



Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 06:23 AM EDT

PDB ID : 5TAY
EMDB ID : EMD-8389
Title : Structure of rabbit RyR1 (ryanodine dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.60 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:

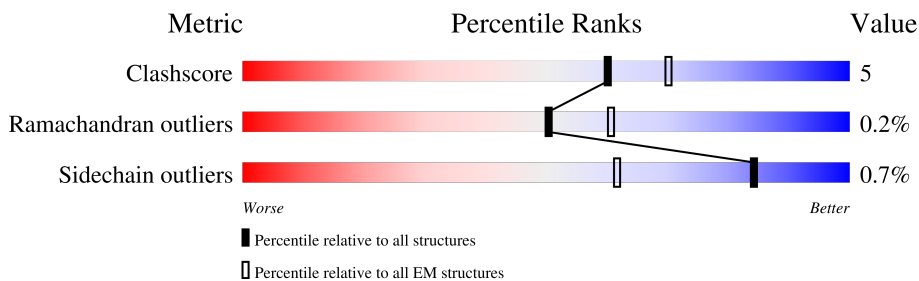
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 4.60 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	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 121276 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
			Total	C	N	O	S		
1	F	107	818	516	144	154	4	0	0
1	A	107	818	516	144	154	4	0	0
1	H	107	818	516	144	154	4	0	0
1	J	107	818	516	144	154	4	0	0

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	4194	29499	18686	5228	5428	157	0	0
2	G	4194	29499	18686	5228	5428	157	0	0
2	I	4194	29499	18686	5228	5428	157	0	0
2	E	4194	29499	18686	5228	5428	157	0	0

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

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

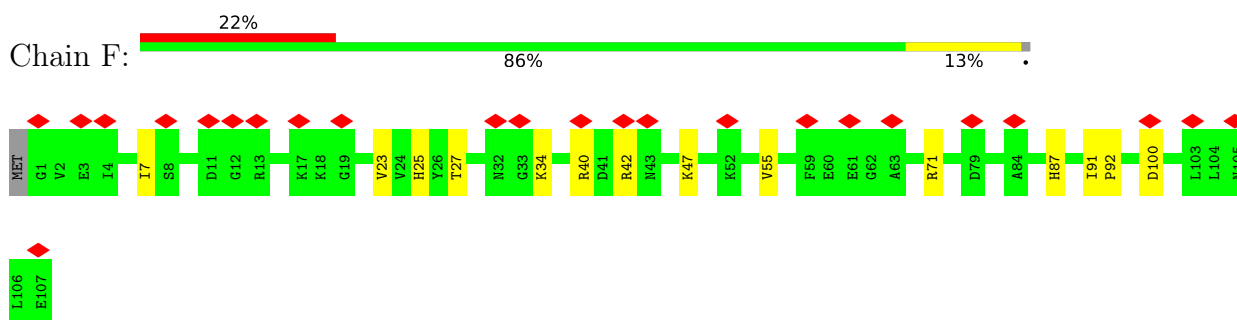
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0

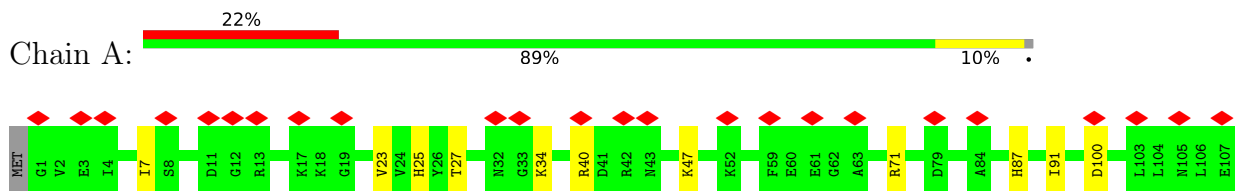
3 Residue-property plots [i](#)

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.

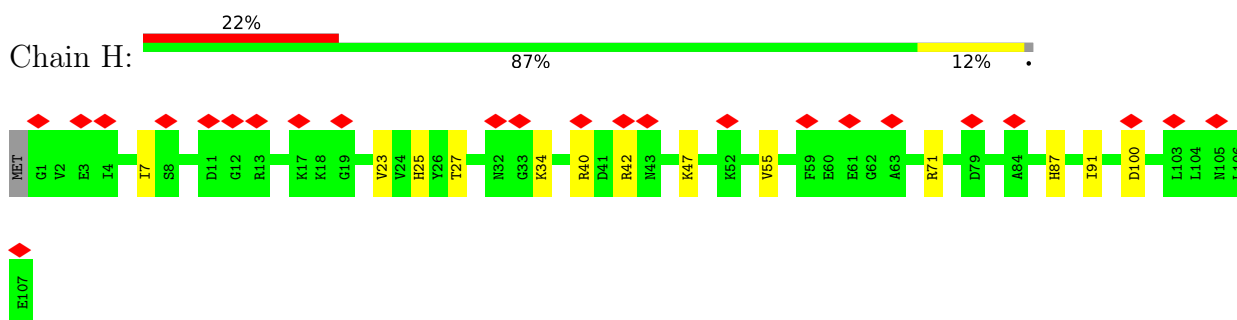
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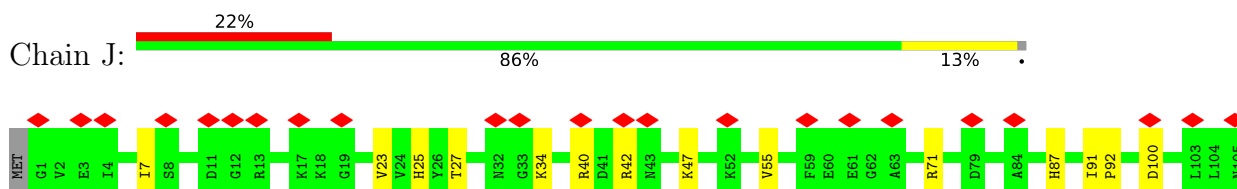
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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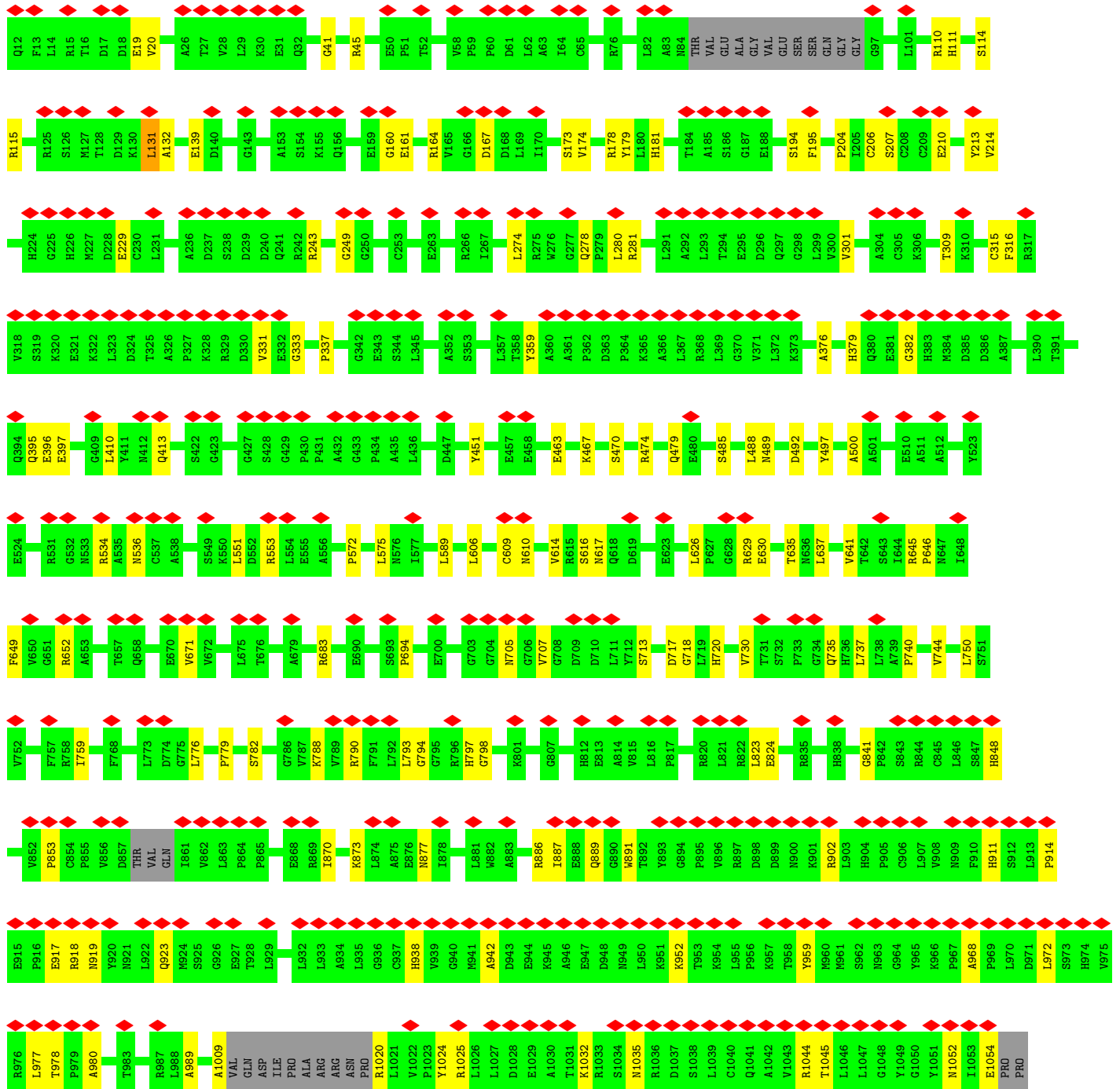
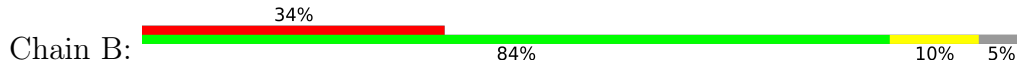


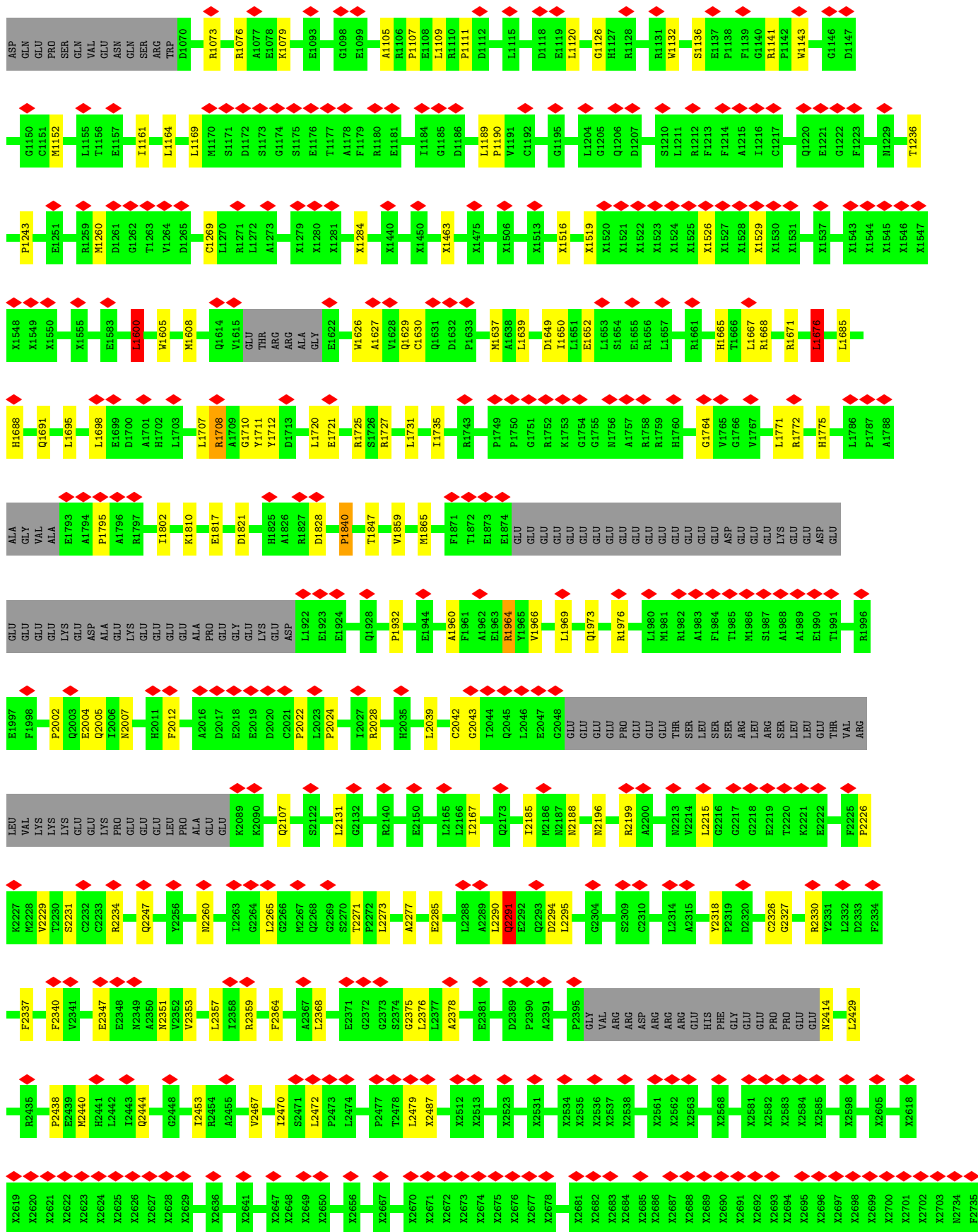
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



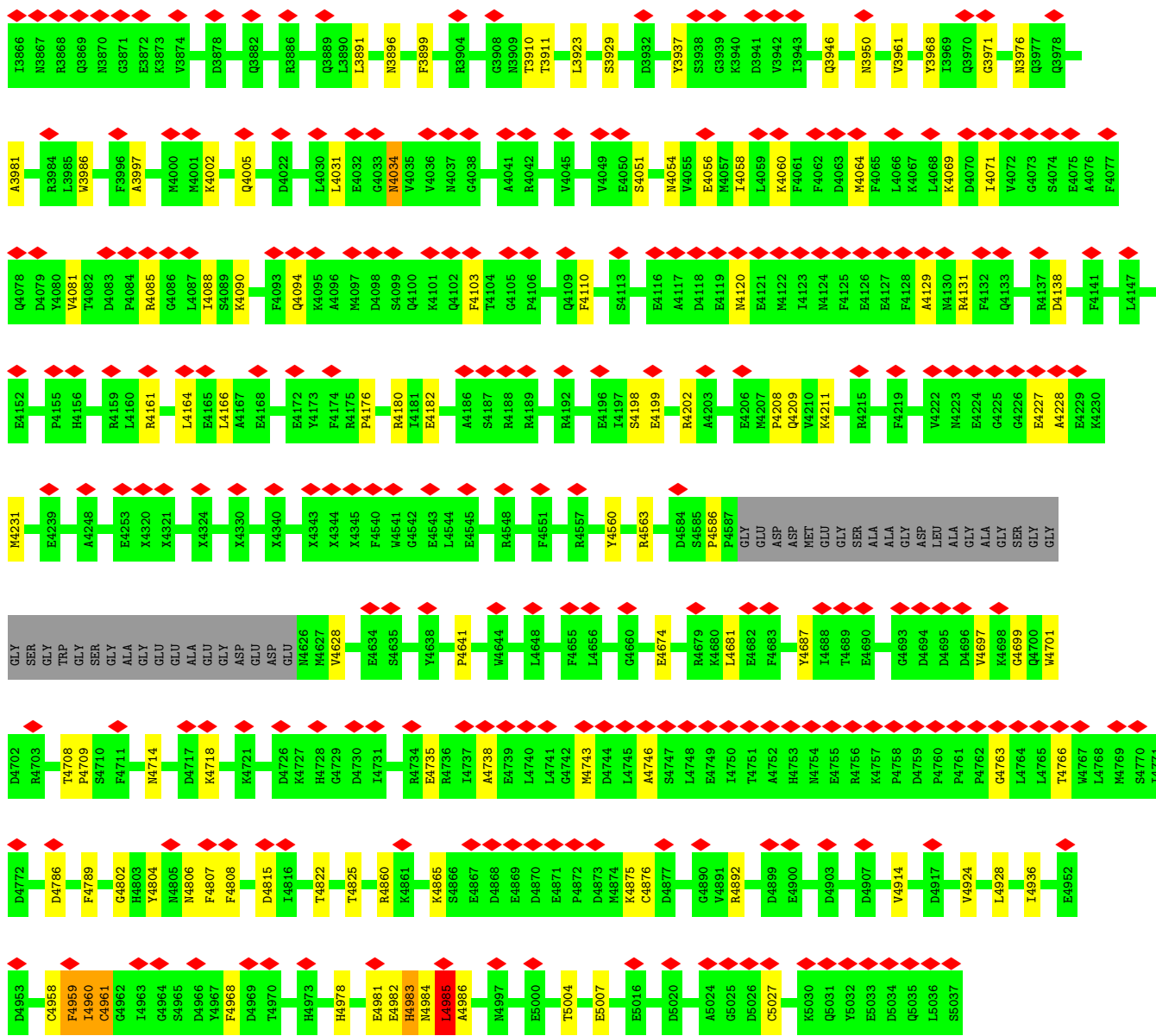
L106
E107

• Molecule 2: Ryanodine receptor 1

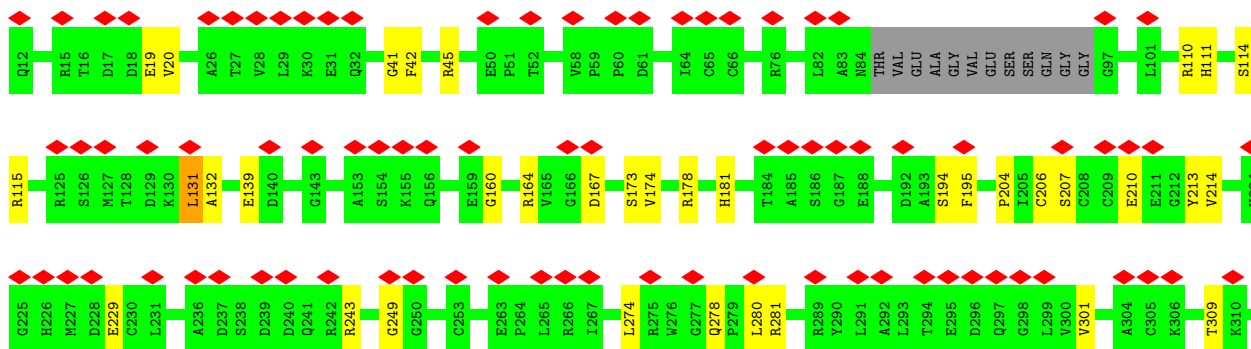
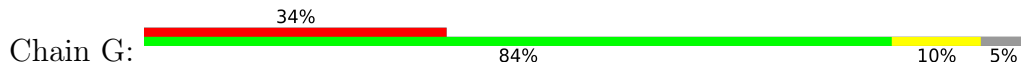


