



Full wwPDB EM Validation Report ⓘ

Oct 5, 2024 – 10:59 AM EDT

PDB ID : 5TAT
EMDB ID : EMD-8384
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA 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 : 4.80 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

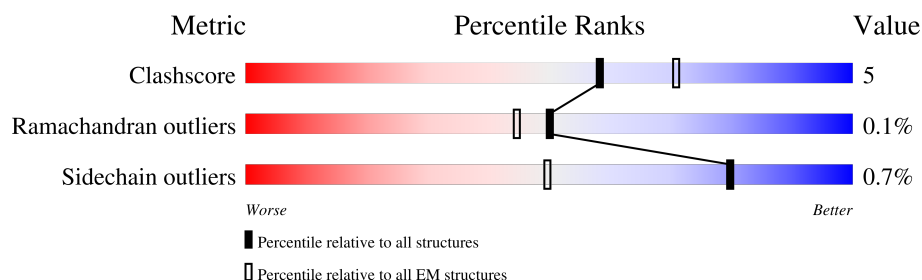
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	<div> <div>36%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	F	108	<div> <div>36%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	H	108	<div> <div>36%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	J	108	<div> <div>37%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	B	4416	<div> <div>39%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
2	E	4416	<div> <div>39%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
2	G	4416	<div> <div>39%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
2	I	4416	<div> <div>39%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

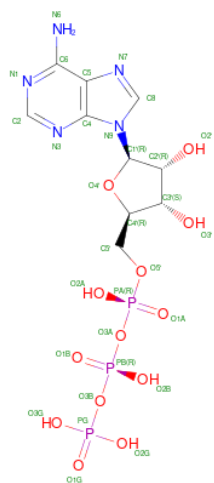
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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		

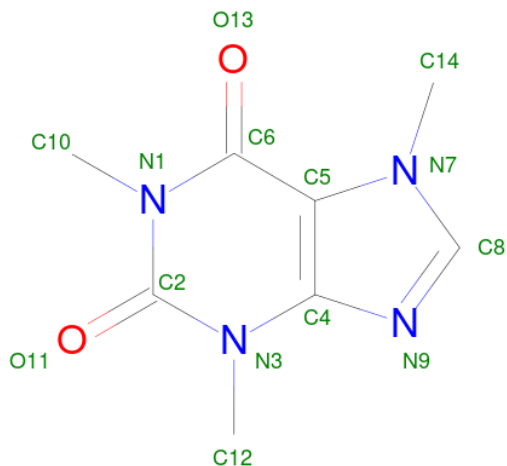
- Molecule 2 is a protein called Ryanodine receptor 1.

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



- Molecule 4 is **CAFFEINE** (three-letter code: CFF) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

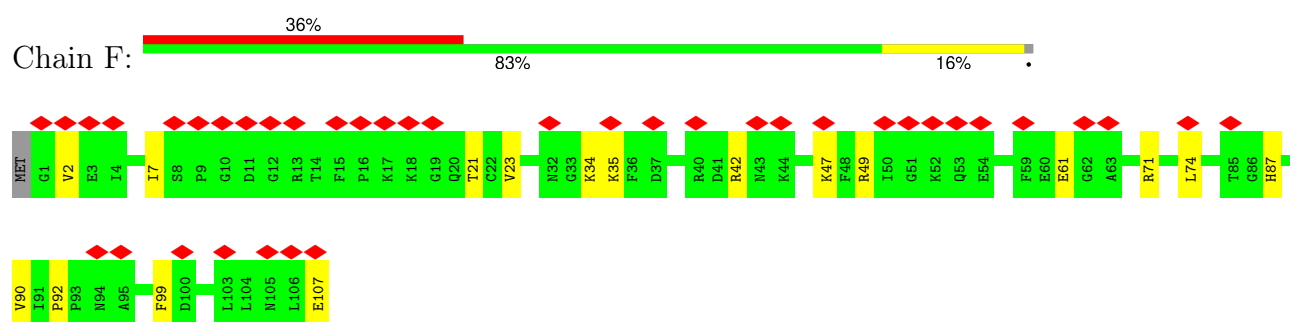
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

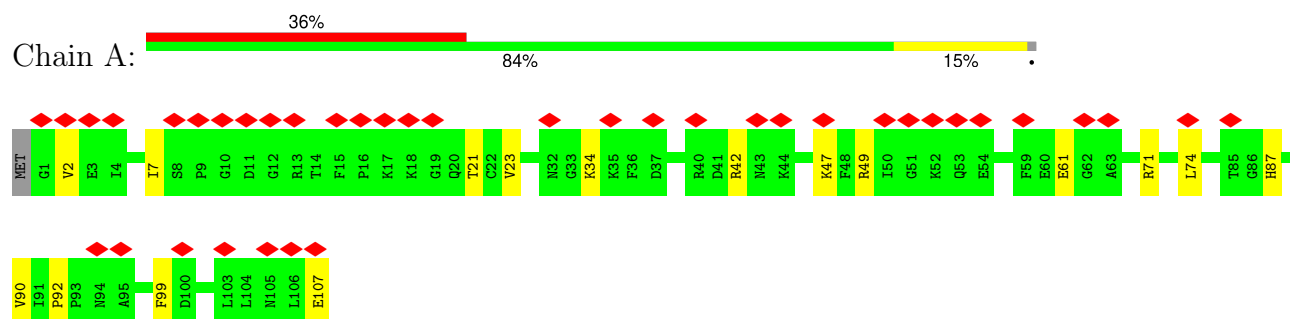
3 Residue-property plots [i](#)

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

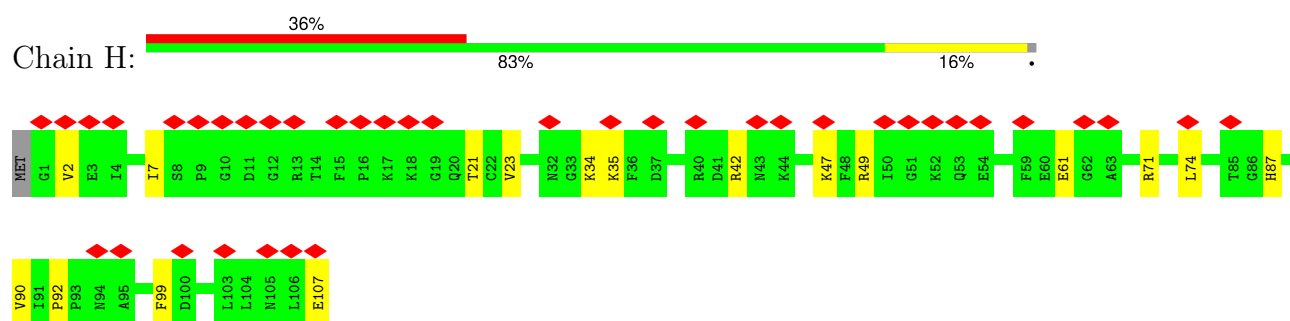
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



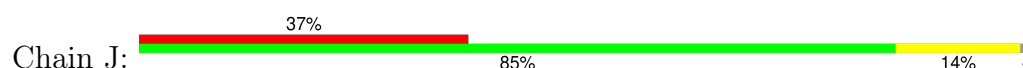
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

