:355:LEU:HB3	2:E:378:LEU:HB3	2.00	0.43
2:B:4016:LYS:HA	2:B:4134:ILE:HD13	2.01	0.42
2:H:21:VAL:HB	2:H:205:ILE:HD11	2.01	0.42
2:K:615:ARG:NH2	2:K:1677:GLY:O	2.52	0.42
2:K:682:LEU:HD13	2:K:787:VAL:HG11	1.99	0.42
2:E:21:VAL:HB	2:E:205:ILE:HD11	2.01	0.42
2:H:682:LEU:HD13	2:H:787:VAL:HG11	1.99	0.42
2:K:1848:THR:HG22	2:K:1852:MET:HE1	2.00	0.42
2:K:4016:LYS:HA	2:K:4134:ILE:HD13	2.01	0.42
3:C:21:ASP:HB2	3:C:28:ILE:HD11	2.00	0.42
2:E:308:HIS:H	2:E:312:THR:HG21	1.83	0.42
2:E:1867:ILE:HG22	2:E:1927:LEU:HD23	2.01	0.42
2:E:4016:LYS:HA	2:E:4134:ILE:HD13	2.01	0.42
3:F:5:LEU:HD21	3:F:74:ALA:HA	2.01	0.42
2:H:942:ALA:N	2:H:1050:GLY:O	2.48	0.42
2:H:1867:ILE:HG22	2:H:1927:LEU:HD23	2.01	0.42
2:H:3625:ARG:HH11	3:I:146:MET:HA	1.85	0.42
2:K:1247:ALA:HA	2:K:1598:GLN:HA	2.01	0.42
2:K:1745:ILE:HD12	2:K:1745:ILE:HA	1.96	0.42
3:L:21:ASP:HB2	3:L:28:ILE:HD11	2.00	0.42
2:B:1247:ALA:HA	2:B:1598:GLN:HA	2.01	0.42
2:B:3625:ARG:HH11	3:C:146:MET:HA	1.85	0.42
2:H:2186:ILE:HD13	2:H:2204:MET:HE2	2.01	0.42
3:I:5:LEU:HD21	3:I:74:ALA:HA	2.01	0.42
3:L:33:LEU:HD22	3:L:64:ILE:HG12	2.02	0.42
2:B:131:LEU:HD23	2:K:2457:ILE:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1448:VAL:HG22	2:B:1554:VAL:HG23	2.01	0.42
3:I:33:LEU:HD22	3:I:64:ILE:HG12	2.02	0.42
2:K:1448:VAL:HG22	2:K:1554:VAL:HG23	2.01	0.42
2:K:4634:THR:HG22	2:K:4636:TYR:H	1.85	0.42
2:B:4129:GLU:HB3	2:B:4130:PRO:HD3	2.02	0.42
2:H:49:LEU:HD11	2:H:191:VAL:HG13	2.02	0.42
2:B:21:VAL:HB	2:B:205:ILE:HD11	2.01	0.42
2:B:942:ALA:N	2:B:1050:GLY:O	2.48	0.42
2:B:4634:THR:HG22	2:B:4636:TYR:H	1.85	0.42
2:H:3930:TRP:CD1	2:K:80:GLU:HG3	2.55	0.42
3:C:5:LEU:HD21	3:C:74:ALA:HA	2.01	0.42
2:K:2186:ILE:HD13	2:K:2204:MET:HE2	2.01	0.42
2:K:3625:ARG:HH11	3:L:146:MET:HA	1.85	0.42
2:E:49:LEU:HD11	2:E:191:VAL:HG13	2.02	0.42
1:J:35:LYS:HD2	2:K:636:ASN:HD21	1.85	0.42
2:K:1867:ILE:HG22	2:K:1927:LEU:HD23	2.01	0.42
2:B:299:LEU:HD23	2:B:299:LEU:H	1.85	0.42
2:B:1465:ASP:OD1	2:B:1465:ASP:N	2.53	0.42
2:B:2186:ILE:HD13	2:B:2204:MET:HE2	2.01	0.42
3:C:33:LEU:HD22	3:C:64:ILE:HG12	2.02	0.42
2:E:1247:ALA:HA	2:E:1598:GLN:HA	2.01	0.42
2:E:1526:LEU:HD23	2:E:1526:LEU:H	1.85	0.42
2:E:4129:GLU:HB3	2:E:4130:PRO:HD3	2.02	0.42
2:H:1686:CYS:HB3	2:H:1783:PHE:HZ	1.85	0.42
2:H:4016:LYS:HA	2:H:4134:ILE:HD13	2.01	0.42
2:K:1686:CYS:HB3	2:K:1783:PHE:HZ	1.85	0.42
3:L:5:LEU:HD21	3:L:74:ALA:HA	2.01	0.42
2:B:80:GLU:HG3	2:K:3930:TRP:CD1	2.55	0.41
2:E:181:HIS:ND1	2:E:182:LEU:O	2.53	0.41
2:E:1848:THR:HG22	2:E:1852:MET:HE1	2.00	0.41
1:G:35:LYS:HD2	2:H:636:ASN:HD21	1.85	0.41
2:K:4031:VAL:HG13	2:K:4148:HIS:HA	2.02	0.41
2:B:1848:THR:HG22	2:B:1852:MET:HE1	2.00	0.41
2:B:3930:TRP:CD1	2:E:80:GLU:HG3	2.55	0.41
1:D:35:LYS:HD2	2:E:636:ASN:HD21	1.85	0.41
2:E:1686:CYS:HB3	2:E:1783:PHE:HZ	1.85	0.41
2:E:3625:ARG:HH11	3:F:146:MET:HA	1.85	0.41
2:H:4031:VAL:HG13	2:H:4148:HIS:HA	2.02	0.41
2:E:35:LEU:HD11	2:E:189:LEU:HD13	2.02	0.41
2:E:2243:ILE:HA	3:F:2:ALA:HB3	2.03	0.41
2:E:3936:ASP:OD1	2:E:3936:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:33:LEU:HD22	3:F:64:ILE:HG12	2.02	0.41
2:H:4634:THR:HG22	2:H:4636:TYR:H	1.85	0.41
2:K:49:LEU:HD11	2:K:191:VAL:HG13	2.02	0.41
2:K:1526:LEU:HD23	2:K:1526:LEU:H	1.85	0.41
2:B:1686:CYS:HB3	2:B:1783:PHE:HZ	1.85	0.41
2:B:2243:ILE:HA	3:C:2:ALA:HB3	2.03	0.41
2:B:2455:ARG:HE	2:B:2459:ARG:HH22	1.68	0.41
2:E:2455:ARG:HE	2:E:2459:ARG:HH22	1.68	0.41
2:H:684:VAL:HG22	2:H:781:VAL:HG23	2.02	0.41
2:H:1745:ILE:HD12	2:H:1745:ILE:HA	1.96	0.41
2:K:181:HIS:ND1	2:K:182:LEU:O	2.53	0.41
2:K:1465:ASP:OD1	2:K:1465:ASP:N	2.53	0.41
2:B:1857:ASP:OD1	2:B:1857:ASP:N	2.53	0.41
2:E:684:VAL:HG22	2:E:781:VAL:HG23	2.02	0.41
2:E:3930:TRP:CD1	2:H:80:GLU:HG3	2.55	0.41
2:H:1247:ALA:HA	2:H:1598:GLN:HA	2.01	0.41
2:H:1465:ASP:OD1	2:H:1465:ASP:N	2.53	0.41
2:H:1526:LEU:HD23	2:H:1526:LEU:H	1.85	0.41
2:K:4129:GLU:HB3	2:K:4130:PRO:HD3	2.02	0.41
2:B:4031:VAL:HG13	2:B:4148:HIS:HA	2.02	0.41
2:B:4700:ASP:HA	2:B:4776:TRP:HE1	1.86	0.41
2:E:4700:ASP:HA	2:E:4776:TRP:HE1	1.86	0.41
2:B:1526:LEU:H	2:B:1526:LEU:HD23	1.85	0.41
2:E:1465:ASP:N	2:E:1465:ASP:OD1	2.53	0.41
2:K:1600:LEU:HD23	2:K:1600:LEU:HA	1.96	0.41
2:K:2455:ARG:HE	2:K:2459:ARG:HH22	1.68	0.41
2:B:49:LEU:HD11	2:B:191:VAL:HG13	2.02	0.41
2:B:167:ASP:N	2:B:167:ASP:OD1	2.50	0.41
2:B:687:ALA:HA	2:B:713:SER:HA	2.03	0.41
2:E:143:GLY:HA2	2:E:147:TRP:HE1	1.86	0.41
2:H:143:GLY:HA2	2:H:147:TRP:HE1	1.86	0.41
2:H:687:ALA:HA	2:H:713:SER:HA	2.03	0.41
2:H:4129:GLU:HB3	2:H:4130:PRO:HD3	2.02	0.41
2:K:299:LEU:HD23	2:K:299:LEU:H	1.85	0.41
2:B:3936:ASP:OD1	2:B:3936:ASP:N	2.53	0.41
2:H:1857:ASP:OD1	2:H:1857:ASP:N	2.53	0.41
2:K:2258:LEU:HD13	2:K:2276:VAL:HG13	2.03	0.41
3:L:17:PHE:CE1	3:L:28:ILE:HD12	2.57	0.41
1:A:35:LYS:HD2	2:B:636:ASN:HD21	1.85	0.40
2:B:35:LEU:HD11	2:B:189:LEU:HD13	2.02	0.40
2:B:1101:ARG:HB3	2:B:1123:VAL:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:663:TYR:HD1	2:E:747:CYS:HB3	1.86	0.40
2:H:1499:ASP:OD1	2:H:1499:ASP:N	2.55	0.40
2:K:143:GLY:HA2	2:K:147:TRP:HE1	1.86	0.40
2:K:638:ILE:HD12	2:K:1638:ALA:HB3	2.03	0.40
2:K:684:VAL:HG22	2:K:781:VAL:HG23	2.02	0.40
2:K:1101:ARG:HB3	2:K:1123:VAL:HG21	2.04	0.40
2:K:1857:ASP:OD1	2:K:1857:ASP:N	2.53	0.40
2:K:4700:ASP:HA	2:K:4776:TRP:HE1	1.86	0.40
2:B:638:ILE:HD12	2:B:1638:ALA:HB3	2.03	0.40
2:B:663:TYR:HD1	2:B:747:CYS:HB3	1.86	0.40
2:E:687:ALA:HA	2:E:713:SER:HA	2.03	0.40
2:E:4634:THR:HG22	2:E:4636:TYR:H	1.85	0.40
2:H:288:GLY:HA3	2:H:405:TYR:CZ	2.56	0.40
2:H:299:LEU:HD23	2:H:299:LEU:H	1.85	0.40
2:H:609:CYS:HB3	2:H:612:VAL:O	2.22	0.40
2:K:35:LEU:HD11	2:K:189:LEU:HD13	2.02	0.40
2:B:143:GLY:HA2	2:B:147:TRP:HE1	1.86	0.40
2:B:684:VAL:HG22	2:B:781:VAL:HG23	2.02	0.40
2:E:3905:THR:HG23	2:E:3906:THR:HG23	2.04	0.40
2:H:181:HIS:ND1	2:H:182:LEU:O	2.53	0.40
2:H:1777:HIS:HB3	2:H:1799:LEU:HD13	2.04	0.40
2:H:1834:SER:HB2	2:H:1837:PHE:HD1	1.87	0.40
2:H:2455:ARG:HE	2:H:2459:ARG:HH22	1.68	0.40
2:K:288:GLY:HA3	2:K:405:TYR:CZ	2.56	0.40
2:K:2284:ASN:HD21	2:K:2287:LEU:HD13	1.87	0.40
2:B:2258:LEU:HD13	2:B:2276:VAL:HG13	2.03	0.40
2:H:2243:ILE:HA	3:I:2:ALA:HB3	2.03	0.40
2:K:687:ALA:HA	2:K:713:SER:HA	2.03	0.40
2:K:3936:ASP:N	2:K:3936:ASP:OD1	2.53	0.40
2:B:288:GLY:HA3	2:B:405:TYR:CZ	2.56	0.40
2:B:336:PRO:HA	2:B:337:PRO:HD3	1.89	0.40
2:B:1557:THR:C	2:B:1559:GLN:H	2.30	0.40
2:B:4039:MET:HE2	2:B:4141:LEU:HD11	2.04	0.40
3:C:17:PHE:CE1	3:C:28:ILE:HD12	2.57	0.40
2:E:609:CYS:HB3	2:E:612:VAL:O	2.22	0.40
2:E:2258:LEU:HD13	2:E:2276:VAL:HG13	2.03	0.40
2:E:4031:VAL:HG13	2:E:4148:HIS:HA	2.02	0.40
3:F:17:PHE:CE1	3:F:28:ILE:HD12	2.57	0.40
2:H:4700:ASP:HA	2:H:4776:TRP:HE1	1.86	0.40
2:K:2243:ILE:HA	3:L:2:ALA:HB3	2.03	0.40
2:K:4039:MET:HE2	2:K:4141:LEU:HD11	2.04	0.40