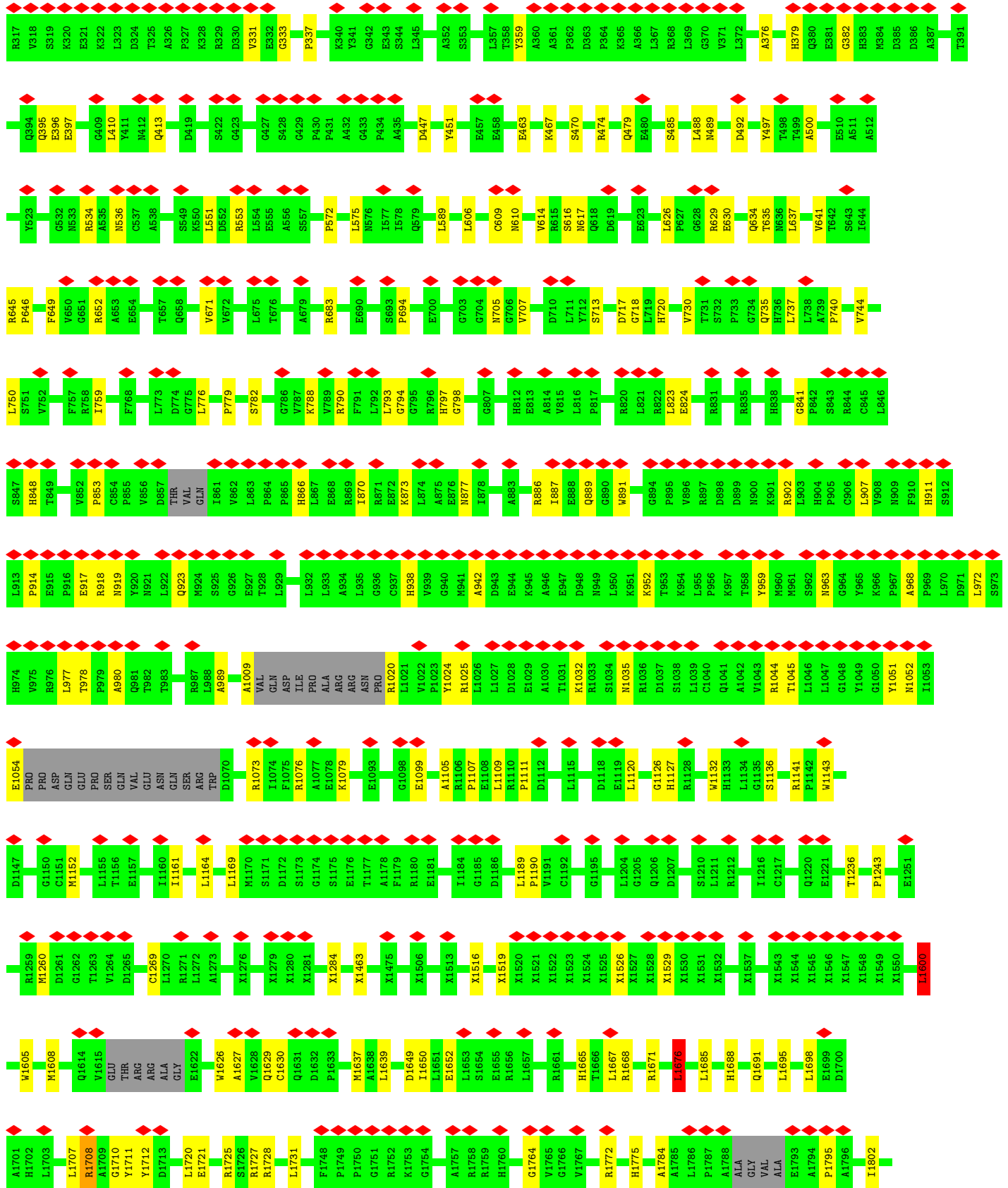


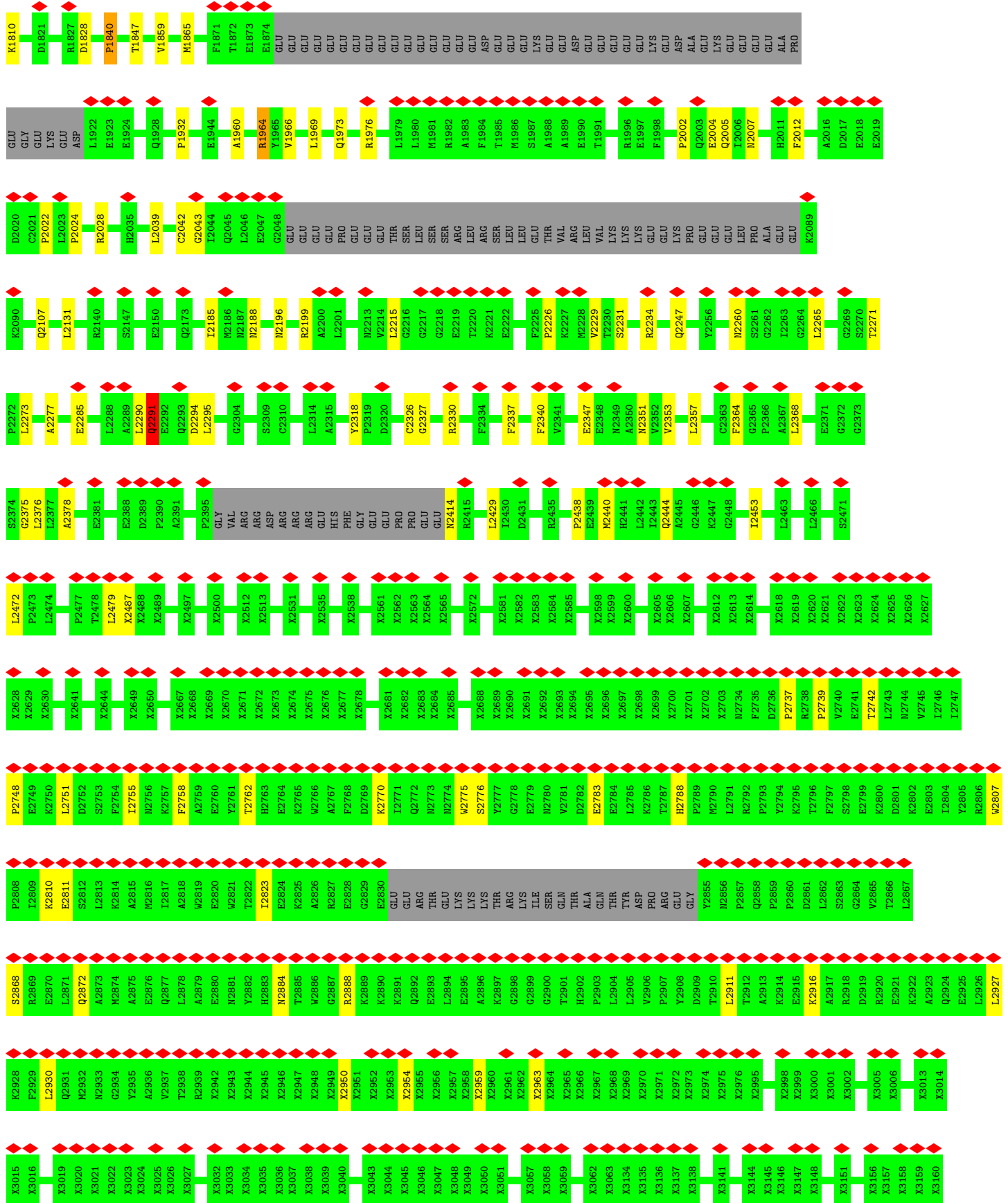
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X3559	X3450	X3451	X3454	X3455	X3456	X3457	X3458	X3459	X3462	X3467	X3468	X3511	X3512	X3514	X3515	X3516	X3517	X3518	X3519	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555																																																										
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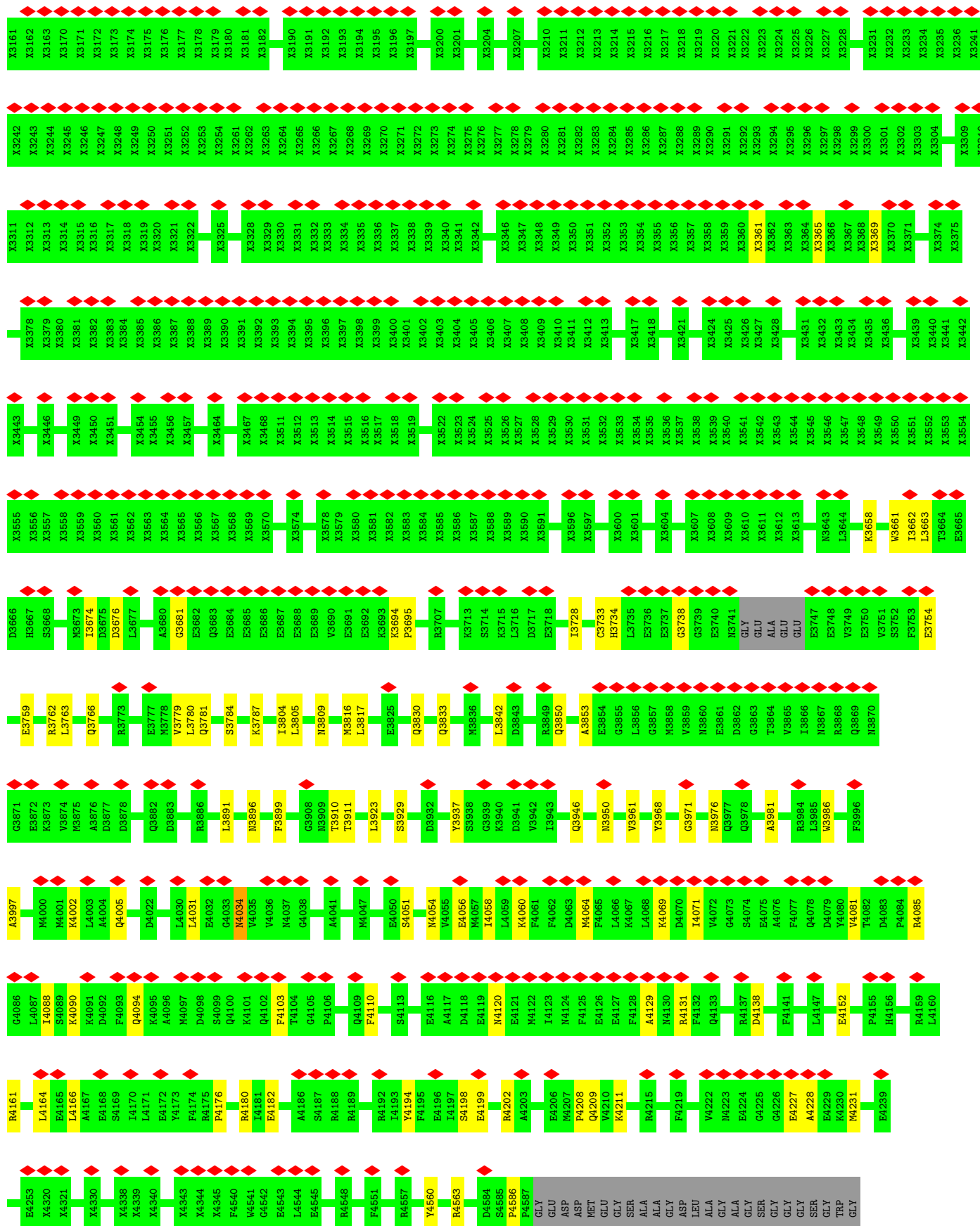


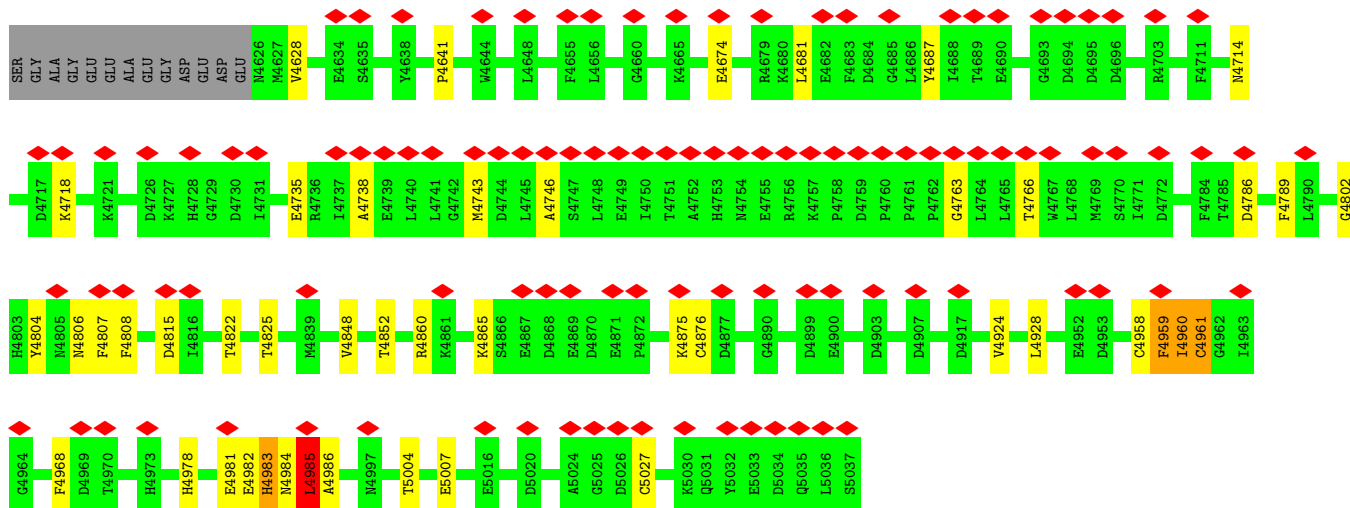
• Molecule 2: Ryanodine receptor 1



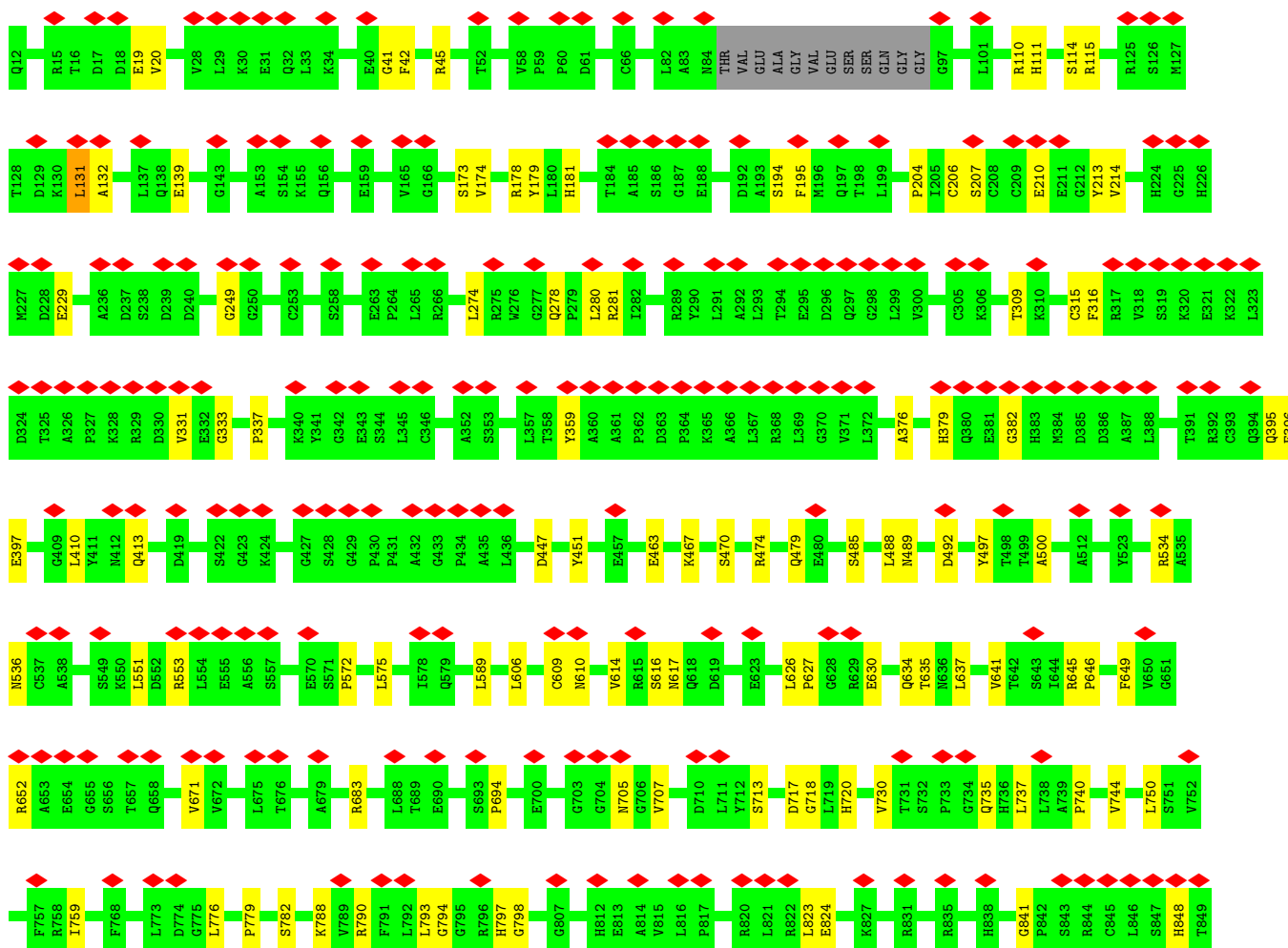
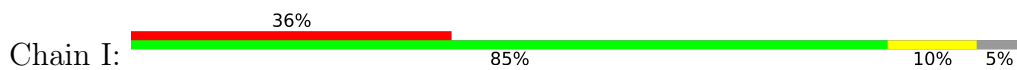


