



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:21 PM UTC

PDB ID : 5T9S / pdb_00005t9s
EMDB ID : EMD-8375
Title : Structure of rabbit RyR1 (Ca²⁺-only dataset, class 4)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-09
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

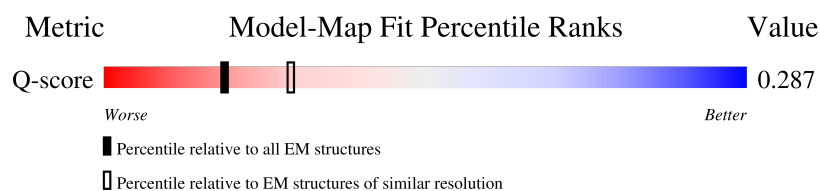
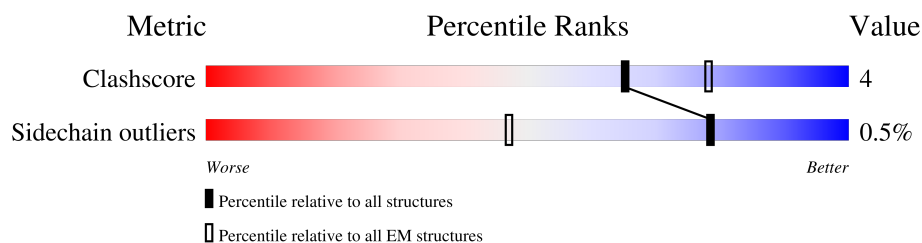
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4676	

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Mol	Chain	Length	Quality of chain			
2	E	4676	32%			
			80%9%11%			
2	G	4676	32%			
			80%9%11%			
2	I	4676	32%			
			80%9%11%			

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

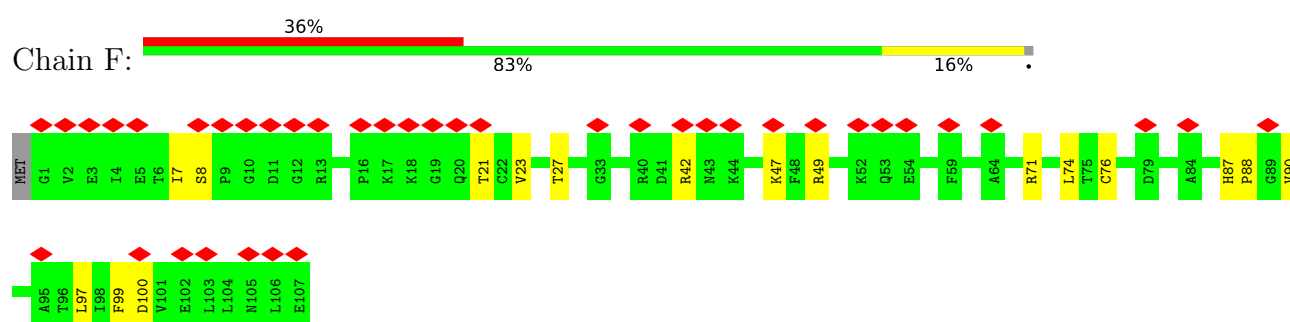
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

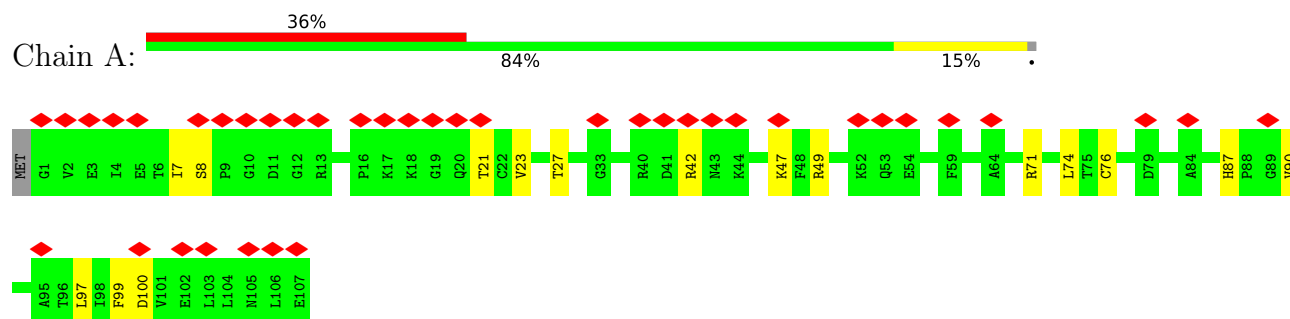
3 Residue-property plots [i](#)

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.

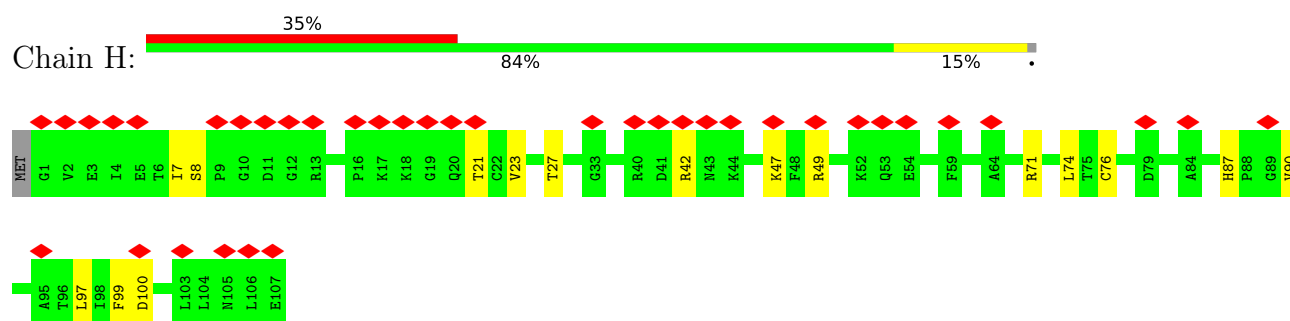
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



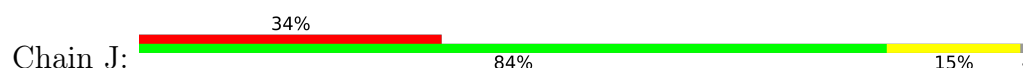
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

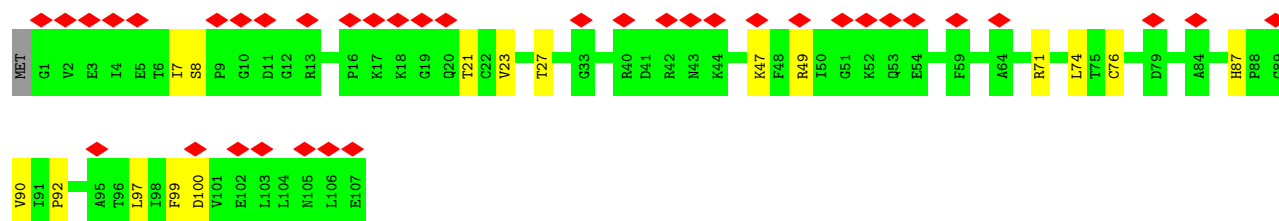


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

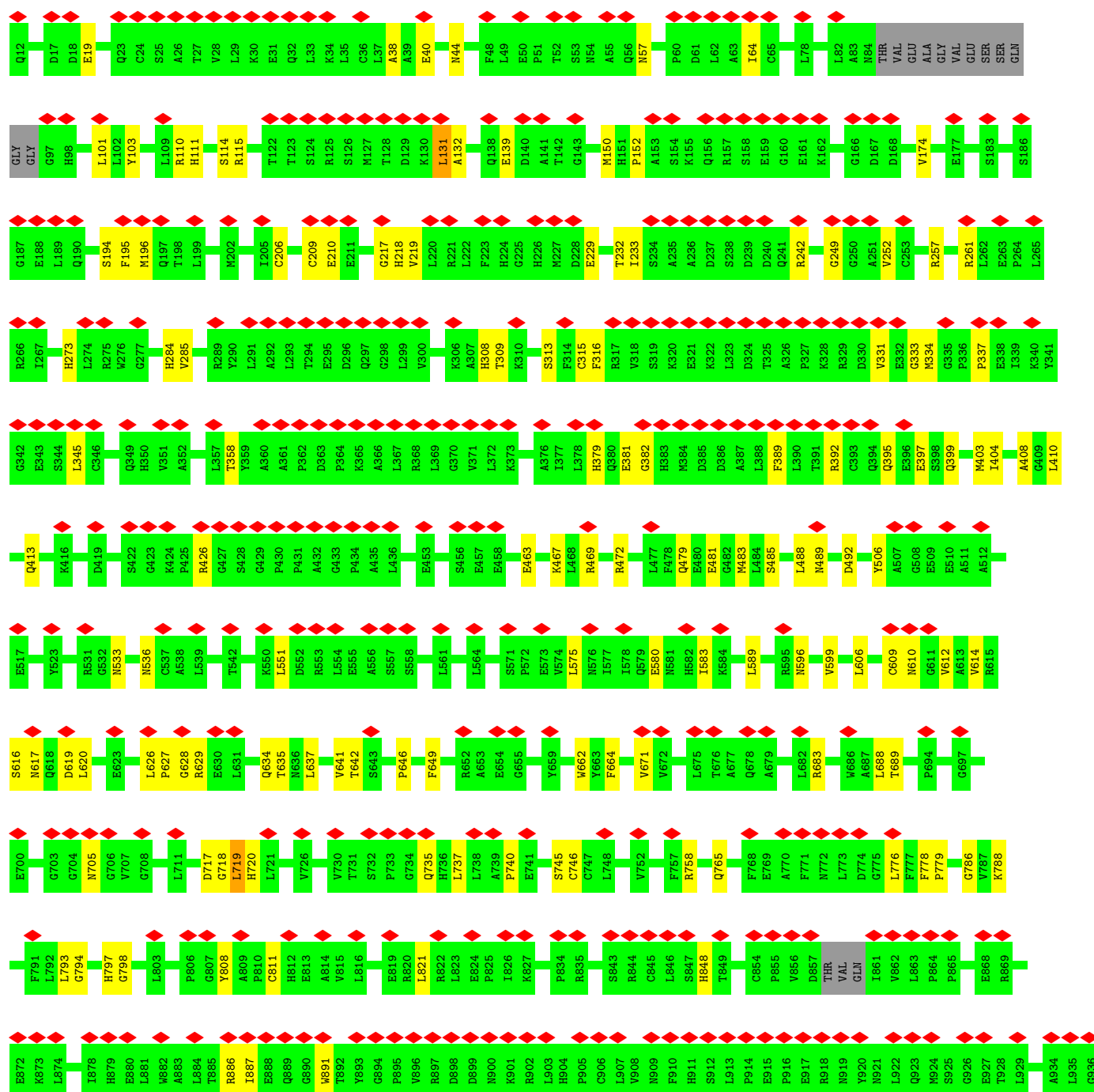
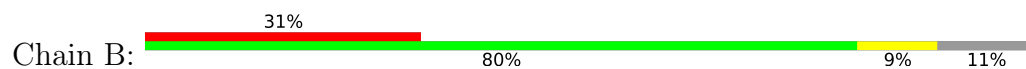


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



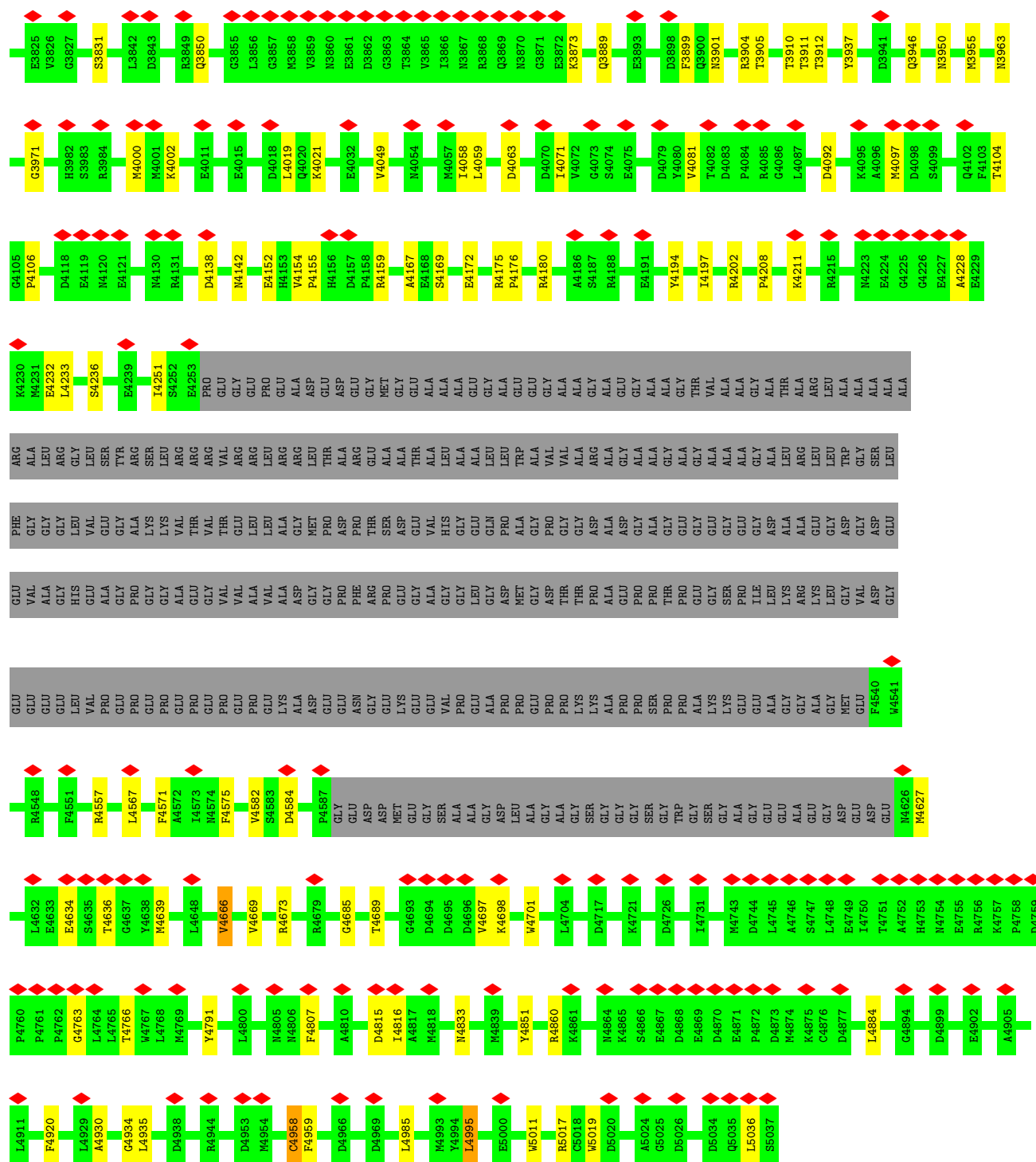


• Molecule 2: Ryanodine receptor 1

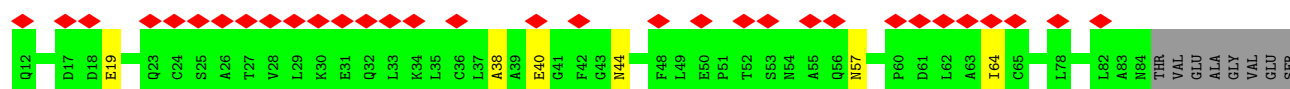
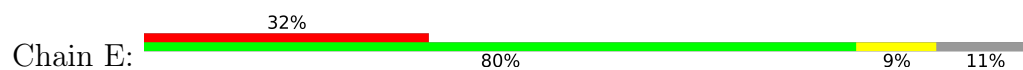