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	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
1	D	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
1	G	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
1	J	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
2	B	3396/3816 (89%)	3335 (98%)	61 (2%)	0	100	100
2	E	3396/3816 (89%)	3335 (98%)	61 (2%)	0	100	100
2	H	3396/3816 (89%)	3335 (98%)	61 (2%)	0	100	100
2	K	3396/3816 (89%)	3335 (98%)	61 (2%)	0	100	100
3	C	127/148 (86%)	124 (98%)	3 (2%)	0	100	100
3	F	127/148 (86%)	124 (98%)	3 (2%)	0	100	100
3	I	127/148 (86%)	124 (98%)	3 (2%)	0	100	100
3	L	127/148 (86%)	124 (98%)	3 (2%)	0	100	100
All	All	14508/16284 (89%)	14228 (98%)	280 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	66/88 (75%)	66 (100%)	0	100	100
1	D	66/88 (75%)	66 (100%)	0	100	100
1	G	66/88 (75%)	66 (100%)	0	100	100
1	J	66/88 (75%)	66 (100%)	0	100	100
2	B	2222/3025 (74%)	2222 (100%)	0	100	100
2	E	2222/3025 (74%)	2222 (100%)	0	100	100
2	H	2222/3025 (74%)	2222 (100%)	0	100	100
2	K	2222/3025 (74%)	2222 (100%)	0	100	100
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	9268/12956 (72%)	9268 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
2	B	56	GLN
2	B	203	ASN
2	B	461	HIS
2	B	617	ASN
2	B	774	ASN
2	B	838	HIS
2	B	919	ASN
2	B	991	ASN
2	B	1144	GLN
2	B	1198	GLN
2	B	1244	GLN
2	B	1298	HIS
2	B	1558	HIS
2	B	1629	GLN
2	B	2128	GLN
2	B	2214	ASN
2	B	2552	ASN
2	B	2585	HIS