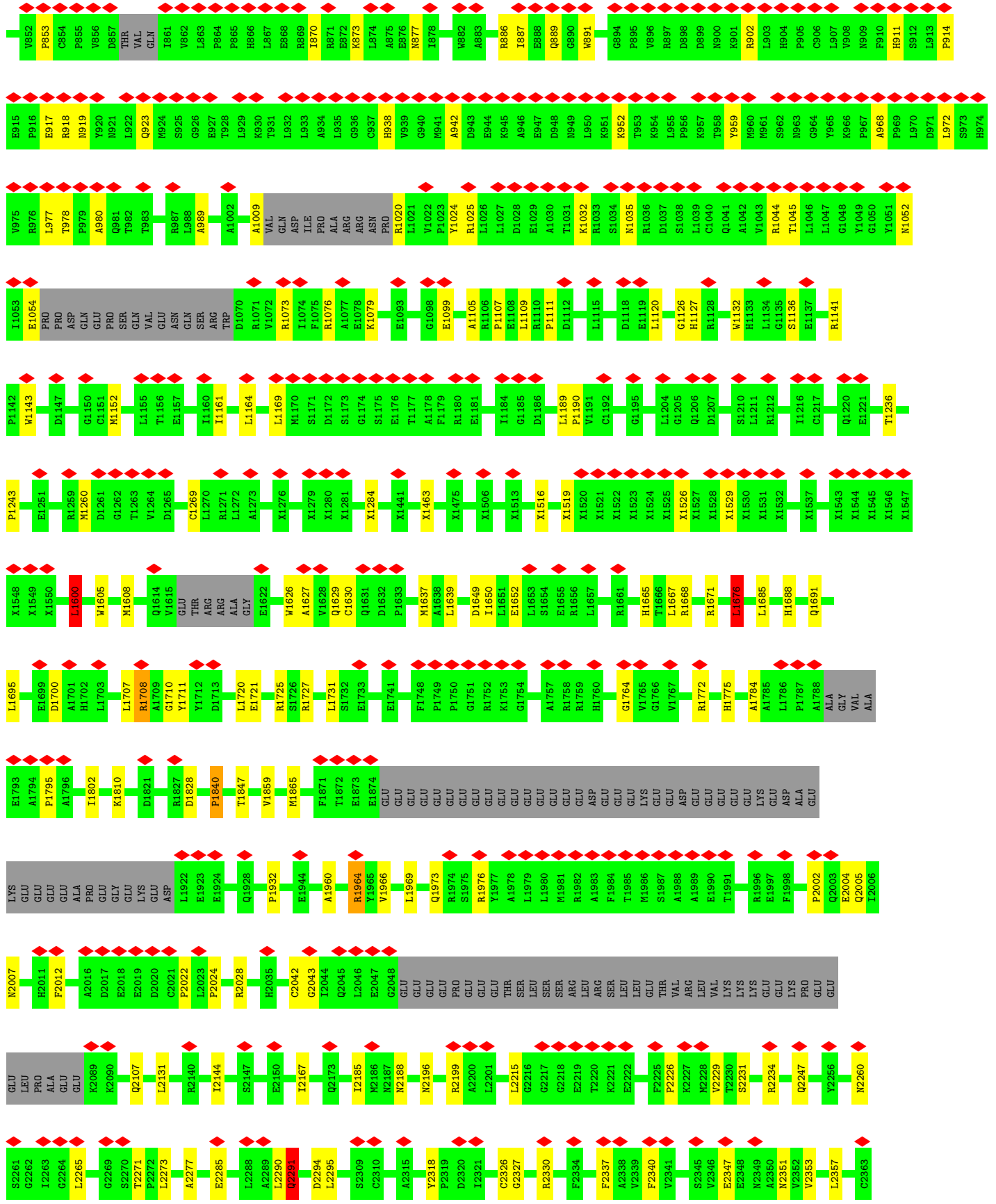


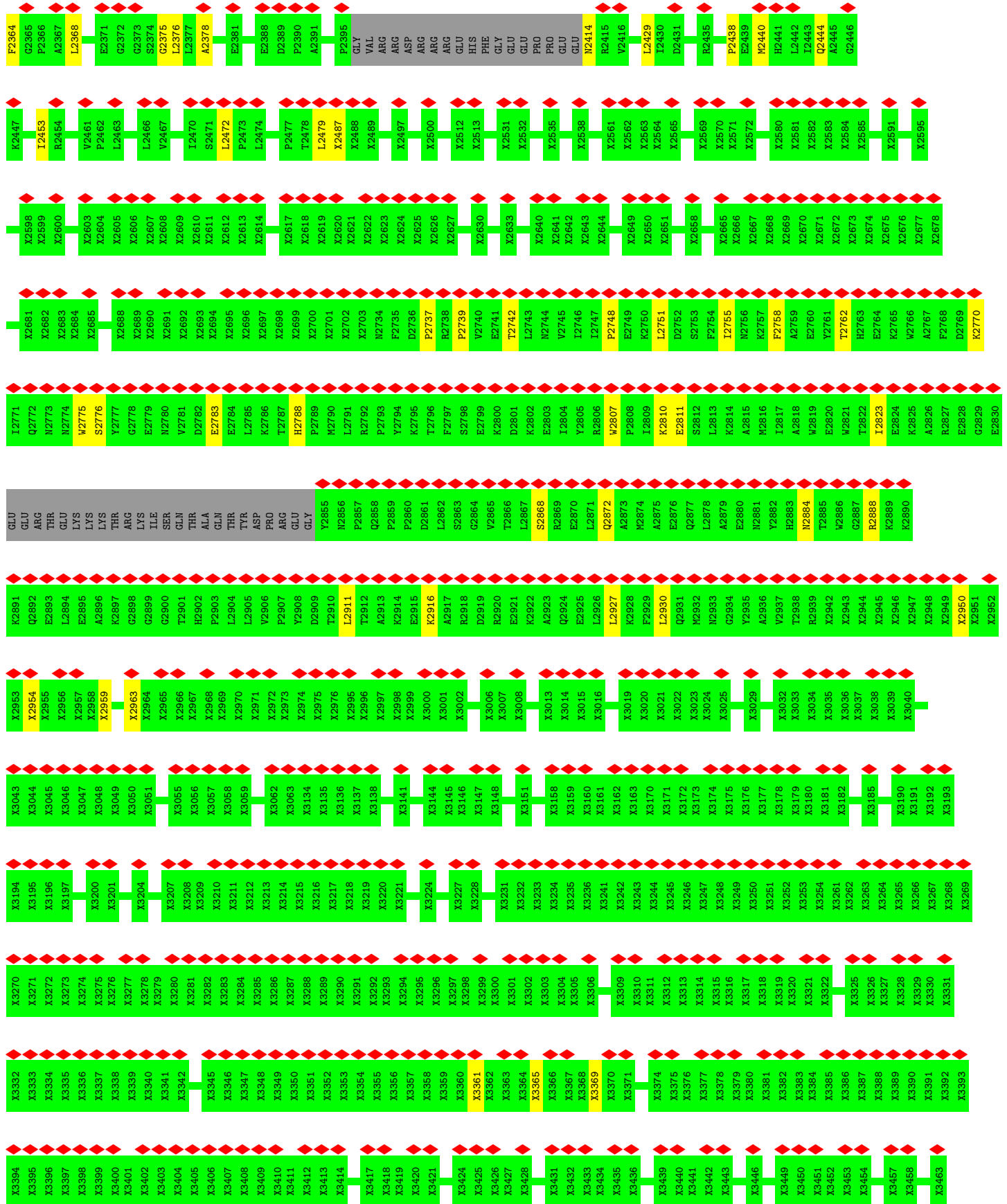




• Molecule 2: Ryanodine receptor 1

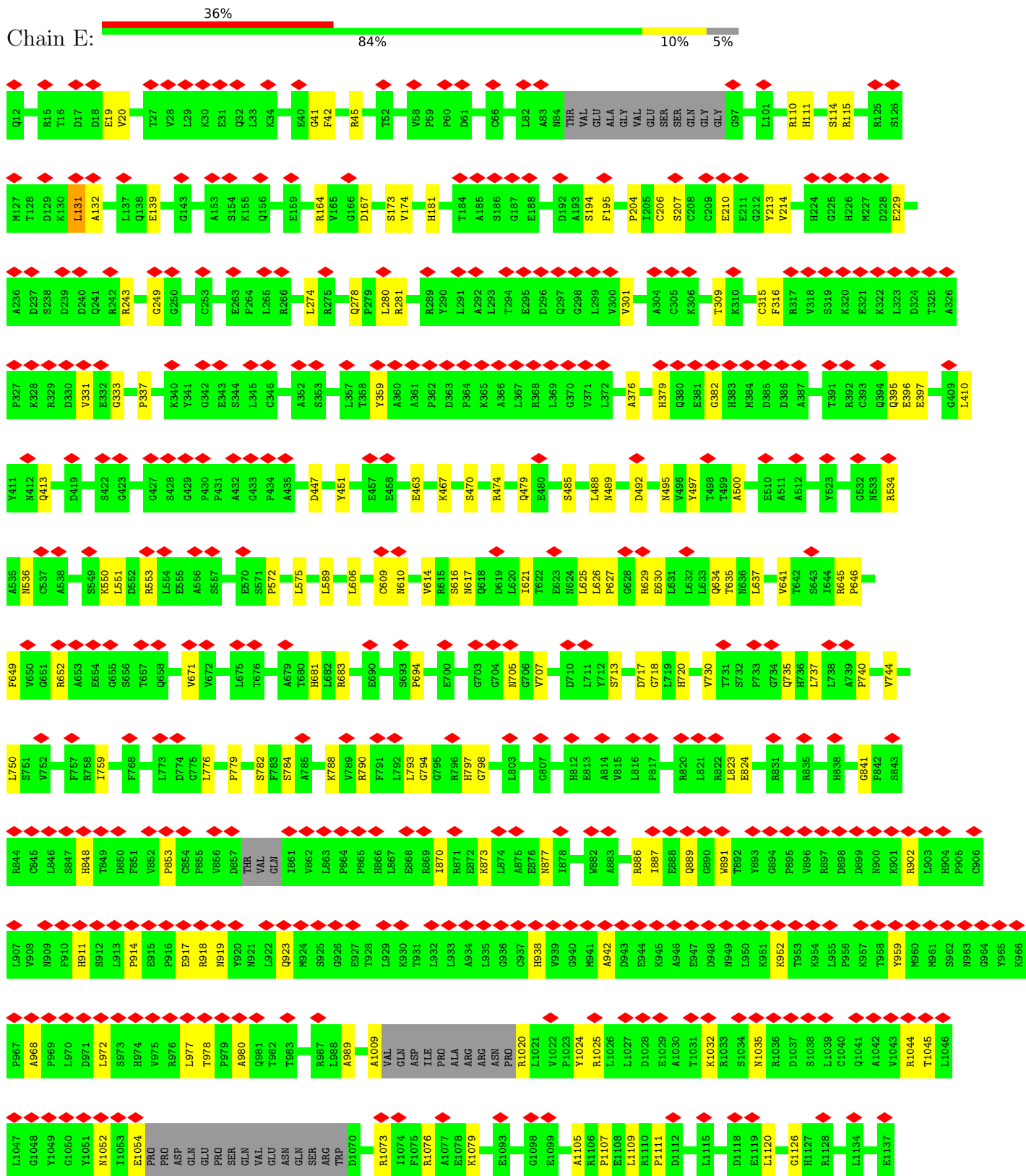


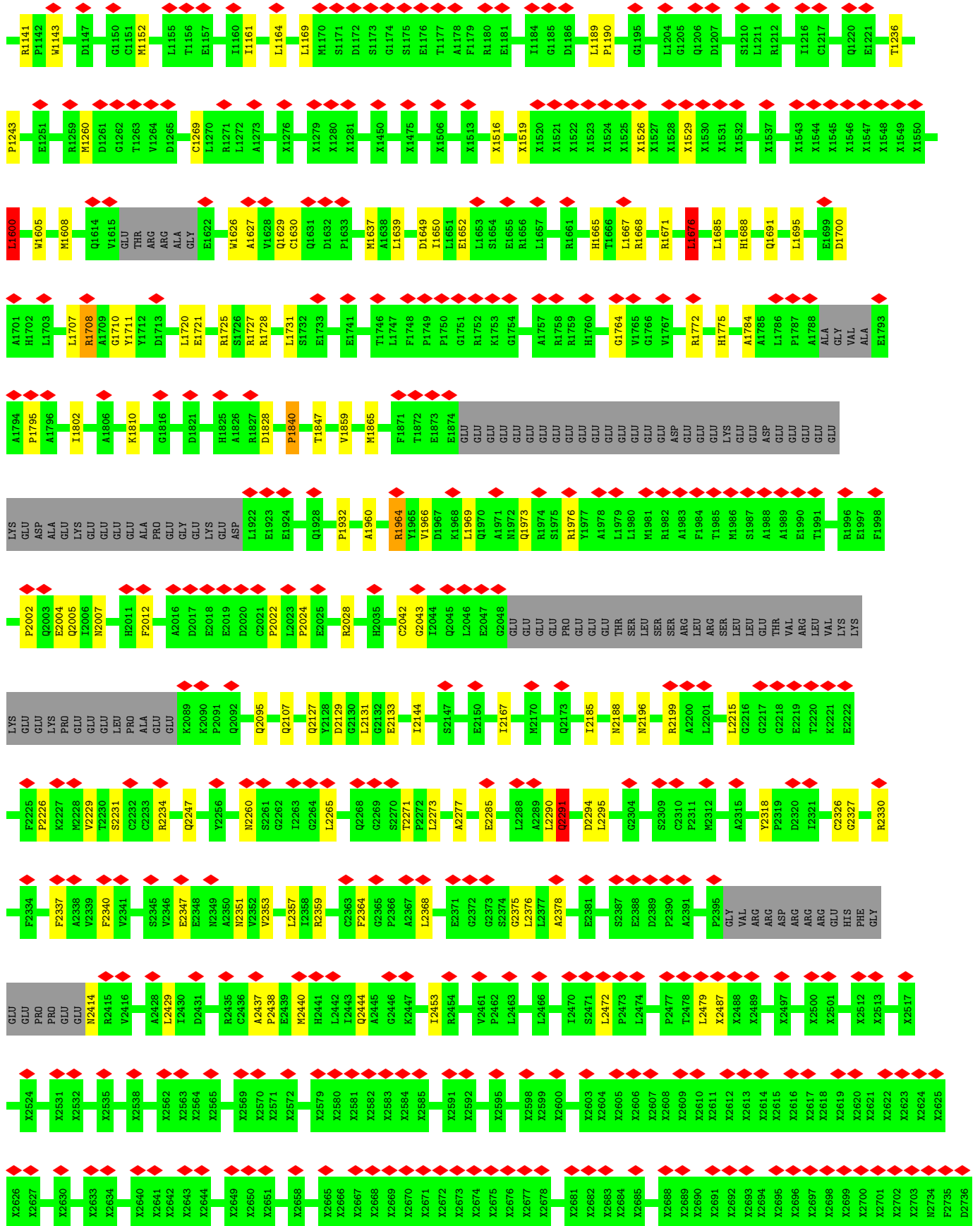




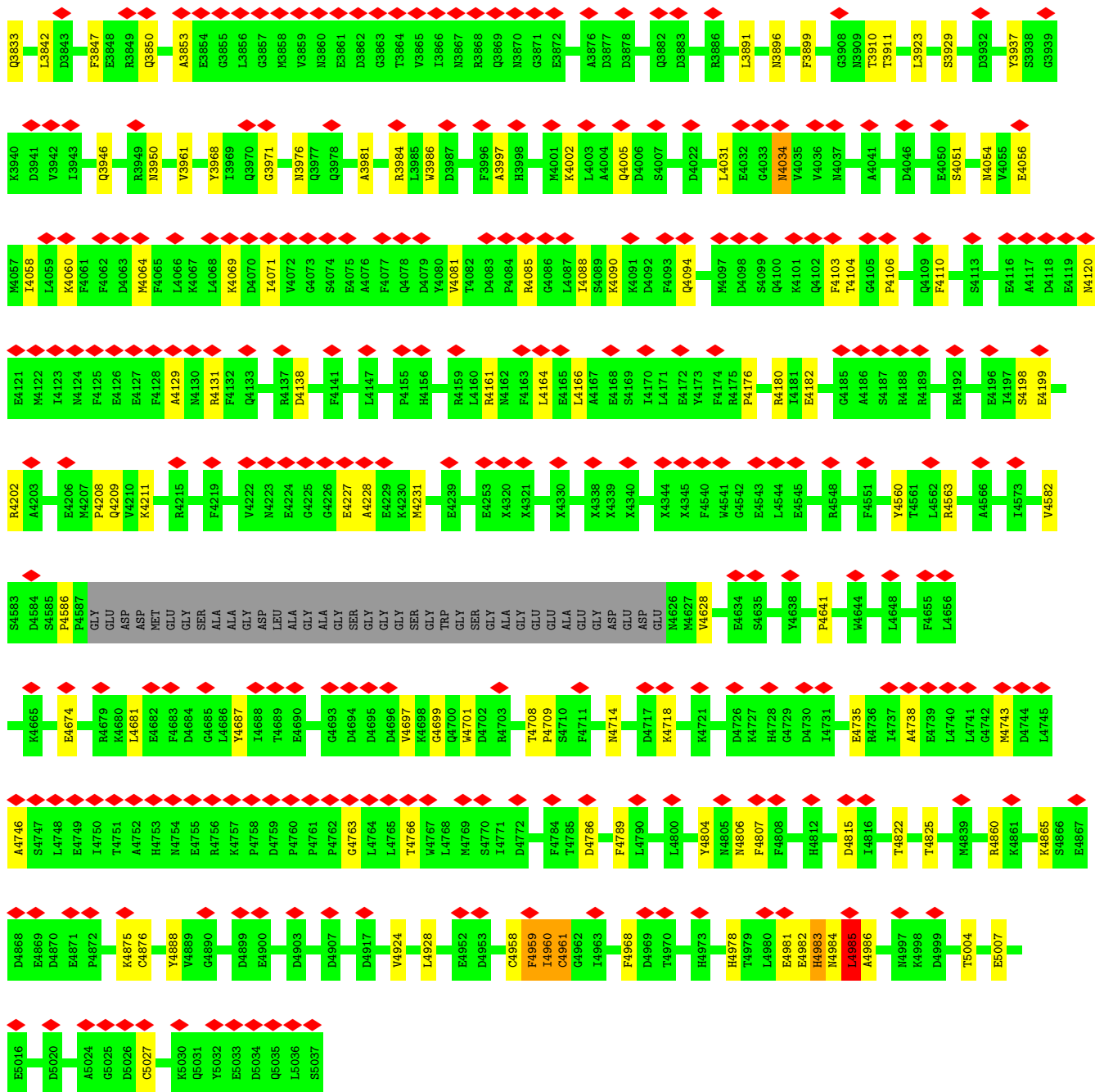
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• Molecule 2: Ryanodine receptor 1





L3716	L3717	L3728	C3733	H3734	L3735	E3736	E3737	G3738	G3739	E3740	N3741	GLU	ALA	ALA	GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3759	K3760	R3761	L3762	L3763	Q3766	R3773	D3675	D3676	L3677	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	R3707	K3713	S3714	K3715	P2737	R2738	P2739	V2740	E2741	T2742	L2743	H2744	V2745	L2746	L2747	P2748	E2749	K2810	L2751	D2752	S2753	F2754	L2755	H2756	F2757	F2758	A2759	E2760	V2761	T2762	H2763	E2764	K2765	K2766	A2767	F2768	D2769	K2770	L2771	Q2772	H2773	H2774	K2775	S2776	Y2777	G2778	E2779	H2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	F2789	H2790	L2791	R2792	F2793	V2794	K2795	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	V2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	GLU	GLU	ARG	THR	THR	THR	GLU	LYS	LYS	LYS	THR	ARG	GLN	ALA	GLN	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	M2933	Q2934	Y2935	A2936	Y2937	T2938	R2939	Y2942	Y2943	Y2944	Y2945	Y2946	Y2947	Y2948	Y2949	Y2950	Y2951	Y2952	Y2953	Y2954	Y2955	Y2956	Y2957	Y2958	Y2959	Y2963	Y2964	Y2965	Y2966	Y2967	Y2968	Y2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3013	X3014	X3015	X3016	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3029	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3055	X3056	X3057	X3058	X3059	X3062	X3110	X3111	X3112	X3113	X3114	X3115	X3116	X3117	X3118	X3119	X3120	X3121	X3122	X3123	X3124	X3125	X3126	X3127	X3128	X3129	X3130	X3131	X3132	X3133	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3144	X3145	X3146	X3147	X3148	X3151	X3155	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3185	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3201	X3204	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3224	X3225	X3226	X3227	X3228	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3424	X3425	X3426	X3427	X3428	X3431	X3432	X3433	X3434	X3435	X3436	X3439	X3440	X3441	X3442	X3443	X3446	X3449	X3450	X3451	X3452	X3453	X3454	X3457	X3458	X3459	X3460	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3574	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3594	X3595	X3596	X3597	X3598	X3599	X3600	X3601	X3604	X3605	X3606	X3607	X3608	X3609	X3610	X3611	X3612	X3613	N3643	L3644	K3658	W3661	L3662	L3663	T3664	E3665	D3666	H3667	S3668	F3669	I3674	D3675	D3676	L3677	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	R3707	K3713	S3714	K3715	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	W2881	Y2882	H2883	M2884	W2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	Q2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	M2933	Q2934	Y2935	A2936	Y2937	T2938	R2939	Y2942	Y2943	Y2944	Y2945	Y2946	Y2947	Y2948	Y2949	Y2950	Y2951	Y2952	Y2953	Y2954	Y2955	Y2956	Y2957	Y2958	Y2959	Y2963	Y2964	Y2965	Y2966	Y2967	Y2968	Y2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3013	X3014	X3015	X3016	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3029	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3055	X3056	X3057	X3058	X3059	X3062	X3110	X3111	X3112	X3113	X3114	X3115	X3116	X3117	X3118	X3119	X3120	X3121	X3122	X3123	X3124	X3125	X3126	X3127	X3128	X3129	X3130	X3131	X3132	X3133	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3144	X3145	X3146	X3147	X3148	X3151	X3155	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3185	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3201	X3204	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3224	X3225	X3226	X3227	X3228	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3424	X3425	X3426	X3427	X3428	X3431	X3432	X3433	X3434	X3435	X3436	X3439	X3440	X3441	X3442	X3443	X3446	X3449	X3450	X3451	X3452	X3453	X3454	X3457	X3458	X3459	X3460	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3574	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3594	X3595	X3596	X3597	X3598	X3599	X3600	X3601	X3604	X3605	X3606	X3607	X3608	X3609	X3610	X3611	X3612	X3613	N3643	L3644	K3658	W3661	L3662	L3663	T3664	E3665	D3666	H3667	S3668	F3669	I3674	D3675	D3676	L3677	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	R3707	K3713	S3714	K3715	L3716	D3717	L3728	C3733	H3734	L3735	E3736	E3737	G3738	G3739	E3740	N3741	GLU	ALA	ALA	GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3759	K3760	R3761	L3762	L3763	Q3766	R3773	D3675	D3676	L3677	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	R3707	K3713	S3714	K3715	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.133	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	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, CA

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	0.30	0/834	0.53	0/1123
1	F	0.30	0/834	0.53	0/1123
1	H	0.30	0/834	0.53	0/1123
1	J	0.30	0/834	0.53	0/1123
2	B	0.30	0/25428	0.54	6/34534 (0.0%)
2	E	0.30	0/25428	0.54	6/34534 (0.0%)
2	G	0.30	0/25428	0.54	6/34534 (0.0%)
2	I	0.30	0/25428	0.54	6/34534 (0.0%)
All	All	0.30	0/105048	0.54	24/142628 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	131	LEU	CA-CB-CG	7.94	133.56	115.30
2	I	131	LEU	CA-CB-CG	7.93	133.53	115.30
2	B	131	LEU	CA-CB-CG	7.92	133.53	115.30
2	G	131	LEU	CA-CB-CG	7.91	133.49	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1676	LEU	CA-CB-CG	6.62	130.52	115.30
2	I	1676	LEU	CA-CB-CG	6.61	130.50	115.30
2	B	1676	LEU	CA-CB-CG	6.60	130.49	115.30
2	G	1676	LEU	CA-CB-CG	6.59	130.46	115.30
2	G	1600	LEU	CA-CB-CG	6.37	129.94	115.30
2	E	1600	LEU	CA-CB-CG	6.35	129.91	115.30
2	B	1600	LEU	CA-CB-CG	6.34	129.88	115.30
2	I	1600	LEU	CA-CB-CG	6.33	129.86	115.30
2	B	4985	LEU	CA-CB-CG	5.79	128.63	115.30
2	I	4985	LEU	CA-CB-CG	5.79	128.62	115.30
2	G	4985	LEU	CA-CB-CG	5.79	128.61	115.30
2	E	4985	LEU	CA-CB-CG	5.77	128.58	115.30
2	E	977	LEU	CA-CB-CG	5.20	127.27	115.30
2	G	977	LEU	CA-CB-CG	5.20	127.25	115.30
2	I	977	LEU	CA-CB-CG	5.19	127.24	115.30
2	B	977	LEU	CA-CB-CG	5.19	127.24	115.30
2	G	2290	LEU	CA-CB-CG	5.17	127.19	115.30
2	E	2290	LEU	CA-CB-CG	5.17	127.18	115.30
2	B	2290	LEU	CA-CB-CG	5.16	127.16	115.30
2	I	2290	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide

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	818	0	824	6	0
1	F	818	0	824	10	0
1	H	818	0	824	9	0
1	J	818	0	824	9	0
2	B	29499	0	24750	264	0
2	E	29499	0	24750	264	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	29499	0	24750	256	0
2	I	29499	0	24750	256	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102296	1050	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 5.