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X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2680	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	P2735	D2736	P2737	P2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	P2754	L2755	N2756	K2757	P2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765						
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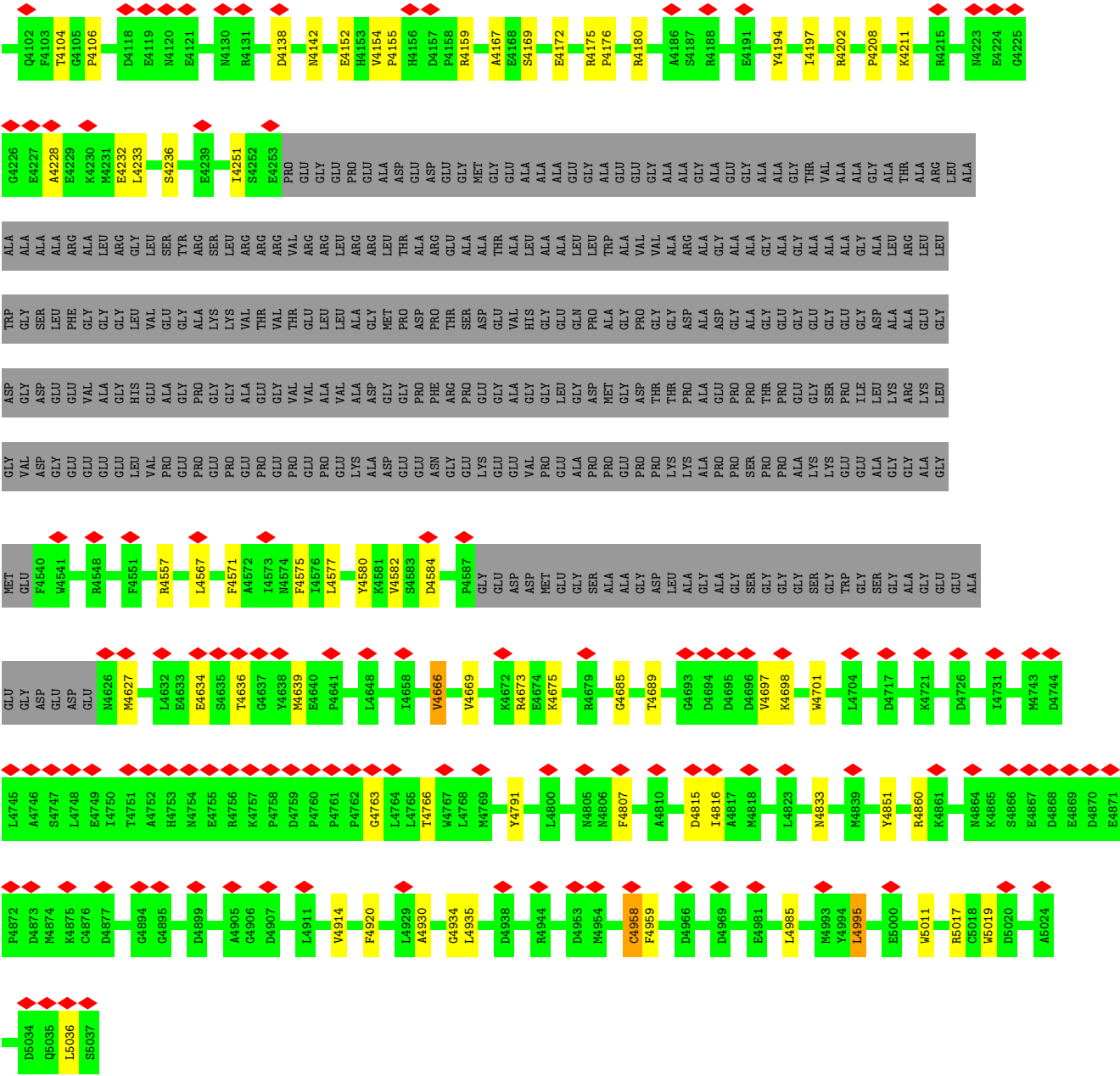
• Molecule 2: Ryanodine receptor 1



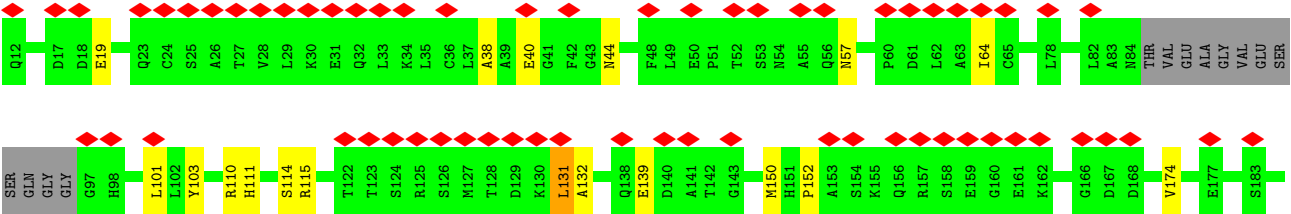
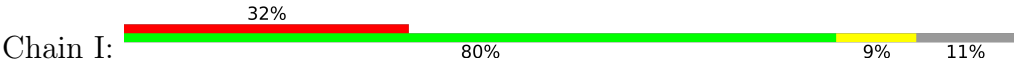
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H797	G798	L803	P806	G807	Y808	A809	P810	C811	H812	E813	A814	V815	L816	E819	T820	L821	R822	L823	E824	P825	I826	K827	R835	S843	R844	C845	L846	S847	H848	T849	R850	C854	P855	V856	D857	THR	VAL	GLN	I861	V862	L863	P864	P865	E868	R869	E872	K873	L874	I878	H879							
E880	L881	W882	A883	L884	T885	R886	L887	E888	Q889	G890	W891	T892	Y893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	M924	S925	G926	T928	L929	L933	A934	L935	C936	C937	H938	V939	G940	M941
A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	M960	M961	S962	N963	G964	Y965	K966	P967	A968	P969	L970	D971	N972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	R987	L988	A989	D999	Q1003	G1004	A1009	VAL	GLN	ASP	ILE	PRO	ALA		

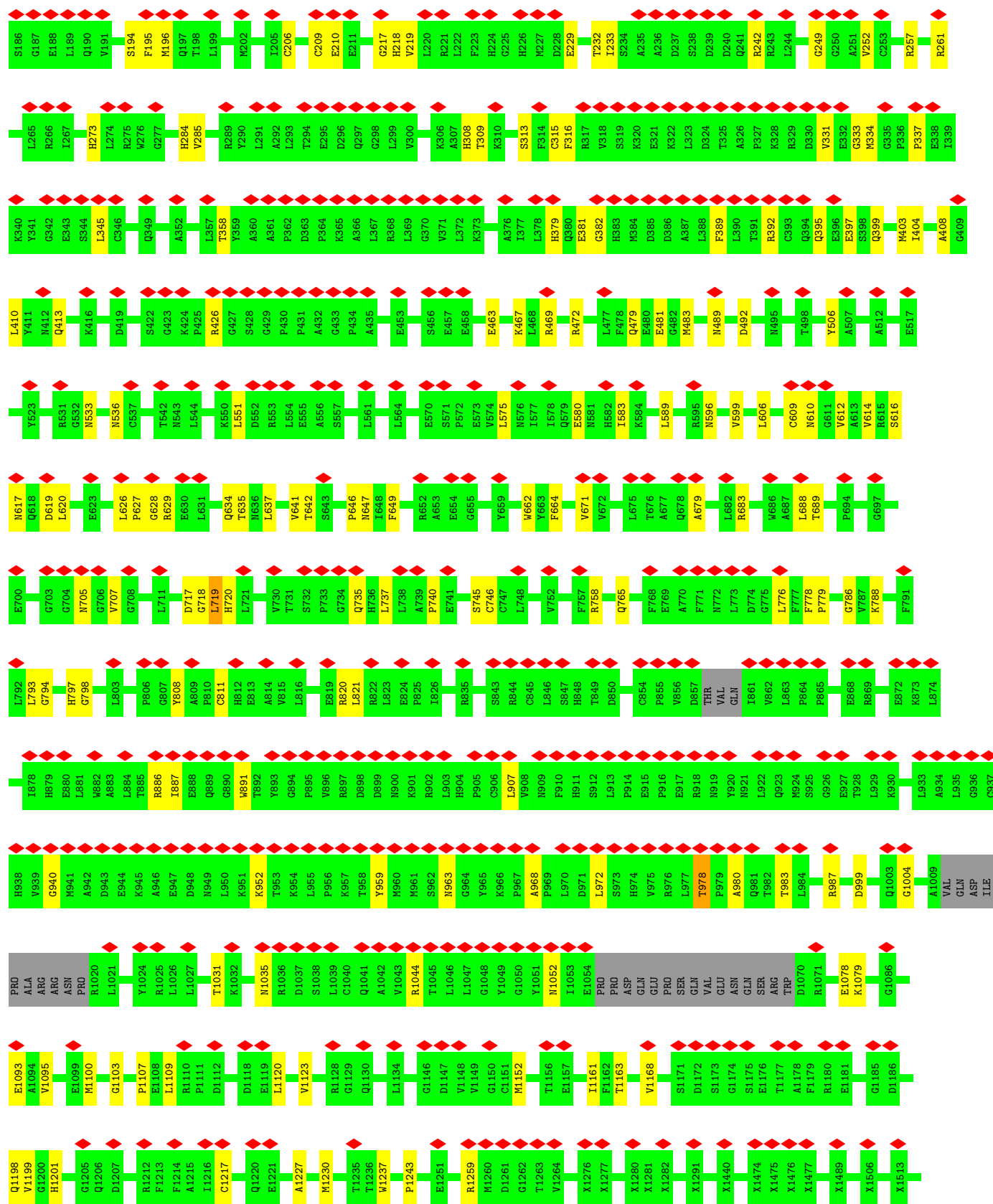


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D3943	E3789	S3668	X3558	X3433	X3355	X3276	X3201	X3043	X2940	E2820	E2760
N3805		D3676	X3559	X3434	X3356	X3277	X3202	X3044	X2941	E2821	V2761
N3806			X3560	X3435	X3357	X3278	X3203	X3045	X2942	T2822	T2762
G3807			X3561	X3436	X3358	X3279	X3204	X3046	X2943	H2763	
M3816			X3562	X3437	X3359	X3280	X3205	X3047	X2944		
L3817			X3563	X3438	X3360	X3281	X3206	X3048	X2945		
D3822			X3564	X3439	X3361	X3282	X3207	X3049	X2946	E2824	E2764
E3825			X3565	X3440	X3362	X3283	X3208	X3050	X2947	K2825	K2765
V3826			X3566	X3441	X3363	X3284	X3209	X3051	X2948	K2826	K2766
G3827			X3567	X3442	X3364	X3285	X3210	X3052	X2949	R2827	A2767
S3831			X3568	X3443	X3365	X3286	X3211	X3053	X2950	E2828	F2768
E4011			X3569	X3444	X3366	X3287	X3212	X3054	X2951	G2829	D2769
E4015			X3570	X3445	X3367	X3288	X3213	X3055	X2952	E2830	K2770
P4018			X3571	X3446	X3368	X3289	X3214			GLU	T2771
L4019			X3572	X3447	X3369	X3290	X3215			GLU	Q2772
Q4020			X3573	X3448	X3370	X3291	X3216			ARG	Q2773
K4021			X3574	X3449	X3371	X3292	X3217			THR	W2774
E4032			X3575	X3450	X3372	X3293	X3218			GLU	W2775
V4049			X3576	X3451	X3373	X3294	X3219			LYS	S2776
M4054			X3577	X3452	X3374	X3295	X3220			LYS	V2777
L4057			X3578	X3453	X3375	X3296	X3221			THR	G2778
L4058			X3579	X3454	X3376	X3297	X3222			ARG	E2779
L4059			X3580	X3455	X3377	X3298	X3223			LYS	I2780
D4063			X3581	X3456	X3378	X3299	X3224			LYS	W2781
D4070			X3582	X3457	X3379	X3300	X3225			ILE	E2782
L4071			X3583	X3458	X3380	X3301				GLN	D2783
V4072			X3584	X3459	X3381	X3302				ALA	E2784
G4073			X3585	X3460	X3382	X3303				GLN	L2785
S4074			X3586	X3461	X3383	X3304				THR	ASP
N3870			X3587	X3462	X3384	X3305				ASP	P2786
E4075			X3588	X3463	X3385	X3306				PIR	K2787
D4079			X3589	X3464	X3386	X3307				ARG	T2788
Y4080			X3590	X3465	X3387	X3308				GLU	H2789
V4081			X3591	X3466	X3388	X3309				GLY	P2790
T4082			X3592	X3467	X3389	X3310				Y2855	H2790
D4083			X3593	X3468	X3390	X3311				N2856	L2791
P4084			X3594	X3469	X3391	X3312				P2857	R2792
L4085			X3595	X3470	X3392	X3313				Q2858	P2793
G4086			X3596	X3471	X3393	X3314				P2859	T2794
L4087			X3597	X3472	X3394	X3315				E2860	K2795
D4092			X3598	X3473	X3395	X3316				D2861	T2796
H4097			X3599	X3474	X3396	X3317				L2862	F2797
D4098			X3600	X3475	X3397	X3318				S2863	S2798
S4099			X3601	X3476	X3398	X3319				G2864	E2799
			X3602	X3477	X3399	X3320				V2865	K2800
			X3603	X3478	X3400	X3321				D2866	D2801
			X3604	X3479	X3401	X3322				L2867	K2802
			X3605	X3480	X3402	X3323				S2868	E2803
			X3606	X3481	X3403	X3324				R2869	T2804
			X3607	X3482	X3404	X3325				E2870	V2805
			X3608	X3483	X3405	X3326				L2871	K2806
			X3609	X3484	X3406	X3327				Q2872	W2807
			X3610	X3485	X3407	X3328				A2873	F2808
			X3611	X3486	X3408	X3329				M2874	T2809
			X3612	X3487	X3409	X3330				K2810	E2811
			X3613	X3488	X3410	X3331				L2811	S2812
			X3614	X3489	X3411	X3332				G2812	L2813
			X3615	X3490	X3412	X3333				Y2815	A2816
			X3616	X3491	X3413	X3334				T2817	
			X3617	X3492	X3414	X3335					
			X3618	X3493	X3415	X3336					
			X3619	X3494	X3416	X3337					
			X3620	X3495	X3417	X3338					
			X3621	X3496	X3418	X3339					
			X3622	X3497	X3419	X3340					
			X3623	X3498	X3420	X3341					
			X3624	X3499	X3421	X3342					
			X3625	X3500	X3422	X3343					
			X3626	X3501	X3423	X3344					
			X3627	X3502	X3424	X3345					
			X3628	X3503	X3425	X3346					
			X3629	X3504	X3426	X3347					
			X3630	X3505	X3427	X3348					
			X3631	X3506	X3428	X3349					
			X3632	X3507	X3429	X3350					
			X3633	X3508	X3430	X3351					
			X3634	X3509	X3431	X3352					
			X3635	X3510	X3432	X3353					
			X3636	X3511	X3433	X3354					
			X3637	X3512	X3434	X3355					
			X3638	X3513	X3435	X3356					
			X3639	X3514	X3436	X3357					
			X3640	X3515	X3437	X3358					
			X3641	X3516	X3438	X3359					
			X3642	X3517	X3439	X3360					
			X3643	X3518	X3440	X3361					
			X3644	X3519	X3441	X3362					
			X3645	X3520	X3442	X3363					
			X3646	X3521	X3443	X3364					
			X3647	X3522	X3444	X3365					
			X3648	X3523	X3445	X3366					
			X3649	X3524	X3446	X3367					
			X3650	X3525	X3447	X3368					
			X3651	X3526	X3448	X3369					
			X3652	X3527	X3449	X3370					
			X3653	X3528	X3450	X3371					
			X3654	X3529	X3451	X3372					
			X3655	X3530	X3452	X3373					
			X3656	X3531	X3453	X3374					
			X3657	X3532	X3454	X3375					
			X3658	X3533	X3455	X3376					
			X3659	X3534	X3456	X3377					
			X3660	X3535	X3457	X3378					
			X3661	X3536	X3458	X3379					
			X3662	X3537	X3459	X3380					
			X3663	X3538	X3460	X3381					
			X3664	X3539	X3461	X3382					
			X3665	X3540	X3462	X3383					
			X3666	X3541	X3463	X3384					
			X3667	X3542	X3464	X3385					
			X3668	X3543	X3465	X3386					
			X3669	X3544	X3466	X3387					
			X3670	X3545	X3467	X3388					
			X3671	X3546	X3468	X3389					
			X3672	X3547	X3469	X3390					
			X3673	X3548	X3470	X3391					
			X3674	X3549	X3471	X3392					
			X3675	X3550	X3472	X3393					
			X3676	X3551	X3473	X3394					
			X3677	X3552	X3474	X3395					
			X3678	X3553	X3475	X3396					
			X3679	X3554	X3476	X3397					
			X3680	X3555	X3477	X3398					
			X3681	X3556	X3478	X3399					
			X3682	X3557	X3479	X3400					
			X3683	X3558	X3480	X3401					
			X3684	X3559	X3481	X3402					
			X3685	X3560	X3482	X3403					
			X3686	X3561	X3483	X3404					
			X3687	X3562	X3484	X3405					
			X3688	X3563	X3485	X3406					
			X3689	X3564	X3486	X3407					
			X3690	X3565	X3487	X3408					
			X3691	X3566	X3488	X3409					
			X3692	X3567	X3489	X3410					
			X3693	X3568	X3490	X3411					
			X3694	X3569	X3491	X3412					
			X3695	X3570	X3492	X3413					
			X3696	X3571	X3493	X3414					
			X3697	X3572	X3494	X3415					
			X3698	X3573	X3495	X3416					
			X3699	X3574	X3496	X3417					
			X3700	X3575	X3497	X3418					
			X3701	X3576	X3498	X3419					
			X3702	X3577	X3499	X3420					
			X3703	X3578	X3500	X3421					
			X3704	X3579	X3501	X3422					
			X3705	X3580	X3502	X3423					
			X3706	X3581	X3503	X3424					
			X3707	X3582	X3504	X3425					
			X3708	X3583	X3505	X3426					
			X3709	X3584	X3506	X3427					
			X3710	X3585	X3507	X3428					
</											