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Mol	Chain	Res	Type
2	B	3700	HIS
2	B	3955	GLN
2	B	4032	ASN
2	B	4648	HIS
2	B	4976	HIS
2	B	4982	ASN
1	D	70	GLN
2	E	56	GLN
2	E	203	ASN
2	E	461	HIS
2	E	617	ASN
2	E	774	ASN
2	E	838	HIS
2	E	991	ASN
2	E	1144	GLN
2	E	1198	GLN
2	E	1244	GLN
2	E	1558	HIS
2	E	1629	GLN
2	E	2030	GLN
2	E	2128	GLN
2	E	2214	ASN
2	E	2552	ASN
2	E	3700	HIS
2	E	3955	GLN
2	E	3972	GLN
2	E	4032	ASN
2	E	4648	HIS
2	E	4981	HIS
2	E	4982	ASN
1	G	70	GLN
2	H	203	ASN
2	H	461	HIS
2	H	465	GLN
2	H	617	ASN
2	H	774	ASN
2	H	838	HIS
2	H	919	ASN
2	H	991	ASN
2	H	1144	GLN
2	H	1198	GLN
2	H	1244	GLN

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Mol	Chain	Res	Type
2	H	1558	HIS
2	H	1629	GLN
2	H	2030	GLN
2	H	2128	GLN
2	H	2214	ASN
2	H	2352	ASN
2	H	2552	ASN
2	H	3451	ASN
2	H	3700	HIS
2	H	3955	GLN
2	H	3972	GLN
2	H	4032	ASN
2	H	4648	HIS
2	H	4981	HIS
2	H	4982	ASN
1	J	70	GLN
2	K	56	GLN
2	K	203	ASN
2	K	461	HIS
2	K	465	GLN
2	K	581	ASN
2	K	617	ASN
2	K	774	ASN
2	K	838	HIS
2	K	919	ASN
2	K	991	ASN
2	K	1198	GLN
2	K	1244	GLN
2	K	1298	HIS
2	K	1558	HIS
2	K	1629	GLN
2	K	2030	GLN
2	K	2128	GLN
2	K	2552	ASN
2	K	3451	ASN
2	K	3700	HIS
2	K	3955	GLN
2	K	4032	ASN
2	K	4196	ASN
2	K	4648	HIS
2	K	4981	HIS
2	K	4982	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	56
2	E	56
2	H	56
2	K	56

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	51.24
1	E	4331:UNK	C	4543:GLU	N	51.24
1	H	4331:UNK	C	4543:GLU	N	51.24
1	K	4331:UNK	C	4543:GLU	N	51.24
1	B	1054:GLU	C	1071:ARG	N	36.98
1	E	1054:GLU	C	1071:ARG	N	36.98
1	H	1054:GLU	C	1071:ARG	N	36.98
1	K	1054:GLU	C	1071:ARG	N	36.98
1	B	854:CYS	C	866:HIS	N	29.09
1	E	854:CYS	C	866:HIS	N	29.09
1	H	854:CYS	C	866:HIS	N	29.09
1	K	854:CYS	C	866:HIS	N	29.09
1	B	3606:UNK	C	3617:HIS	N	28.52
1	E	3606:UNK	C	3617:HIS	N	28.52
1	H	3606:UNK	C	3617:HIS	N	28.52
1	K	3606:UNK	C	3617:HIS	N	28.52
1	B	4245:GLN	C	4315:UNK	N	27.59
1	E	4245:GLN	C	4315:UNK	N	27.59
1	H	4245:GLN	C	4315:UNK	N	27.59
1	K	4245:GLN	C	4315:UNK	N	27.59
1	B	2700:UNK	C	2736:ASP	N	25.87
1	E	2700:UNK	C	2736:ASP	N	25.87
1	H	2700:UNK	C	2736:ASP	N	25.87
1	K	2700:UNK	C	2736:ASP	N	25.87
1	B	2830:GLU	C	2855:TYR	N	23.98
1	E	2830:GLU	C	2855:TYR	N	23.98
1	H	2830:GLU	C	2855:TYR	N	23.98
1	K	2830:GLU	C	2855:TYR	N	23.98
1	B	84:ASN	C	97:GLY	N	23.34
1	E	84:ASN	C	97:GLY	N	23.34
1	H	84:ASN	C	97:GLY	N	23.34
1	K	84:ASN	C	97:GLY	N	23.34
1	B	2939:ARG	C	2956:UNK	N	23.02
1	E	2939:ARG	C	2956:UNK	N	23.02
1	H	2939:ARG	C	2956:UNK	N	23.02
1	K	2939:ARG	C	2956:UNK	N	23.02
1	B	3555:UNK	C	3565:UNK	N	22.27
1	E	3555:UNK	C	3565:UNK	N	22.27
1	H	3555:UNK	C	3565:UNK	N	22.27
1	K	3555:UNK	C	3565:UNK	N	22.27
1	B	1299:GLN	C	1428:LEU	N	21.92
1	E	1299:GLN	C	1428:LEU	N	21.92
1	H	1299:GLN	C	1428:LEU	N	21.92

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	1299:GLN	C	1428:LEU	N	21.92
1	B	3574:UNK	C	3586:UNK	N	21.88
1	E	3574:UNK	C	3586:UNK	N	21.88
1	H	3574:UNK	C	3586:UNK	N	21.88
1	K	3574:UNK	C	3586:UNK	N	21.88
1	B	4737:GLU	C	4769:ILE	N	20.65
1	E	4737:GLU	C	4769:ILE	N	20.65
1	H	4737:GLU	C	4769:ILE	N	20.65
1	K	4737:GLU	C	4769:ILE	N	20.65
1	B	2385:ILE	C	2418:HIS	N	18.54
1	E	2385:ILE	C	2418:HIS	N	18.54
1	H	2385:ILE	C	2418:HIS	N	18.54
1	K	2385:ILE	C	2418:HIS	N	18.54
1	B	3358:UNK	C	3365:UNK	N	17.90
1	E	3358:UNK	C	3365:UNK	N	17.90
1	H	3358:UNK	C	3365:UNK	N	17.90
1	K	3358:UNK	C	3365:UNK	N	17.90
1	B	2046:GLN	C	2092:LEU	N	17.87
1	E	2046:GLN	C	2092:LEU	N	17.87
1	H	2046:GLN	C	2092:LEU	N	17.87
1	K	2046:GLN	C	2092:LEU	N	17.87
1	B	2653:UNK	C	2664:UNK	N	17.50
1	E	2653:UNK	C	2664:UNK	N	17.50
1	H	2653:UNK	C	2664:UNK	N	17.50
1	K	2653:UNK	C	2664:UNK	N	17.50
1	B	3193:UNK	C	3202:UNK	N	17.22
1	E	3193:UNK	C	3202:UNK	N	17.22
1	H	3193:UNK	C	3202:UNK	N	17.22
1	K	3193:UNK	C	3202:UNK	N	17.22
1	B	3733:GLU	C	3747:SER	N	15.80
1	E	3733:GLU	C	3747:SER	N	15.80
1	H	3733:GLU	C	3747:SER	N	15.80
1	K	3733:GLU	C	3747:SER	N	15.80
1	B	3385:UNK	C	3399:PHE	N	15.58
1	E	3385:UNK	C	3399:PHE	N	15.58
1	H	3385:UNK	C	3399:PHE	N	15.58
1	K	3385:UNK	C	3399:PHE	N	15.58
1	B	3062:UNK	C	3146:UNK	N	15.38
1	E	3062:UNK	C	3146:UNK	N	15.38
1	H	3062:UNK	C	3146:UNK	N	15.38
1	K	3062:UNK	C	3146:UNK	N	15.38
1	B	3238:UNK	C	3278:UNK	N	14.98