All (1050) 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:B:4968:PHE:HE2	2:B:4978:HIS:CE1	1.29	1.49
2:I:4968:PHE:HE2	2:I:4978:HIS:CE1	1.29	1.48
2:E:4968:PHE:HE2	2:E:4978:HIS:CE1	1.29	1.48
2:G:4968:PHE:HE2	2:G:4978:HIS:CE1	1.29	1.48
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.09	1.41
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.09	1.39
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.09	1.39
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.09	1.39
2:G:4968:PHE:CE2	2:G:4978:HIS:HE1	1.56	1.16
2:E:4968:PHE:CE2	2:E:4978:HIS:HE1	1.56	1.05
2:I:4968:PHE:CE2	2:I:4978:HIS:HE1	1.56	1.02
2:B:4968:PHE:CE2	2:B:4978:HIS:HE1	1.56	1.02
2:G:4968:PHE:CD2	2:G:4978:HIS:ND1	2.30	1.00
2:I:4968:PHE:CD2	2:I:4978:HIS:ND1	2.30	1.00
2:B:4968:PHE:CD2	2:B:4978:HIS:ND1	2.30	0.99
2:E:4968:PHE:CD2	2:E:4978:HIS:ND1	2.30	0.98
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.35	0.94
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.35	0.94
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.35	0.93
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.35	0.93
2:G:4968:PHE:CD2	2:G:4978:HIS:CE1	2.72	0.77
2:B:4231:MET:SD	2:B:4960:ILE:HD12	2.32	0.70
2:G:4231:MET:SD	2:G:4960:ILE:HD12	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4231:MET:SD	2:I:4960:ILE:HD12	2.32	0.69
2:E:4231:MET:SD	2:E:4960:ILE:HD12	2.32	0.69
2:B:379:HIS:HD2	2:B:382:GLY:H	1.42	0.68
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.92	0.68
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.92	0.68
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.92	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.42	0.67
2:I:379:HIS:HD2	2:I:382:GLY:H	1.42	0.67
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.92	0.67
2:I:4968:PHE:CD2	2:I:4978:HIS:CE1	2.72	0.67
2:B:626:LEU:HD23	2:B:630:GLU:H	1.60	0.67
2:I:626:LEU:HD23	2:I:630:GLU:H	1.60	0.66
2:G:379:HIS:HD2	2:G:382:GLY:H	1.42	0.66
2:E:4968:PHE:HD2	2:E:4978:HIS:ND1	1.90	0.66
2:G:626:LEU:HD23	2:G:630:GLU:H	1.60	0.66
2:E:626:LEU:HD23	2:E:630:GLU:H	1.60	0.66
2:G:111:HIS:HD2	2:G:114:SER:H	1.42	0.66
2:B:111:HIS:HD2	2:B:114:SER:H	1.42	0.66
2:I:111:HIS:HD2	2:I:114:SER:H	1.42	0.66
2:G:4968:PHE:HD2	2:G:4978:HIS:ND1	1.90	0.65
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.30	0.65
2:I:4968:PHE:HD2	2:I:4978:HIS:ND1	1.90	0.65
2:E:4968:PHE:CD2	2:E:4978:HIS:CE1	2.72	0.64
2:E:111:HIS:HD2	2:E:114:SER:H	1.42	0.64
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.30	0.64
2:B:179:TYR:OH	2:E:2359:ARG:NH1	2.31	0.63
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.30	0.63
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.30	0.63
2:B:4968:PHE:HD2	2:B:4978:HIS:ND1	1.90	0.63
2:E:4968:PHE:HE2	2:E:4978:HIS:HE1	0.67	0.62
2:I:132:ALA:HA	2:I:194:SER:HB2	1.82	0.62
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.65	0.62
2:G:132:ALA:HA	2:G:194:SER:HB2	1.82	0.62
2:B:132:ALA:HA	2:B:194:SER:HB2	1.82	0.61
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.65	0.61
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.65	0.61
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.83	0.61
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.34	0.61
2:E:132:ALA:HA	2:E:194:SER:HB2	1.82	0.61
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.65	0.61
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.34	0.61
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.61
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.83	0.61
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.34	0.61
2:G:4182:GLU:OE2	2:G:4983:HIS:CE1	2.54	0.61
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.83	0.60
2:B:4182:GLU:OE2	2:B:4983:HIS:CE1	2.54	0.60
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.83	0.60
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.34	0.60
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.84	0.60
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.60
2:E:4982:GLU:HG3	2:E:5027:CYS:SG	2.42	0.60
2:E:4182:GLU:OE2	2:E:4983:HIS:CE1	2.54	0.60
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.83	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.60
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.84	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.84	0.60
2:G:4982:GLU:HG3	2:G:5027:CYS:SG	2.42	0.60
2:I:4182:GLU:OE2	2:I:4983:HIS:CE1	2.54	0.60
2:B:4968:PHE:HE2	2:B:4978:HIS:HE1	0.67	0.59
2:B:4982:GLU:HG3	2:B:5027:CYS:SG	2.42	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.35	0.59
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.35	0.59
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.83	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.85	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.85	0.59
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.83	0.59
2:I:4982:GLU:HG3	2:I:5027:CYS:SG	2.42	0.59
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.85	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.85	0.58
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.35	0.58
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.84	0.58
2:B:4968:PHE:CD2	2:B:4978:HIS:CE1	2.72	0.58
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.86	0.58
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.36	0.58
2:I:4968:PHE:HE2	2:I:4978:HIS:HE1	0.67	0.58
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.69	0.58
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.21	0.58
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.69	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.86	0.58
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.86	0.58
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.21	0.58
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.36	0.58
2:B:2359:ARG:NH1	2:I:179:TYR:OH	2.36	0.58
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.69	0.58
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.86	0.57
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.36	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.57
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.36	0.57
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.37	0.57
2:B:4056:GLU:HG3	2:B:4166:LEU:HD21	1.87	0.57
2:G:4056:GLU:HG3	2:G:4166:LEU:HD21	1.87	0.57
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.86	0.57
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.38	0.57
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.21	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.57
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.69	0.57
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.87	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.69	0.57
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.35	0.57
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.69	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.57
2:I:4056:GLU:HG3	2:I:4166:LEU:HD21	1.87	0.57
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.87	0.57
2:G:2107:GLN:HG3	2:G:3681:GLY:HA2	1.87	0.57
2:G:4968:PHE:HE2	2:G:4978:HIS:HE1	0.67	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.69	0.57
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.87	0.57
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.86	0.57
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.38	0.56
2:I:4180:ARG:HH22	2:I:4981:GLU:HA	1.70	0.56
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.88	0.56
2:E:4056:GLU:HG3	2:E:4166:LEU:HD21	1.87	0.56
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.38	0.56
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.38	0.56
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.87	0.56
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.87	0.56
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.86	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.69	0.56
2:I:2107:GLN:HG3	2:I:3681:GLY:HA2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.38	0.56
2:E:3734:HIS:O	2:E:3738:GLY:N	2.39	0.56
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.56
2:B:4180:ARG:HH22	2:B:4981:GLU:HA	1.70	0.56
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.38	0.56
2:I:744:VAL:HG22	2:I:759:ILE:HG12	1.88	0.56
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.71	0.56
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.87	0.56
2:G:3734:HIS:O	2:G:3738:GLY:N	2.39	0.56
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.87	0.56
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.38	0.56
2:G:4180:ARG:HH22	2:G:4981:GLU:HA	1.70	0.56
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.88	0.56
2:E:359:TYR:HA	2:E:376:ALA:HA	1.88	0.56
2:E:2107:GLN:HG3	2:E:3681:GLY:HA2	1.87	0.56
2:G:359:TYR:HA	2:G:376:ALA:HA	1.88	0.56
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.87	0.56
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.87	0.56
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.38	0.56
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.71	0.56
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.38	0.56
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.87	0.56
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.38	0.56
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.38	0.56
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.87	0.56
2:B:395:GLN:HG3	2:B:397:GLU:H	1.71	0.56
2:B:744:VAL:HG22	2:B:759:ILE:HG12	1.88	0.56
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.56
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.21	0.56
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.71	0.55
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.71	0.55
2:G:744:VAL:HG22	2:G:759:ILE:HG12	1.88	0.55
2:G:395:GLN:HG3	2:G:397:GLU:H	1.71	0.55
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.87	0.55
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.71	0.55
2:I:395:GLN:HG3	2:I:397:GLU:H	1.71	0.55
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.71	0.55
2:E:609:CYS:SG	2:E:610:ASN:N	2.80	0.55
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.87	0.55
2:B:1009:ALA:O	2:B:1020:ARG:N	2.40	0.55
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.87	0.55
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.55
2:B:2107:GLN:HG3	2:B:3681:GLY:HA2	1.87	0.55
2:E:744:VAL:HG22	2:E:759:ILE:HG12	1.88	0.55
2:G:4161:ARG:HD3	2:G:4164:LEU:HD12	1.89	0.55
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.89	0.55
2:B:4982:GLU:OE1	2:B:4982:GLU:HA	2.07	0.55
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.87	0.55
2:I:359:TYR:HA	2:I:376:ALA:HA	1.88	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.80	0.55
2:I:1009:ALA:O	2:I:1020:ARG:N	2.40	0.55
2:I:4982:GLU:OE1	2:I:4982:GLU:HA	2.07	0.55
2:E:4180:ARG:HH22	2:E:4981:GLU:HA	1.70	0.55
2:B:359:TYR:HA	2:B:376:ALA:HA	1.88	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:I:730:VAL:O	2:I:735:GLN:NE2	2.40	0.54
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.90	0.54
2:E:1009:ALA:O	2:E:1020:ARG:N	2.40	0.54
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.54
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.40	0.54
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.40	0.54
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.54
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.89	0.54
2:B:315:CYS:SG	2:B:316:PHE:N	2.81	0.54
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.90	0.54
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.89	0.54
2:G:609:CYS:SG	2:G:610:ASN:N	2.80	0.54
2:I:4161:ARG:HD3	2:I:4164:LEU:HD12	1.89	0.54
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.90	0.54
2:B:609:CYS:SG	2:B:610:ASN:N	2.80	0.54
2:G:730:VAL:O	2:G:735:GLN:NE2	2.40	0.54
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.41	0.54
2:E:730:VAL:O	2:E:735:GLN:NE2	2.40	0.54
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.71	0.54
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.90	0.54
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.41	0.54
2:G:315:CYS:SG	2:G:316:PHE:N	2.81	0.54
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.41	0.54
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.90	0.54
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.41	0.54
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.89	0.54
2:E:4982:GLU:OE1	2:E:4982:GLU:HA	2.07	0.54
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.90	0.54
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.54
2:B:730:VAL:O	2:B:735:GLN:NE2	2.40	0.54
2:B:4161:ARG:HD3	2:B:4164:LEU:HD12	1.89	0.54
2:I:315:CYS:SG	2:I:316:PHE:N	2.81	0.54
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.90	0.54
2:E:395:GLN:HG3	2:E:397:GLU:H	1.71	0.54
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.37	0.54
2:B:614:VAL:HG22	2:B:616:SER:H	1.73	0.54
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.71	0.54
2:G:1009:ALA:O	2:G:1020:ARG:N	2.40	0.54
2:G:4982:GLU:OE1	2:G:4982:GLU:HA	2.07	0.54
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.41	0.54
2:E:315:CYS:SG	2:E:316:PHE:N	2.81	0.54
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.72	0.54
2:B:853:PRO:HB3	2:B:1024:TYR:H	1.72	0.54
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.90	0.54
2:G:853:PRO:HB3	2:G:1024:TYR:H	1.72	0.54
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.89	0.54
2:E:2479:LEU:O	2:E:2487:UNK:N	2.41	0.54
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.41	0.53
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.90	0.53
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.37	0.53
2:I:2479:LEU:O	2:I:2487:UNK:N	2.41	0.53
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.53
2:E:4031:LEU:HB3	2:E:4034:ASN:HB2	1.90	0.53
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.90	0.53
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.73	0.53
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.81	0.53
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.90	0.53
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.89	0.53
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.40	0.53
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.40	0.53
2:E:614:VAL:HG22	2:E:616:SER:H	1.73	0.53
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.90	0.53
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.89	0.53
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.90	0.53
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.90	0.53
2:E:4161:ARG:HD3	2:E:4164:LEU:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4031:LEU:HB3	2:G:4034:ASN:HB2	1.90	0.53
2:I:4031:LEU:HB3	2:I:4034:ASN:HB2	1.90	0.53
2:E:2347:GLU:O	2:E:2351:ASN:N	2.41	0.53
2:B:4031:LEU:HB3	2:B:4034:ASN:HB2	1.90	0.53
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.41	0.53
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.41	0.53
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.74	0.53
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.74	0.53
2:B:2479:LEU:O	2:B:2487:UNK:N	2.41	0.53
2:I:3733:CYS:HA	2:I:3766:GLN:HG2	1.91	0.53
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.81	0.53
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.72	0.53
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.73	0.53
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.90	0.53
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.74	0.53
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.73	0.52
2:B:3734:HIS:O	2:B:3738:GLY:N	2.39	0.52
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.91	0.52
2:I:614:VAL:HG22	2:I:616:SER:H	1.73	0.52
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.42	0.52
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.89	0.52
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.91	0.52
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.91	0.52
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.92	0.52
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.74	0.52
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	1.92	0.52
2:E:1516:UNK:N	2:E:1529:UNK:O	2.43	0.52
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.91	0.52
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.37	0.52
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.42	0.52
2:B:3733:CYS:HA	2:B:3766:GLN:HG2	1.91	0.52
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	1.92	0.52
2:G:1516:UNK:N	2:G:1529:UNK:O	2.42	0.52
2:I:1516:UNK:N	2:I:1529:UNK:O	2.42	0.52
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	1.92	0.52
2:B:1516:UNK:N	2:B:1529:UNK:O	2.42	0.52
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.92	0.52
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.73	0.52
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	1.92	0.52
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.91	0.52
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.92	0.52
2:G:2479:LEU:O	2:G:2487:UNK:N	2.41	0.52
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.91	0.52
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.91	0.52
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.92	0.52
2:E:3733:CYS:HA	2:E:3766:GLN:HG2	1.91	0.52
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.75	0.52
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.92	0.52
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.92	0.52
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.91	0.52
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.92	0.52
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.91	0.52
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.74	0.52
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.91	0.52
2:B:3968:TYR:O	2:B:3976:ASN:ND2	2.43	0.52
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.92	0.52
2:I:3734:HIS:O	2:I:3738:GLY:N	2.39	0.52
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.74	0.52
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.75	0.51
1:J:34:LYS:HE3	2:I:634:GLN:HB3	1.93	0.51
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.93	0.51
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.93	0.51
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.92	0.51
2:G:331:VAL:HG12	2:G:333:GLY:H	1.76	0.51
2:I:331:VAL:HG12	2:I:333:GLY:H	1.76	0.51
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.74	0.51
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.74	0.51
2:G:614:VAL:HG22	2:G:616:SER:H	1.73	0.51
2:G:3968:TYR:O	2:G:3976:ASN:ND2	2.43	0.51
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.93	0.51
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.93	0.51
2:G:3733:CYS:HA	2:G:3766:GLN:HG2	1.91	0.51
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.81	0.51
2:G:160:GLY:O	2:I:3984:ARG:NH2	2.39	0.51
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.81	0.51
2:I:3968:TYR:O	2:I:3976:ASN:ND2	2.43	0.51
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.76	0.51
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.93	0.51
2:B:2353:VAL:O	2:B:2357:LEU:N	2.44	0.51
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.75	0.51
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.75	0.51
2:I:2353:VAL:O	2:I:2357:LEU:N	2.44	0.51
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.44	0.51
1:A:27:THR:HB	1:A:100:ASP:HB3	1.94	0.51
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.44	0.51
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.93	0.51
2:E:331:VAL:HG12	2:E:333:GLY:H	1.76	0.51
2:E:2353:VAL:O	2:E:2357:LEU:N	2.44	0.51
2:E:3968:TYR:O	2:E:3976:ASN:ND2	2.43	0.51
2:B:331:VAL:HG12	2:B:333:GLY:H	1.76	0.50
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.37	0.50
2:G:2347:GLU:O	2:G:2351:ASN:N	2.41	0.50
2:G:2353:VAL:O	2:G:2357:LEU:N	2.44	0.50
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	1.93	0.50
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.44	0.50
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.93	0.50
2:I:41:GLY:O	2:I:45:ARG:NH1	2.45	0.50
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.76	0.50
1:F:27:THR:HB	1:F:100:ASP:HB3	1.93	0.50
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.42	0.50
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.44	0.50
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	1.93	0.50
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.91	0.50
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.94	0.50
2:E:41:GLY:O	2:E:45:ARG:NH1	2.45	0.50
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.44	0.50
2:B:41:GLY:O	2:B:45:ARG:NH1	2.45	0.50
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.94	0.50
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.91	0.50
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.92	0.50
2:I:2347:GLU:O	2:I:2351:ASN:N	2.41	0.50
2:B:160:GLY:O	2:E:3984:ARG:NH2	2.43	0.50
1:J:27:THR:HB	1:J:100:ASP:HB3	1.93	0.50
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.77	0.50
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.94	0.50
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.77	0.50
2:G:41:GLY:O	2:G:45:ARG:NH1	2.45	0.49
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.44	0.49
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	1.93	0.49
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.77	0.49
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.76	0.49
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.94	0.49
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.77	0.49
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.77	0.49
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.77	0.49
2:B:4090:LYS:O	2:B:4094:GLN:N	2.46	0.49
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.94	0.49
2:E:776:LEU:HG	2:E:848:HIS:HA	1.95	0.49
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.78	0.49
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.78	0.49
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.77	0.49
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.95	0.49
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.95	0.49
1:H:27:THR:HB	1:H:100:ASP:HB3	1.93	0.49
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.95	0.49
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.95	0.49
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.95	0.49
2:G:3997:ALA:HA	2:G:4058:ILE:HD11	1.95	0.49
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.29	0.49
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.95	0.49
2:I:2868:SER:O	2:I:2872:GLN:N	2.45	0.49
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.77	0.49
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.78	0.49
2:B:776:LEU:HG	2:B:848:HIS:HA	1.95	0.49
2:B:4822:THR:O	2:B:4825:THR:OG1	2.30	0.49
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.95	0.49
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.95	0.49
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.78	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.41	0.49
2:G:794:GLY:H	2:G:798:GLY:HA3	1.78	0.49
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.95	0.49
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.95	0.48
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.94	0.48
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.78	0.48
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	1.93	0.48
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.95	0.48
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.94	0.48
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.96	0.48
2:I:794:GLY:H	2:I:798:GLY:HA3	1.78	0.48
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.96	0.48
2:B:794:GLY:H	2:B:798:GLY:HA3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3997:ALA:HA	2:B:4058:ILE:HD11	1.95	0.48
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.96	0.48
2:G:776:LEU:HG	2:G:848:HIS:HA	1.95	0.48
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.76	0.48
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.44	0.48
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.94	0.48
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.42	0.48
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.96	0.48
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.94	0.48
2:I:3997:ALA:HA	2:I:4058:ILE:HD11	1.95	0.48
2:E:794:GLY:H	2:E:798:GLY:HA3	1.78	0.48
2:E:2868:SER:O	2:E:2872:GLN:N	2.45	0.48
2:E:4090:LYS:O	2:E:4094:GLN:N	2.46	0.48
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.96	0.48
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.95	0.48
2:G:396:GLU:OE2	2:G:451:TYR:OH	2.29	0.48
2:G:4090:LYS:O	2:G:4094:GLN:N	2.46	0.48
2:I:776:LEU:HG	2:I:848:HIS:HA	1.95	0.48
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.96	0.48
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.48
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.94	0.48
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.96	0.48
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.78	0.48
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.96	0.48
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.96	0.48
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.95	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.29	0.48
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.95	0.48
2:E:4822:THR:O	2:E:4825:THR:OG1	2.30	0.48
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.96	0.48
2:B:1650:ILE:HG13	2:B:1707:LEU:HD21	1.96	0.48
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.95	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.95	0.48
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.78	0.48
2:B:978:THR:HB	2:B:980:ALA:H	1.80	0.47
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.96	0.47
2:G:4822:THR:O	2:G:4825:THR:OG1	2.30	0.47
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.94	0.47
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.95	0.47
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.95	0.47
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:396:GLU:OE2	2:E:451:TYR:OH	2.29	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.95	0.47
2:E:3997:ALA:HA	2:E:4058:ILE:HD11	1.95	0.47
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.78	0.47
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.97	0.47
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.79	0.47
2:I:4090:LYS:O	2:I:4094:GLN:N	2.46	0.47
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.46	0.47
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.96	0.47
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.96	0.47
2:E:1650:ILE:HG13	2:E:1707:LEU:HD21	1.96	0.47
2:E:2375:GLY:HA3	2:E:2378:ALA:HB3	1.97	0.47
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.95	0.47
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.96	0.47
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.96	0.47
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.47
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.96	0.47
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.97	0.47
2:G:2868:SER:O	2:G:2872:GLN:N	2.45	0.47
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.97	0.47
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.97	0.47
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.95	0.47
2:B:2375:GLY:HA3	2:B:2378:ALA:HB3	1.97	0.47
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.49	0.47
2:I:978:THR:HB	2:I:980:ALA:H	1.80	0.47
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.97	0.47
2:E:978:THR:HB	2:E:980:ALA:H	1.80	0.47
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.96	0.47
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.43	0.47
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.96	0.47
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.49	0.47
2:I:1650:ILE:HG13	2:I:1707:LEU:HD21	1.96	0.47
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.97	0.47
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.49	0.47
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.48	0.47
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.96	0.47