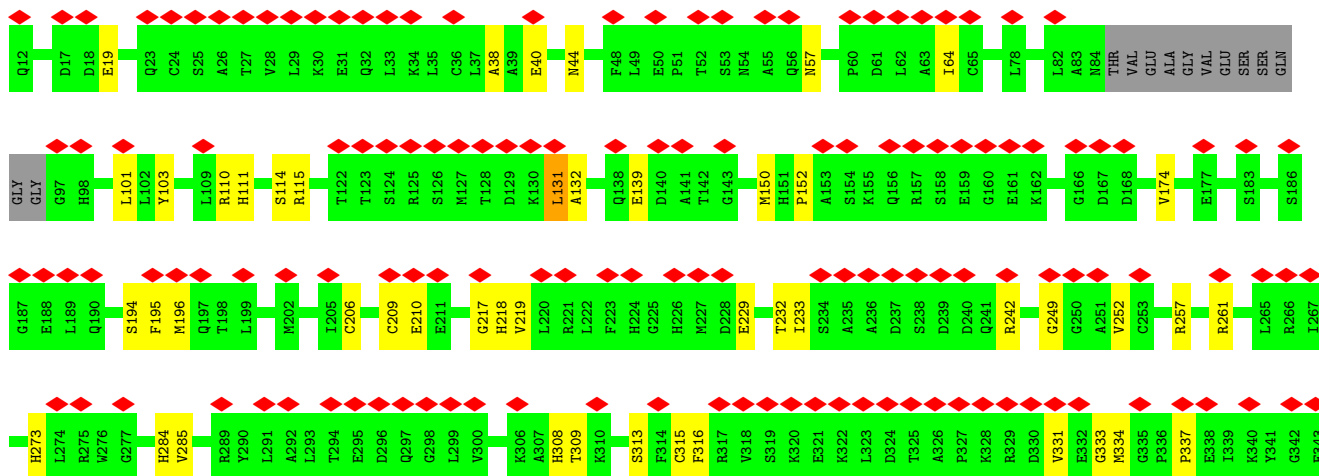
• Molecule 2: Ryanodine receptor 1



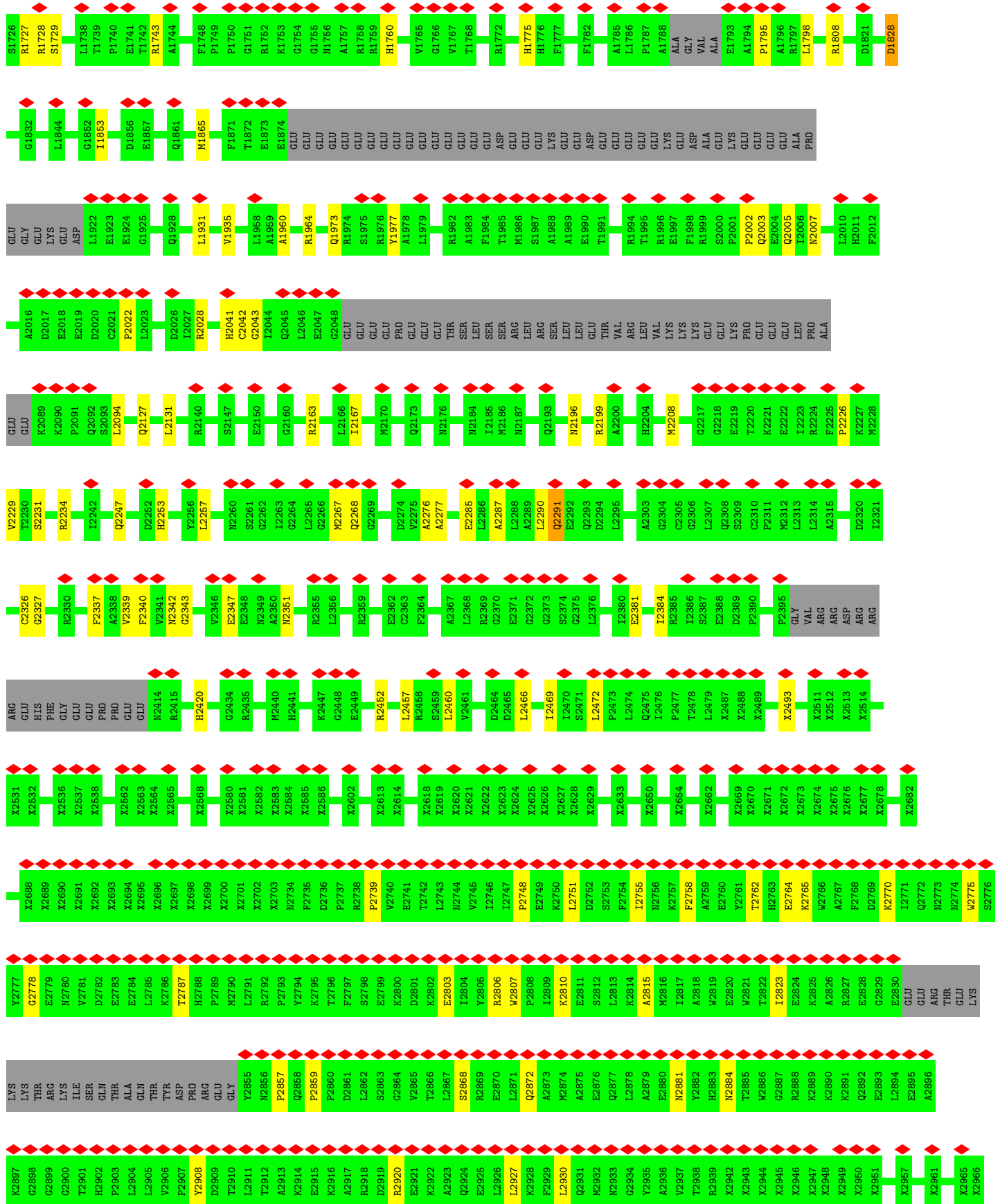




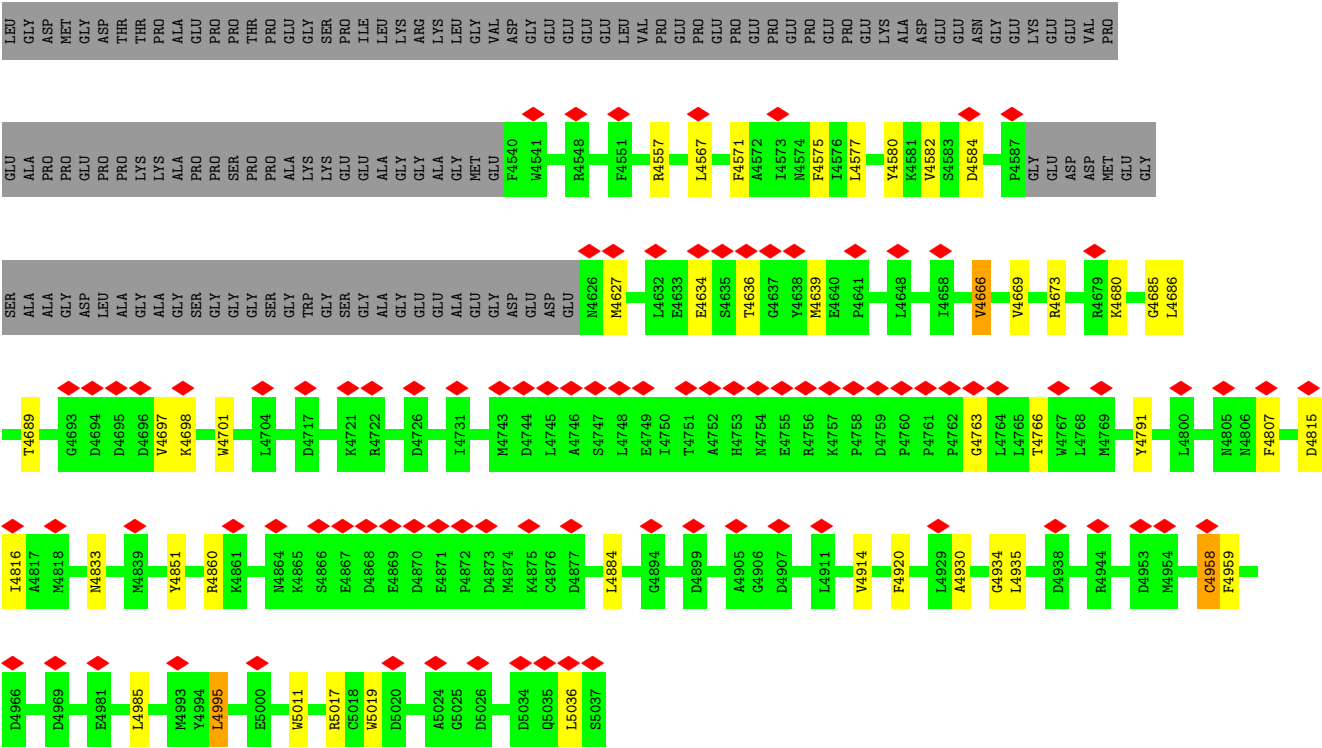
GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	T2855	T2856	P2857	Q2858	P2859	P2860	L2861	S2863	G2864	T2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	T2882	H2883	N2884	T2885	W2886	G2887	R2888	L2889	K2890	L2891
X2892	E2893	L2894	E2895	X2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	K2921	K2922	A2923	Q2924	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	
X2957	X2961	X2965	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3006	X3013	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3026	X3027	X3032	X3035	X3036	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3053	X3054	X3055									
X3058	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3144	X3145	X3148	X3149	X3153	X3154	X3155	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3177	X3178	X3179	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3204	X3207	X3208	X3211	X3212	X3213	X3214	X3215	X3216											
X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3284	X3285	X3286	X3287	X3288	X3289	X3290		
X3291	X3292	X3293	X3294	X3295	X3296	X3301	X3306	X3309	X3313	X3314	X3315	X3318	X3321	X3322	X3325	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368								
X3369	X3370	X3371	X3372	X3373	X3374	X3378	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3402	X3403	X3406	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3424	X3425	X3432	X3433	X3434	X3435	X3436	X3439	X3440	X3443	X3446										
X3449	X3450	X3453	X3454	X3457	X3463	X3464	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3538	X3539	X3540	X3547	X3548	X3549	X3550	X3551	X3552	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	X3592	X3593	X3597	X3600	X3605	X3608	X3609	X3610	X3611	X3612	X3613	T3639	N3643	L3644	P3645	F3653	A3659	L3662	E3665	D3666	H3667	S3668	D3676	K3679	A3680	G3681	E3682	Q3683	E3684	E3685													
E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	T3711	E3712	K3713	S3714	K3715	L3716	D3717	E3718	D3719	Y3720	E3737	G3738	C3739	E3740	K3741	GLY	GLU	ALA	GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	T3772	E3773	K3778	V3779	L3780	Q3781	S3784	K3787	G3788	E3789	L3805	N3806	G3807	K3815	M3816	L3817								
D3822	E3825	V3826	G3827	S3831	L3842	D3843	Q3850	G3855	L3856	G3857	M3858	V3859	N3860	E3861	D3862	G3863	T3864	V3865	L3866	R3867	R3868	Q3869	N3870	G3871	E3872	K3873	E3893	D3898	F3899	Q3900	N3901	R3904	T3905	T3910	T3911	T3912	Y3937	D3941	Q3946	F4103	T4104	G4105	P4106	D4118	E4119													
R3984	D3987	M4000	M4001	K4002	E4011	E4015	D4018	L4019	Q4020	K4021	E4032	V4049	N4054	M4057	I4058	L4059	D4063	D4070	I4071	V4072	S4074	E4075	D4079	Y4080	V4081	T4082	D4083	P4084	R4085	G4086	L4087	D4092	M4097	D4098	S4099	Q4102	F4103	T4104	G4105	P4106	D4118	E4119																
N4120	E4121	N4130	R4131	D4138	N4142	E4152	H4153	V4154	P4155	H4156	P4157	P4158	R4159	A4167	E4168	S4169	E4172	R4175	P4176	R4180	A4186	S4187	R4188	E4191	Y4194	I4197	R4202	P4208	K4211	R4215	M4223	E4224	G4225	G4226	E4227	A4228	E4229	F4230	H4231	L4232	L4233																	











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	0.141	Depositor
Minimum map value	-0.064	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/834	0.45	0/1123
1	F	0.20	0/834	0.45	0/1123
1	H	0.20	0/834	0.45	0/1123
1	J	0.20	0/834	0.45	0/1123
2	B	0.21	0/25428	0.52	5/34534 (0.0%)
2	E	0.21	0/25428	0.52	5/34534 (0.0%)
2	G	0.21	0/25428	0.52	5/34534 (0.0%)
2	I	0.21	0/25428	0.52	5/34534 (0.0%)
All	All	0.21	0/105048	0.52	20/142628 (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
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	68

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1828	ASP	CA-C-N	5.96	125.97	119.89
2	I	1828	ASP	C-N-CA	5.96	125.97	119.89
2	E	1828	ASP	CA-C-N	5.96	125.96	119.89
2	E	1828	ASP	C-N-CA	5.96	125.96	119.89
2	G	1828	ASP	CA-C-N	5.95	125.96	119.89
2	G	1828	ASP	C-N-CA	5.95	125.96	119.89
2	B	1828	ASP	CA-C-N	5.90	125.91	119.89
2	B	1828	ASP	C-N-CA	5.90	125.91	119.89
2	E	4639	MET	CA-C-N	5.16	134.38	121.80
2	E	4639	MET	C-N-CA	5.16	134.38	121.80
2	G	4639	MET	CA-C-N	5.15	134.37	121.80
2	G	4639	MET	C-N-CA	5.15	134.37	121.80
2	I	4639	MET	CA-C-N	5.15	134.36	121.80
2	I	4639	MET	C-N-CA	5.15	134.36	121.80
2	B	4639	MET	CA-C-N	5.12	134.31	121.80
2	B	4639	MET	C-N-CA	5.12	134.31	121.80
2	G	131	LEU	CA-CB-CG	5.06	134.00	116.30
2	E	131	LEU	CA-CB-CG	5.05	133.96	116.30
2	I	131	LEU	CA-CB-CG	5.04	133.96	116.30
2	B	131	LEU	CA-CB-CG	5.04	133.94	116.30

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	4958	CYS	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	4958	CYS	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	4958	CYS	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	4958	CYS	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	8	0
1	F	818	0	824	9	0
1	H	818	0	824	8	0
1	J	818	0	824	9	0
2	B	29369	0	24721	223	0
2	E	29369	0	24721	219	0
2	G	29369	0	24719	217	0
2	I	29369	0	24721	221	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	120756	0	102178	898	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 4.