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3238:UNK	C	3278:UNK	N	14.98
1	H	3238:UNK	C	3278:UNK	N	14.98
1	K	3238:UNK	C	3278:UNK	N	14.98
1	B	2978:UNK	C	2999:UNK	N	14.76
1	E	2978:UNK	C	2999:UNK	N	14.76
1	H	2978:UNK	C	2999:UNK	N	14.76
1	K	2978:UNK	C	2999:UNK	N	14.76
1	B	3461:VAL	C	3509:UNK	N	13.70
1	E	3461:VAL	C	3509:UNK	N	13.70
1	H	3461:VAL	C	3509:UNK	N	13.70
1	K	3461:VAL	C	3509:UNK	N	13.70
1	B	3018:UNK	C	3032:UNK	N	12.78
1	E	3018:UNK	C	3032:UNK	N	12.78
1	H	3018:UNK	C	3032:UNK	N	12.78
1	K	3018:UNK	C	3032:UNK	N	12.78
1	B	2014:LYS	C	2023:PRO	N	12.65
1	E	2014:LYS	C	2023:PRO	N	12.65
1	H	2014:LYS	C	2023:PRO	N	12.65
1	K	2014:LYS	C	2023:PRO	N	12.65
1	B	2683:UNK	C	2688:UNK	N	12.62
1	E	2683:UNK	C	2688:UNK	N	12.62
1	H	2683:UNK	C	2688:UNK	N	12.62
1	K	2683:UNK	C	2688:UNK	N	12.62
1	B	2571:ALA	C	2579:MET	N	12.58
1	E	2571:ALA	C	2579:MET	N	12.58
1	H	2571:ALA	C	2579:MET	N	12.58
1	K	2571:ALA	C	2579:MET	N	12.58
1	B	3166:UNK	C	3173:UNK	N	12.43
1	E	3166:UNK	C	3173:UNK	N	12.43
1	H	3166:UNK	C	3173:UNK	N	12.43
1	K	3166:UNK	C	3173:UNK	N	12.43
1	B	3308:UNK	C	3320:UNK	N	12.24
1	E	3308:UNK	C	3320:UNK	N	12.24
1	H	3308:UNK	C	3320:UNK	N	12.24
1	K	3308:UNK	C	3320:UNK	N	12.24
1	B	361:ALA	C	372:LEU	N	12.09
1	E	361:ALA	C	372:LEU	N	12.09
1	H	361:ALA	C	372:LEU	N	12.09
1	K	361:ALA	C	372:LEU	N	12.09
1	B	2629:PHE	C	2641:UNK	N	12.03
1	E	2629:PHE	C	2641:UNK	N	12.03
1	H	2629:PHE	C	2641:UNK	N	12.03

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	2629:PHE	C	2641:UNK	N	12.03
1	B	4090:LYS	C	4109:UNK	N	11.95
1	E	4090:LYS	C	4109:UNK	N	11.95
1	H	4090:LYS	C	4109:UNK	N	11.95
1	K	4090:LYS	C	4109:UNK	N	11.95
1	B	1750:PRO	C	1760:ARG	N	11.65
1	E	1750:PRO	C	1760:ARG	N	11.65
1	H	1750:PRO	C	1760:ARG	N	11.65
1	K	1750:PRO	C	1760:ARG	N	11.65
1	B	3544:UNK	C	3548:UNK	N	11.53
1	E	3544:UNK	C	3548:UNK	N	11.53
1	H	3544:UNK	C	3548:UNK	N	11.53
1	K	3544:UNK	C	3548:UNK	N	11.53
1	B	3217:UNK	C	3225:UNK	N	11.39
1	E	3217:UNK	C	3225:UNK	N	11.39
1	H	3217:UNK	C	3225:UNK	N	11.39
1	K	3217:UNK	C	3225:UNK	N	11.39
1	B	1501:VAL	C	1510:SER	N	11.35
1	E	1501:VAL	C	1510:SER	N	11.35
1	H	1501:VAL	C	1510:SER	N	11.35
1	K	1501:VAL	C	1510:SER	N	11.35
1	B	3047:UNK	C	3051:UNK	N	11.02
1	E	3047:UNK	C	3051:UNK	N	11.02
1	H	3047:UNK	C	3051:UNK	N	11.02
1	K	3047:UNK	C	3051:UNK	N	11.02
1	B	1788:PRO	C	1794:GLU	N	10.90
1	E	1788:PRO	C	1794:GLU	N	10.90
1	H	1788:PRO	C	1794:GLU	N	10.90
1	K	1788:PRO	C	1794:GLU	N	10.90
1	B	4114:UNK	C	4122:GLU	N	10.72
1	E	4114:UNK	C	4122:GLU	N	10.72
1	H	4114:UNK	C	4122:GLU	N	10.72
1	K	4114:UNK	C	4122:GLU	N	10.72
1	B	1871:VAL	C	1924:GLU	N	10.67
1	E	1871:VAL	C	1924:GLU	N	10.67
1	H	1871:VAL	C	1924:GLU	N	10.67
1	K	1871:VAL	C	1924:GLU	N	10.67
1	B	3335:UNK	C	3346:UNK	N	10.58
1	E	3335:UNK	C	3346:UNK	N	10.58
1	H	3335:UNK	C	3346:UNK	N	10.58
1	K	3335:UNK	C	3346:UNK	N	10.58
1	B	3288:UNK	C	3292:UNK	N	10.44

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3288:UNK	C	3292:UNK	N	10.44
1	H	3288:UNK	C	3292:UNK	N	10.44
1	K	3288:UNK	C	3292:UNK	N	10.44
1	B	323:LEU	C	328:LYS	N	10.40
1	E	323:LEU	C	328:LYS	N	10.40
1	H	323:LEU	C	328:LYS	N	10.40
1	K	323:LEU	C	328:LYS	N	10.40
1	B	4585:PRO	C	4626:VAL	N	10.08
1	E	4585:PRO	C	4626:VAL	N	10.08
1	H	4585:PRO	C	4626:VAL	N	10.08
1	K	4585:PRO	C	4626:VAL	N	10.08
1	B	2535:ALA	C	2549:LEU	N	9.70
1	E	2535:ALA	C	2549:LEU	N	9.70
1	H	2535:ALA	C	2549:LEU	N	9.70
1	K	2535:ALA	C	2549:LEU	N	9.70
1	B	2478:PRO	C	2491:MET	N	9.63
1	E	2478:PRO	C	2491:MET	N	9.63
1	H	2478:PRO	C	2491:MET	N	9.63
1	K	2478:PRO	C	2491:MET	N	9.63
1	B	3526:UNK	C	3534:UNK	N	9.43
1	E	3526:UNK	C	3534:UNK	N	9.43
1	H	3526:UNK	C	3534:UNK	N	9.43
1	K	3526:UNK	C	3534:UNK	N	9.43
1	B	2263:GLY	C	2267:GLY	N	8.79
1	E	2263:GLY	C	2267:GLY	N	8.79
1	H	2263:GLY	C	2267:GLY	N	8.79
1	K	2263:GLY	C	2267:GLY	N	8.79
1	B	3861:ILE	C	3866:GLY	N	8.58
1	E	3861:ILE	C	3866:GLY	N	8.58
1	H	3861:ILE	C	3866:GLY	N	8.58
1	K	3861:ILE	C	3866:GLY	N	8.58
1	B	2216:LEU	C	2225:ARG	N	7.09
1	E	2216:LEU	C	2225:ARG	N	7.09
1	H	2216:LEU	C	2225:ARG	N	7.09
1	K	2216:LEU	C	2225:ARG	N	7.09
1	B	4219:GLU	C	4225:LYS	N	6.52
1	E	4219:GLU	C	4225:LYS	N	6.52
1	H	4219:GLU	C	4225:LYS	N	6.52
1	K	4219:GLU	C	4225:LYS	N	6.52
1	B	1275:ARG	C	1282:SER	N	6.22
1	E	1275:ARG	C	1282:SER	N	6.22
1	H	1275:ARG	C	1282:SER	N	6.22