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.79	0.47
2:E:645:ARG:N	2:E:824:GLU:O	2.42	0.47
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.97	0.47
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.49	0.47
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:HIS:CD2	2:B:114:SER:H	2.29	0.46
2:B:4865:LYS:HG3	2:B:4875:LYS:HZ3	1.79	0.46
2:G:485:SER:HA	2:G:488:LEU:HB2	1.96	0.46
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.79	0.46
2:I:2375:GLY:HA3	2:I:2378:ALA:HB3	1.97	0.46
2:E:1865:MET:SD	2:E:1865:MET:N	2.89	0.46
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.98	0.46
2:B:1865:MET:SD	2:B:1865:MET:N	2.88	0.46
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.46	0.46
2:G:2375:GLY:HA3	2:G:2378:ALA:HB3	1.97	0.46
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.96	0.46
2:E:485:SER:HA	2:E:488:LEU:HB2	1.96	0.46
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.98	0.46
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.48	0.46
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.96	0.46
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.98	0.46
2:I:2364:PHE:HD1	2:I:2429:LEU:HD21	1.81	0.46
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.48	0.46
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.96	0.46
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.97	0.46
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.48	0.46
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.81	0.46
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.48	0.46
2:E:2364:PHE:HD1	2:E:2429:LEU:HD21	1.81	0.46
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.79	0.46
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.84	0.46
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.97	0.46
2:B:2868:SER:O	2:B:2872:GLN:N	2.45	0.46
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.81	0.46
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.84	0.46
2:G:1650:ILE:HG13	2:G:1707:LEU:HD21	1.96	0.46
2:G:1865:MET:SD	2:G:1865:MET:N	2.88	0.46
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.97	0.46
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.96	0.46
2:B:485:SER:HA	2:B:488:LEU:HB2	1.96	0.46
2:B:2364:PHE:HD1	2:B:2429:LEU:HD21	1.81	0.46
2:G:978:THR:HB	2:G:980:ALA:H	1.79	0.46
2:G:2364:PHE:HD1	2:G:2429:LEU:HD21	1.80	0.46
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.84	0.46
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.34	0.46
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:485:SER:HA	2:I:488:LEU:HB2	1.96	0.46
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.97	0.45
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.98	0.45
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.34	0.45
2:I:1865:MET:SD	2:I:1865:MET:N	2.88	0.45
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.81	0.45
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.47	0.45
2:B:4958:CYS:HB2	2:B:4961:CYS:H	1.82	0.45
2:G:2291:GLN:HE21	2:G:2294:ASP:H	1.65	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.48	0.45
2:E:2291:GLN:HE21	2:E:2294:ASP:H	1.64	0.45
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.97	0.45
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.98	0.45
2:B:4069:LYS:HG3	2:B:4129:ALA:HB1	1.99	0.45
2:G:4069:LYS:HG3	2:G:4129:ALA:HB1	1.99	0.45
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.14	0.45
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.99	0.45
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.34	0.45
2:I:4005:GLN:HE21	2:I:4110:PHE:HE1	1.63	0.45
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.97	0.45
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.97	0.45
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.99	0.45
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.98	0.45
2:E:4005:GLN:HE21	2:E:4110:PHE:HE1	1.63	0.45
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.14	0.45
2:B:4005:GLN:HE21	2:B:4110:PHE:HE1	1.63	0.45
2:G:278:GLN:N	2:G:315:CYS:SG	2.90	0.45
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.75	0.45
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.81	0.45
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.46	0.45
2:I:213:TYR:CG	2:I:337:PRO:HB2	2.52	0.45
2:I:4069:LYS:HG3	2:I:4129:ALA:HB1	1.99	0.45
2:I:4958:CYS:HB2	2:I:4961:CYS:H	1.82	0.45
2:E:4069:LYS:HG3	2:E:4129:ALA:HB1	1.99	0.45
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.99	0.45
2:B:164:ARG:N	2:B:167:ASP:OD2	2.43	0.45
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.98	0.45
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	1.99	0.45
2:I:206:CYS:SG	2:I:207:SER:N	2.90	0.45
2:I:2291:GLN:HE21	2:I:2294:ASP:H	1.65	0.45
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.97	0.45
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.98	0.45
2:B:2291:GLN:HE21	2:B:2294:ASP:H	1.64	0.45
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.48	0.45
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.97	0.45
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.47	0.45
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.99	0.45
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	1.99	0.45
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.84	0.45
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.97	0.45
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.46	0.45
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.75	0.45
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.81	0.45
2:G:213:TYR:CG	2:G:337:PRO:HB2	2.52	0.45
2:G:4005:GLN:HE21	2:G:4110:PHE:HE1	1.63	0.45
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.99	0.45
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.30	0.45
2:B:213:TYR:CG	2:B:337:PRO:HB2	2.52	0.45
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.30	0.45
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.30	0.45
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.99	0.45
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.81	0.45
2:E:4958:CYS:HB2	2:E:4961:CYS:H	1.82	0.45
2:B:4959:PHE:O	2:B:4959:PHE:CD1	2.71	0.44
2:B:4960:ILE:HG12	2:B:4985:LEU:HD23	2.00	0.44
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.99	0.44
2:E:2959:UNK:O	2:E:2963:UNK:N	2.50	0.44
2:I:652:ARG:HB2	2:I:750:LEU:HD13	1.99	0.44
2:I:4960:ILE:HG12	2:I:4985:LEU:HD23	2.00	0.44
2:E:206:CYS:SG	2:E:207:SER:N	2.90	0.44
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.99	0.44
2:B:278:GLN:N	2:B:315:CYS:SG	2.90	0.44
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.34	0.44
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	1.99	0.44
2:G:2959:UNK:O	2:G:2963:UNK:N	2.50	0.44
2:G:3759:GLU:O	2:G:3763:LEU:N	2.48	0.44
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.81	0.44
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.14	0.44
2:B:645:ARG:N	2:B:824:GLU:O	2.42	0.44
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.99	0.44
2:G:206:CYS:SG	2:G:207:SER:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.14	0.44
2:G:652:ARG:HB2	2:G:750:LEU:HD13	2.00	0.44
2:G:4960:ILE:HG12	2:G:4985:LEU:HD23	2.00	0.44
2:I:278:GLN:N	2:I:315:CYS:SG	2.90	0.44
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.75	0.44
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.99	0.44
2:E:3759:GLU:O	2:E:3763:LEU:N	2.48	0.44
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.99	0.44
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.34	0.44
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.99	0.44
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.98	0.44
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	1.99	0.44
2:I:551:LEU:HD21	2:I:589:LEU:HD13	2.00	0.44
2:E:551:LEU:HD21	2:E:589:LEU:HD13	2.00	0.44
2:E:606:LEU:O	2:E:617:ASN:ND2	2.51	0.44
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	1.99	0.44
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.70	0.44
2:B:606:LEU:O	2:B:617:ASN:ND2	2.51	0.44
2:B:652:ARG:HB2	2:B:750:LEU:HD13	1.99	0.44
2:G:551:LEU:HD21	2:G:589:LEU:HD13	2.00	0.44
2:G:1720:LEU:HD12	2:G:1847:THR:HG23	1.99	0.44
2:I:4822:THR:O	2:I:4825:THR:OG1	2.30	0.44
2:E:213:TYR:CG	2:E:337:PRO:HB2	2.52	0.44
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.98	0.44
2:E:793:LEU:HB2	2:E:797:HIS:H	1.83	0.44
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.99	0.44
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.75	0.44
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.30	0.44
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.91	0.44
2:B:2959:UNK:O	2:B:2963:UNK:N	2.50	0.44
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.51	0.44
2:G:4959:PHE:O	2:G:4959:PHE:CD1	2.71	0.44
2:I:641:VAL:HG21	2:I:705:ASN:HA	2.00	0.44
2:I:911:HIS:O	2:I:918:ARG:NH2	2.48	0.44
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.48	0.44
2:I:2959:UNK:O	2:I:2963:UNK:N	2.50	0.44
2:I:4984:ASN:C	2:I:4986:ALA:H	2.21	0.44
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.99	0.44
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	2.00	0.44
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.00	0.44
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.51	0.44
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	2.00	0.44
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.51	0.44
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.46	0.44
2:E:4960:ILE:HG12	2:E:4985:LEU:HD23	2.00	0.44
1:F:34:LYS:HE3	2:E:634:GLN:HB3	2.00	0.43
2:B:1695:LEU:HB3	2:B:1810:LYS:HZ2	1.83	0.43
2:I:606:LEU:O	2:I:617:ASN:ND2	2.51	0.43
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.70	0.43
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.82	0.43
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.91	0.43
1:F:23:VAL:HG22	1:F:47:LYS:HG2	2.00	0.43
2:G:606:LEU:O	2:G:617:ASN:ND2	2.51	0.43
2:G:1132:TRP:HE1	2:G:1136:SER:HG	1.61	0.43
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.48	0.43
2:B:243:ARG:NH1	2:B:301:VAL:O	2.49	0.43
2:B:793:LEU:HB2	2:B:797:HIS:H	1.83	0.43
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.99	0.43
2:B:4209:GLN:HE22	2:B:4560:TYR:HE2	1.66	0.43
2:B:4984:ASN:C	2:B:4986:ALA:H	2.21	0.43
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.91	0.43
2:G:4209:GLN:HE22	2:G:4560:TYR:HE2	1.66	0.43
2:I:4209:GLN:HE22	2:I:4560:TYR:HE2	1.66	0.43
1:J:23:VAL:HG22	1:J:47:LYS:HG2	2.01	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.90	0.43
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.00	0.43
2:B:4563:ARG:NH1	2:B:4815:ASP:OD1	2.52	0.43
2:B:4968:PHE:HD2	2:B:4978:HIS:HD1	1.47	0.43
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.99	0.43
2:G:4958:CYS:HB2	2:G:4961:CYS:H	1.82	0.43
2:I:1720:LEU:HD12	2:I:1847:THR:HG23	1.99	0.43
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.00	0.43
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.99	0.43
2:E:652:ARG:HB2	2:E:750:LEU:HD13	1.99	0.43
2:E:4586:PRO:HB3	2:E:4628:VAL:HG21	2.01	0.43
2:B:551:LEU:HD21	2:B:589:LEU:HD13	2.00	0.43
2:G:889:GLN:O	2:G:902:ARG:NH1	2.52	0.43
2:G:914:PRO:HD2	2:G:917:GLU:HB2	2.00	0.43
2:G:2775:TRP:HZ3	2:G:2783:GLU:HA	1.84	0.43
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.00	0.43
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1132:TRP:HE1	2:I:1136:SER:HG	1.65	0.43
2:I:4563:ARG:NH1	2:I:4815:ASP:OD1	2.52	0.43
2:E:914:PRO:HD2	2:E:917:GLU:HB2	2.00	0.43
2:E:919:ASN:O	2:E:923:GLN:N	2.52	0.43
2:E:1720:LEU:HD12	2:E:1847:THR:HG23	1.99	0.43
2:E:4209:GLN:HE22	2:E:4560:TYR:HE2	1.67	0.43
1:H:23:VAL:HG22	1:H:47:LYS:HG2	2.01	0.43
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.84	0.43
2:B:889:GLN:O	2:B:902:ARG:NH1	2.52	0.43
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.99	0.43
2:G:641:VAL:HG21	2:G:705:ASN:HA	2.00	0.43
2:E:2775:TRP:HZ3	2:E:2783:GLU:HA	1.84	0.43
2:E:4984:ASN:C	2:E:4986:ALA:H	2.21	0.43
2:B:2440:MET:O	2:B:2444:GLN:N	2.51	0.43
2:G:4563:ARG:NH1	2:G:4815:ASP:OD1	2.52	0.43
2:E:889:GLN:O	2:E:902:ARG:NH1	2.52	0.43
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.51	0.43
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.34	0.43
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.00	0.43
2:G:4198:SER:OG	2:G:4199:GLU:N	2.52	0.43
2:G:4984:ASN:C	2:G:4986:ALA:H	2.21	0.43
2:I:4071:ILE:HG13	2:I:4103:PHE:HZ	1.84	0.43
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.84	0.43
1:J:55:VAL:HA	2:I:1784:ALA:HA	2.00	0.43
2:B:870:ILE:HD12	2:B:873:LYS:HB2	2.01	0.43
2:B:911:HIS:O	2:B:918:ARG:NH2	2.48	0.43
2:B:1966:VAL:HA	2:B:1969:LEU:HB3	2.01	0.43
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.00	0.43
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.84	0.43
2:G:1695:LEU:HB3	2:G:1810:LYS:HZ2	1.83	0.43
2:G:1966:VAL:HA	2:G:1969:LEU:HB3	2.01	0.43
2:G:4586:PRO:HB3	2:G:4628:VAL:HG21	2.01	0.43
2:I:793:LEU:HB2	2:I:797:HIS:H	1.83	0.43
2:I:2440:MET:O	2:I:2444:GLN:N	2.51	0.43
2:I:4198:SER:OG	2:I:4199:GLU:N	2.52	0.43
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.30	0.43
2:E:243:ARG:NH1	2:E:301:VAL:O	2.49	0.43
2:E:870:ILE:HD12	2:E:873:LYS:HB2	2.01	0.43
1:A:23:VAL:HG22	1:A:47:LYS:HG2	2.01	0.43
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.52	0.43
2:B:4936:ILE:HG21	2:I:4927:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:790:ARG:HG2	2:G:1627:ALA:HA	2.01	0.43
2:G:793:LEU:HB2	2:G:797:HIS:H	1.83	0.43
2:G:2440:MET:O	2:G:2444:GLN:N	2.51	0.43
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.54	0.43
2:I:1695:LEU:HB3	2:I:1810:LYS:HZ2	1.83	0.43
2:E:1966:VAL:HA	2:E:1969:LEU:HB3	2.01	0.43
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	2.01	0.43
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	2.00	0.43
2:B:919:ASN:O	2:B:923:GLN:N	2.52	0.42
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	2.01	0.42
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	2.01	0.42
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.01	0.42
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.44	0.42
2:I:790:ARG:HG2	2:I:1627:ALA:HA	2.01	0.42
2:I:2758:PHE:O	2:I:2762:THR:N	2.46	0.42
2:E:1708:ARG:HG2	2:E:1711:TYR:CD2	2.54	0.42
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.01	0.42
2:E:4563:ARG:NH1	2:E:4815:ASP:OD1	2.52	0.42
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.99	0.42
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.54	0.42
2:B:4071:ILE:HG13	2:B:4103:PHE:HZ	1.84	0.42
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	2.01	0.42
2:I:1966:VAL:HA	2:I:1969:LEU:HB3	2.01	0.42
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	2.01	0.42
2:E:649:PHE:HB3	2:E:776:LEU:HD13	2.01	0.42
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.00	0.42
2:E:4198:SER:OG	2:E:4199:GLU:N	2.52	0.42
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.29	0.42
2:B:914:PRO:HD2	2:B:917:GLU:HB2	2.00	0.42
2:G:20:VAL:HG12	2:G:204:PRO:HA	2.01	0.42
2:G:919:ASN:O	2:G:923:GLN:N	2.52	0.42
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.85	0.42
2:G:4071:ILE:HG13	2:G:4103:PHE:HZ	1.84	0.42
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.27	0.42
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.84	0.42
2:I:919:ASN:O	2:I:923:GLN:N	2.52	0.42
2:I:2775:TRP:HZ3	2:I:2783:GLU:HA	1.84	0.42
2:I:3754:GLU:HG3	2:I:4718:LYS:HD2	2.01	0.42
2:E:2144:ILE:H	2:E:2144:ILE:HG13	1.79	0.42
2:E:2742:THR:OG1	2:E:2811:GLU:OE1	2.34	0.42
2:E:3754:GLU:HG3	2:E:4718:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:ASN:HA	2:B:492:ASP:HB2	2.01	0.42
2:B:649:PHE:HB3	2:B:776:LEU:HD13	2.02	0.42
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.93	0.42
2:B:4051:SER:OG	2:B:4054:ASN:OD1	2.37	0.42
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.00	0.42
2:G:4051:SER:OG	2:G:4054:ASN:OD1	2.37	0.42
2:I:20:VAL:HG12	2:I:204:PRO:HA	2.01	0.42
2:I:889:GLN:O	2:I:902:ARG:NH1	2.52	0.42
2:I:914:PRO:HD2	2:I:917:GLU:HB2	2.00	0.42
2:I:4051:SER:OG	2:I:4054:ASN:OD1	2.37	0.42
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.47	0.42
2:E:2440:MET:O	2:E:2444:GLN:N	2.51	0.42
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.54	0.42
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.85	0.42
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.52	0.42
2:G:649:PHE:HB3	2:G:776:LEU:HD13	2.01	0.42
2:I:649:PHE:HB3	2:I:776:LEU:HD13	2.01	0.42
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.54	0.42
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.84	0.42
2:E:1695:LEU:HB3	2:E:1810:LYS:HZ2	1.83	0.42
2:E:2776:SER:O	2:E:2788:HIS:N	2.52	0.42
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.52	0.42
2:E:4071:ILE:HG13	2:E:4103:PHE:HZ	1.84	0.42
1:H:34:LYS:HE3	2:G:634:GLN:HB3	2.02	0.42
2:B:790:ARG:HG2	2:B:1627:ALA:HA	2.01	0.42
2:B:3754:GLU:HG3	2:B:4718:LYS:HD2	2.01	0.42
2:B:4586:PRO:HB3	2:B:4628:VAL:HG21	2.01	0.42
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.84	0.42
2:G:645:ARG:N	2:G:824:GLU:O	2.42	0.42
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.93	0.42
2:E:280:LEU:HD21	2:E:316:PHE:HE2	1.85	0.42
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.01	0.42
2:B:2215:LEU:HD23	2:B:2260:ASN:HB3	2.02	0.42
2:B:2775:TRP:HZ3	2:B:2783:GLU:HA	1.84	0.42
2:B:4198:SER:OG	2:B:4199:GLU:N	2.52	0.42
2:B:4708:THR:HA	2:B:4709:PRO:HD3	1.94	0.42
2:G:489:ASN:HA	2:G:492:ASP:HB2	2.01	0.42
2:G:2012:PHE:CG	2:G:2022:PRO:HD3	2.55	0.42
2:G:2776:SER:O	2:G:2788:HIS:N	2.52	0.42
2:I:181:HIS:CE1	2:I:195:PHE:HB2	2.55	0.42
2:E:181:HIS:CE1	2:E:195:PHE:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.00	0.42
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.93	0.42
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	2.01	0.42
2:B:181:HIS:CE1	2:B:195:PHE:HB2	2.55	0.42
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.55	0.42
2:I:1708:ARG:HG2	2:I:1711:TYR:CD2	2.54	0.42
2:I:3842:LEU:O	2:I:3929:SER:OG	2.38	0.42
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	2.02	0.42
2:E:20:VAL:HG12	2:E:204:PRO:HA	2.01	0.42
2:E:788:LYS:HG2	2:E:1629:GLN:HA	2.02	0.42
2:E:2012:PHE:CG	2:E:2022:PRO:HD3	2.55	0.42
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.55	0.42
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.02	0.42
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.55	0.42
2:B:3842:LEU:O	2:B:3929:SER:OG	2.38	0.42
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.02	0.42
2:G:870:ILE:HD12	2:G:873:LYS:HB2	2.01	0.42
2:G:1708:ARG:HG2	2:G:1711:TYR:CD2	2.54	0.42
2:G:3754:GLU:HG3	2:G:4718:LYS:HD2	2.01	0.42
2:G:3842:LEU:O	2:G:3929:SER:OG	2.38	0.42
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.52	0.42
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.85	0.42
2:I:4586:PRO:HB3	2:I:4628:VAL:HG21	2.01	0.42
1:F:25:HIS:HB3	1:F:40:ARG:HD3	2.02	0.42
1:F:87:HIS:H	1:F:91:ILE:HB	1.85	0.42
2:B:20:VAL:HG12	2:B:204:PRO:HA	2.01	0.42
2:B:1189:LEU:HD12	2:B:1190:PRO:HD2	2.02	0.42
2:B:2950:UNK:O	2:B:2954:UNK:N	2.53	0.42
2:B:4804:TYR:HB3	2:B:4806:ASN:HD22	1.85	0.42
2:G:243:ARG:NH1	2:G:301:VAL:O	2.49	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.85	0.42
2:G:3759:GLU:HA	2:G:3762:ARG:HB2	2.02	0.42
2:I:870:ILE:HD12	2:I:873:LYS:HB2	2.01	0.42
2:I:2012:PHE:CG	2:I:2022:PRO:HD3	2.55	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.42
2:E:2215:LEU:HD23	2:E:2260:ASN:HB3	2.02	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:E:4708:THR:HA	2:E:4709:PRO:HD3	1.94	0.42
1:H:25:HIS:HB3	1:H:40:ARG:HD3	2.02	0.41
1:J:25:HIS:HB3	1:J:40:ARG:HD3	2.02	0.41
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1132:TRP:HE1	2:B:1136:SER:HG	1.68	0.41
2:B:1284:UNK:HA	2:B:1463:UNK:HA	2.02	0.41
2:G:181:HIS:CE1	2:G:195:PHE:HB2	2.55	0.41
2:G:788:LYS:HG2	2:G:1629:GLN:HA	2.02	0.41
2:G:2185:ILE:HA	2:G:2188:ASN:ND2	2.35	0.41
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.01	0.41
2:G:2950:UNK:O	2:G:2954:UNK:N	2.53	0.41
2:E:3759:GLU:HA	2:E:3762:ARG:HB2	2.02	0.41
2:E:4960:ILE:HD13	2:E:4960:ILE:HA	1.83	0.41
1:H:87:HIS:H	1:H:91:ILE:HB	1.85	0.41
2:B:3365:UNK:O	2:B:3369:UNK:N	2.53	0.41
2:B:4231:MET:CE	2:B:4960:ILE:HD12	2.51	0.41
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.41
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.02	0.41
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	2.01	0.41
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.01	0.41
2:E:278:GLN:N	2:E:315:CYS:SG	2.90	0.41
2:E:489:ASN:HA	2:E:492:ASP:HB2	2.01	0.41
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	2.02	0.41
2:B:4735:GLU:HA	2:B:4738:ALA:HB3	2.02	0.41
2:G:4231:MET:CE	2:G:4960:ILE:HD12	2.50	0.41
2:I:2742:THR:OG1	2:I:2811:GLU:OE1	2.34	0.41
2:I:2950:UNK:O	2:I:2954:UNK:N	2.53	0.41
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.01	0.41
2:E:2185:ILE:HA	2:E:2188:ASN:HD21	1.85	0.41
2:B:2776:SER:O	2:B:2788:HIS:N	2.52	0.41
2:G:164:ARG:N	2:G:167:ASP:OD2	2.43	0.41
2:G:173:SER:HB3	2:G:178:ARG:H	1.85	0.41
2:G:280:LEU:HD21	2:G:316:PHE:HE2	1.85	0.41
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	2.03	0.41
2:G:5004:THR:H	2:G:5007:GLU:HB2	1.86	0.41
2:I:173:SER:HB3	2:I:178:ARG:H	1.85	0.41
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.93	0.41
2:I:2185:ILE:HA	2:I:2188:ASN:ND2	2.35	0.41
2:I:3759:GLU:HA	2:I:3762:ARG:HB2	2.02	0.41
2:E:173:SER:OG	2:E:174:VAL:N	2.54	0.41
2:E:2950:UNK:O	2:E:2954:UNK:N	2.53	0.41
2:E:4804:TYR:HB3	2:E:4806:ASN:HD22	1.85	0.41
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	2.03	0.41
2:B:3759:GLU:O	2:B:3763:LEU:N	2.48	0.41
2:B:5004:THR:H	2:B:5007:GLU:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:280:LEU:HD21	2:I:316:PHE:HE2	1.85	0.41
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.44	0.41
2:I:1189:LEU:HD12	2:I:1190:PRO:HD2	2.02	0.41
2:I:2215:LEU:HD23	2:I:2260:ASN:HB3	2.02	0.41
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.84	0.41
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.55	0.41
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	2.03	0.41
2:I:4804:TYR:HB3	2:I:4806:ASN:HD22	1.85	0.41
2:I:4928:LEU:HD13	2:I:4928:LEU:HA	1.91	0.41
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.52	0.41
2:B:173:SER:HB3	2:B:178:ARG:H	1.85	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CD2	2.54	0.41
2:B:4697:VAL:O	2:B:4701:TRP:N	2.52	0.41
2:B:4914:VAL:HG23	2:E:4888:TYR:CD1	2.55	0.41
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	2.01	0.41
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.41
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.52	0.41
2:I:4231:MET:CE	2:I:4960:ILE:HD12	2.51	0.41
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	2.03	0.41
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.84	0.41
2:E:3842:LEU:O	2:E:3929:SER:OG	2.38	0.41
2:E:4231:MET:CE	2:E:4960:ILE:HD12	2.51	0.41
1:F:92:PRO:HD3	2:E:627:PRO:HB2	2.02	0.41
2:B:173:SER:OG	2:B:174:VAL:N	2.54	0.41
2:B:788:LYS:HG2	2:B:1629:GLN:HA	2.02	0.41
2:G:911:HIS:O	2:G:918:ARG:NH2	2.48	0.41
2:I:2185:ILE:HA	2:I:2188:ASN:HD21	1.85	0.41
2:I:2776:SER:O	2:I:2788:HIS:N	2.52	0.41
2:I:3361:UNK:O	2:I:3365:UNK:N	2.54	0.41
2:E:2437:ALA:HA	2:E:2438:PRO:HD3	1.94	0.41
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.02	0.41
2:B:1817:GLU:O	2:B:1821:ASP:N	2.50	0.41
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.84	0.41
2:G:1189:LEU:HD12	2:G:1190:PRO:HD2	2.02	0.41
2:G:2039:LEU:HA	2:G:2042:CYS:HB3	2.03	0.41
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	2.02	0.41
2:G:3361:UNK:O	2:G:3365:UNK:N	2.54	0.41
2:G:4060:LYS:NZ	2:G:4064:MET:SD	2.94	0.41
2:I:173:SER:OG	2:I:174:VAL:N	2.54	0.41
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.85	0.41
1:A:25:HIS:HB3	1:A:40:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:H	1:A:91:ILE:HB	1.85	0.41
1:J:87:HIS:H	1:J:91:ILE:HB	1.85	0.41
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.03	0.41
2:B:2039:LEU:HA	2:B:2042:CYS:HB3	2.03	0.41
2:B:2185:ILE:HA	2:B:2188:ASN:HD21	1.85	0.41
2:B:3361:UNK:O	2:B:3365:UNK:N	2.54	0.41
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	2.02	0.41
2:G:173:SER:OG	2:G:174:VAL:N	2.54	0.41
2:G:1284:UNK:HA	2:G:1463:UNK:HA	2.02	0.41
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.03	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.93	0.41
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	2.03	0.41
2:I:489:ASN:HA	2:I:492:ASP:HB2	2.01	0.41
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	2.03	0.41
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.54	0.41
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	2.02	0.41
2:I:3676:ASP:N	2:I:3676:ASP:OD1	2.52	0.41
2:I:4060:LYS:NZ	2:I:4064:MET:SD	2.94	0.41
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	2.03	0.41
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.30	0.41
2:I:4735:GLU:HA	2:I:4738:ALA:HB3	2.02	0.41
2:E:2129:ASP:O	2:E:2133:GLU:N	2.49	0.41
2:E:4051:SER:OG	2:E:4054:ASN:OD1	2.37	0.41
2:E:4060:LYS:NZ	2:E:4064:MET:SD	2.94	0.41
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	2.02	0.41
2:E:4697:VAL:O	2:E:4701:TRP:N	2.52	0.41
2:E:5004:THR:H	2:E:5007:GLU:HB2	1.86	0.41
2:B:2012:PHE:CG	2:B:2022:PRO:HD3	2.55	0.41
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	2.02	0.41
2:B:3677:LEU:O	2:B:3698:LEU:N	2.54	0.41
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	2.03	0.41
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	2.03	0.41
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.02	0.41
2:G:2185:ILE:HA	2:G:2188:ASN:HD21	1.85	0.41
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	2.02	0.41
2:I:788:LYS:HG2	2:I:1629:GLN:HA	2.02	0.41
2:I:2144:ILE:H	2:I:2144:ILE:HG13	1.79	0.41
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.54	0.41
1:A:34:LYS:HD3	2:B:629:ARG:HD2	2.03	0.40
2:B:280:LEU:HD21	2:B:316:PHE:HE2	1.85	0.40
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.87	0.40
2:G:866:HIS:O	2:G:1051:TYR:OH	2.28	0.40
2:G:2215:LEU:HD23	2:G:2260:ASN:HB3	2.02	0.40
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.40
2:E:911:HIS:O	2:E:918:ARG:NH2	2.48	0.40
2:E:1189:LEU:HD12	2:E:1190:PRO:HD2	2.02	0.40
2:E:3658:LYS:HA	2:E:3661:TRP:CE2	2.56	0.40
2:E:4735:GLU:HA	2:E:4738:ALA:HB3	2.02	0.40
2:B:3658:LYS:HA	2:B:3661:TRP:CE2	2.56	0.40
2:G:907:LEU:O	2:G:963:ASN:ND2	2.42	0.40
2:I:1284:UNK:HA	2:I:1463:UNK:HA	2.02	0.40
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.02	0.40
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.87	0.40
2:E:164:ARG:N	2:E:167:ASP:OD2	2.43	0.40
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.02	0.40
2:E:495:ASN:HD21	2:E:550:LYS:HE3	1.87	0.40
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	2.03	0.40
1:H:55:VAL:HA	2:G:1784:ALA:HA	2.04	0.40
2:B:3694:LYS:HA	2:B:3695:PRO:HD3	1.93	0.40
2:B:3847:PHE:HA	2:B:3850:GLN:HG2	2.04	0.40
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.55	0.40
2:G:4735:GLU:HA	2:G:4738:ALA:HB3	2.02	0.40
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.03	0.40
2:E:2185:ILE:HA	2:E:2188:ASN:ND2	2.35	0.40
2:E:3361:UNK:O	2:E:3365:UNK:N	2.54	0.40
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.55	0.40
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	2.04	0.40
2:B:2185:ILE:HA	2:B:2188:ASN:ND2	2.35	0.40
2:B:3759:GLU:HA	2:B:3762:ARG:HB2	2.02	0.40
2:G:3676:ASP:N	2:G:3676:ASP:OD1	2.52	0.40
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.40	0.40
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.03	0.40
2:I:5004:THR:H	2:I:5007:GLU:HB2	1.86	0.40
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.04	0.40
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.02	0.40
2:E:3847:PHE:HA	2:E:3850:GLN:HG2	2.04	0.40
2:B:2467:VAL:HA	2:B:2470:ILE:HD12	2.03	0.40
2:B:4060:LYS:NZ	2:B:4064:MET:SD	2.94	0.40
2:G:4804:TYR:HB3	2:G:4806:ASN:HD22	1.85	0.40
2:I:645:ARG:N	2:I:824:GLU:O	2.42	0.40
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:621:ILE:O	2:E:625:LEU:N	2.52	0.40
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.03	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	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2892 (89%)	337 (10%)	6 (0%)	47	81
2	E	3235/4416 (73%)	2894 (90%)	335 (10%)	6 (0%)	47	81
2	G	3235/4416 (73%)	2895 (90%)	334 (10%)	6 (0%)	47	81
2	I	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	47	81
All	All	13360/18096 (74%)	11944 (89%)	1392 (10%)	24 (0%)	50	81