All (898) 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:426:ARG:HB2	2:B:506:TYR:HA	1.78	0.66
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.78	0.66
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.78	0.66
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.78	0.65
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.77	0.64
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.80	0.64
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.80	0.63
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.80	0.63
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.31	0.63
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.31	0.63
2:E:627:PRO:O	2:E:629:ARG:NH1	2.32	0.63
2:I:627:PRO:O	2:I:629:ARG:NH1	2.32	0.63
2:B:627:PRO:O	2:B:629:ARG:NH1	2.32	0.62
2:G:627:PRO:O	2:G:629:ARG:NH1	2.32	0.62
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.80	0.62
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.82	0.62
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.82	0.62
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.33	0.62
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.30	0.61
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.33	0.61
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.33	0.61
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.82	0.61
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.82	0.61
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.83	0.61
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.83	0.61
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.83	0.61
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.83	0.61
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.83	0.61
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.33	0.61
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.83	0.61
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.83	0.60
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.30	0.60
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.83	0.60
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.82	0.60
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.82	0.60
2:G:1703:LEU:HB3	2:G:1708:ARG:HH21	1.67	0.60
2:E:379:HIS:HD2	2:E:382:GLY:H	1.49	0.60
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.82	0.60
2:E:4251:ILE:O	2:E:4557:ARG:NH1	2.35	0.60
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.84	0.60
2:G:4251:ILE:O	2:G:4557:ARG:NH1	2.35	0.60
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1703:LEU:HB3	2:B:1708:ARG:HH21	1.67	0.59
2:E:111:HIS:HD2	2:E:114:SER:H	1.48	0.59
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.66	0.59
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.83	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.30	0.59
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.82	0.59
2:B:111:HIS:HD2	2:B:114:SER:H	1.48	0.59
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.84	0.59
2:E:1703:LEU:HB3	2:E:1708:ARG:HH21	1.67	0.59
2:B:379:HIS:HD2	2:B:382:GLY:H	1.49	0.59
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.59
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.66	0.59
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.83	0.59
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.85	0.59
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.83	0.59
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.83	0.59
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.84	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.66	0.59
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.59
2:B:4251:ILE:O	2:B:4557:ARG:NH1	2.35	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.76	0.59
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.84	0.59
2:B:614:VAL:HG22	2:B:616:SER:H	1.68	0.59
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.85	0.59
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.85	0.59
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.85	0.59
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.66	0.59
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.36	0.59
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.85	0.59
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.85	0.58
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.58
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.85	0.58
2:I:4251:ILE:O	2:I:4557:ARG:NH1	2.35	0.58
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.22	0.58
2:G:379:HIS:HD2	2:G:382:GLY:H	1.49	0.58
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.86	0.58
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.85	0.58
2:I:1703:LEU:HB3	2:I:1708:ARG:HH21	1.67	0.58
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.85	0.58
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:614:VAL:HG22	2:E:616:SER:H	1.68	0.58
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.86	0.58
2:I:4233:LEU:HA	2:I:4236:SER:HB3	1.86	0.58
2:G:111:HIS:HD2	2:G:114:SER:H	1.49	0.58
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.86	0.58
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.86	0.58
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.37	0.58
2:G:609:CYS:SG	2:G:610:ASN:N	2.76	0.58
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.86	0.58
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.22	0.58
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.86	0.58
2:I:614:VAL:HG22	2:I:616:SER:H	1.68	0.58
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.22	0.58
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.37	0.58
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.36	0.58
2:I:101:LEU:HB3	2:I:150:MET:HE1	1.86	0.58
2:I:111:HIS:HD2	2:I:114:SER:H	1.48	0.58
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.85	0.58
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.58
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.58
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.37	0.58
2:I:379:HIS:HD2	2:I:382:GLY:H	1.49	0.58
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.86	0.57
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.85	0.57
2:G:101:LEU:HB3	2:G:150:MET:HE1	1.86	0.57
2:G:4233:LEU:HA	2:G:4236:SER:HB3	1.86	0.57
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.35	0.57
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.85	0.57
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.37	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.76	0.57
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.35	0.57
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.70	0.57
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.87	0.57
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.86	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.36	0.57
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.38	0.57
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.36	0.57
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.38	0.57
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.38	0.57
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.70	0.57
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.38	0.57
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.30	0.57
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.38	0.57
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.87	0.57
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.57
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.38	0.57
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.87	0.57
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.70	0.56
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.38	0.56
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.87	0.56
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.56
2:E:4233:LEU:HA	2:E:4236:SER:HB3	1.86	0.56
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.87	0.56
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.38	0.56
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.38	0.56
2:B:4233:LEU:HA	2:B:4236:SER:HB3	1.86	0.56
2:E:101:LEU:HB3	2:E:150:MET:HE1	1.86	0.56
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.86	0.56
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.38	0.56
2:G:614:VAL:HG22	2:G:616:SER:H	1.68	0.56
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.87	0.56
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.39	0.56
2:E:626:LEU:HG	2:E:628:GLY:H	1.70	0.56
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.88	0.56
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.38	0.56
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.38	0.56
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.35	0.56
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.88	0.56
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.88	0.56
2:E:217:GLY:O	2:E:261:ARG:NH1	2.39	0.56
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.88	0.56
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.39	0.56
2:G:626:LEU:HG	2:G:628:GLY:H	1.70	0.56
2:B:217:GLY:O	2:B:261:ARG:NH1	2.39	0.56
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.39	0.56
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.38	0.56
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.89	0.55
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.39	0.55
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.55
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.40	0.55
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.87	0.55
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.39	0.55
2:B:309:THR:O	2:B:313:SER:OG	2.24	0.55
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.39	0.55
2:I:626:LEU:HG	2:I:628:GLY:H	1.70	0.55
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.39	0.55
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.89	0.55
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.55
2:G:217:GLY:O	2:G:261:ARG:NH1	2.39	0.55
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.35	0.55
2:B:626:LEU:HG	2:B:628:GLY:H	1.70	0.55
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.87	0.55
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.87	0.55
2:I:217:GLY:O	2:I:261:ARG:NH1	2.39	0.55
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.40	0.55
2:G:132:ALA:HA	2:G:194:SER:HB2	1.88	0.55
2:B:609:CYS:SG	2:B:610:ASN:N	2.76	0.55
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.89	0.55
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.40	0.55
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.39	0.55
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.72	0.55
2:I:309:THR:O	2:I:313:SER:OG	2.24	0.55
2:G:309:THR:O	2:G:313:SER:OG	2.24	0.55
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.40	0.55
2:G:4152:GLU:OE2	2:G:4180:ARG:NH1	2.40	0.55
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.39	0.54
2:E:132:ALA:HA	2:E:194:SER:HB2	1.88	0.54
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.89	0.54
2:I:132:ALA:HA	2:I:194:SER:HB2	1.88	0.54
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.40	0.54
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.90	0.54
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.73	0.54
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.90	0.54
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.89	0.54
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.72	0.54
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.89	0.54
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.90	0.54
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.72	0.54
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.72	0.54
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.41	0.54
2:B:132:ALA:HA	2:B:194:SER:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:309:THR:O	2:E:313:SER:OG	2.24	0.54
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.90	0.54
2:E:4152:GLU:OE2	2:E:4180:ARG:NH1	2.40	0.54
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.91	0.53
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.40	0.53
2:I:4152:GLU:OE2	2:I:4180:ARG:NH1	2.40	0.53
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.73	0.53
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.73	0.53
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.41	0.53
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.90	0.53
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.90	0.53
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.41	0.53
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.91	0.53
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.91	0.53
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.82	0.53
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.41	0.53
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.91	0.53
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.91	0.53
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.90	0.53
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.42	0.53
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.82	0.53
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.90	0.53
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.82	0.53
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.42	0.53
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.91	0.52
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.42	0.52
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.92	0.52
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.91	0.52
2:B:4071:ILE:HG21	2:B:4097:MET:HE1	1.91	0.52
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.91	0.52
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.92	0.52
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.91	0.52
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.92	0.52
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.52
2:G:4958:CYS:SG	2:G:4959:PHE:N	2.82	0.52
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.92	0.52
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.34	0.52
2:I:1973:GLN:O	2:I:1977:TYR:N	2.43	0.52
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.92	0.52
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.42	0.52
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.82	0.52
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.92	0.52
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.91	0.52
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.92	0.52
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.91	0.52
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.92	0.52
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.91	0.52
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.91	0.52
2:I:4071:ILE:HG21	2:I:4097:MET:HE1	1.92	0.52
2:B:1973:GLN:O	2:B:1977:TYR:N	2.43	0.52
2:B:4958:CYS:SG	2:B:4959:PHE:N	2.82	0.52
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.52
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.91	0.52
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.73	0.52
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.92	0.52
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.91	0.52
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.91	0.52
2:E:395:GLN:HG3	2:E:397:GLU:H	1.75	0.52
2:G:4071:ILE:HG21	2:G:4097:MET:HE1	1.92	0.52
2:B:1729:SER:HB3	2:B:2163:ARG:HH11	1.75	0.52
2:B:4884:LEU:HD11	2:I:4914:VAL:HG21	1.92	0.52
2:E:4071:ILE:HG21	2:E:4097:MET:HE1	1.92	0.52
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.91	0.52
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.92	0.52
2:I:1729:SER:HB3	2:I:2163:ARG:HH11	1.75	0.52
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.91	0.52
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.75	0.52
2:E:315:CYS:SG	2:E:316:PHE:N	2.83	0.52
2:E:4958:CYS:SG	2:E:4959:PHE:N	2.82	0.52
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.92	0.51
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.92	0.51
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.91	0.51
2:I:395:GLN:HG3	2:I:397:GLU:H	1.75	0.51
2:G:315:CYS:SG	2:G:316:PHE:N	2.83	0.51
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.93	0.51
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.75	0.51
2:B:315:CYS:SG	2:B:316:PHE:N	2.83	0.51
2:B:395:GLN:HG3	2:B:397:GLU:H	1.75	0.51
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.91	0.51
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.75	0.51
2:I:315:CYS:SG	2:I:316:PHE:N	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.92	0.51
2:E:765:GLN:NE2	2:E:1521:UNK:O	2.43	0.51
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.92	0.51
2:G:1973:GLN:O	2:G:1977:TYR:N	2.43	0.51
2:G:395:GLN:HG3	2:G:397:GLU:H	1.75	0.51
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.92	0.51
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.91	0.51
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.92	0.51
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.92	0.51
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.75	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.51
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.92	0.51
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.44	0.51
2:E:4172:GLU:HA	2:E:4175:ARG:HE	1.76	0.51
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.44	0.51
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.92	0.51
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.44	0.51
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.92	0.51
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.44	0.51
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.44	0.51
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.93	0.51
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.44	0.50
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.92	0.50
2:E:2908:TYR:OH	2:E:2920:ARG:NE	2.44	0.50
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.93	0.50
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.44	0.50
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.92	0.50
2:E:1973:GLN:O	2:E:1977:TYR:N	2.43	0.50
2:I:4958:CYS:SG	2:I:4959:PHE:N	2.82	0.50
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.50
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.44	0.50
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.94	0.50
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.50
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.94	0.50
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.94	0.50
2:G:4172:GLU:HA	2:G:4175:ARG:HE	1.76	0.50
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.40	0.50
2:B:1622:GLU:N	2:B:1627:ALA:O	2.45	0.50
2:B:4172:GLU:HA	2:B:4175:ARG:HE	1.76	0.50
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.76	0.50
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.94	0.50
2:E:1729:SER:HB3	2:E:2163:ARG:HH11	1.75	0.50
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.50
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.94	0.50
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.93	0.50
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.94	0.50
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.76	0.50
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	1.94	0.50
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.77	0.50
2:G:1729:SER:HB3	2:G:2163:ARG:HH11	1.75	0.50
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.94	0.50
2:B:689:THR:H	2:B:778:PHE:HE2	1.60	0.50
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.77	0.50
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.94	0.50
2:E:689:THR:H	2:E:778:PHE:HE2	1.60	0.49
2:I:689:THR:H	2:I:778:PHE:HE2	1.60	0.49
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.94	0.49
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.77	0.49
2:E:38:ALA:HB1	2:E:64:ILE:HG13	1.94	0.49
2:E:408:ALA:HB2	2:E:483:MET:HE1	1.94	0.49
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.93	0.49
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.77	0.49
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.92	0.49
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.94	0.49
2:G:689:THR:H	2:G:778:PHE:HE2	1.60	0.49
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	1.94	0.49
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.95	0.49
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.93	0.49
2:E:1259:ARG:NH2	2:E:1595:LEU:O	2.46	0.49
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.76	0.49
2:G:606:LEU:O	2:G:617:ASN:ND2	2.45	0.49
2:G:2347:GLU:O	2:G:2351:ASN:N	2.45	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.45	0.49
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.94	0.49
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	1.94	0.49
2:I:2347:GLU:O	2:I:2351:ASN:N	2.45	0.49
2:G:38:ALA:HB1	2:G:64:ILE:HG13	1.95	0.49
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.94	0.49
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.94	0.49
2:G:4251:ILE:HD12	2:G:4557:ARG:HA	1.94	0.49
2:B:331:VAL:HG12	2:B:333:GLY:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:ALA:HB2	2:B:483:MET:HE1	1.94	0.49
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.95	0.49
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.94	0.49
2:B:4251:ILE:HD12	2:B:4557:ARG:HA	1.94	0.49
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.94	0.49
2:E:2347:GLU:O	2:E:2351:ASN:N	2.45	0.49
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.46	0.49
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.93	0.49
2:I:1622:GLU:N	2:I:1627:ALA:O	2.45	0.49
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.77	0.49
2:B:38:ALA:HB1	2:B:64:ILE:HG13	1.95	0.49
2:B:195:PHE:HB3	2:B:196:MET:HG2	1.95	0.49
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.94	0.49
2:B:233:ILE:HD11	2:B:242:ARG:HH21	1.77	0.49
2:B:1259:ARG:NH2	2:B:1595:LEU:O	2.46	0.49
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.93	0.49
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.95	0.49
2:G:765:GLN:NE2	2:G:1521:UNK:O	2.46	0.49
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.94	0.49
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	1.94	0.49
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.95	0.49
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.95	0.49
2:I:606:LEU:O	2:I:617:ASN:ND2	2.46	0.49
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.95	0.49
2:G:1622:GLU:N	2:G:1627:ALA:O	2.45	0.49
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.77	0.49
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.95	0.48
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.77	0.48
2:E:606:LEU:O	2:E:617:ASN:ND2	2.45	0.48
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.94	0.48
2:E:4251:ILE:HD12	2:E:4557:ARG:HA	1.94	0.48
2:I:765:GLN:NE2	2:I:1521:UNK:O	2.46	0.48
2:I:4172:GLU:HA	2:I:4175:ARG:HE	1.76	0.48
2:G:111:HIS:CD2	2:G:114:SER:H	2.29	0.48
2:G:1259:ARG:NH2	2:G:1595:LEU:O	2.46	0.48
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.95	0.48
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.95	0.48
2:B:111:HIS:CD2	2:B:114:SER:H	2.29	0.48
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.94	0.48
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.95	0.48
2:I:233:ILE:HD11	2:I:242:ARG:HH21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.95	0.48
2:G:408:ALA:HB2	2:G:483:MET:HE1	1.94	0.48
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.95	0.48
2:B:606:LEU:O	2:B:617:ASN:ND2	2.45	0.48
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.96	0.48
2:E:233:ILE:HD11	2:E:242:ARG:HH21	1.77	0.48
2:I:38:ALA:HB1	2:I:64:ILE:HG13	1.94	0.48
2:I:408:ALA:HB2	2:I:483:MET:HE1	1.94	0.48
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.95	0.48
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.94	0.48
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.48
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.94	0.48
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.95	0.48
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.95	0.48
2:E:195:PHE:HB3	2:E:196:MET:HG2	1.95	0.48
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.95	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.29	0.48
2:I:257:ARG:O	2:I:284:HIS:NE2	2.36	0.48
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.77	0.48
2:G:331:VAL:HG12	2:G:333:GLY:H	1.77	0.48
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.95	0.48
2:E:331:VAL:HG12	2:E:333:GLY:H	1.77	0.48
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.96	0.48