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	1275:ARG	C	1282:SER	N	6.22
1	B	4863:LYS	C	4872:MET	N	5.66
1	E	4863:LYS	C	4872:MET	N	5.66
1	H	4863:LYS	C	4872:MET	N	5.66
1	K	4863:LYS	C	4872:MET	N	5.66
1	B	1478:ASP	C	1482:ASN	N	5.62
1	E	1478:ASP	C	1482:ASN	N	5.62
1	H	1478:ASP	C	1482:ASN	N	5.62
1	K	1478:ASP	C	1482:ASN	N	5.62
1	B	2527:PHE	C	2528:LEU	N	3.17
1	E	2527:PHE	C	2528:LEU	N	3.17
1	H	2527:PHE	C	2528:LEU	N	3.17
1	K	2527:PHE	C	2528:LEU	N	3.17

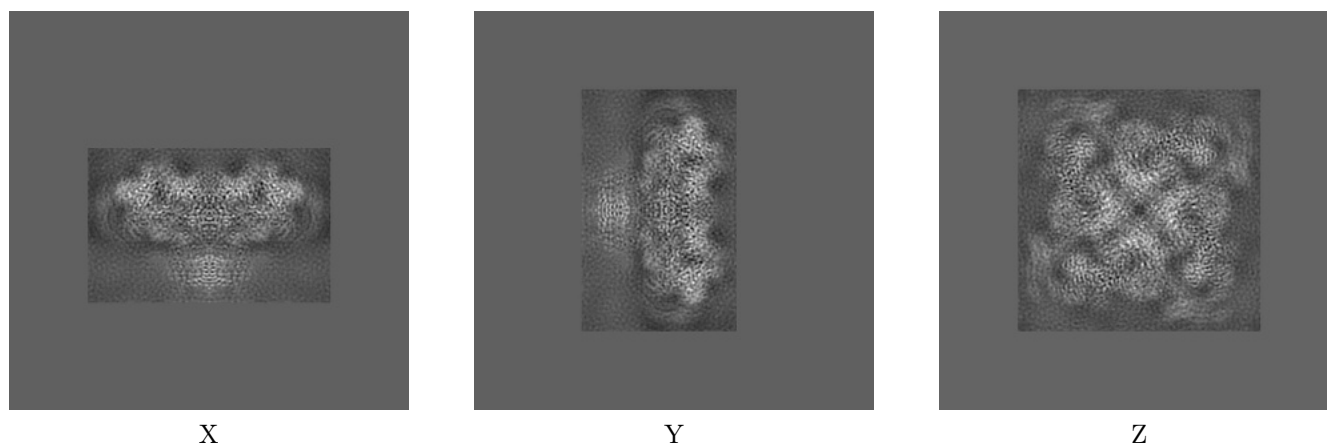
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22016. 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](#)

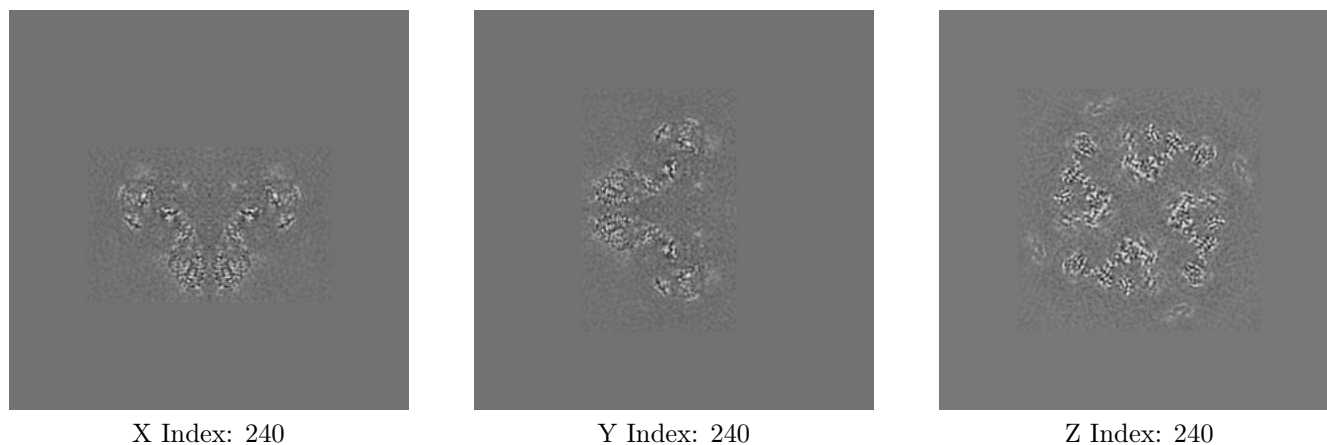
6.1.1 Primary map



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

6.2 Central slices [i](#)

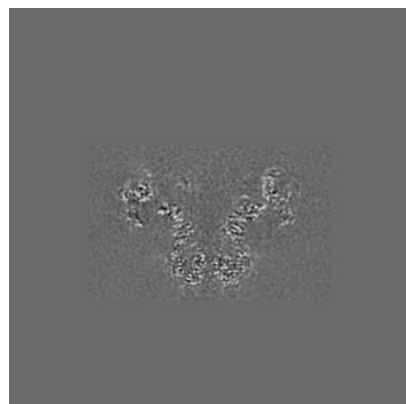
6.2.1 Primary map



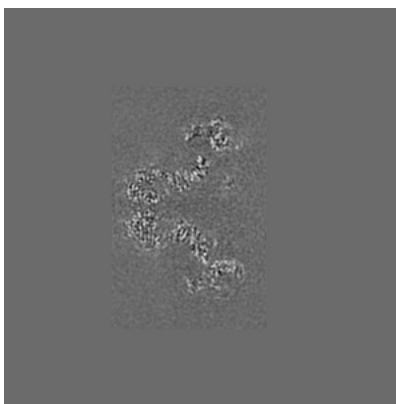
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

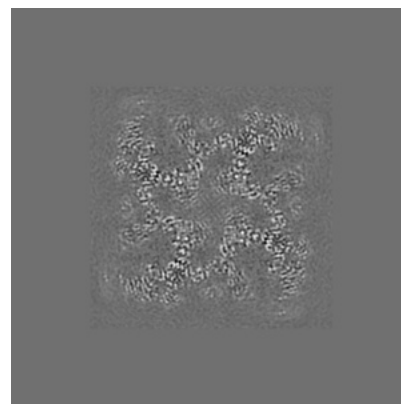
6.3.1 Primary map



X Index: 236



Y Index: 236

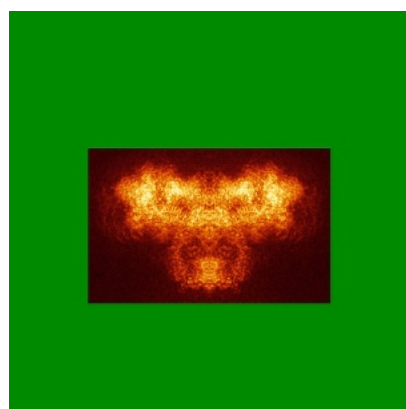


Z Index: 265

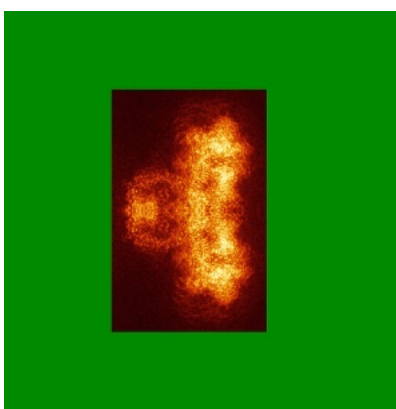
The images above show the largest variance slices of the map in three orthogonal directions.