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	E	4985	LEU
2	B	1840	PRO
2	B	4985	LEU
2	G	1840	PRO

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Mol	Chain	Res	Type
2	G	4985	LEU
2	I	1840	PRO
2	I	4985	LEU
2	E	1840	PRO
2	B	1932	PRO
2	B	2291	GLN
2	B	4641	PRO
2	G	1932	PRO
2	G	2291	GLN
2	G	4641	PRO
2	I	1932	PRO
2	I	2291	GLN
2	I	4641	PRO
2	E	1932	PRO
2	E	2291	GLN
2	E	4641	PRO

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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	84	90

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3663	LEU
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4959	PHE
2	B	4960	ILE
2	B	4961	CYS
2	B	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3663	LEU
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4959	PHE
2	G	4960	ILE
2	G	4961	CYS
2	G	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG

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Mol	Chain	Res	Type
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3663	LEU
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4959	PHE
2	I	4960	ILE
2	I	4961	CYS
2	I	4983	HIS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3663	LEU
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4959	PHE
2	E	4960	ILE
2	E	4961	CYS
2	E	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN

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Mol	Chain	Res	Type
2	B	71	GLN
2	B	113	HIS
2	B	224	HIS
2	B	379	HIS
2	B	383	HIS
2	B	413	GLN
2	B	479	GLN
2	B	797	HIS
2	B	921	ASN
2	B	1041	GLN
2	B	1598	GLN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	2041	HIS
2	B	2127	GLN
2	B	2291	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	3994	HIS
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4142	ASN
2	B	4209	GLN
2	B	4806	ASN
2	G	57	ASN
2	G	71	GLN
2	G	111	HIS
2	G	113	HIS
2	G	224	HIS
2	G	379	HIS
2	G	383	HIS
2	G	413	GLN

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Mol	Chain	Res	Type
2	G	479	GLN
2	G	797	HIS
2	G	921	ASN
2	G	1041	GLN
2	G	1598	GLN
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	1973	GLN
2	G	2041	HIS
2	G	2127	GLN
2	G	2291	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	3994	HIS
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4142	ASN
2	G	4209	GLN
2	G	4806	ASN
2	I	57	ASN
2	I	71	GLN
2	I	111	HIS
2	I	113	HIS
2	I	224	HIS
2	I	379	HIS
2	I	383	HIS
2	I	413	GLN
2	I	479	GLN
2	I	797	HIS
2	I	921	ASN
2	I	1041	GLN
2	I	1158	ASN

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Mol	Chain	Res	Type
2	I	1598	GLN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	2041	HIS
2	I	2127	GLN
2	I	2291	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	3994	HIS
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4209	GLN
2	I	4806	ASN
2	E	57	ASN
2	E	71	GLN
2	E	111	HIS
2	E	113	HIS
2	E	224	HIS
2	E	379	HIS
2	E	383	HIS
2	E	413	GLN
2	E	479	GLN
2	E	797	HIS
2	E	921	ASN
2	E	1041	GLN
2	E	1598	GLN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1760	HIS
2	E	1775	HIS
2	E	2041	HIS

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Mol	Chain	Res	Type
2	E	2127	GLN
2	E	2291	GLN
2	E	3809	ASN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	3994	HIS
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4130	ASN
2	E	4142	ASN
2	E	4209	GLN
2	E	4806	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	14
2	G	14
2	I	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.85
1	G	4345:UNK	C	4540:PHE	N	73.85
1	I	4345:UNK	C	4540:PHE	N	73.85
1	E	4345:UNK	C	4540:PHE	N	73.85
1	B	3613:UNK	C	3639:THR	N	45.57
1	G	3613:UNK	C	3639:THR	N	45.57
1	I	3613:UNK	C	3639:THR	N	45.57
1	E	3613:UNK	C	3639:THR	N	45.57
1	B	4253:GLU	C	4320:UNK	N	29.50
1	G	4253:GLU	C	4320:UNK	N	29.50
1	I	4253:GLU	C	4320:UNK	N	29.50
1	E	4253:GLU	C	4320:UNK	N	29.50
1	B	3163:UNK	C	3170:UNK	N	15.85
1	G	3163:UNK	C	3170:UNK	N	15.85
1	I	3163:UNK	C	3170:UNK	N	15.85
1	E	3163:UNK	C	3170:UNK	N	15.85
1	B	3063:UNK	C	3134:UNK	N	15.15
1	G	3063:UNK	C	3134:UNK	N	15.15
1	I	3063:UNK	C	3134:UNK	N	15.15
1	E	3063:UNK	C	3134:UNK	N	15.15
1	B	3468:UNK	C	3511:UNK	N	14.46
1	G	3468:UNK	C	3511:UNK	N	14.46
1	I	3468:UNK	C	3511:UNK	N	14.46
1	E	3468:UNK	C	3511:UNK	N	14.46

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2703:UNK	C	2734:ASN	N	13.26
1	G	2703:UNK	C	2734:ASN	N	13.26
1	I	2703:UNK	C	2734:ASN	N	13.26
1	E	2703:UNK	C	2734:ASN	N	13.26
1	B	3236:UNK	C	3241:UNK	N	13.11
1	G	3236:UNK	C	3241:UNK	N	13.11
1	I	3236:UNK	C	3241:UNK	N	13.11
1	E	3236:UNK	C	3241:UNK	N	13.11
1	B	1564:UNK	C	1573:MET	N	12.51
1	G	1564:UNK	C	1573:MET	N	12.51
1	I	1564:UNK	C	1573:MET	N	12.51
1	E	1564:UNK	C	1573:MET	N	12.51
1	B	2976:UNK	C	2995:UNK	N	12.28
1	G	2976:UNK	C	2995:UNK	N	12.28
1	I	2976:UNK	C	2995:UNK	N	12.28
1	E	2976:UNK	C	2995:UNK	N	12.28
1	B	3254:UNK	C	3261:UNK	N	8.55
1	G	3254:UNK	C	3261:UNK	N	8.55
1	I	3254:UNK	C	3261:UNK	N	8.55
1	E	3254:UNK	C	3261:UNK	N	8.55
1	B	1297:UNK	C	1430:UNK	N	5.58
1	G	1297:UNK	C	1430:UNK	N	5.58
1	I	1297:UNK	C	1430:UNK	N	5.58
1	E	1297:UNK	C	1430:UNK	N	5.58
1	B	2479:LEU	C	2487:UNK	N	3.51
1	G	2479:LEU	C	2487:UNK	N	3.51
1	I	2479:LEU	C	2487:UNK	N	3.51
1	E	2479:LEU	C	2487:UNK	N	3.51
1	B	2939:ARG	C	2942:UNK	N	3.39
1	G	2939:ARG	C	2942:UNK	N	3.39
1	I	2939:ARG	C	2942:UNK	N	3.39
1	E	2939:ARG	C	2942:UNK	N	3.39

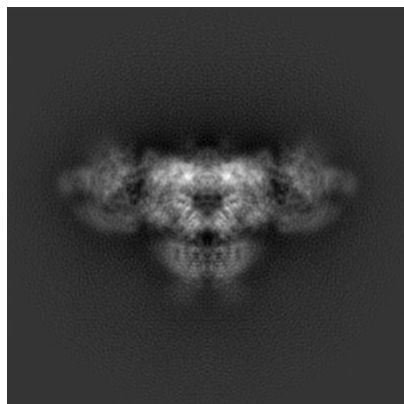
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8389. These allow visual inspection of the internal detail of the map and identification of artifacts.