2:E:1622:GLU:N	2:E:1627:ALA:O	2.45	0.48
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.94	0.48
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.94	0.48
2:G:2908:TYR:OH	2:G:2920:ARG:NE	2.44	0.48
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.96	0.48
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.94	0.48
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.96	0.48
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.95	0.48
2:I:1259:ARG:NH2	2:I:1595:LEU:O	2.46	0.48
2:I:4228:ALA:O	2:I:4232:GLU:N	2.46	0.48
2:E:793:LEU:HD12	2:E:797:HIS:HB2	1.96	0.48
2:I:331:VAL:HG12	2:I:333:GLY:H	1.77	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
2:I:4251:ILE:HD12	2:I:4557:ARG:HA	1.94	0.48
2:G:195:PHE:HB3	2:G:196:MET:HG2	1.95	0.48
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.95	0.48
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.96	0.48
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:233:ILE:HD11	2:G:242:ARG:HH21	1.77	0.48
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.46	0.48
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.95	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.29	0.48
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.48
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.95	0.48
2:B:257:ARG:O	2:B:284:HIS:NE2	2.36	0.47
2:I:642:THR:HG23	2:I:1613:LEU:HD12	1.96	0.47
2:B:642:THR:HG23	2:B:1613:LEU:HD12	1.96	0.47
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.95	0.47
2:I:793:LEU:HD12	2:I:797:HIS:HB2	1.96	0.47
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.46	0.47
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.30	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.47
2:I:195:PHE:HB3	2:I:196:MET:HG2	1.95	0.47
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.94	0.47
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.97	0.47
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.97	0.47
2:B:3901:ASN:OD1	2:B:3904:ARG:NH1	2.46	0.47
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.97	0.47
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.96	0.47
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	1.97	0.47
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.34	0.47
2:E:3901:ASN:OD1	2:E:3904:ARG:NH1	2.46	0.47
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	1.97	0.47
2:B:793:LEU:HD12	2:B:797:HIS:HB2	1.96	0.47
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.95	0.47
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.96	0.47
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	1.97	0.47
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.96	0.47
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	1.97	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.47
2:I:232:THR:HB	2:I:252:VAL:HG11	1.96	0.47
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.97	0.47
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.96	0.47
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.96	0.47
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.96	0.47
2:G:4228:ALA:O	2:G:4232:GLU:N	2.46	0.47
2:E:232:THR:HB	2:E:252:VAL:HG11	1.96	0.47
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:232:THR:HB	2:G:252:VAL:HG11	1.96	0.47
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.40	0.47
2:G:2758:PHE:O	2:G:2762:THR:N	2.45	0.47
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.96	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:4228:ALA:O	2:B:4232:GLU:N	2.46	0.47
2:G:793:LEU:HD12	2:G:797:HIS:HB2	1.96	0.47
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.97	0.47
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.97	0.47
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.97	0.47
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.96	0.47
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.96	0.47
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.97	0.46
2:B:232:THR:HB	2:B:252:VAL:HG11	1.96	0.46
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.96	0.46
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.97	0.46
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.34	0.46
2:E:4571:PHE:O	2:E:4575:PHE:N	2.48	0.46
2:G:1171:SER:HG	2:G:1175:SER:H	1.63	0.46
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.46	0.46
2:E:642:THR:HG23	2:E:1613:LEU:HD12	1.96	0.46
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.97	0.46
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.97	0.46
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.29	0.46
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.96	0.46
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.81	0.46
2:I:2908:TYR:OH	2:I:2920:ARG:NE	2.44	0.46
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.97	0.46
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.97	0.46
2:B:2868:SER:O	2:B:2872:GLN:N	2.47	0.46
2:B:4571:PHE:O	2:B:4575:PHE:N	2.48	0.46
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.81	0.46
2:G:3905:THR:HA	2:G:3912:THR:HG23	1.97	0.46
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.97	0.46
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.29	0.46
2:I:358:THR:HG21	2:I:382:GLY:HA2	1.98	0.46
2:I:3905:THR:HA	2:I:3912:THR:HG23	1.97	0.46
2:E:358:THR:HG21	2:E:382:GLY:HA2	1.98	0.46
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.98	0.46
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.81	0.46
2:B:2908:TYR:OH	2:B:2920:ARG:NE	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3905:THR:HA	2:E:3912:THR:HG23	1.97	0.46
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.81	0.46
2:G:4571:PHE:O	2:G:4575:PHE:N	2.48	0.46
2:B:485:SER:O	2:B:489:ASN:N	2.42	0.46
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.97	0.46
2:G:642:THR:HG23	2:G:1613:LEU:HD12	1.96	0.46
2:G:662:TRP:HZ3	2:G:811:CYS:HA	1.81	0.46
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.97	0.45
2:E:662:TRP:HZ3	2:E:811:CYS:HA	1.81	0.45
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.34	0.45
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.41	0.45
2:G:358:THR:HG21	2:G:382:GLY:HA2	1.98	0.45
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.97	0.45
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.81	0.45
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.29	0.45
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.98	0.45
2:E:4697:VAL:O	2:E:4701:TRP:N	2.49	0.45
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.45
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.98	0.45
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.34	0.45
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.45
2:B:358:THR:HG21	2:B:382:GLY:HA2	1.98	0.45
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.97	0.45
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.97	0.45
2:E:4914:VAL:HG21	2:G:4884:LEU:HD11	1.98	0.45
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.27	0.45
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.98	0.45
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.97	0.45
2:E:999:ASP:O	2:E:1004:GLY:N	2.50	0.45
2:I:1991:THR:O	2:I:1995:THR:OG1	2.32	0.45
2:I:4571:PHE:O	2:I:4575:PHE:N	2.48	0.45
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.97	0.45
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.98	0.45
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.97	0.45
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.97	0.45
2:I:2758:PHE:O	2:I:2762:THR:N	2.45	0.45
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.99	0.45
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.81	0.45
2:E:2765:LYS:HA	2:E:2859:PRO:HG3	1.99	0.45
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.81	0.45
2:I:999:ASP:O	2:I:1004:GLY:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2868:SER:O	2:I:2872:GLN:N	2.47	0.45
2:I:3901:ASN:OD1	2:I:3904:ARG:NH1	2.46	0.45
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.34	0.45
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.97	0.45
2:B:3905:THR:HA	2:B:3912:THR:HG23	1.97	0.45
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.99	0.45
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.99	0.45
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.99	0.45
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.34	0.45
2:E:488:LEU:O	2:E:492:ASP:N	2.45	0.45
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.97	0.45
2:E:1031:THR:O	2:E:1035:ASN:N	2.46	0.45
2:G:999:ASP:O	2:G:1004:GLY:N	2.50	0.45
2:G:2765:LYS:HA	2:G:2859:PRO:HG3	1.99	0.45
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.99	0.45
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.97	0.45
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.81	0.45
2:B:1269:CYS:HA	2:B:1473:UNK:HA	1.99	0.45
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.99	0.45
2:I:662:TRP:HZ3	2:I:811:CYS:HA	1.81	0.45
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.99	0.45
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.99	0.45
2:B:999:ASP:O	2:B:1004:GLY:N	2.50	0.45
2:B:1865:MET:SD	2:B:1865:MET:N	2.90	0.45
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.34	0.45
2:G:3901:ASN:OD1	2:G:3904:ARG:NH1	2.46	0.45
2:B:1031:THR:O	2:B:1035:ASN:N	2.46	0.44
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.27	0.44
2:E:1865:MET:SD	2:E:1865:MET:N	2.90	0.44
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.98	0.44
2:B:2457:LEU:HD23	2:B:2460:LEU:HD12	1.98	0.44
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.44
2:G:683:ARG:HG2	2:G:717:ASP:HB3	2.00	0.44
2:G:2868:SER:O	2:G:2872:GLN:N	2.47	0.44
2:B:683:ARG:HG2	2:B:717:ASP:HB3	2.00	0.44
2:E:257:ARG:O	2:E:284:HIS:NE2	2.36	0.44
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.99	0.44
2:I:2457:LEU:HD23	2:I:2460:LEU:HD12	1.98	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	2.00	0.44
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.97	0.44
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:662:TRP:HZ3	2:B:811:CYS:HA	1.81	0.44
2:B:1163:THR:HA	2:B:1168:VAL:HA	2.00	0.44
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.98	0.44
2:I:2765:LYS:HA	2:I:2859:PRO:HG3	1.99	0.44
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.97	0.44
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.98	0.44
2:E:2457:LEU:HD23	2:E:2460:LEU:HD12	1.98	0.44
2:I:1865:MET:SD	2:I:1865:MET:N	2.90	0.44
1:H:21:THR:HA	1:H:49:ARG:HA	2.00	0.44
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.42	0.44
2:E:629:ARG:HD3	2:E:634:GLN:HG2	2.00	0.44
2:E:1163:THR:HA	2:E:1168:VAL:HA	2.00	0.44
2:I:1694:LEU:O	2:I:1712:TYR:OH	2.27	0.44
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	2.00	0.44
2:E:4228:ALA:O	2:E:4232:GLU:N	2.46	0.44
2:I:4697:VAL:O	2:I:4701:TRP:N	2.49	0.44
2:G:399:GLN:HG2	2:G:403:MET:HE3	2.00	0.44
2:G:488:LEU:O	2:G:492:ASP:N	2.45	0.44
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.34	0.44
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.00	0.44
2:B:2765:LYS:HA	2:B:2859:PRO:HG3	1.99	0.44
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.41	0.44
2:I:683:ARG:HG2	2:I:717:ASP:HB3	2.00	0.44
2:I:4059:LEU:HD11	2:I:4167:ALA:HB2	2.00	0.44
2:G:629:ARG:HD3	2:G:634:GLN:HG2	2.00	0.44
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.99	0.44
2:G:1163:THR:HA	2:G:1168:VAL:HA	2.00	0.44
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.00	0.44
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.34	0.44
1:F:21:THR:HA	1:F:49:ARG:HA	2.00	0.44
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.99	0.44
2:E:4930:ALA:O	2:E:4934:GLY:N	2.51	0.44
2:G:1865:MET:SD	2:G:1865:MET:N	2.90	0.44
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	2.00	0.44
2:G:4697:VAL:O	2:G:4701:TRP:N	2.49	0.44
1:J:21:THR:HA	1:J:49:ARG:HA	2.00	0.43
2:E:683:ARG:HG2	2:E:717:ASP:HB3	2.00	0.43
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.42	0.43
2:B:488:LEU:O	2:B:492:ASP:N	2.45	0.43
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.50	0.43
2:I:1163:THR:HA	2:I:1168:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4930:ALA:O	2:I:4934:GLY:N	2.51	0.43
2:G:4930:ALA:O	2:G:4934:GLY:N	2.51	0.43
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.99	0.43
2:B:765:GLN:NE2	2:B:1521:UNK:O	2.51	0.43
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.99	0.43
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.00	0.43
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.00	0.43
2:B:629:ARG:HD3	2:B:634:GLN:HG2	2.00	0.43
2:E:1171:SER:HG	2:E:1175:SER:H	1.63	0.43
2:E:1760:HIS:CE1	2:E:2041:HIS:HA	2.54	0.43
2:G:3787:LYS:HB2	2:G:3831:SER:HA	2.01	0.43
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	2.00	0.43
2:I:1760:HIS:CE1	2:I:2041:HIS:HA	2.54	0.43
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.99	0.43
2:G:2457:LEU:HD23	2:G:2460:LEU:HD12	1.98	0.43
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.99	0.43
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	2.00	0.43
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.42	0.43
2:I:3787:LYS:HB2	2:I:3831:SER:HA	2.01	0.43
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.41	0.43
2:G:1636:MET:HE2	2:G:1638:ALA:HB2	2.01	0.43
2:B:1760:HIS:CE1	2:B:2041:HIS:HA	2.54	0.43
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.48	0.43
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	2.00	0.43
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.34	0.43
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	2.01	0.43
2:I:629:ARG:HD3	2:I:634:GLN:HG2	2.00	0.43
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	2.01	0.43
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.52	0.43
1:A:21:THR:HA	1:A:49:ARG:HA	2.00	0.43
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	2.00	0.43
2:E:907:LEU:O	2:E:963:ASN:ND2	2.38	0.43
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	2.01	0.43
2:I:4995:LEU:HD11	2:I:5011:TRP:HB2	2.01	0.43
2:G:209:CYS:HA	2:G:334:MET:HE2	2.01	0.43
2:G:983:THR:O	2:G:987:ARG:N	2.51	0.43
2:B:4930:ALA:O	2:B:4934:GLY:N	2.51	0.43
2:E:4232:GLU:OE1	2:E:5019:TRP:NE1	2.52	0.43
2:I:647:ASN:ND2	2:I:820:ARG:O	2.43	0.43
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	2.01	0.43
2:E:2381:GLU:HA	2:E:2384:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.41	0.42
2:I:209:CYS:HA	2:I:334:MET:HE2	2.01	0.42
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	2.01	0.42
2:I:2742:THR:OG1	2:I:2811:GLU:OE1	2.35	0.42
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.36	0.42
2:G:4059:LEU:HD11	2:G:4167:ALA:HB2	2.00	0.42
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	2.01	0.42
2:B:4995:LEU:HD11	2:B:5011:TRP:HB2	2.01	0.42
2:E:2758:PHE:O	2:E:2762:THR:N	2.45	0.42
2:E:4851:TYR:HD2	2:E:4920:PHE:HD1	1.68	0.42
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	2.01	0.42
2:I:907:LEU:O	2:I:963:ASN:ND2	2.38	0.42
2:I:983:THR:O	2:I:987:ARG:N	2.51	0.42
2:I:2778:GLY:HA3	2:I:2787:THR:HB	2.02	0.42
2:I:4092:ASP:OD1	2:I:4092:ASP:N	2.53	0.42
2:G:1760:HIS:CE1	2:G:2041:HIS:HA	2.54	0.42
2:B:4697:VAL:O	2:B:4701:TRP:N	2.49	0.42
2:E:4059:LEU:HD11	2:E:4167:ALA:HB2	2.00	0.42
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.49	0.42
2:E:1636:MET:HE2	2:E:1638:ALA:HB2	2.01	0.42
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	2.01	0.42
2:G:218:HIS:HB3	2:G:392:ARG:HD3	2.02	0.42
2:G:4851:TYR:HD2	2:G:4920:PHE:HD1	1.67	0.42
2:B:218:HIS:HB3	2:B:392:ARG:HD3	2.02	0.42
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.53	0.42
2:I:379:HIS:CD2	2:I:381:GLU:H	2.38	0.42
2:I:2381:GLU:HA	2:I:2384:ILE:HD12	2.01	0.42
1:J:71:ARG:HH22	2:I:679:ALA:HB2	1.85	0.42
2:E:983:THR:O	2:E:987:ARG:N	2.51	0.42
2:I:683:ARG:NH1	2:I:707:VAL:O	2.45	0.42
2:G:379:HIS:CD2	2:G:381:GLU:H	2.38	0.42
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.85	0.42
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.53	0.42
2:B:209:CYS:HA	2:B:334:MET:HE2	2.01	0.42
2:B:2381:GLU:HA	2:B:2384:ILE:HD12	2.01	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.42
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.53	0.42
2:B:4092:ASP:OD1	2:B:4092:ASP:N	2.53	0.42
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.34	0.42
2:E:209:CYS:HA	2:E:334:MET:HE2	2.01	0.42
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.53	0.42
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	2.02	0.42
2:B:1636:MET:HE2	2:B:1638:ALA:HB2	2.01	0.42
2:B:4059:LEU:HD11	2:B:4167:ALA:HB2	2.00	0.42
2:B:4851:TYR:HD2	2:B:4920:PHE:HD1	1.68	0.42
2:E:3787:LYS:HB2	2:E:3831:SER:HA	2.01	0.42
2:E:4092:ASP:N	2:E:4092:ASP:OD1	2.53	0.42
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	2.00	0.42
2:I:218:HIS:HB3	2:I:392:ARG:HD3	2.02	0.42
2:G:257:ARG:O	2:G:284:HIS:NE2	2.36	0.42
2:G:1031:THR:O	2:G:1035:ASN:N	2.46	0.42
2:B:978:THR:HB	2:B:980:ALA:H	1.85	0.42
2:E:1694:LEU:O	2:E:1712:TYR:OH	2.27	0.42
2:E:4685:GLY:HA3	2:E:4689:THR:HB	2.02	0.42
2:I:4851:TYR:HD2	2:I:4920:PHE:HD1	1.68	0.42
2:G:2778:GLY:HA3	2:G:2787:THR:HB	2.02	0.42
2:B:4021:LYS:HG3	2:B:4142:ASN:HD22	1.85	0.41
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	2.02	0.41
2:E:1078:GLU:HG3	2:E:1237:TRP:HE1	1.85	0.41
2:E:4000:MET:HE1	2:E:4058:ILE:HG23	2.02	0.41
2:E:4021:LYS:HG3	2:E:4142:ASN:HD22	1.85	0.41
2:G:940:GLY:O	2:G:1052:ASN:N	2.53	0.41
2:G:4685:GLY:HA3	2:G:4689:THR:HB	2.02	0.41
2:B:379:HIS:CD2	2:B:381:GLU:H	2.38	0.41
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.03	0.41
2:B:3787:LYS:HB2	2:B:3831:SER:HA	2.01	0.41
2:E:218:HIS:HB3	2:E:392:ARG:HD3	2.02	0.41
2:E:4995:LEU:HD11	2:E:5011:TRP:HB2	2.01	0.41
2:I:1078:GLU:HG3	2:I:1237:TRP:HE1	1.85	0.41
2:I:4232:GLU:OE1	2:I:5019:TRP:NE1	2.52	0.41
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.03	0.41
2:G:978:THR:HB	2:G:980:ALA:H	1.85	0.41
2:G:2381:GLU:HA	2:G:2384:ILE:HD12	2.01	0.41
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.86	0.41
2:G:4995:LEU:HD11	2:G:5011:TRP:HB2	2.01	0.41
2:E:2778:GLY:HA3	2:E:2787:THR:HB	2.02	0.41
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.85	0.41
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.85	0.41
2:I:1636:MET:HE2	2:I:1638:ALA:HB2	2.01	0.41
2:I:4000:MET:HE1	2:I:4058:ILE:HG23	2.02	0.41
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:612:VAL:HG12	2:B:2167:ILE:HA	2.03	0.41
2:B:4000:MET:HE1	2:B:4058:ILE:HG23	2.02	0.41
2:E:379:HIS:CD2	2:E:381:GLU:H	2.38	0.41
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	2.02	0.41
2:I:612:VAL:HG12	2:I:2167:ILE:HA	2.03	0.41
2:I:1227:ALA:HB1	2:I:1230:MET:HG3	2.02	0.41
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.53	0.41
2:G:273:HIS:CE1	2:G:337:PRO:HB3	2.56	0.41
2:G:612:VAL:HG12	2:G:2167:ILE:HA	2.02	0.41
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.93	0.41
2:B:273:HIS:CE1	2:B:337:PRO:HB3	2.56	0.41
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.41	0.41
2:B:940:GLY:O	2:B:1052:ASN:N	2.53	0.41
2:B:1078:GLU:HG3	2:B:1237:TRP:HE1	1.85	0.41
2:B:1641:ILE:HA	2:B:1642:PRO:HD3	1.92	0.41
2:B:4232:GLU:OE1	2:B:5019:TRP:NE1	2.52	0.41
2:E:273:HIS:CE1	2:E:337:PRO:HB3	2.56	0.41
2:E:2868:SER:O	2:E:2872:GLN:N	2.47	0.41
2:I:273:HIS:CE1	2:I:337:PRO:HB3	2.56	0.41
2:I:978:THR:HB	2:I:980:ALA:H	1.85	0.41
2:I:1031:THR:O	2:I:1035:ASN:N	2.46	0.41
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.03	0.41
2:B:793:LEU:HD22	2:B:821:LEU:HD13	2.03	0.41
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.53	0.41
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.53	0.41
2:B:3365:UNK:O	2:B:3369:UNK:N	2.54	0.41
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.03	0.41
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.86	0.41
2:I:793:LEU:HD22	2:I:821:LEU:HD13	2.03	0.41
2:I:4685:GLY:HA3	2:I:4689:THR:HB	2.02	0.41
2:G:2094:LEU:HD23	2:G:2127:GLN:HE22	1.86	0.41
2:B:786:GLY:HA2	2:B:1631:GLN:HA	2.03	0.41
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.86	0.41
2:B:4685:GLY:HA3	2:B:4689:THR:HB	2.02	0.41
2:E:489:ASN:HA	2:E:492:ASP:HB2	2.03	0.41
2:E:683:ARG:NH1	2:E:707:VAL:O	2.45	0.41
2:G:793:LEU:HD22	2:G:821:LEU:HD13	2.03	0.41
2:G:3362:UNK:O	2:G:3366:UNK:N	2.54	0.41
2:B:1227:ALA:HB1	2:B:1230:MET:HG3	2.02	0.41
2:E:2212:VAL:O	2:E:2216:GLY:N	2.48	0.41
2:E:3362:UNK:O	2:E:3366:UNK:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	2.02	0.41
2:I:786:GLY:HA2	2:I:1631:GLN:HA	2.03	0.41
2:I:940:GLY:O	2:I:1052:ASN:N	2.53	0.41
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.85	0.41
2:I:3362:UNK:O	2:I:3366:UNK:N	2.54	0.41
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.86	0.41
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.85	0.41
2:G:489:ASN:HA	2:G:492:ASP:HB2	2.03	0.41
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.03	0.41
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.53	0.41
1:F:27:THR:HB	1:F:100:ASP:HB3	2.03	0.41
2:B:2024:PRO:O	2:B:2028:ARG:NE	2.48	0.41
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.85	0.41
2:E:612:VAL:HG12	2:E:2167:ILE:HA	2.03	0.41
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.53	0.41
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.41
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.19	0.41
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.03	0.41
2:I:4884:LEU:HD11	2:G:4914:VAL:HG21	2.03	0.41
2:G:2290:LEU:HG	2:G:2291:GLN:H	1.86	0.41
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	2.02	0.41
1:J:27:THR:HB	1:J:100:ASP:HB3	2.03	0.41
2:E:776:LEU:HG	2:E:848:HIS:HA	2.03	0.41
2:E:793:LEU:HD22	2:E:821:LEU:HD13	2.03	0.41
2:E:794:GLY:H	2:E:798:GLY:HA3	1.86	0.41
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.03	0.41
2:I:2290:LEU:HG	2:I:2291:GLN:H	1.86	0.41
2:I:4021:LYS:HG3	2:I:4142:ASN:HD22	1.86	0.41
1:H:27:THR:HB	1:H:100:ASP:HB3	2.03	0.40
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.03	0.40
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	2.02	0.40
2:B:2778:GLY:HA3	2:B:2787:THR:HB	2.02	0.40
2:E:2094:LEU:HD23	2:E:2127:GLN:HE22	1.86	0.40
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.03	0.40
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	2.04	0.40
2:I:1595:LEU:HD23	2:I:1595:LEU:HA	1.97	0.40
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.40	0.40
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	2.02	0.40
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.40
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.86	0.40
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:HB	1:A:100:ASP:HB3	2.03	0.40
2:B:489:ASN:HA	2:B:492:ASP:HB2	2.03	0.40
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.03	0.40
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.40	0.40
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.04	0.40
2:G:794:GLY:H	2:G:798:GLY:HA3	1.86	0.40
2:G:3842:LEU:O	2:G:3929:SER:OG	2.40	0.40
2:G:4021:LYS:HG3	2:G:4142:ASN:HD22	1.86	0.40
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.19	0.40
2:B:794:GLY:H	2:B:798:GLY:HA3	1.86	0.40
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.03	0.40
2:B:2212:VAL:O	2:B:2216:GLY:N	2.48	0.40
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.02	0.40
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.86	0.40
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.03	0.40
2:I:489:ASN:HA	2:I:492:ASP:HB2	2.03	0.40
2:I:2094:LEU:HD23	2:I:2127:GLN:HE22	1.86	0.40
2:I:2212:VAL:O	2:I:2216:GLY:N	2.48	0.40
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.03	0.40
2:B:776:LEU:HG	2:B:848:HIS:HA	2.03	0.40
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.03	0.40
2:E:3365:UNK:O	2:E:3369:UNK:N	2.55	0.40
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	2.03	0.40
2:I:3365:UNK:O	2:I:3369:UNK:N	2.55	0.40
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.04	0.40
2:G:1078:GLU:HG3	2:G:1237:TRP:HE1	1.85	0.40
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.03	0.40
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.86	0.40
2:G:4000:MET:HE1	2:G:4058:ILE:HG23	2.02	0.40
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.03	0.40
2:B:2290:LEU:HG	2:B:2291:GLN:H	1.86	0.40
2:B:2517:UNK:O	2:B:2521:UNK:N	2.55	0.40
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.04	0.40
2:I:794:GLY:H	2:I:798:GLY:HA3	1.86	0.40
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	2.04	0.40
2:G:3365:UNK:O	2:G:3369:UNK:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	59/89 (66%)	59 (100%)	0	100	100
1	J	71/89 (80%)	71 (100%)	0	100	100
2	B	2486/3202 (78%)	2473 (100%)	13 (0%)	81	81
2	E	2440/3202 (76%)	2428 (100%)	12 (0%)	81	81
2	G	2493/3202 (78%)	2480 (100%)	13 (0%)	81	81
2	I	2467/3202 (77%)	2455 (100%)	12 (0%)	81	81
All	All	10192/13164 (77%)	10142 (100%)	50 (0%)	78	81