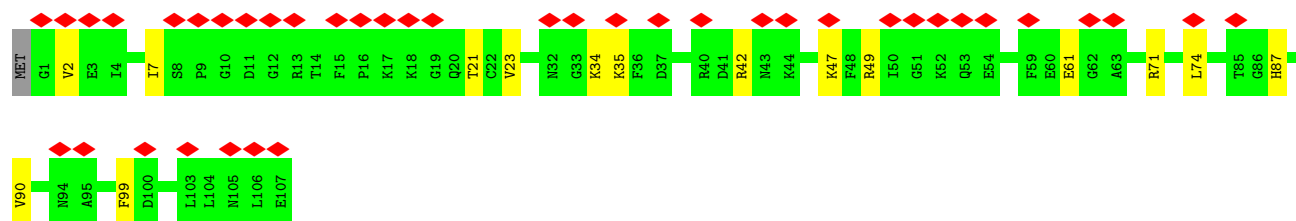


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

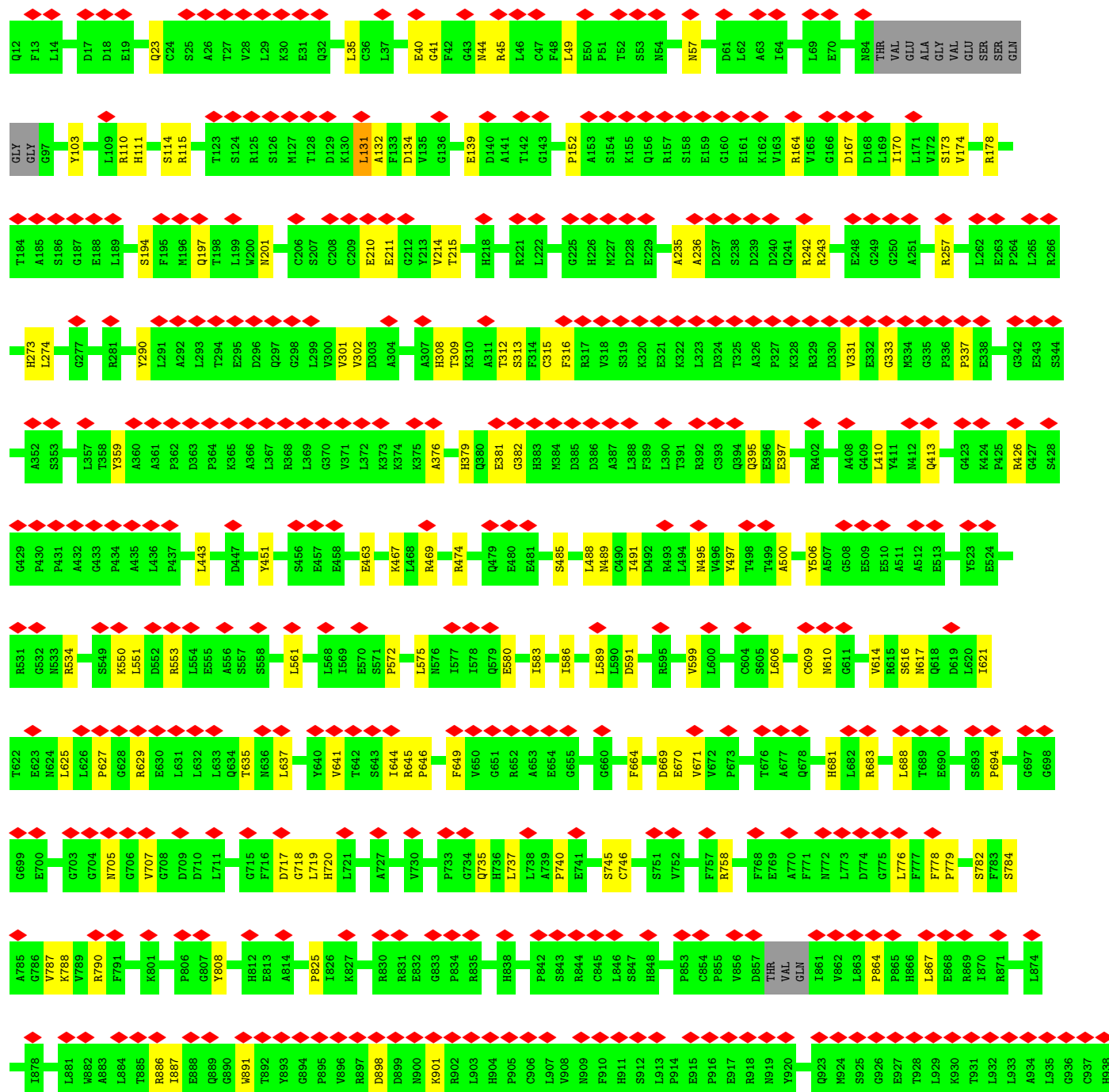
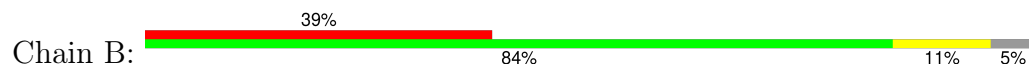