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

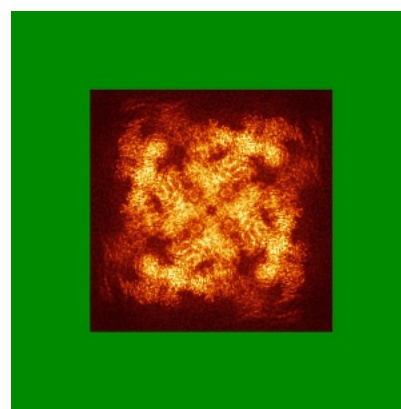
6.4.1 Primary map



X



Y

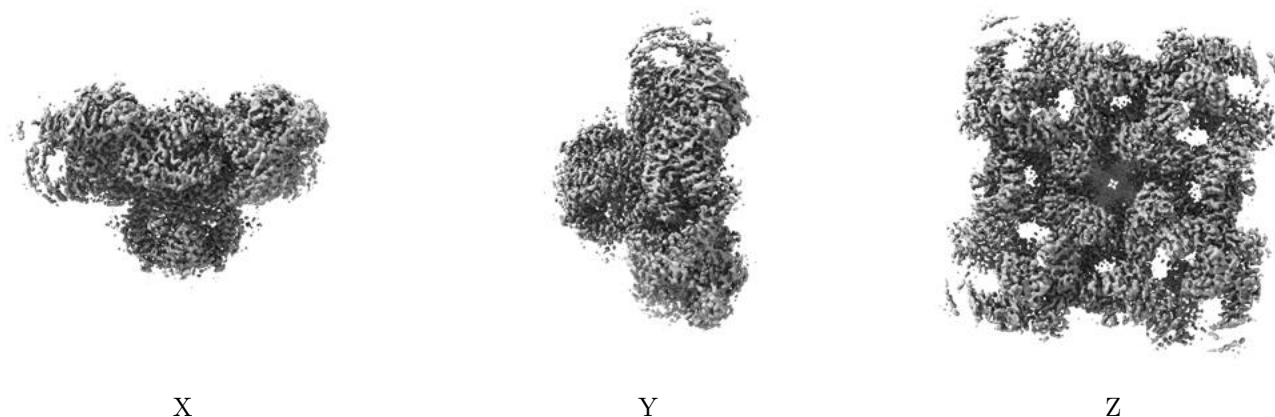


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

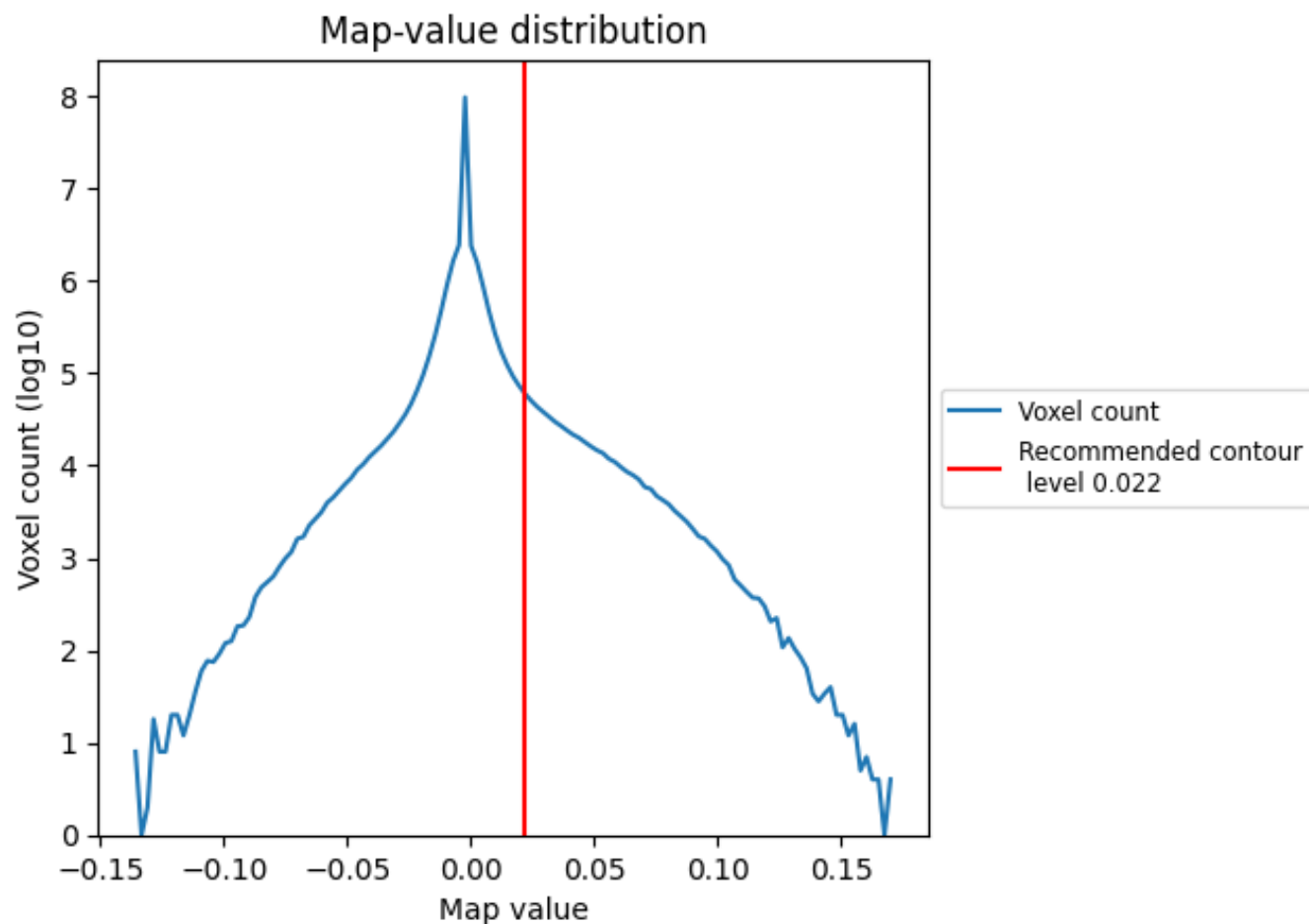
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

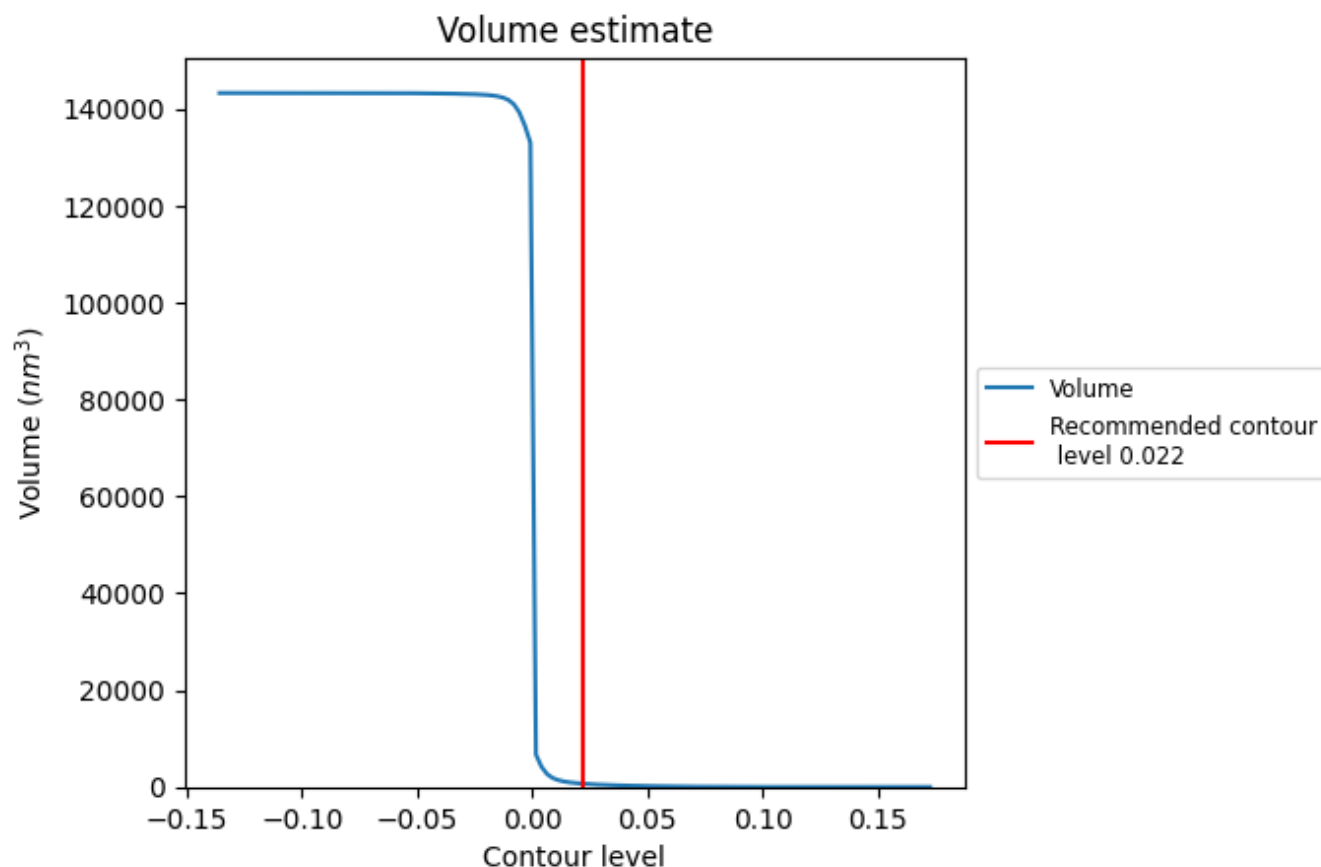
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