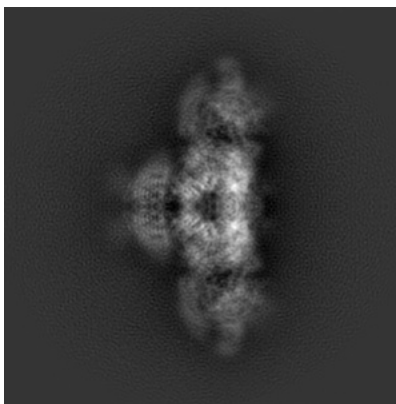
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

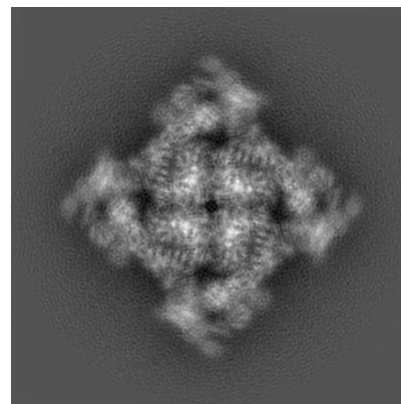
6.1.1 Primary map



X

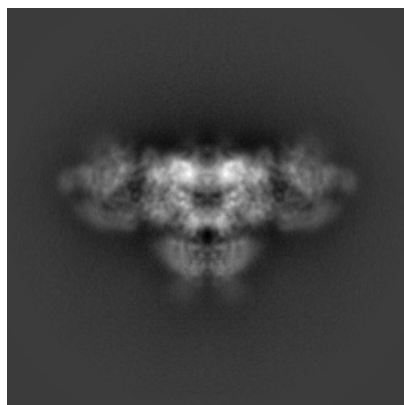


Y

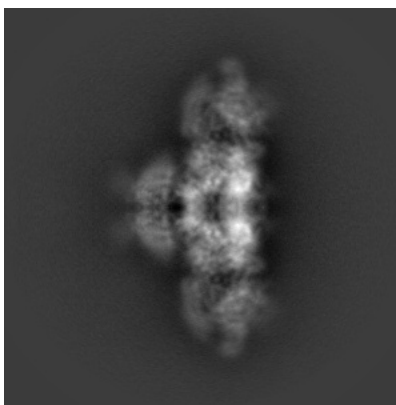


Z

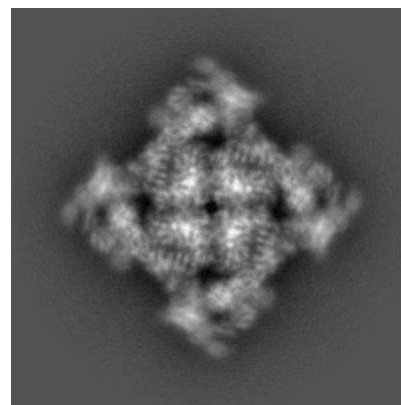
6.1.2 Raw map



X



Y

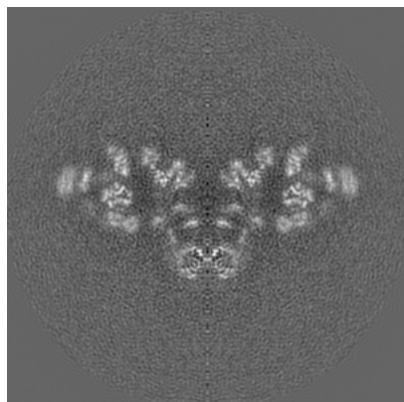


Z

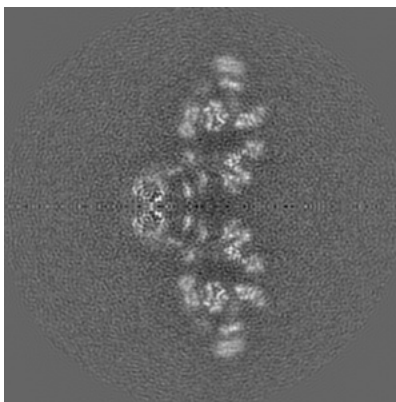
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

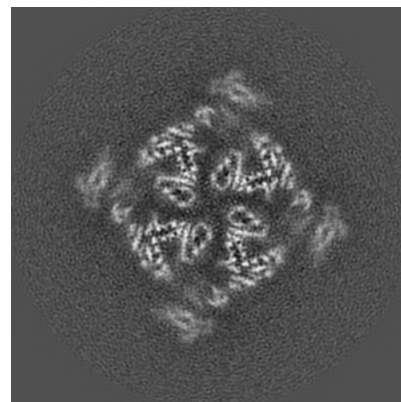
6.2.1 Primary map



X Index: 200

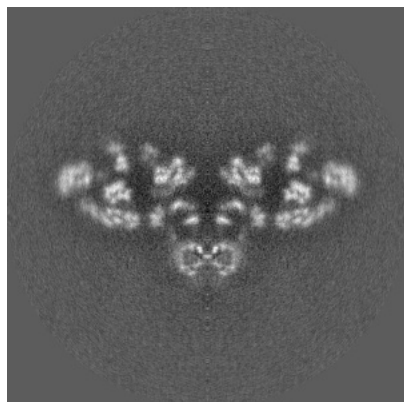


Y Index: 200

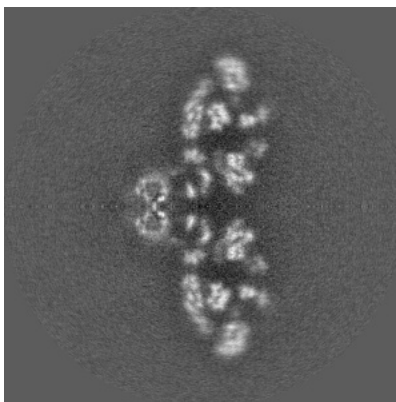


Z Index: 200

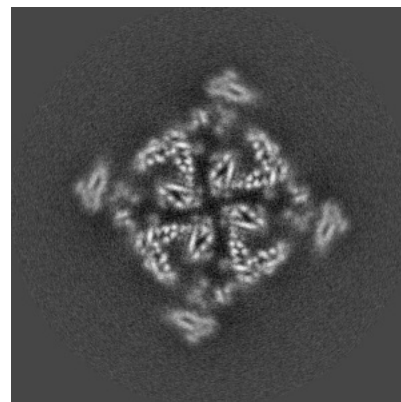
6.2.2 Raw map



X Index: 200



Y Index: 200

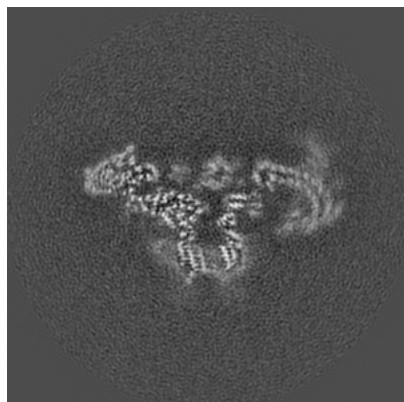


Z Index: 200

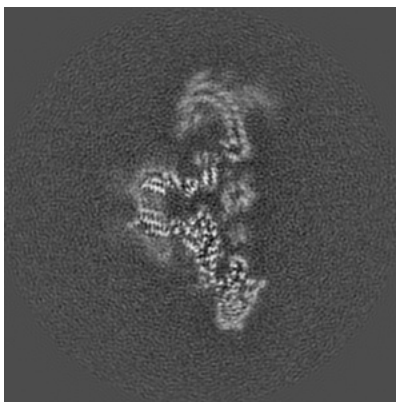
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

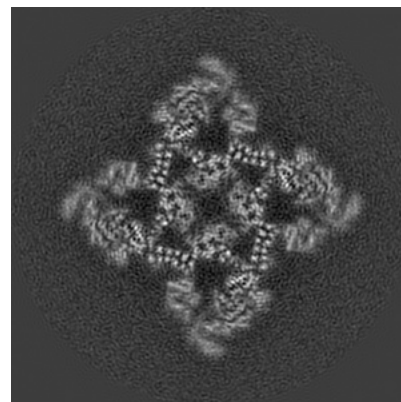
6.3.1 Primary map



X Index: 225

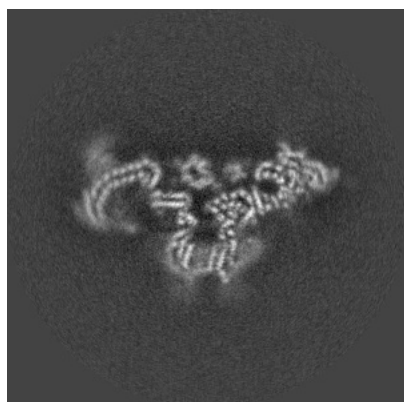


Y Index: 175

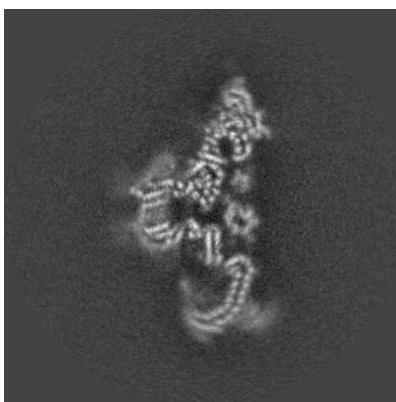


Z Index: 226

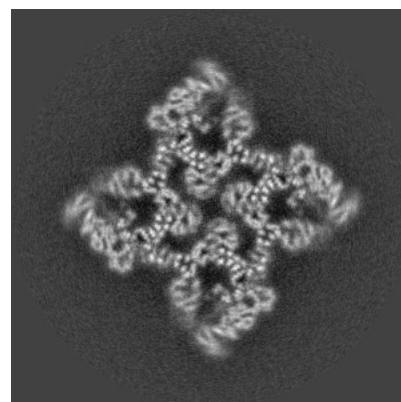
6.3.2 Raw map



X Index: 175



Y Index: 225

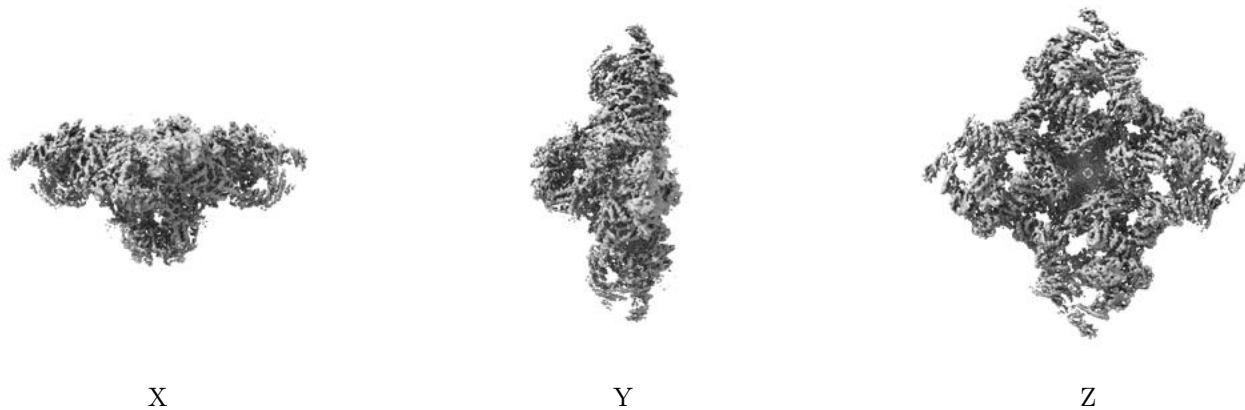


Z Index: 234

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

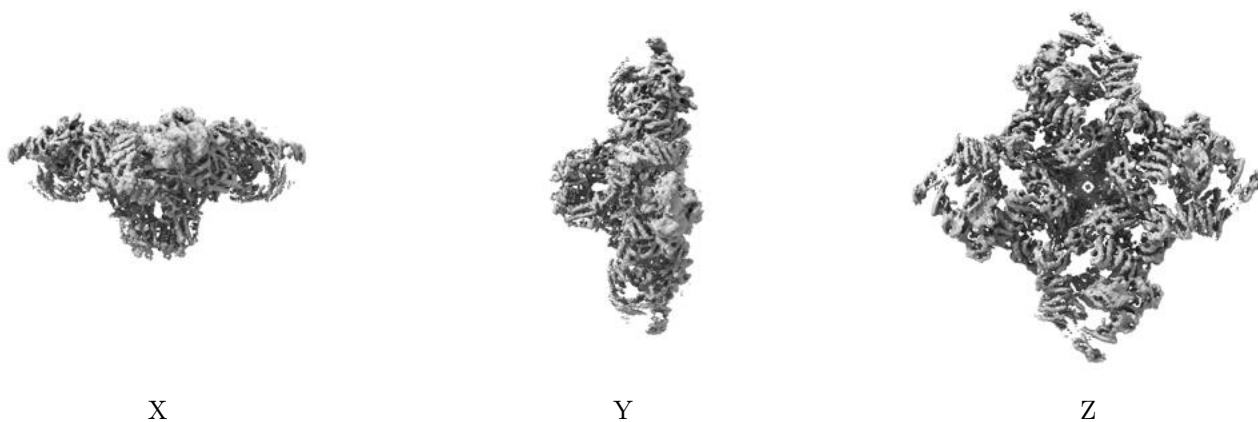
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

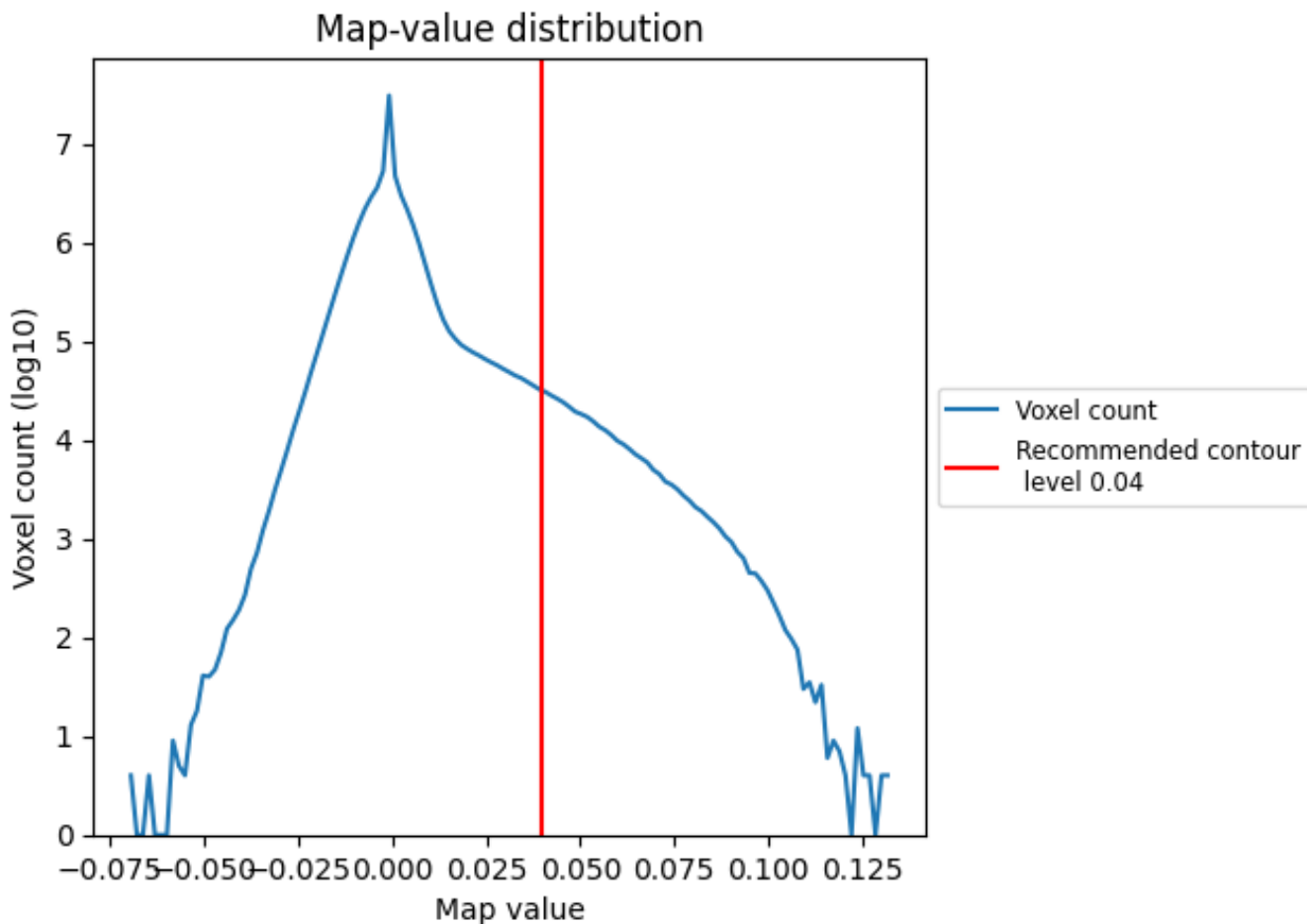
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

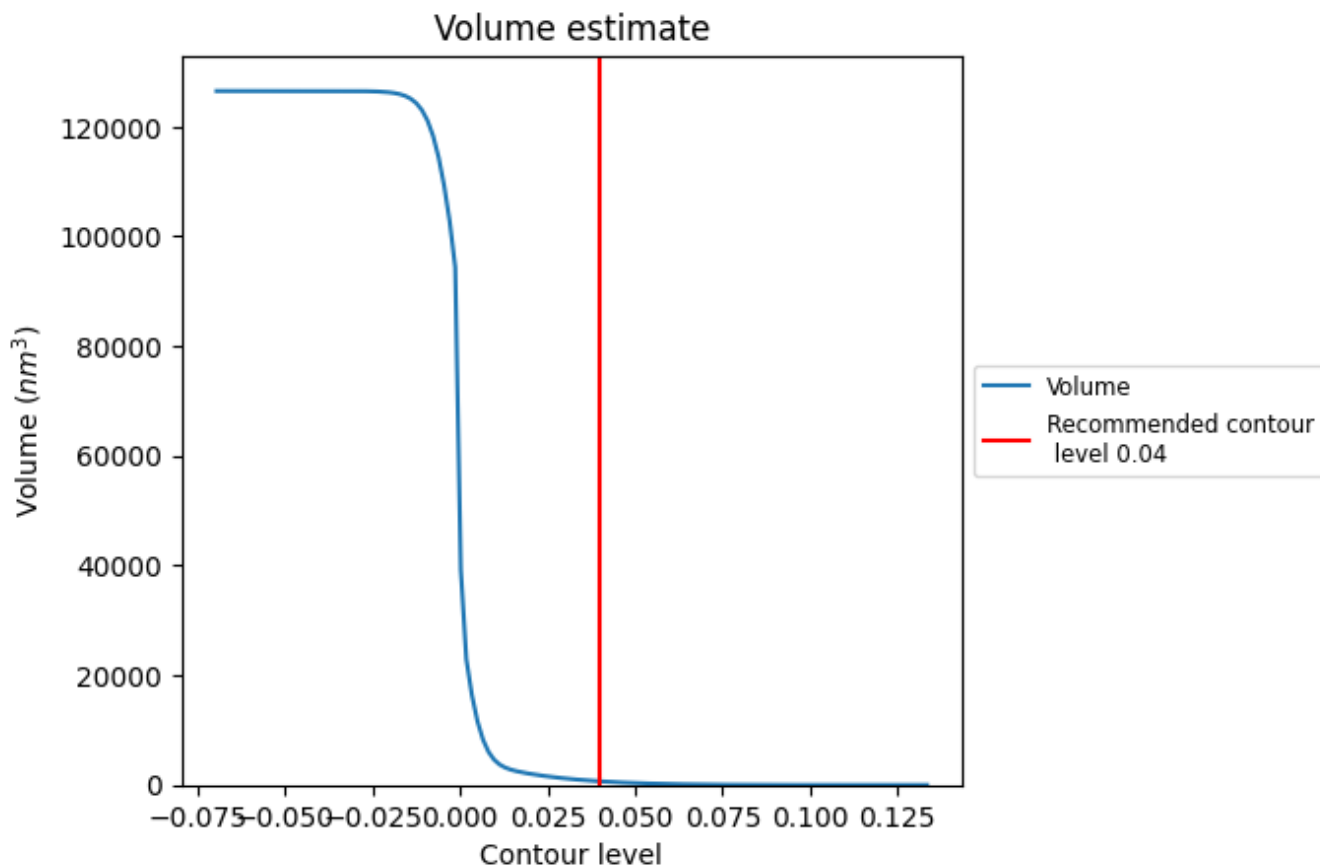
This section contains the results of statistical analysis of the map.