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

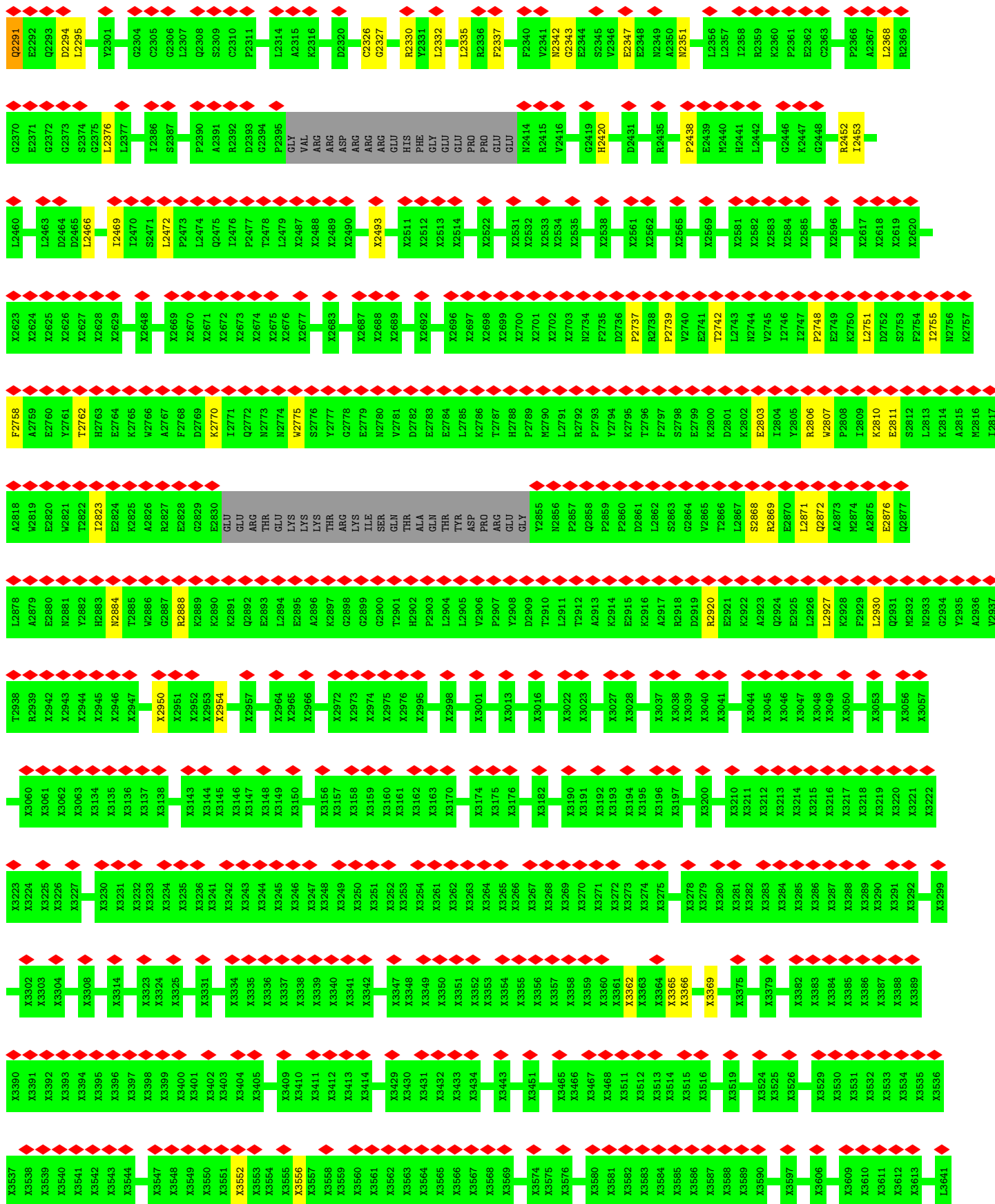




• Molecule 2: Ryanodine receptor 1









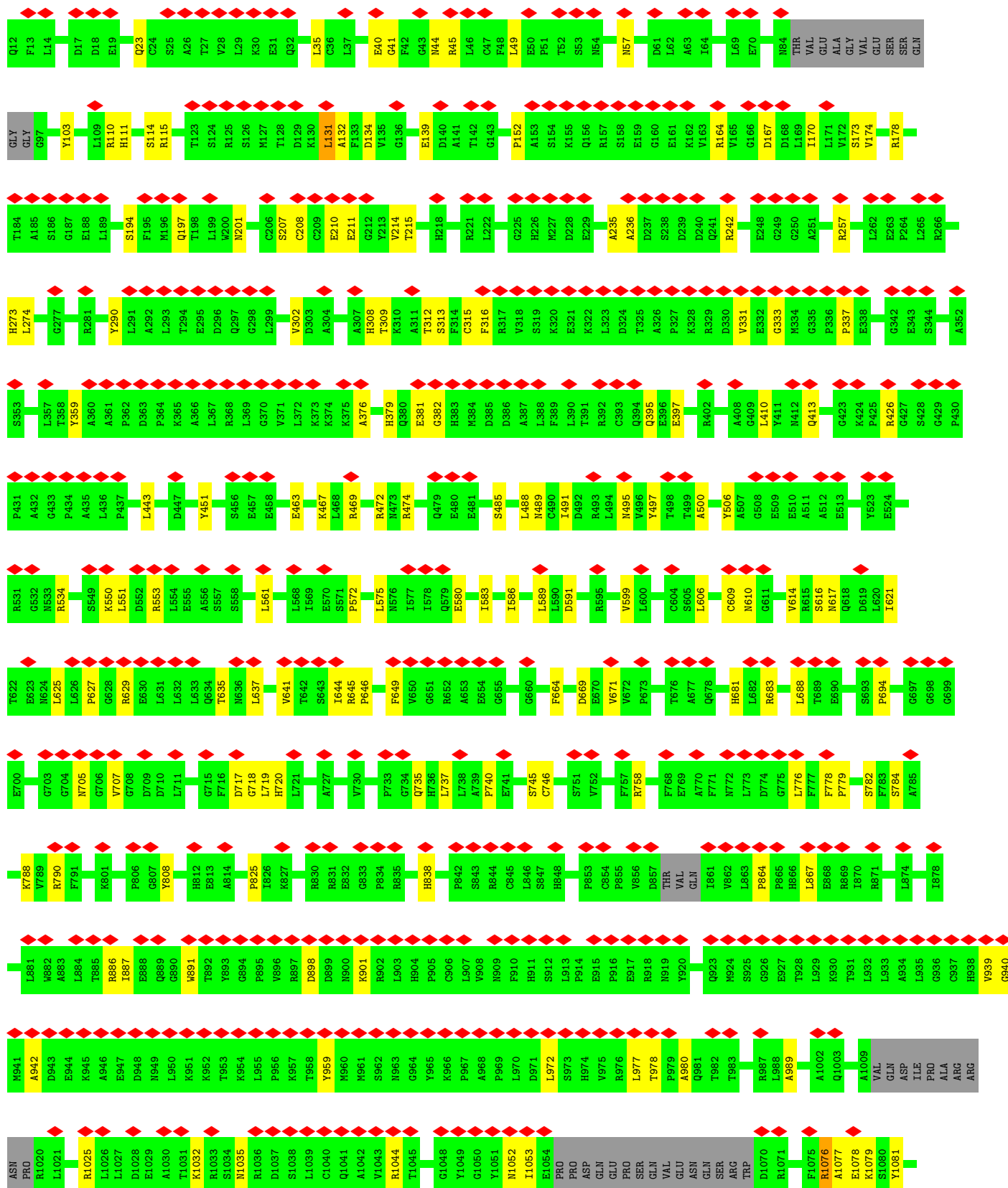
Chain I:





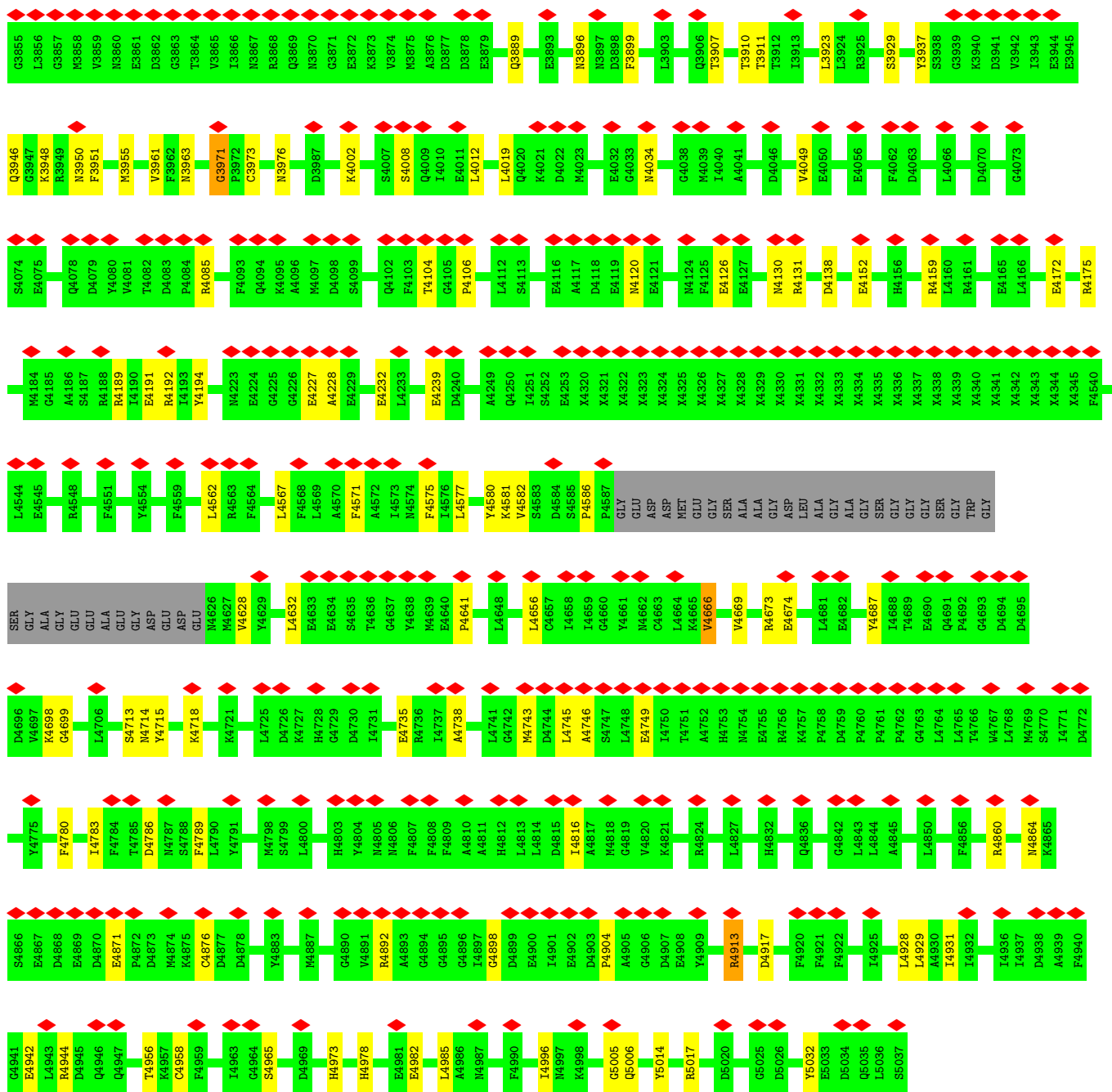




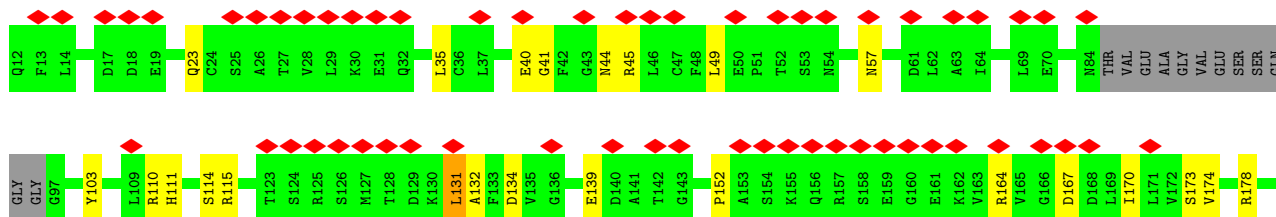
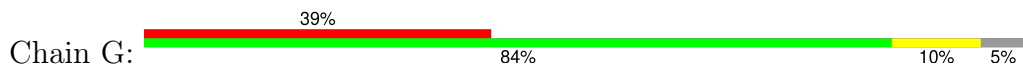




GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3757	V3758	E3762	S3768	R3769	L3770	H3771	T3772	R3773	V3779	L3780	Q3781	S3784	K3787	G3788	E3789	T3790	L3798	L3806	G3807	G3808	N3809	L3817	K3821	D3822	K3823	K3824	G3827	Q3830	Q3833	L3842	D3843	L3849	E3854	K3658	W3661	I3662	L3663	T3664	E3665	D3666	H3667	S3668	F3669	R3672	D3676	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	R3707	T3711	E3712	K3713	S3714	K3715	L3716	D3717	E3718	D3719	Y3720	M3723	A3724	Y3725	H3734	L3735	E3736	E3737	G3738	G3739	E3740	N3741	GLY	GLU	ALA	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
K3543	K3544	K3547	K3548	K3549	K3550	K3551	K3552	K3553	K3554	K3555	K3556	K3557	K3558	K3559	K3560	K3561	K3562	K3563	K3564	K3565	K3566	K3567	K3568	K3569	K3574	K3575	K3576	K3580	K3581	K3582	K3583	K3584	K3585	K3586	K3587	K3588	K3589	K3590	K3597	K3606	K3609	K3610	K3611	K3612	K3613	L3641	V3642	L3643	L3644	F3653	K3396	K3397	K3398	K3399	K3400	K3401	K3402	K3403	K3404	K3405	K3409	K3410	K3411	K3412	K3413	K3414	K3429	K3430	K3431	K3432	K3433	K3434	K3443	K3451	K3465	K3466	K3467	K3468	K3511	K3512	K3513	K3514	K3515	K3516	K3519	K3524	K3525	K3526	K3529	K3530	K3531	K3532	K3533	K3534	K3535	K3536	K3537	K3538	K3539	K3540	K3541	K3542	K3314	K3323	K3324	K3325	K3331	K3334	K3335	K3336	K3337	K3338	K3339	K3340	K3341	K3342	K3347	K3348	K3349	K3350	K3351	K3352	K3353	K3354	K3355	K3356	K3357	K3358	K3359	K3361	K3362	K3363	K3364	K3365	K3366	K3369	K3375	K3379	K3382	K3383	K3384	K3385	K3386	K3387	K3388	K3389	K3391	K3392	K3399	K3302	K3303	K3304	K3395	K3230	K3231	K3232	K3233	K3234	K3235	K3236	K3241	K3242	K3243	K3244	K3245	K3246	K3247	K3248	K3249	K3250	K3251	K3252	K3253	K3254	K3261	K3262	K3263	K3264	K3266	K3267	K3268	K3269	K3270	K3271	K3272	K3273	K3274	K3275	K3278	K3279	K3280	K3281	K3282	K3283	K3284	K3285	K3286	K3287	K3288	K3289	K3290	K3291	K3292	K3299	K3302	K3303	K3304	K3395	X3136	X3137	X3138	X3143	X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3174	X3175	X3176	X3182	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X2945	X2946	X2947	X2950	X2951	X2952	X2957	X2964	X2965	X2966	X2972	X2973	X2974	X2975	X2976	X2995	X2998	X3001	X3013	X3016	X3022	X3023	X3027	X3028	X3037	X3038	X3039	X3040	X3041	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3053	X3056	X3057	X3060	X3061	X3062	X3063	X3066	X3134	X3135	H2883	N2884	T2885	W2886	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	Q2898	G2899	Q2900	T2901	H2902	T2903	L2904	L2905	V2906	T2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	N2932	N2933	Q2934	V2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	K2683	K2684	K2685	W2686	R2688	K2689	K2690	Q2692	E2693	L2694	E2695	A2696	K2697	Q2698	G2699	I2699	L2699	T2699	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	K2788	T2789	M2790	X2701	X2702	X2703	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	P2768	D2769	K2770	I2771	Q2772	N2773	THR	N2774	L2775	S2776	Y2777	Q2778	E2779	L2780	THR	E2782	E2783	E2784	L2785	K2786	T2787	K2788	P2789	M2790	X2701	X2702	X2703	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2628	X2629	X2648	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2683	X2687	X2688	X2689	X2692	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2466	I2469	S2470	S2471	L2472	P2473	L2474	Q2475	L2476	Q2475	L2476	P2477	L2478	L2479	X2487	X2488	X2489	X2490	X2493	X2511	X2512	X2513	X2514	X2522	X2531	X2532	X2533	X2534	X2535	X2538	X2561	X2562	X2565	X2569	X2581	X2582	X2583	X2584	X2585	X2596	X2617	X2618	X2619	X2620	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2648	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2683	X2687	X2688	X2689	X2692	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2263	E2264	K2265	W2266	A2267	P2268	D2269	K2270	I2271	Q2272	N2273	THR	N2274	L2275	S2276	Y2277	Q2278	E2279	L2280	THR	E2282	E2283	E2284	L2285	K2286	T2287	K2288	P2289	M2290	X2201	X2202	X2203	X2204	X2205	X2206	T2207	V2208	D2209	T2210	L2211	T2212	A2213	K2214	E2215	K2216	A2217	R2218	D2219	R2220	E2221	K2222	A2223	Q2224	E2225	L2226	L2227	K2228	F2229	L2230	Q2231	N2232	N2233	Q2234	V2235	A2236	V2237	T2238	R2239	X2242	X2243	X2244	K2263	K2264	K2265	K2266	K2267	K2268	K2269	K2270	K2271	K2272	K2273	K2274	K2275	K2276	K2277	K2278	K2279	K2280	K2281	K2282	K2283	K2284	K2285	K2286	K2287	K2288	K2289	K2290	K2291	K2292	K2293	K2294	K2295	K2296	K2297	K2298	K2299	K2300	K2301	K2302	K2303	K2304	K2305	K2306	K2307	K2308	K2309	K2310	K2311	K2312	K2313	K2314	K2315	K2316	K2317	K2318	K2319	K2320	K2321	K2322	K2323	K2324	K2325	K2326	K2327	K2328	K2329	K2330	K2331	K2332	K2333	K2334	K2335	K2336	K2337	K2338	K2339	K2340	K2341	K2342	K2347	K2348	K2349	K2350	K2351	K2352	K2353	K2354	K2355	K2356	K2357	K2358	K2359	K2361	K2362	K2363	K2364	K2366	K2367	K2368	K2369	K2370	K2371	K2372	K2373	K2374	K2375	K3278	K3279	K3280	K3281	K3282	K3283	K3284	K3285	K3286	K3287	K3288	K3289	K3290	K3291	K329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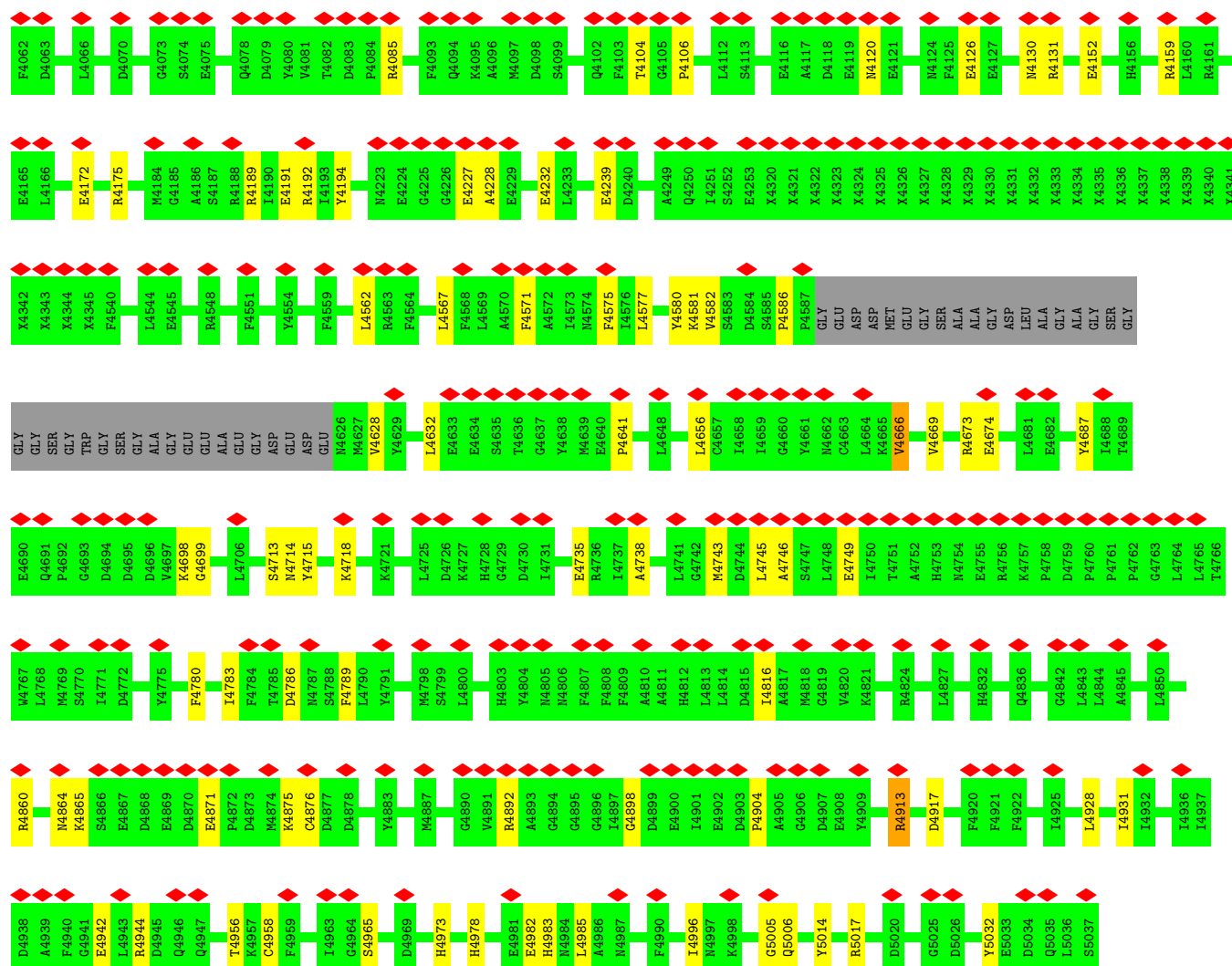
• Molecule 2: Ryanodine receptor 1