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	688	LEU
2	B	719	LEU
2	B	978	THR
2	B	1600	LEU
2	B	1676	LEU
2	B	2339	VAL
2	B	3805	LEU
2	B	4081	VAL
2	B	4154	VAL
2	B	4197	ILE
2	B	4985	LEU

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Mol	Chain	Res	Type
2	B	4995	LEU
2	E	131	LEU
2	E	688	LEU
2	E	719	LEU
2	E	978	THR
2	E	1600	LEU
2	E	2339	VAL
2	E	3805	LEU
2	E	4081	VAL
2	E	4154	VAL
2	E	4197	ILE
2	E	4985	LEU
2	E	4995	LEU
2	I	131	LEU
2	I	688	LEU
2	I	719	LEU
2	I	978	THR
2	I	1676	LEU
2	I	2339	VAL
2	I	3805	LEU
2	I	4081	VAL
2	I	4154	VAL
2	I	4197	ILE
2	I	4985	LEU
2	I	4995	LEU
2	G	131	LEU
2	G	688	LEU
2	G	719	LEU
2	G	978	THR
2	G	1600	LEU
2	G	1676	LEU
2	G	2339	VAL
2	G	3805	LEU
2	G	4081	VAL
2	G	4154	VAL
2	G	4197	ILE
2	G	4985	LEU
2	G	4995	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (206) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	31	GLN
1	F	87	HIS
1	A	31	GLN
1	A	87	HIS
1	H	31	GLN
1	J	31	GLN
1	J	87	HIS
2	B	57	ASN
2	B	105	HIS
2	B	111	HIS
2	B	113	HIS
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	405	HIS
2	B	413	GLN
2	B	479	GLN
2	B	725	HIS
2	B	765	GLN
2	B	797	HIS
2	B	1719	HIS
2	B	1760	HIS
2	B	1949	GLN
2	B	1973	GLN
2	B	2127	GLN
2	B	2184	ASN
2	B	2260	ASN
2	B	2773	ASN
2	B	3781	GLN
2	B	3814	GLN
2	B	3830	GLN
2	B	3850	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3994	HIS
2	B	4034	ASN
2	B	4037	ASN
2	B	4054	ASN
2	B	4109	GLN
2	B	4120	ASN
2	B	4142	ASN
2	B	4204	GLN

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Mol	Chain	Res	Type
2	B	4246	GLN
2	B	4553	ASN
2	B	4707	ASN
2	B	4728	HIS
2	B	4776	GLN
2	B	4864	ASN
2	B	4947	GLN
2	B	4949	GLN
2	B	4973	HIS
2	B	4984	ASN
2	B	5003	HIS
2	B	5015	GLN
2	B	5031	GLN
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	399	GLN
2	E	405	HIS
2	E	412	ASN
2	E	413	GLN
2	E	461	HIS
2	E	479	GLN
2	E	725	HIS
2	E	765	GLN
2	E	797	HIS
2	E	877	ASN
2	E	1760	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	1970	GLN
2	E	1973	GLN
2	E	2127	GLN
2	E	2260	ASN
2	E	2877	GLN
2	E	3781	GLN
2	E	3814	GLN
2	E	3830	GLN
2	E	3850	GLN
2	E	3889	GLN

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Mol	Chain	Res	Type
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3994	HIS
2	E	4034	ASN
2	E	4037	ASN
2	E	4054	ASN
2	E	4109	GLN
2	E	4120	ASN
2	E	4142	ASN
2	E	4204	GLN
2	E	4246	GLN
2	E	4553	ASN
2	E	4707	ASN
2	E	4776	GLN
2	E	4864	ASN
2	E	4949	GLN
2	E	4984	ASN
2	E	5003	HIS
2	E	5031	GLN
2	I	23	GLN
2	I	57	ASN
2	I	105	HIS
2	I	111	HIS
2	I	113	HIS
2	I	203	ASN
2	I	273	HIS
2	I	379	HIS
2	I	405	HIS
2	I	413	GLN
2	I	461	HIS
2	I	479	GLN
2	I	725	HIS
2	I	765	GLN
2	I	797	HIS
2	I	1206	GLN
2	I	1220	GLN
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	1861	GLN

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Mol	Chain	Res	Type
2	I	1970	GLN
2	I	1973	GLN
2	I	2127	GLN
2	I	2260	ASN
2	I	2877	GLN
2	I	3781	GLN
2	I	3814	GLN
2	I	3830	GLN
2	I	3850	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3994	HIS
2	I	4034	ASN
2	I	4037	ASN
2	I	4054	ASN
2	I	4109	GLN
2	I	4120	ASN
2	I	4142	ASN
2	I	4204	GLN
2	I	4246	GLN
2	I	4553	ASN
2	I	4707	ASN
2	I	4776	GLN
2	I	4864	ASN
2	I	4947	GLN
2	I	4949	GLN
2	I	4984	ASN
2	I	5003	HIS
2	I	5031	GLN
2	G	57	ASN
2	G	105	HIS
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	405	HIS
2	G	413	GLN
2	G	461	HIS
2	G	479	GLN

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Mol	Chain	Res	Type
2	G	725	HIS
2	G	765	GLN
2	G	797	HIS
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	1970	GLN
2	G	2005	GLN
2	G	2127	GLN
2	G	2260	ASN
2	G	2877	GLN
2	G	3814	GLN
2	G	3830	GLN
2	G	3850	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3994	HIS
2	G	4034	ASN
2	G	4037	ASN
2	G	4054	ASN
2	G	4109	GLN
2	G	4120	ASN
2	G	4142	ASN
2	G	4204	GLN
2	G	4246	GLN
2	G	4553	ASN
2	G	4707	ASN
2	G	4776	GLN
2	G	4864	ASN
2	G	4947	GLN
2	G	4949	GLN
2	G	4984	ASN
2	G	5015	GLN
2	G	5031	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	12
2	G	12
2	I	12
2	E	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	44.23
1	G	3613:UNK	C	3639:THR	N	43.95
1	I	3613:UNK	C	3639:THR	N	43.88
1	E	3613:UNK	C	3639:THR	N	43.84

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3163:UNK	C	3170:UNK	N	16.60
1	I	3163:UNK	C	3170:UNK	N	16.60
1	G	3163:UNK	C	3170:UNK	N	16.59
1	B	3163:UNK	C	3170:UNK	N	16.55
1	B	3468:UNK	C	3511:UNK	N	15.45
1	G	3468:UNK	C	3511:UNK	N	15.42
1	E	3468:UNK	C	3511:UNK	N	15.40
1	I	3468:UNK	C	3511:UNK	N	15.40
1	B	3063:UNK	C	3134:UNK	N	14.93
1	E	3063:UNK	C	3134:UNK	N	14.90
1	I	3063:UNK	C	3134:UNK	N	14.90
1	G	3063:UNK	C	3134:UNK	N	14.90
1	I	2703:UNK	C	2734:ASN	N	14.22
1	E	2703:UNK	C	2734:ASN	N	14.16
1	G	2703:UNK	C	2734:ASN	N	14.10
1	B	2703:UNK	C	2734:ASN	N	13.86
1	E	3236:UNK	C	3241:UNK	N	13.47
1	I	3236:UNK	C	3241:UNK	N	13.47
1	B	3236:UNK	C	3241:UNK	N	13.46
1	G	3236:UNK	C	3241:UNK	N	13.46
1	I	1564:UNK	C	1573:MET	N	12.78
1	G	1564:UNK	C	1573:MET	N	12.68
1	E	1564:UNK	C	1573:MET	N	12.67
1	B	1564:UNK	C	1573:MET	N	12.65
1	B	2976:UNK	C	2995:UNK	N	12.08
1	E	2976:UNK	C	2995:UNK	N	12.07
1	I	2976:UNK	C	2995:UNK	N	12.07
1	G	2976:UNK	C	2995:UNK	N	12.07
1	E	3254:UNK	C	3261:UNK	N	8.41
1	I	3254:UNK	C	3261:UNK	N	8.41
1	G	3254:UNK	C	3261:UNK	N	8.40
1	B	3254:UNK	C	3261:UNK	N	8.34
1	I	1297:UNK	C	1430:UNK	N	5.95
1	B	1297:UNK	C	1430:UNK	N	5.94
1	E	1297:UNK	C	1430:UNK	N	5.94
1	G	1297:UNK	C	1430:UNK	N	5.94
1	B	2479:LEU	C	2487:UNK	N	3.52
1	B	2939:ARG	C	2942:UNK	N	3.51
1	E	2939:ARG	C	2942:UNK	N	3.44
1	I	2939:ARG	C	2942:UNK	N	3.43
1	G	2939:ARG	C	2942:UNK	N	3.41
1	G	2479:LEU	C	2487:UNK	N	3.26

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	2479:LEU	C	2487:UNK	N	3.22
1	I	2479:LEU	C	2487:UNK	N	3.21

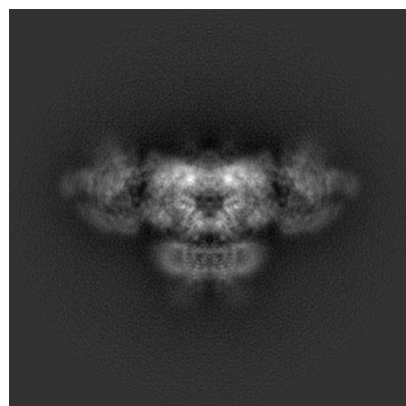
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8375. These allow visual inspection of the internal detail of the map and identification of artifacts.

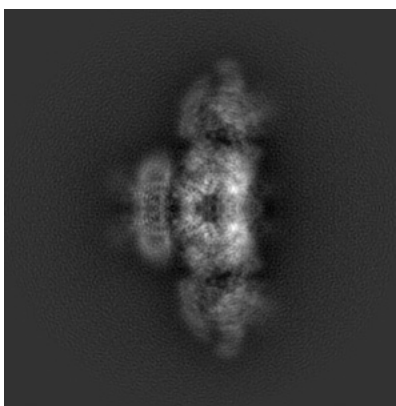
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

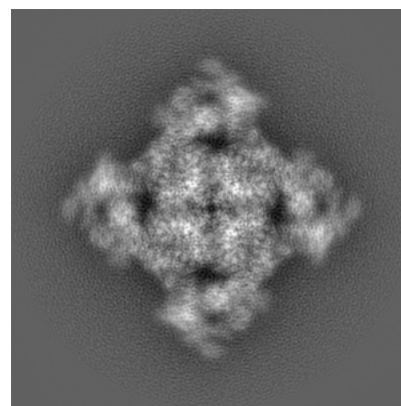
6.1.1 Primary map



X

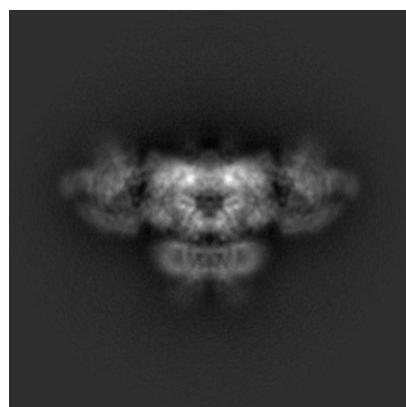


Y

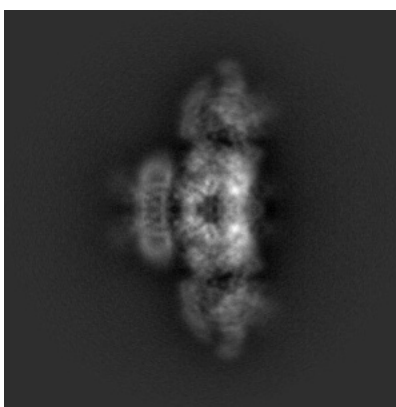


Z

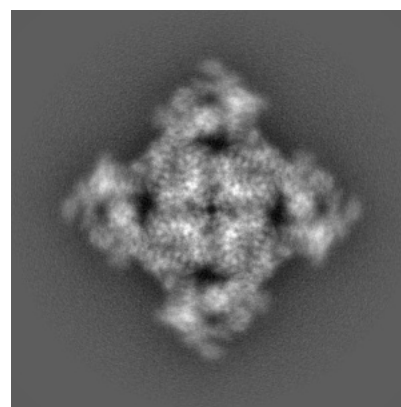
6.1.2 Raw map



X



Y

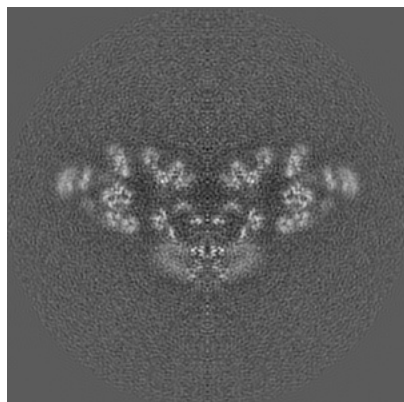


Z

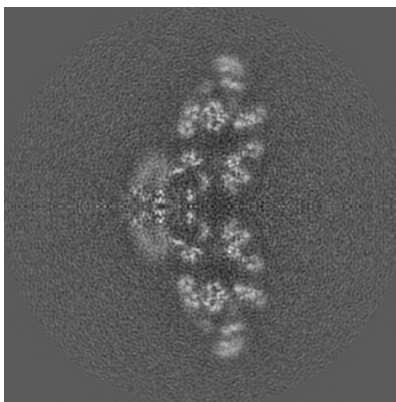
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

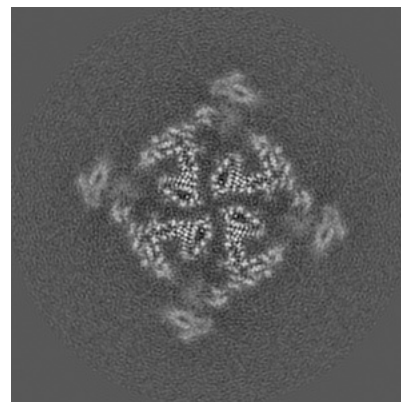
6.2.1 Primary map



X Index: 200

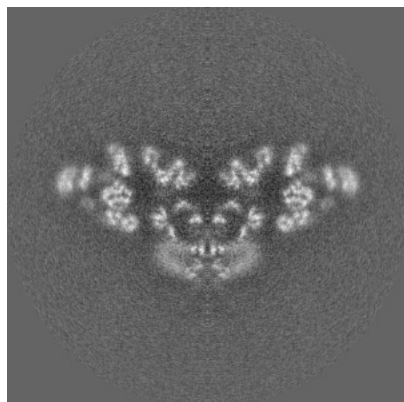


Y Index: 200

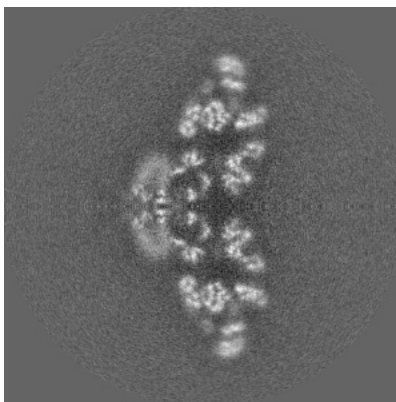


Z Index: 200

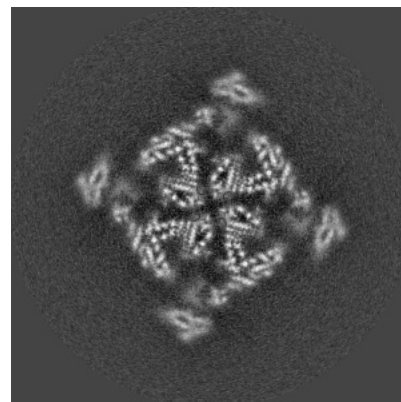
6.2.2 Raw map



X Index: 200



Y Index: 200

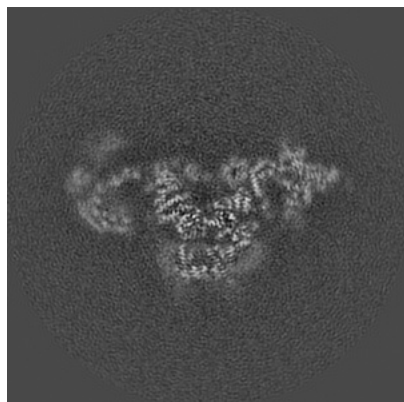


Z Index: 200

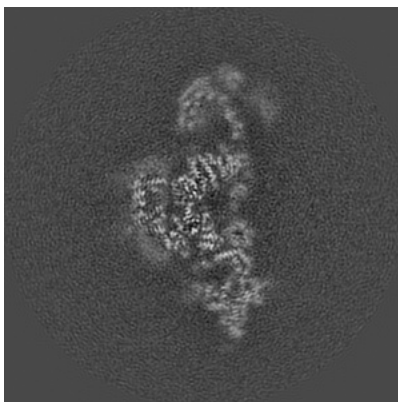
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