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.

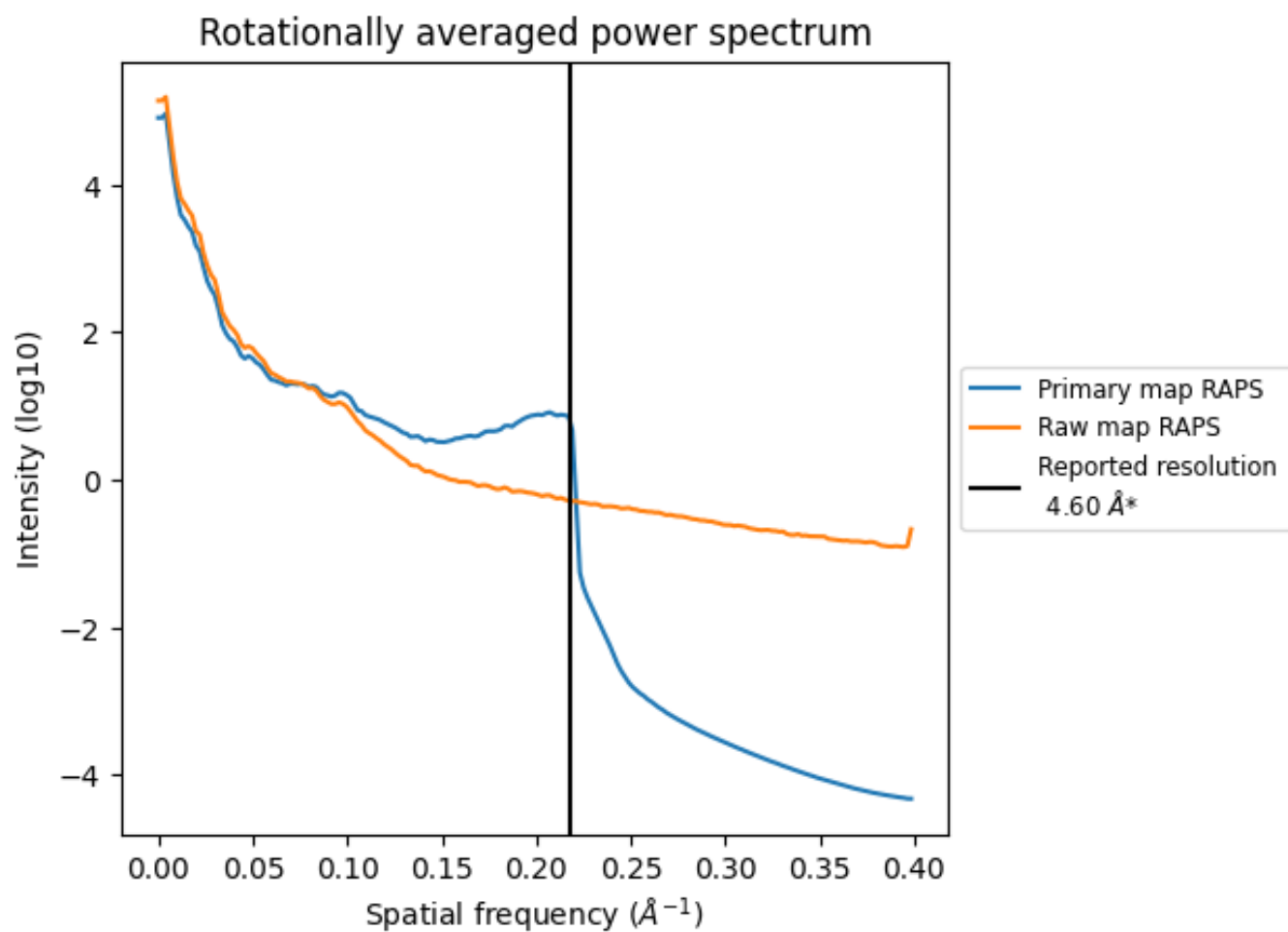
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 666 nm^3 ; this corresponds to an approximate mass of 601 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 i

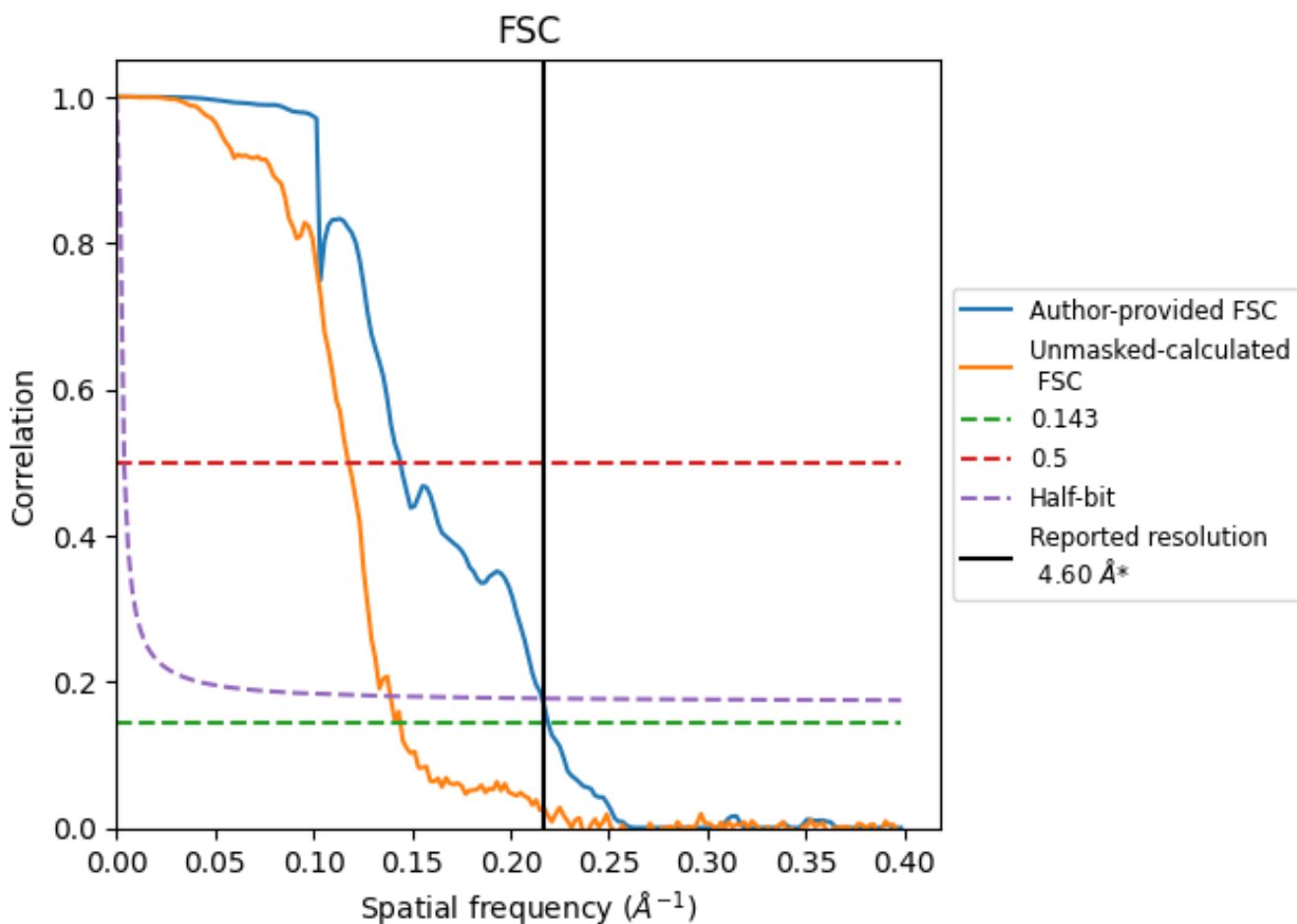


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 \AA^{-1}

8.2 Resolution estimates [i](#)

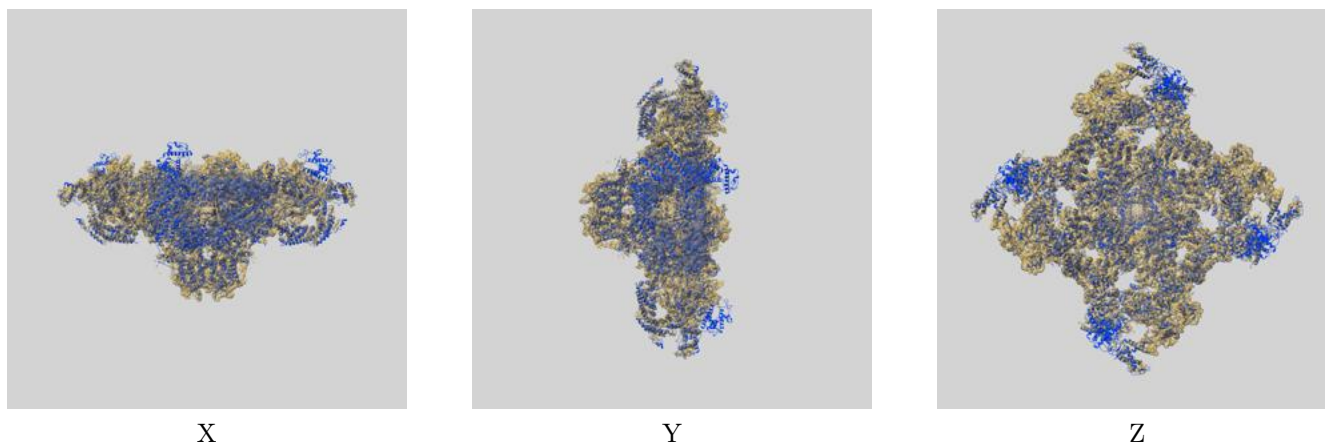
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.56	6.94	4.63
Unmasked-calculated*	6.93	8.49	7.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.93 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

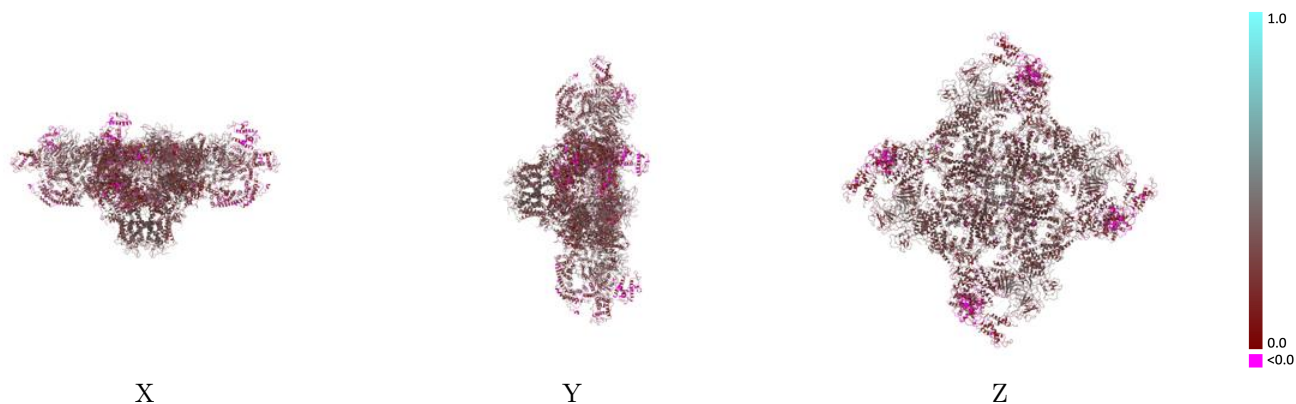
This section contains information regarding the fit between EMDB map EMD-8389 and PDB model 5TAY. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



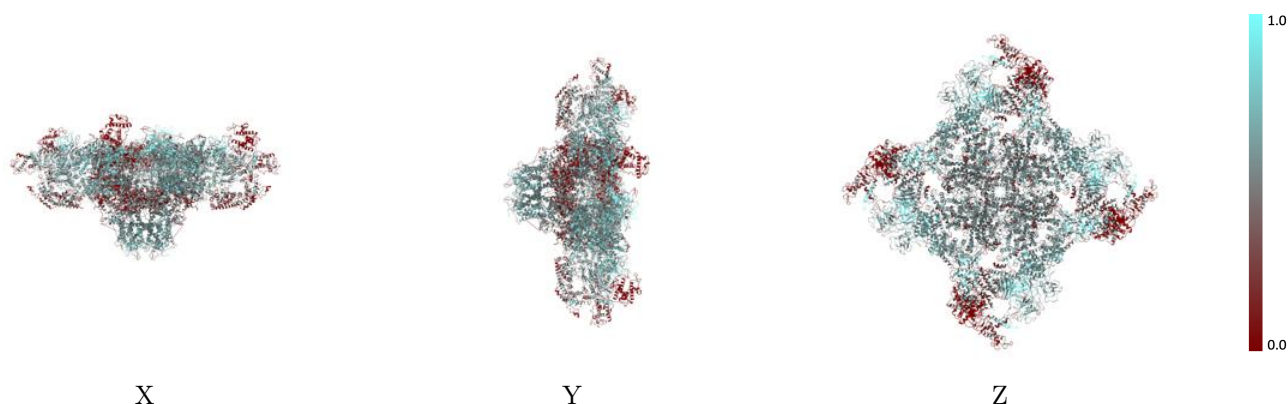
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



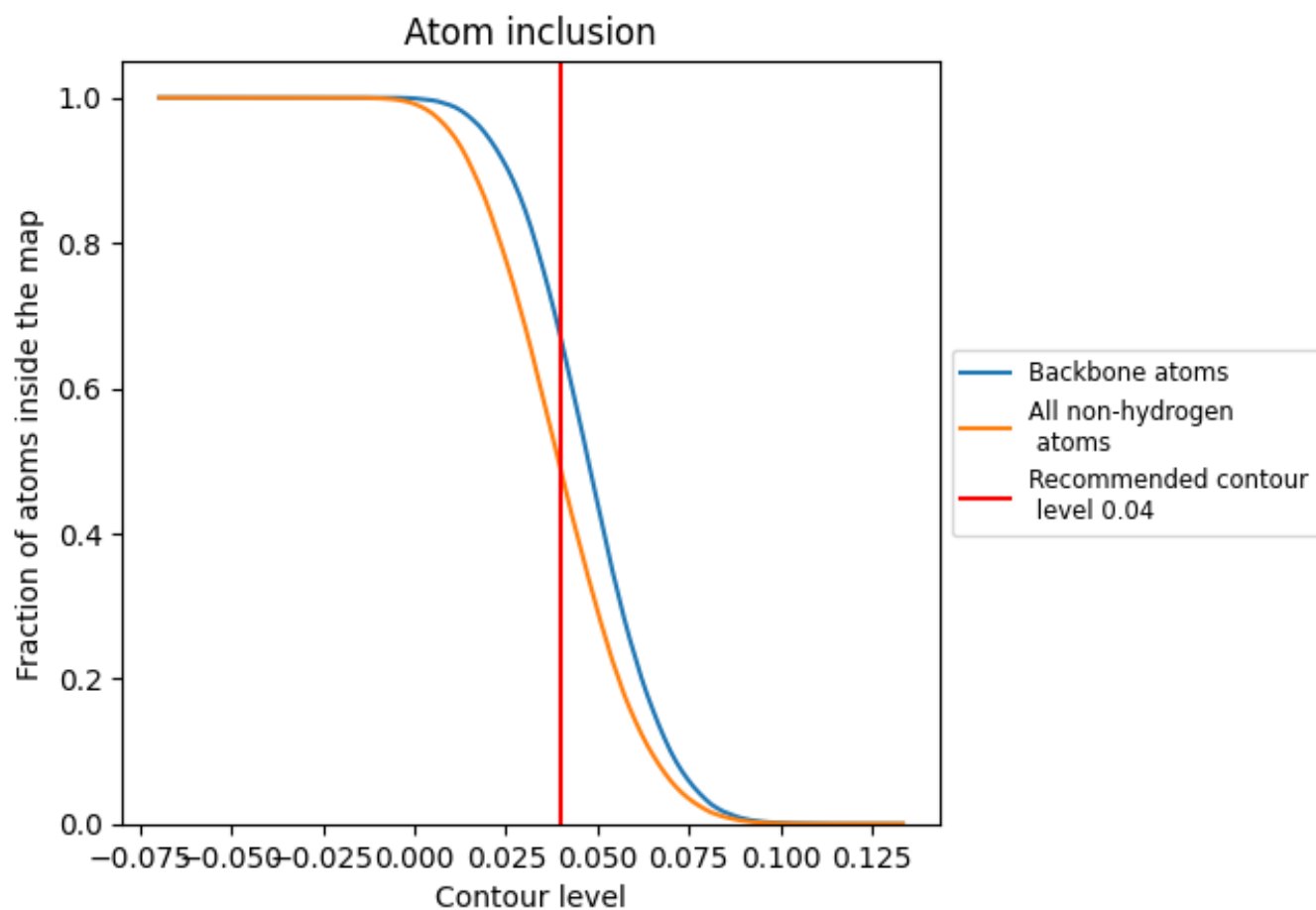
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4873	0.2640
A	0.5658	0.3270
B	0.4909	0.2670
E	0.4802	0.2570
F	0.5670	0.3310
G	0.4887	0.2650
H	0.5670	0.3300
I	0.4808	0.2590
J	0.5645	0.3280