V3942	R3849	T3664	X3324	X3234	X3143	X2950	G2987	A2767
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E3945	G3855	D3666	X3331	X3236	X3145	X2952	R2889	D2769
G3946	H3856	H3667	X3334	X3242	X3146	X2957	K2890	K2770
G3947	L3857	F3668	X3335	X3243	X3147	X2964	K2891	I2771
K3948	F3857	F3669	X3336	X3244	X3148	X2965	Q2892	Q2772
K3949	E3750	R3672	X3337	X3245	X3149	X2966	E2893	H2773
N3950	V3751	M3673	X3338	X3246	X3150	X2972	L2894	H2774
F3951	F3752	I3674	X3339	X3247	X3156	X2977	E2895	K2775
M3955	D3675	D3676	X3340	X3248	X3157	X2978	A2896	S2776
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	E3755	G3681	X3342	X3250	X3159	X2974	Q2898	G2778
	E3756	E3682	X3343	X3251	X3160	X2975	G2899	E2779
	E3757	X3564	X3344	X3252	X3161	X2976	Q2900	H2780
	K3758	X3565	X3347	X3253	X3162	X2995	T2901	V2781
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	S3768	X3567	X3349	X3261	X3170	X3001	P2903	E2783
	R3769	X3568	X3350	X3262	X3174	X3002	L2904	E2784
	H3770	X3569	X3351	X3263	X3175	X3003	L2905	L2785
	T3772	X3574	X3352	X3264	X3176	X3004	V2906	K2786
	R3773	X3575	X3353	X3265	X3182	X3005	P2907	L2787
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	L3780	X3580	X3355	X3267	X3191	X3007	D2909	F2789
	Q3781	X3581	X3356	X3268	X3192	X3008	T2910	H2790
	S3784	X3582	X3357	X3269	X3193	X3009	L2911	L2791
	K3787	X3583	X3358	X3270	X3194	X3010	T2912	R2792
	G3788	X3584	X3359	X3271	X3195	X3011	A2913	F2793
	E3789	X3585	X3360	X3272	X3196	X3012	K2914	V2794
	T3790	X3586	X3361	X3273	X3197	X3013	E2915	K2795
	L3798	X3587	X3362	X3274	X3198	X3014	K2916	T2796
	L3805	X3588	X3363	X3275	X3199	X3015	A2917	F2797
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	G3807	X3590	X3365	X3277	X3201	X3017	D2919	K2799
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	N3809	X3592	X3367	X3279	X3203	X3019	E2921	D2801
	L3817	X3593	X3368	X3280	X3204	X3020	K2922	K2802
	K3821	X3594	X3369	X3281	X3205	X3021	A2923	E2803
	D3822	X3595	X3370	X3282	X3206	X3022	Q2924	E2804
	K3823	X3596	X3371	X3283	X3207	X3023	E2925	T2805
	K3824	X3597	X3372	X3284	X3208	X3024	Q2926	K2806
	G3827	X3598	X3373	X3285	X3209	X3025	E2927	L2807
	Q3830	X3599	X3374	X3286	X3210	X3026	K2928	P2808
	Q3833	X3600	X3375	X3287	X3211	X3027	F2929	M2874
	L3842	X3601	X3376	X3288	X3212	X3028	L2930	K2810
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		X3604	X3379	X3291	X3215	X3031	A2873	S2813
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		X3606	X3381	X3293	X3217	X3033	E2876	K2814
		X3607	X3382	X3294	X3218	X3034	Q2877	A2815
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		X3609	X3384	X3296	X3220	X3036	F2929	L2817
		X3610	X3385	X3297	X3221	X3037	L2930	A2818
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		X3621	X3396	X3308	X3302	X3048	M2874	
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		X3625	X3400	X3312	X3306	X3052	L2878	
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		X3633	X3408	X3320	X3314	X3060	L2930	
		X3634	X3409	X3321	X3315	X3061	Q2876	
		X3635	X3410	X3322	X3316	X3062	A2873	
		X3636	X3411	X3323	X3317	X3063	M2874	
		X3637	X3412	X3324	X3318	X3064	E2875	
		X3638	X3413	X3325	X3319	X3065	A2876	
		X3639	X3414	X3326	X3320	X3066	Q2877	
		X3640	X3415	X3327	X3321	X3067	L2878	
		X3641	X3416	X3328	X3322	X3068	N2933	
		X3642	X3417	X3329	X3323	X3069	Q2934	
		X3643	X3418	X3330	X3324	X3070	E2935	
		X3644	X3419	X3331	X3325	X3071	L2936	
		X3645	X3420	X3332	X3326	X3072	K2928	
		X3646	X3421	X3333	X3327	X3073	F2929	
		X3647	X3422	X3334	X3328	X3074	L2930	
		X3648	X3423	X3335	X3329	X3075	Q2876	
		X3649	X3424	X3336	X3330	X3076	A2873	
		X3650	X3425	X3337	X3331	X3077	M2874	
		X3651	X3426	X3338	X3332	X3078	E2875	
		X3652	X3427	X3339	X3333	X3079	A2876	
		X3653	X3428	X3340	X3334	X3080	Q2877	
		X3654	X3429	X3341	X3335	X3081	L2878	
		X3655	X3430	X3342	X3336	X3082	N2933	
		X3656	X3431	X3343	X3337	X3083	Q2934	
		X3657	X3432	X3344	X3338	X3084	E2935	
		X3658	X3433	X3345	X3339	X3085	L2926	
		X3659	X3434	X3346	X3340	X3086	E2927	
		X3660	X3435	X3347	X3341	X3087	K2928	
		X3661	X3436	X3348	X3342	X3088	F2929	
		X3662	X3437	X3349	X3343	X3089	L2930	
		X3663	X3438	X3350	X3344	X3090	Q2876	
		X3664	X3439	X3351	X3345	X3091	A2873	
		X3665	X3440	X3352	X3346	X3092	M2874	
		X3666	X3441	X3353	X3347	X3093	E2875	
		X3667	X3442	X3354	X3348	X3094	A2876	
		X3668	X3443	X3355	X3349	X3095	Q2877	
		X3669	X3444	X3356	X3350	X3096	L2878	
		X3670	X3445	X3357	X3351	X3097	N2933	
		X3671	X3446	X3358	X3352	X3098	Q2934	
		X3672	X3447	X3359	X3353	X3099	E2935	
		X3673	X3448	X3360	X3354	X3100	L2926	
		X3674	X3449	X3361	X3355	X3101	E2927	
		X3675	X3450	X3362	X3356	X3102	K2928	
		X3676	X3451	X3363	X3357	X3103	F2929	
		X3677	X3452	X3364	X3358	X3104	L2930	
		X3678	X3453	X3365	X3359	X3105	Q2876	
		X3679	X3454	X3366	X3360	X3106	A2873	
		X3680	X3455	X3367	X3361	X3107	M2874	
		X3681	X3456	X3368	X3362	X3108	E2875	
		X3682	X3457	X3369	X3363	X3109	A2876	
		X3683	X3458	X3370	X3364	X3110	Q2877	
		X3684	X3459	X3371	X3365	X3111	L2878	
		X3685	X3460	X3372	X3366	X3112	N2933	
		X3686	X3461	X3373	X3367	X3113	Q2934	
		X3687	X3462	X3374	X3368	X3114	E2935	
		X3688	X3463	X3375	X3369	X3115	L2926	
		X3689	X3464	X3376	X3370	X3116	E2927	
		X3690	X3465	X3377	X3371	X3117	K2928	
		X3691	X3466	X3378	X3372	X3118	F2929	
		X3692	X3467	X3379	X3373	X3119	L2930	
		X3693	X3468	X3380	X3374	X3120	Q2876	
		X3694	X3469	X3381	X3375	X3121	A2873	
		X3695	X3470	X3382	X3376	X3122	M2874	
		X3696	X3471	X3383	X3377	X3123	E2875	
		X3697	X3472	X3384	X3378	X3124	A2876	
		X3698	X3473	X3385	X3379	X3125	Q2877	
		X3699	X3474	X3386	X3380	X3126	L2878	
		X3700	X3475	X3387	X3381	X3127	N2933	
		X3701	X3476	X3388	X3382	X3128	Q2934	
		X3702	X3477	X3389	X3383	X3129	E2935	
		X3703	X3478	X3390	X3384	X3130	L2926	
		X3704	X3479	X3391	X3385	X3131	E2927	
		X3705	X3480	X3392	X3386	X3132	K2928	
		X3706	X3481	X3393	X3387	X3133	F2929	
		X3707	X3482	X3394	X3388	X3134	L2930	
		X3708	X3483	X3395	X3389	X3135	Q2876	
		X3709	X3484	X3396	X3390	X3136	A2873	
		X3710	X3485	X3397	X3391	X3137	M2874	
		X3711	X3486	X3398	X3392	X3138	E2875	
		X3712	X3487	X3399	X3393	X3139	A2876	
		X3713	X3488	X3400	X3394	X3140	Q2877	
		X3714	X3489	X3401	X3395	X3141	L2878	
		X3715	X3490	X3402	X3396	X3142	N2933	
		X3716	X3491	X3403	X3397	X3143	Q2934	
		X3717	X3492	X3404	X3398	X3144	E2935	
		X3718	X3493	X3405	X3399	X3145	L2926	
		X3719	X3494	X3406	X3400	X3146	E2927	
		X3720	X3495	X3407	X3401	X3147	K2928	
		X3721	X3496	X3408	X3402	X3148	F2929	
		X3722	X3497	X3409	X3403	X3149	L2930	
		X3723	X3498	X3410	X3404	X3150	Q2876	
		X372						