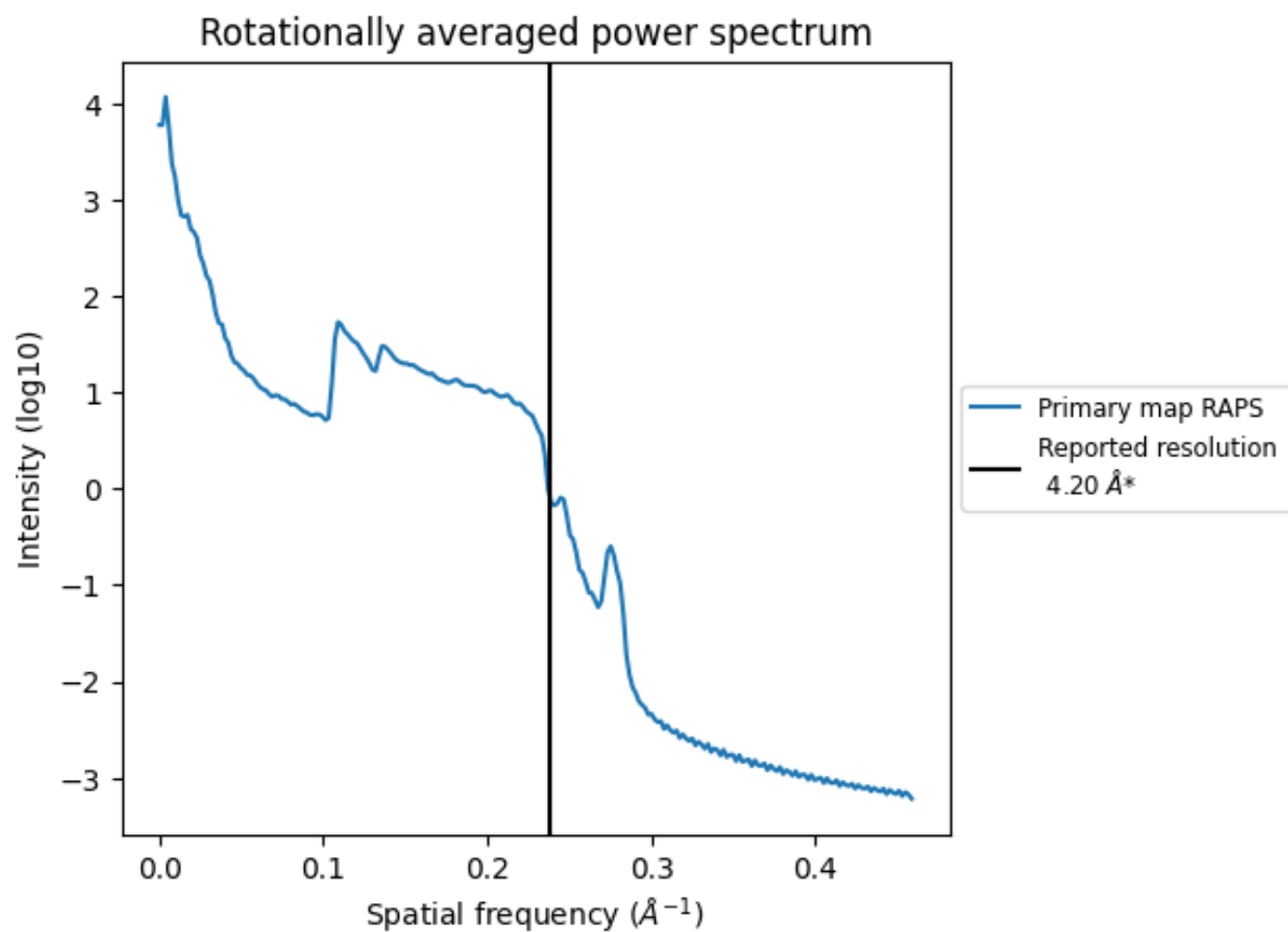
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 672 nm³; this corresponds to an approximate mass of 607 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

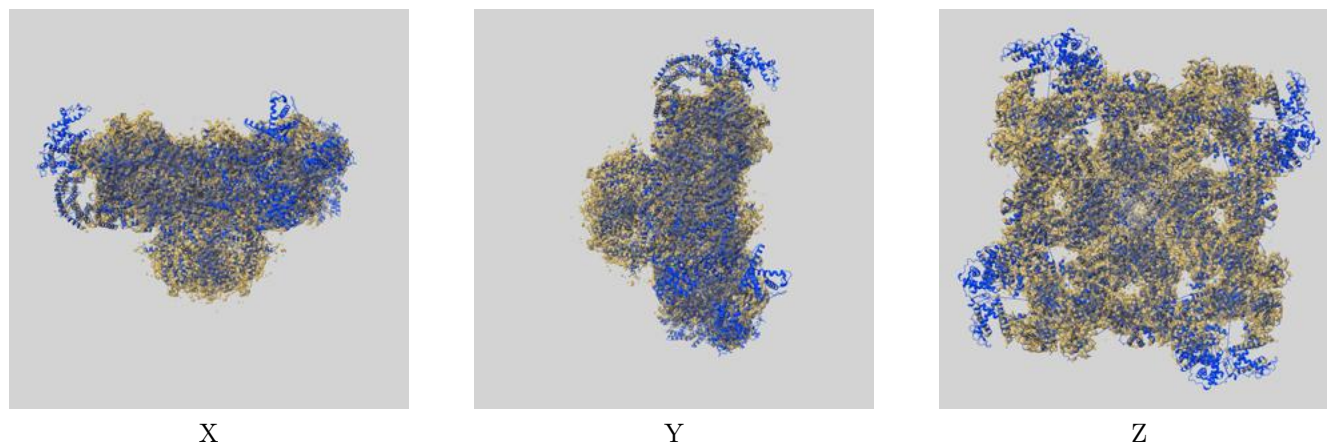
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