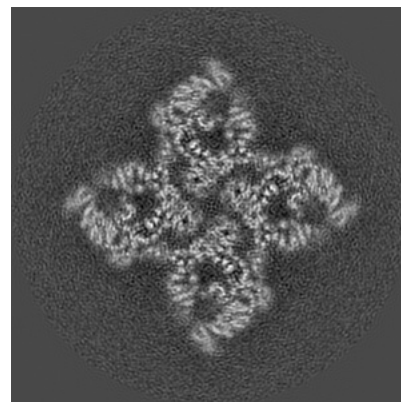
6.3.1 Primary map



X Index: 184

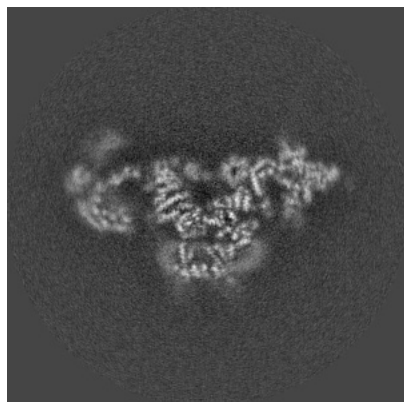


Y Index: 184

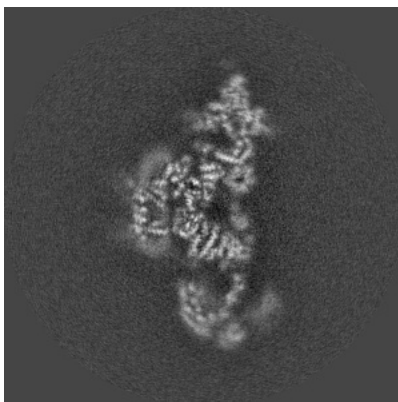


Z Index: 233

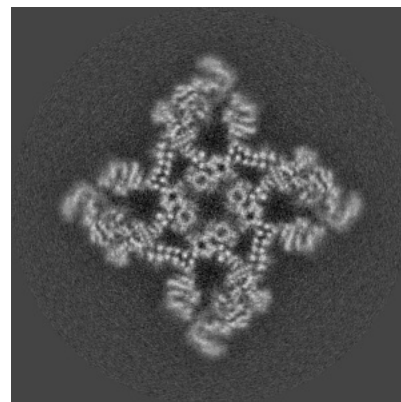
6.3.2 Raw map



X Index: 184



Y Index: 216

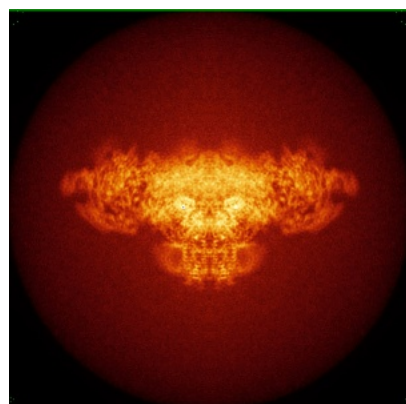


Z Index: 228

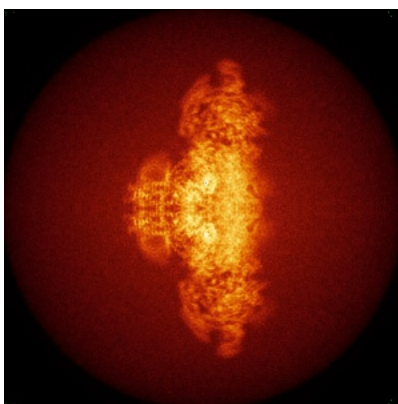
The images above show the largest variance slices of the map in three orthogonal directions.

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

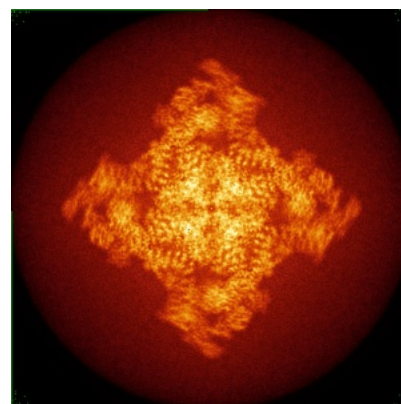
6.4.1 Primary map



X



Y

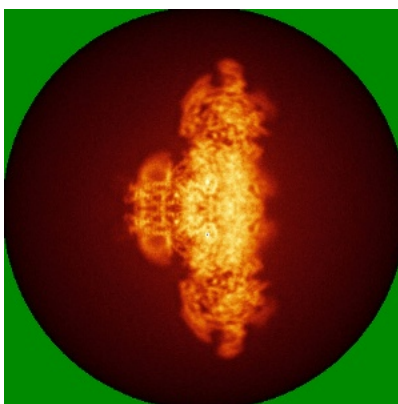


Z

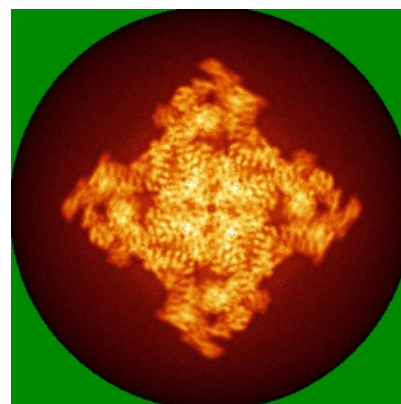
6.4.2 Raw map



X



Y

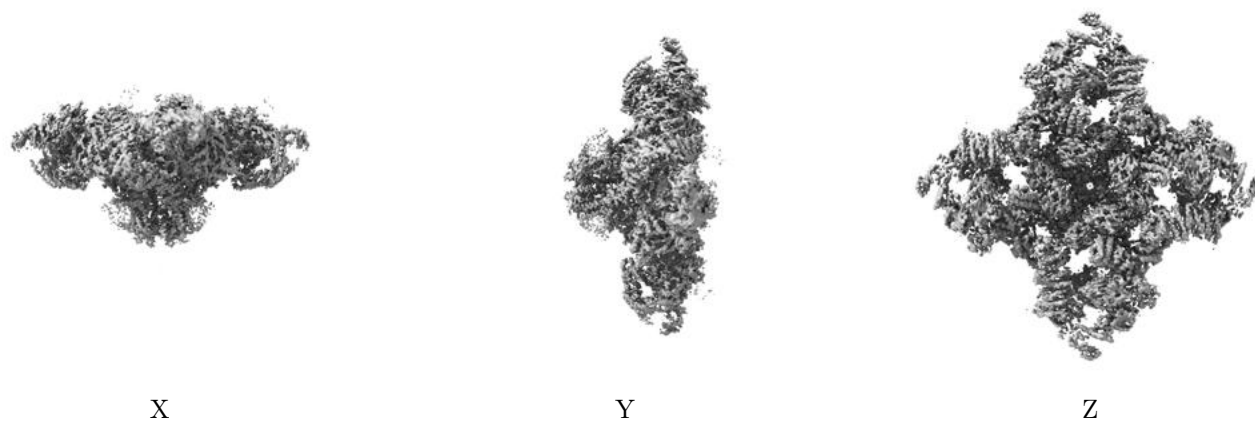


Z

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

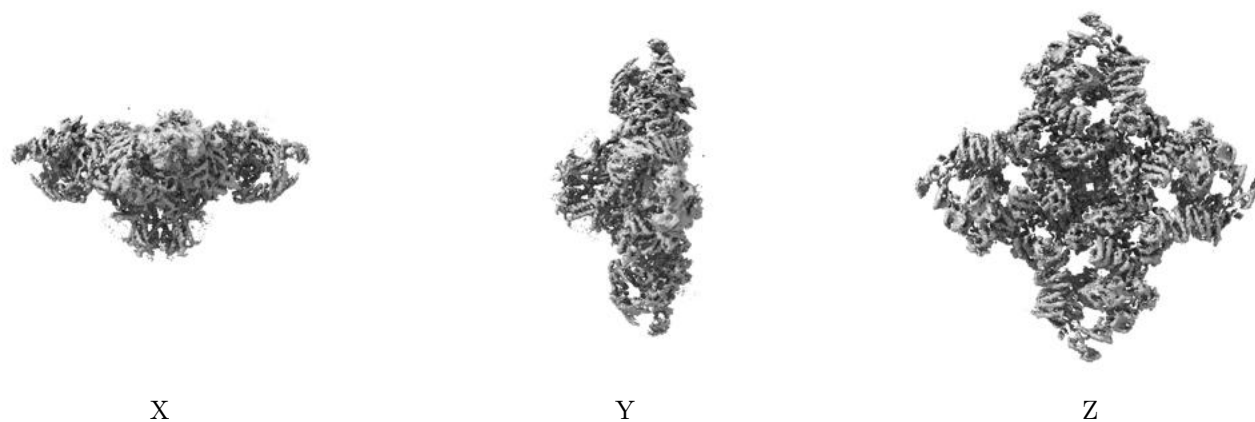
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 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.

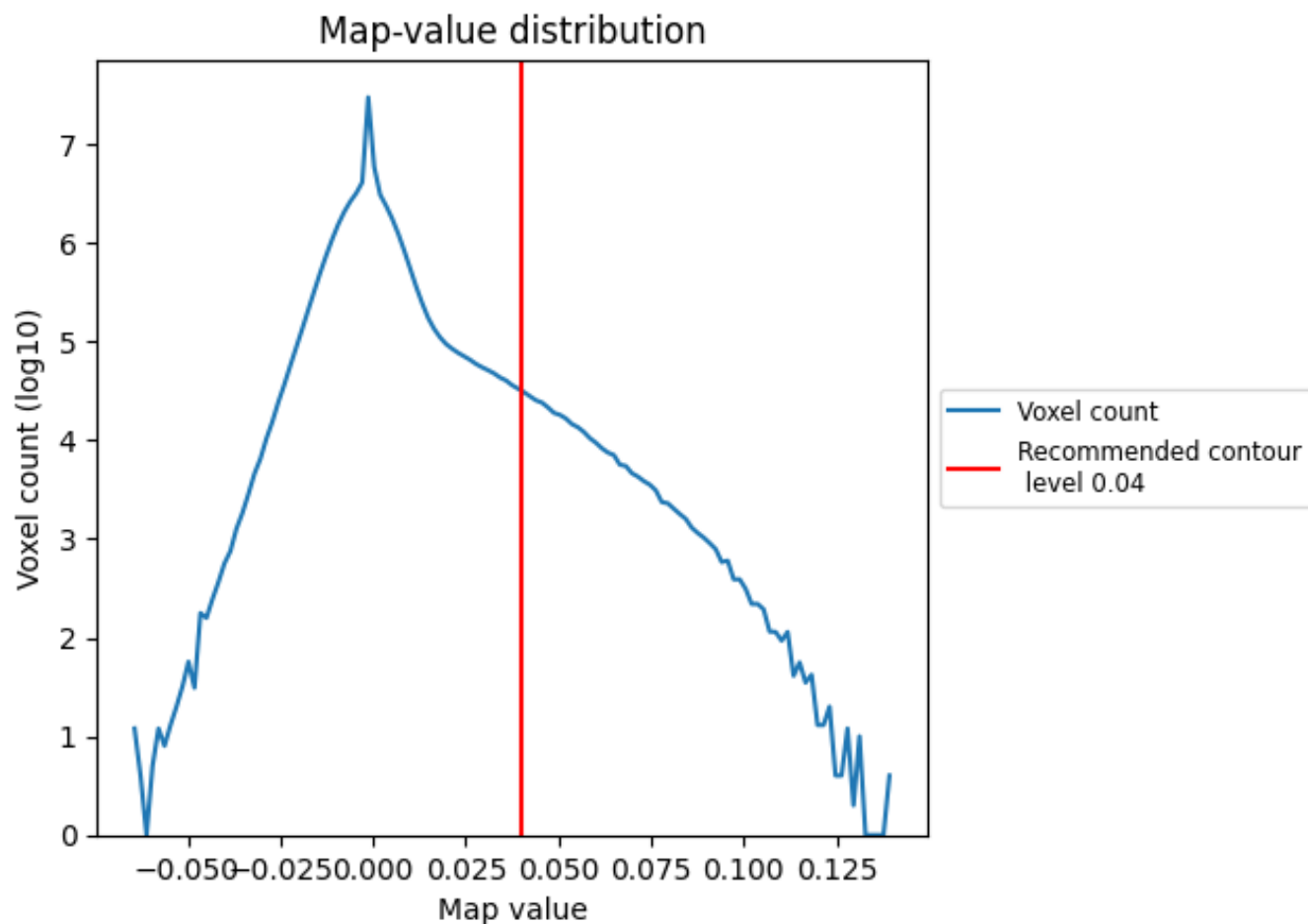
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

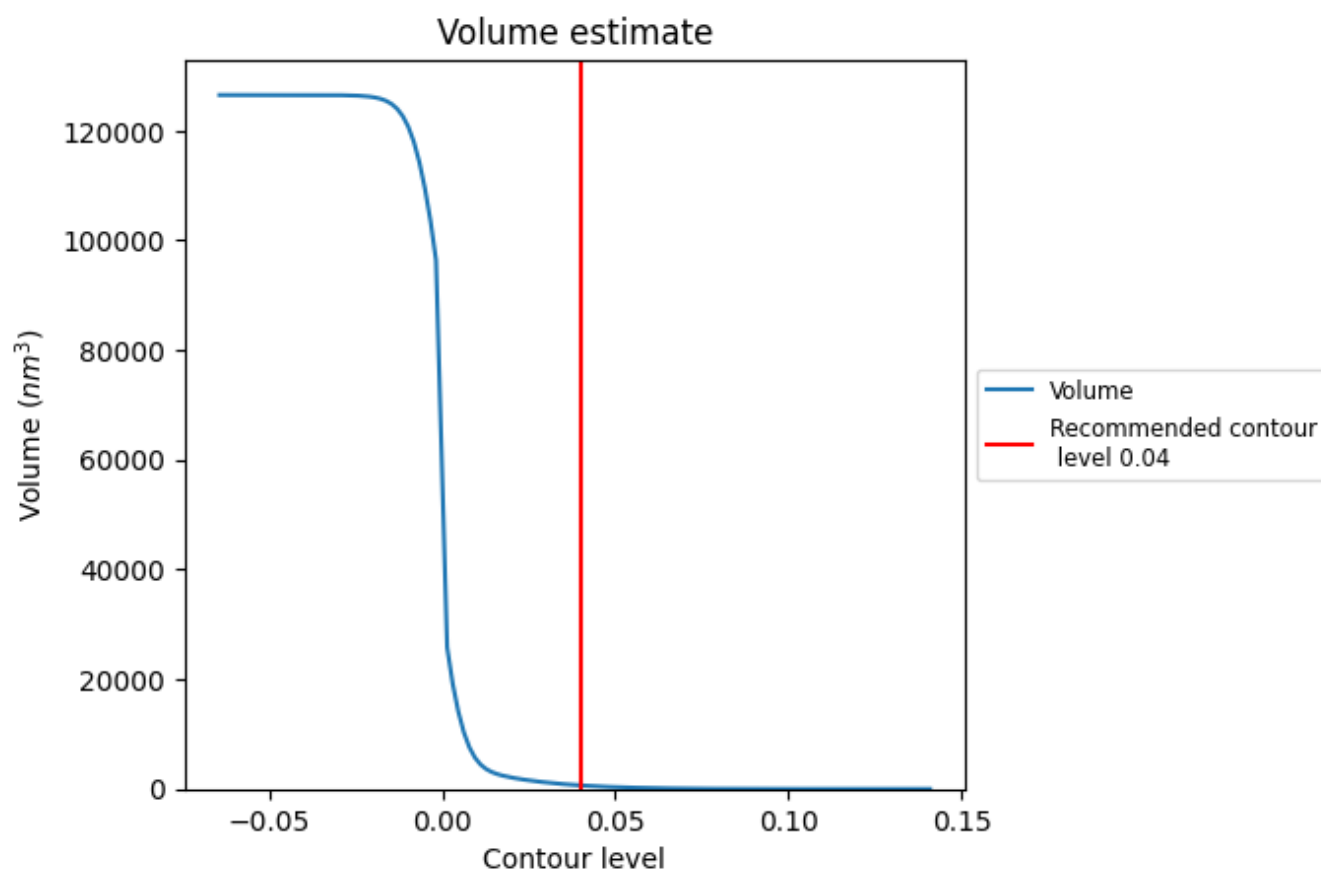
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