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	0.095	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	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: CFF, ATP, 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	0.31	0/834	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.29	0/25428	0.53	6/34534 (0.0%)
2	E	0.29	0/25428	0.53	6/34534 (0.0%)
2	G	0.29	0/25428	0.53	6/34534 (0.0%)
2	I	0.29	0/25428	0.53	6/34534 (0.0%)
All	All	0.29	0/105048	0.53	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	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	LEU	CA-CB-CG	8.17	134.09	115.30
2	E	131	LEU	CA-CB-CG	8.17	134.09	115.30
2	I	131	LEU	CA-CB-CG	8.17	134.08	115.30
2	G	131	LEU	CA-CB-CG	8.16	134.08	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1600	LEU	CA-CB-CG	7.04	131.49	115.30
2	G	1600	LEU	CA-CB-CG	7.04	131.49	115.30
2	B	1600	LEU	CA-CB-CG	7.03	131.47	115.30
2	I	1600	LEU	CA-CB-CG	7.00	131.39	115.30
2	I	1676	LEU	CA-CB-CG	6.44	130.12	115.30
2	G	1676	LEU	CA-CB-CG	6.44	130.11	115.30
2	E	1676	LEU	CA-CB-CG	6.43	130.10	115.30
2	B	1676	LEU	CA-CB-CG	6.42	130.07	115.30
2	G	4985	LEU	CA-CB-CG	6.31	129.82	115.30
2	B	4985	LEU	CA-CB-CG	6.31	129.81	115.30
2	I	4985	LEU	CA-CB-CG	6.30	129.78	115.30
2	E	4985	LEU	CA-CB-CG	6.29	129.76	115.30
2	G	977	LEU	CA-CB-CG	6.18	129.51	115.30
2	I	977	LEU	CA-CB-CG	6.18	129.50	115.30
2	E	977	LEU	CA-CB-CG	6.17	129.50	115.30
2	B	977	LEU	CA-CB-CG	6.17	129.48	115.30
2	B	688	LEU	CA-CB-CG	6.01	129.12	115.30
2	I	688	LEU	CA-CB-CG	6.01	129.11	115.30
2	E	688	LEU	CA-CB-CG	6.00	129.10	115.30
2	G	688	LEU	CA-CB-CG	5.99	129.08	115.30

There are no chirality outliers.