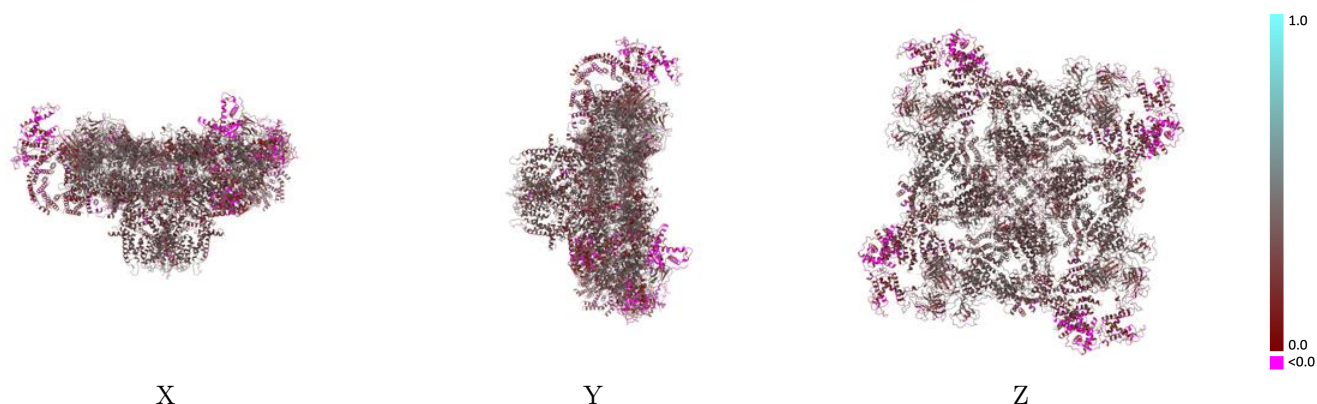
This section contains information regarding the fit between EMDB map EMD-22016 and PDB model 6X33. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



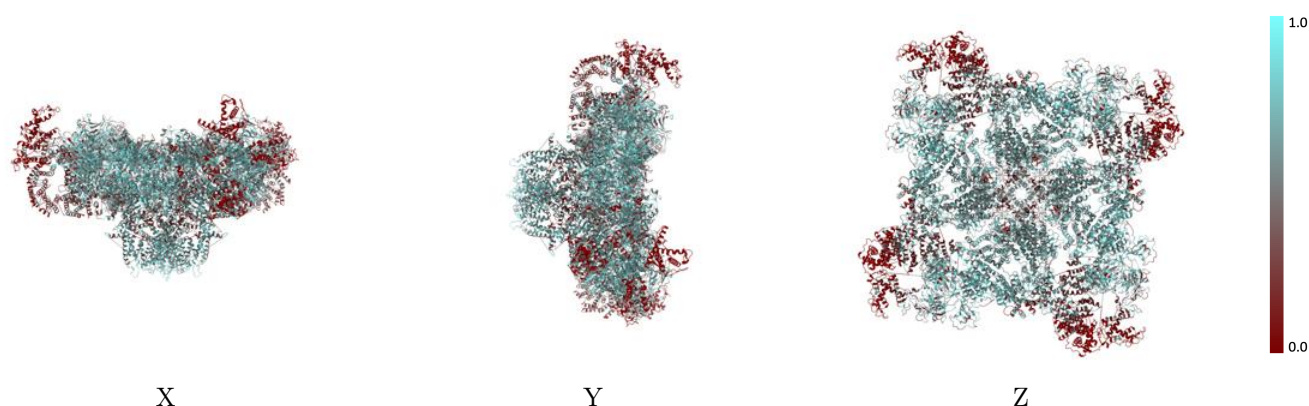
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



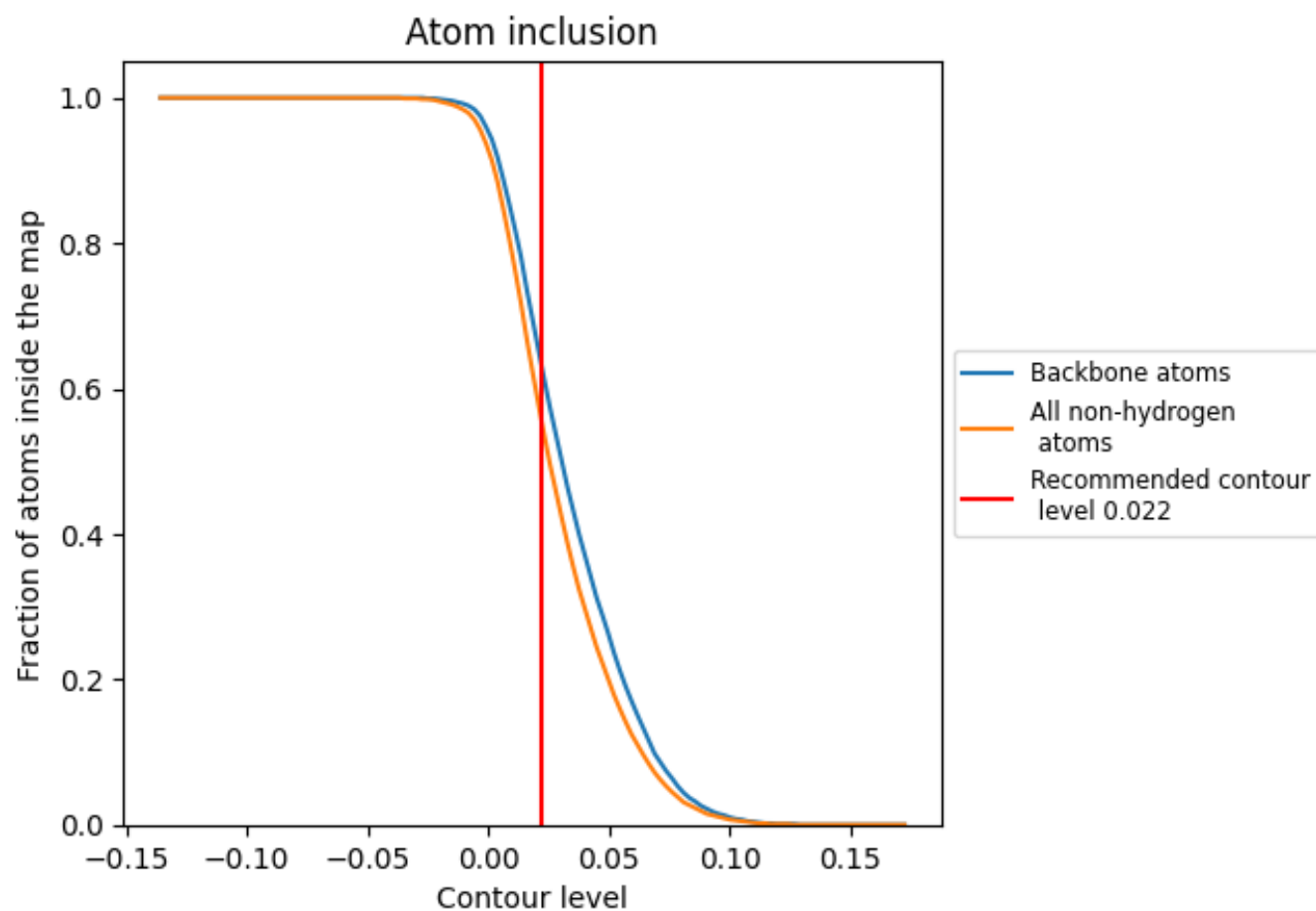
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5580	0.3230
A	0.6020	0.3810
B	0.5610	0.3230
C	0.4110	0.2760
D	0.6020	0.3780
E	0.5610	0.3230
F	0.4110	0.2740
G	0.6010	0.3780
H	0.5610	0.3230
I	0.4110	0.2720
J	0.6020	0.3790
K	0.5620	0.3220
L	0.4110	0.2750

1.0

0.0

<0.0