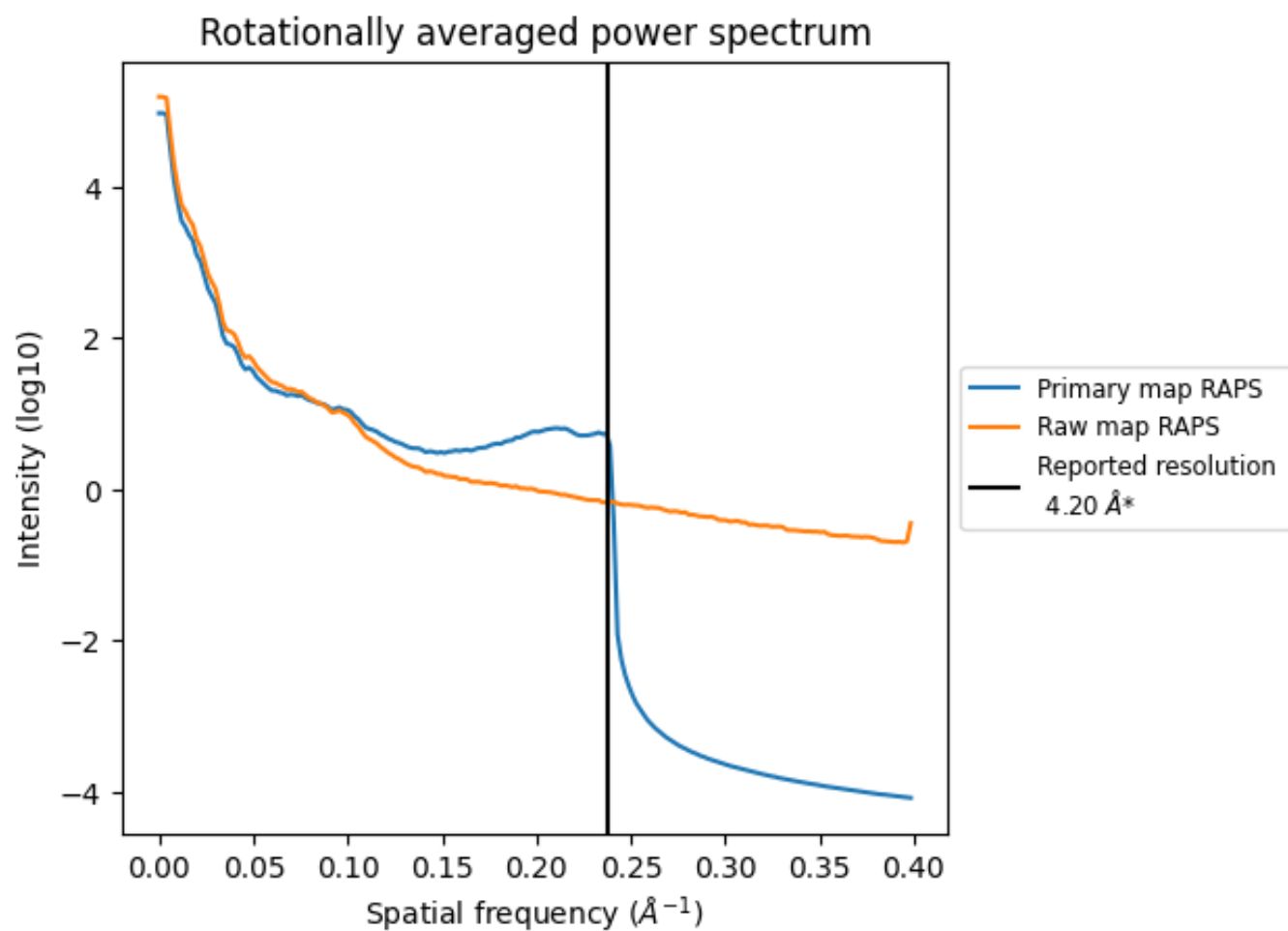
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 651 nm³; this corresponds to an approximate mass of 588 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

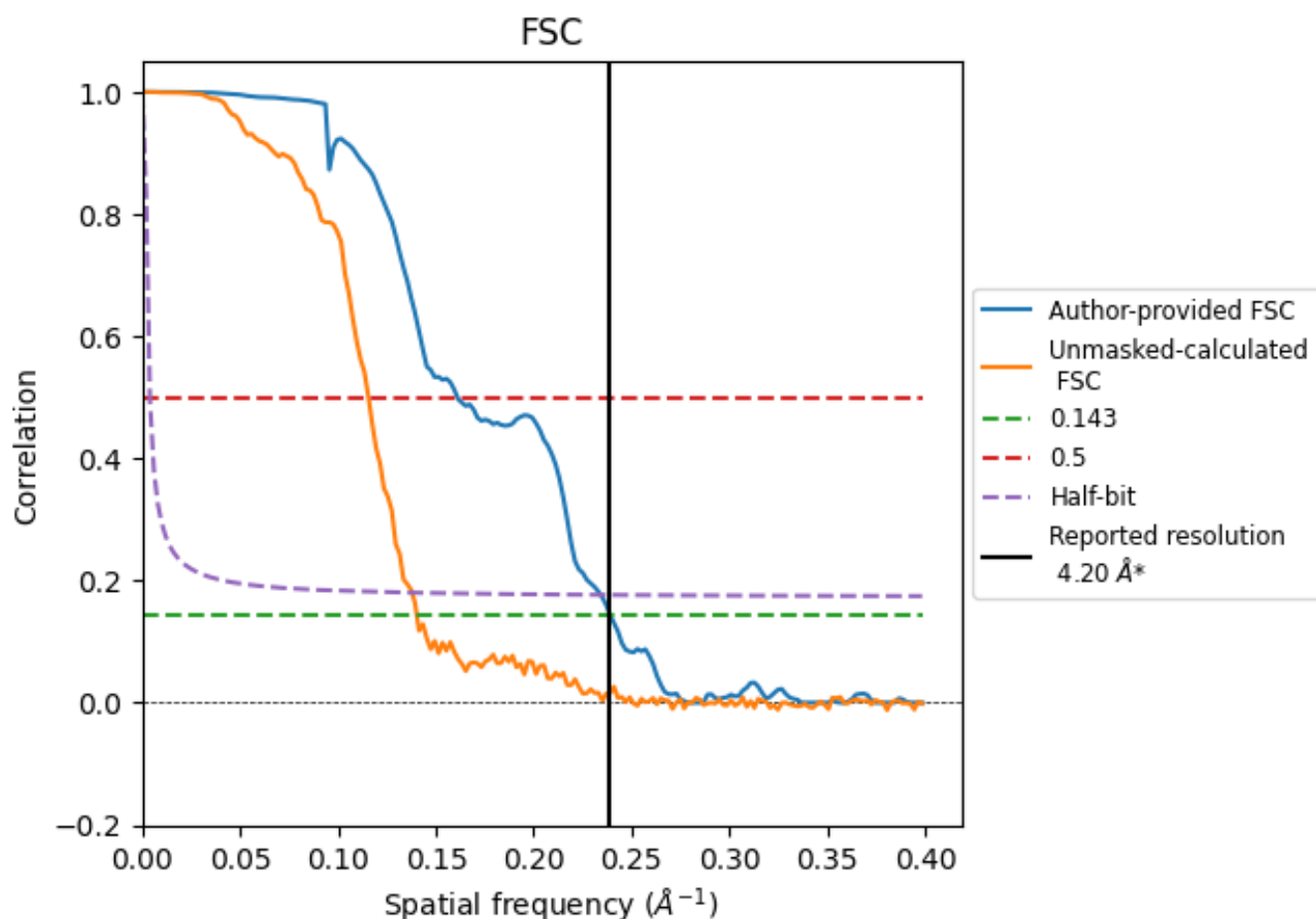


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [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 $0.238 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

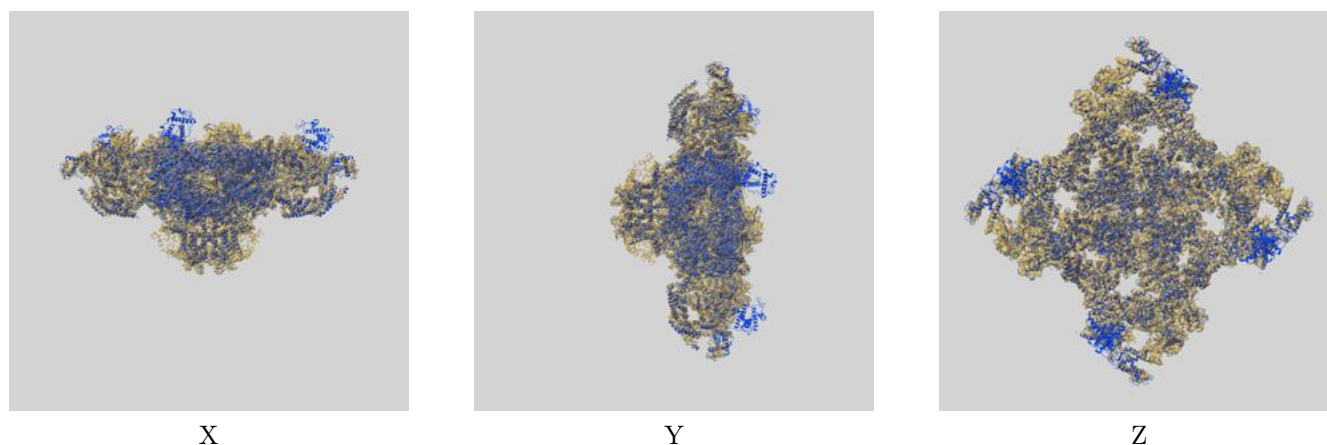
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	6.21	4.27
Unmasked-calculated*	7.13	8.65	7.26

*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 7.13 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

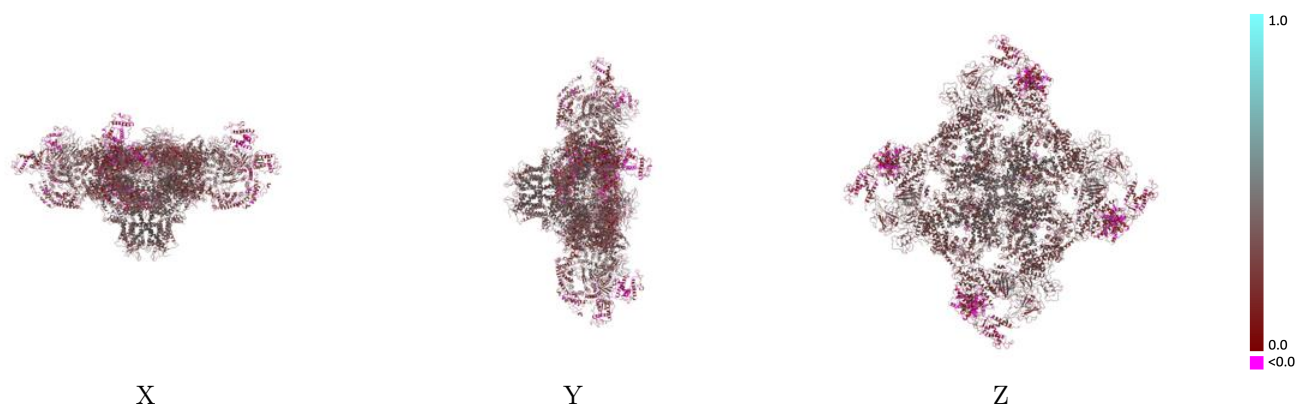
This section contains information regarding the fit between EMDB map EMD-8375 and PDB model 5T9S. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



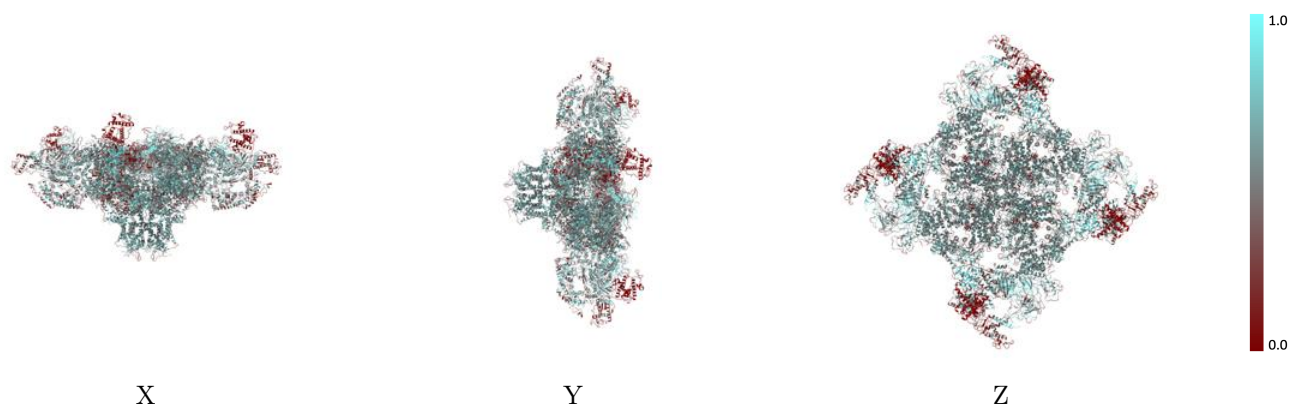
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



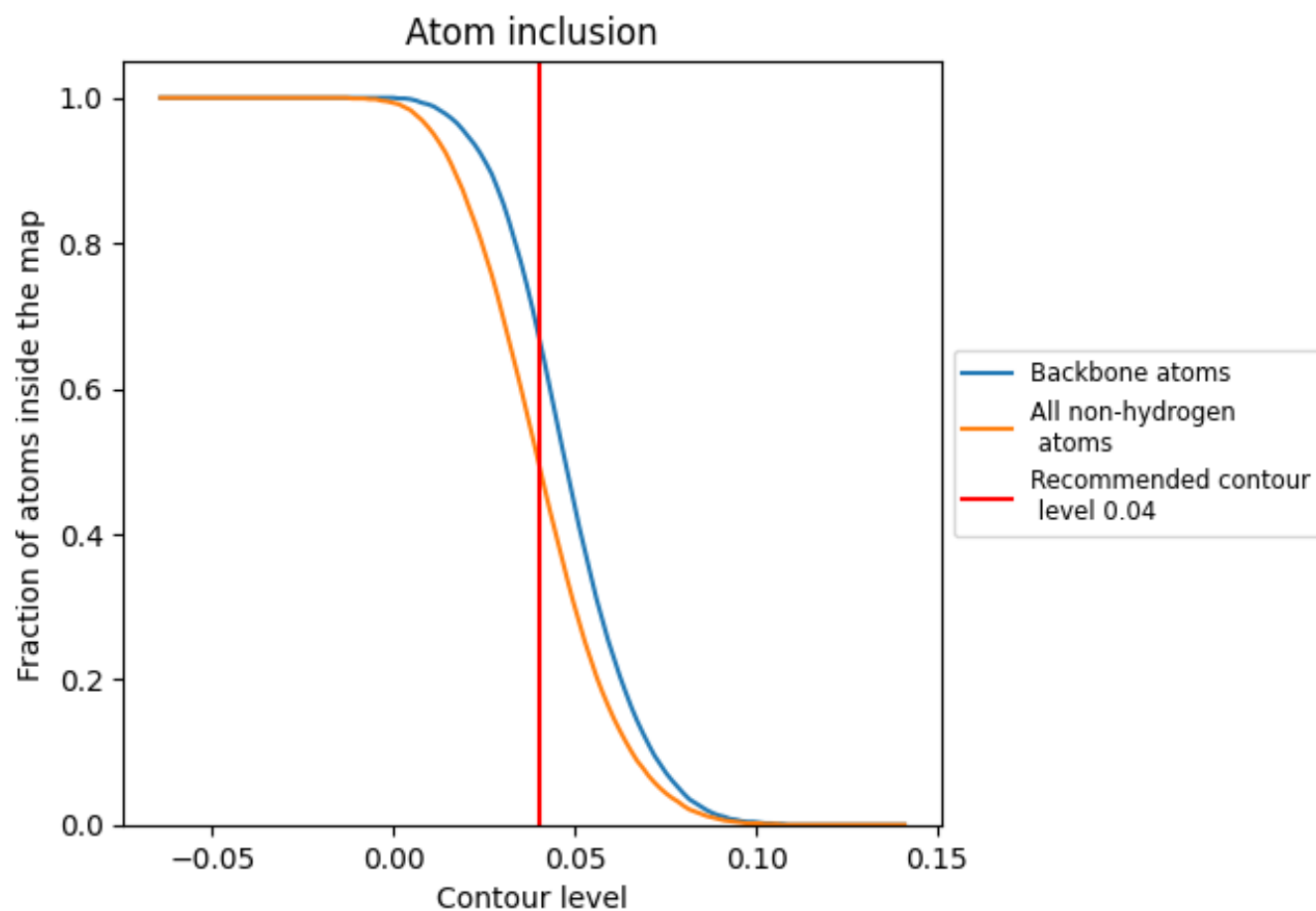
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	0.4980	0.2870
A	0.4780	0.3000
B	0.5030	0.2900
E	0.4950	0.2850
F	0.4780	0.3050
G	0.5000	0.2870
H	0.4840	0.3060
I	0.4950	0.2850
J	0.4840	0.2990

1.0

0.0

<0.0