All (56) 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	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	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	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	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	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	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	10	0
1	F	818	0	824	11	0
1	H	818	0	824	11	0
1	J	818	0	824	9	0
2	B	29499	0	24741	252	0
2	E	29499	0	24741	250	0
2	G	29499	0	24741	251	0
2	I	29499	0	24741	253	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102348	1016	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 (1016) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.78	0.66
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.78	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.45	0.65
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.30	0.65
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.78	0.65
2:E:4958:CYS:O	3:E:5101:ATP:N6	2.30	0.65
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.79	0.64
2:B:4958:CYS:O	3:B:5101:ATP:N6	2.30	0.64
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.30	0.64
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.63	0.64
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.79	0.64
2:B:379:HIS:HD2	2:B:382:GLY:H	1.45	0.64
2:G:4958:CYS:O	3:G:5101:ATP:N6	2.30	0.64
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.81	0.63
2:E:379:HIS:HD2	2:E:382:GLY:H	1.45	0.63
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.79	0.63
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.30	0.63
2:I:4958:CYS:O	3:I:5101:ATP:N6	2.30	0.63
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.81	0.63
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.62	0.63
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.81	0.63
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.80	0.63
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.30	0.63
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.80	0.63
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.81	0.63
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.80	0.63
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.62	0.63
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.81	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.81	0.62
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.81	0.62
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.62
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.82	0.62
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.81	0.62
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.62	0.62
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.79	0.62
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.81	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.62
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.62
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.62
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.81	0.62
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.80	0.62
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.81	0.62
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.82	0.62
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.81	0.62
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.81	0.61
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.61
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:379:HIS:HD2	2:G:382:GLY:H	1.45	0.61
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.80	0.61
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.83	0.61
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.83	0.61
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.61
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.82	0.61
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.61
2:I:173:SER:HB3	2:I:178:ARG:H	1.66	0.61
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.83	0.61
2:G:173:SER:HB3	2:G:178:ARG:H	1.66	0.61
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.81	0.61
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.60
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.82	0.60
2:B:173:SER:HB3	2:B:178:ARG:H	1.66	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.60
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.84	0.60
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.67	0.60
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.67	0.60
2:I:359:TYR:HA	2:I:376:ALA:HA	1.84	0.59
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.84	0.59
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.67	0.59
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.84	0.59
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.67	0.59
2:E:173:SER:HB3	2:E:178:ARG:H	1.66	0.59
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.68	0.59
2:B:359:TYR:HA	2:B:376:ALA:HA	1.84	0.59
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.84	0.59
2:B:2347:GLU:O	2:B:2351:ASN:N	2.32	0.59
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.36	0.59
2:E:4996:ILE:HG12	4:E:5102:CFF:H123	1.85	0.59
2:I:4996:ILE:HG12	4:I:5102:CFF:H123	1.85	0.59
2:B:4996:ILE:HG12	4:B:5102:CFF:H123	1.85	0.59
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.68	0.59
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.68	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.85	0.58
2:G:359:TYR:HA	2:G:376:ALA:HA	1.84	0.58
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.36	0.58
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.36	0.58
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.85	0.58
2:G:4996:ILE:HG12	4:G:5102:CFF:H123	1.85	0.58
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.36	0.58
2:E:359:TYR:HA	2:E:376:ALA:HA	1.84	0.58
2:G:331:VAL:HG12	2:G:333:GLY:H	1.68	0.58
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.86	0.58
2:G:2347:GLU:O	2:G:2351:ASN:N	2.32	0.58
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.86	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.37	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.57
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.57
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.77	0.57
2:G:683:ARG:NH1	2:G:707:VAL:O	2.37	0.57
2:G:3770:LEU:HD23	2:G:3772:THR:HG22	1.86	0.57
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.37	0.57
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.37	0.57
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.85	0.57
2:E:3770:LEU:HD23	2:E:3772:THR:HG22	1.86	0.57
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.77	0.57
2:B:3770:LEU:HD23	2:B:3772:THR:HG22	1.86	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.57
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.77	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.69	0.57
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.77	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.57
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.38	0.57
2:B:614:VAL:HG22	2:B:616:SER:H	1.70	0.57
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.69	0.57
2:I:614:VAL:HG22	2:I:616:SER:H	1.70	0.57
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.57
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.69	0.57
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.69	0.57
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.38	0.57
2:I:331:VAL:HG12	2:I:333:GLY:H	1.68	0.57
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.86	0.57
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.38	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.38	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.57
2:I:3770:LEU:HD23	2:I:3772:THR:HG22	1.87	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.56
2:I:132:ALA:HA	2:I:194:SER:HB2	1.87	0.56
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.38	0.56
2:E:331:VAL:HG12	2:E:333:GLY:H	1.68	0.56
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.87	0.56
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.88	0.56
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.70	0.56
2:I:2347:GLU:O	2:I:2351:ASN:N	2.32	0.56
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.70	0.56
2:G:132:ALA:HA	2:G:194:SER:HB2	1.88	0.56
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.38	0.56
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.70	0.56
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.38	0.56
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.38	0.56
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.56
2:B:331:VAL:HG12	2:B:333:GLY:H	1.68	0.56
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.88	0.56
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.88	0.56
2:E:132:ALA:HA	2:E:194:SER:HB2	1.88	0.56
2:B:4904:PRO:HB3	2:B:4913:ARG:HD2	1.88	0.56
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.88	0.56
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.70	0.56
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	1.88	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.88	0.56
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.88	0.56
2:I:683:ARG:NH1	2:I:707:VAL:O	2.37	0.56
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.39	0.56
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.56
2:G:614:VAL:HG22	2:G:616:SER:H	1.70	0.56
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.39	0.56
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.88	0.56
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.38	0.56
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.39	0.55
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.39	0.55
2:E:4904:PRO:HB3	2:E:4913:ARG:HD2	1.88	0.55
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.70	0.55
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.88	0.55
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.88	0.55
2:E:2347:GLU:O	2:E:2351:ASN:N	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.55	0.55
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	1.88	0.55
2:B:683:ARG:NH1	2:B:707:VAL:O	2.37	0.55
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	1.88	0.55
2:I:4944:ARG:HH22	2:G:4942:GLU:HA	1.72	0.55
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.88	0.55
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.89	0.55
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.89	0.55
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.89	0.55
2:B:4944:ARG:HH22	2:I:4942:GLU:HA	1.72	0.55
2:I:4904:PRO:HB3	2:I:4913:ARG:HD2	1.88	0.55
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	1.88	0.55
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.89	0.55
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.88	0.55
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.55	0.55
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.88	0.55
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.87	0.55
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.89	0.55
2:E:683:ARG:NH1	2:E:707:VAL:O	2.37	0.55
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.40	0.54
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.89	0.54
1:J:34:LYS:HD3	2:I:629:ARG:HD2	1.89	0.54
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.41	0.54
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.88	0.54
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.90	0.54
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.89	0.54
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.40	0.54
2:G:4904:PRO:HB3	2:G:4913:ARG:HD2	1.88	0.54
2:B:4189:ARG:NH1	2:B:5032:TYR:OH	2.39	0.54
2:B:4942:GLU:HA	2:E:4944:ARG:HH22	1.73	0.54
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.55	0.54
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.89	0.54
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.89	0.54
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.40	0.54
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.41	0.54
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.89	0.54
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.89	0.54
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.89	0.54
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.40	0.54
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.89	0.54
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.41	0.54
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.41	0.54
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.89	0.54
2:I:4189:ARG:NH1	2:I:5032:TYR:OH	2.39	0.54
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.90	0.54
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.90	0.54
2:E:4942:GLU:HA	2:G:4944:ARG:HH22	1.72	0.54
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.88	0.54
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.90	0.54
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.41	0.54
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.89	0.54
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.41	0.54
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.90	0.54
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.55	0.54
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.89	0.54
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.41	0.54
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.40	0.54
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.90	0.54
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.89	0.54
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.90	0.54
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.40	0.54
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.90	0.53
2:B:669:ASP:OD2	2:B:790:ARG:NH2	2.41	0.53
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.91	0.53
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.40	0.53
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.91	0.53
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.90	0.53
2:G:4189:ARG:NH1	2:G:5032:TYR:OH	2.39	0.53
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.91	0.53
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.89	0.53
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.89	0.53
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.36	0.53
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.91	0.53
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.42	0.53
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.89	0.53
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.91	0.53
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.89	0.53
2:E:1457:UNK:N	2:E:1497:UNK:O	2.42	0.53
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.89	0.53
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.42	0.53
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:GLN:HB3	2:E:201:ASN:HB2	1.91	0.53
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.91	0.53
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.91	0.53
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.42	0.53
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.27	0.53
2:I:1457:UNK:N	2:I:1497:UNK:O	2.42	0.53
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.89	0.53
2:B:978:THR:HB	2:B:980:ALA:H	1.74	0.53
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.91	0.53
2:E:978:THR:HB	2:E:980:ALA:H	1.74	0.53
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.90	0.53
2:B:23:GLN:HB3	2:B:201:ASN:HB2	1.91	0.52
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.82	0.52
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.90	0.52
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.42	0.52
2:G:1457:UNK:N	2:G:1497:UNK:O	2.42	0.52
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.92	0.52
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.92	0.52
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.92	0.52
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.90	0.52
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.92	0.52
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.75	0.52
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.36	0.52
2:G:23:GLN:HB3	2:G:201:ASN:HB2	1.91	0.52
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.82	0.52
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.90	0.52
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.36	0.52
2:E:4189:ARG:NH1	2:E:5032:TYR:OH	2.39	0.52
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.92	0.52
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.75	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.74	0.52
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.27	0.52
2:E:2332:LEU:HD13	2:E:2335:LEU:HD12	1.92	0.52
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.92	0.52
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.75	0.52
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.27	0.52
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.92	0.52
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.92	0.52
2:G:669:ASP:OD2	2:G:790:ARG:NH2	2.41	0.52
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.91	0.52
2:G:4152:GLU:OE1	2:G:4192:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1457:UNK:N	2:B:1497:UNK:O	2.42	0.52
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.92	0.52
1:A:34:LYS:HD3	2:B:629:ARG:HD2	1.90	0.51
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.91	0.51
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.92	0.51
2:I:4152:GLU:OE1	2:I:4192:ARG:NH2	2.43	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.74	0.51
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.92	0.51
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.76	0.51
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.92	0.51
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.75	0.51
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.93	0.51
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.75	0.51
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.91	0.51
2:G:2332:LEU:HD13	2:G:2335:LEU:HD12	1.92	0.51
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.76	0.51
2:B:4152:GLU:OE1	2:B:4192:ARG:NH2	2.43	0.51
2:I:23:GLN:HB3	2:I:201:ASN:HB2	1.91	0.51
2:E:111:HIS:HD2	2:E:114:SER:H	1.59	0.51
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.93	0.51
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.92	0.51
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.93	0.51
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.75	0.51
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.76	0.51
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.76	0.51
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.92	0.51
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.93	0.51
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.92	0.51
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.75	0.51
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.92	0.51
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.93	0.51
2:E:669:ASP:OD2	2:E:790:ARG:NH2	2.41	0.51
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.92	0.51
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.44	0.51
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.44	0.51
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.76	0.51
2:E:485:SER:O	2:E:489:ASN:N	2.41	0.51
2:E:4152:GLU:OE1	2:E:4192:ARG:NH2	2.43	0.51
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.92	0.51
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.27	0.51
2:B:236:ALA:HA	2:B:242:ARG:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.75	0.51
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.92	0.51
2:G:111:HIS:HD2	2:G:114:SER:H	1.59	0.51
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.75	0.51
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.76	0.51
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.93	0.51
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.92	0.51
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.44	0.51
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.44	0.51
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.93	0.50
2:E:236:ALA:HA	2:E:242:ARG:HD2	1.93	0.50
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.93	0.50
2:B:111:HIS:HD2	2:B:114:SER:H	1.59	0.50
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.44	0.50
2:I:2332:LEU:HD13	2:I:2335:LEU:HD12	1.92	0.50
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.94	0.50
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.93	0.50
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.40	0.50
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.92	0.50
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.93	0.50
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.44	0.50
2:B:2332:LEU:HD13	2:B:2335:LEU:HD12	1.92	0.50
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.94	0.50
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.94	0.50
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.94	0.50
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.93	0.50
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.75	0.50
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.92	0.50
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.94	0.50
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.75	0.50
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.92	0.50
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.44	0.50
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.45	0.50
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.75	0.50
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.44	0.50
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.45	0.50
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.45	0.50
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.93	0.50
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.50
2:I:309:THR:O	2:I:313:SER:OG	2.30	0.50
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.43	0.50
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.44	0.50
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.50
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.45	0.50
2:I:111:HIS:HD2	2:I:114:SER:H	1.59	0.50
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.92	0.50
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.94	0.50
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.75	0.50
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.82	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.43	0.50
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.94	0.50
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.82	0.50
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.92	0.50
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.40	0.50
2:B:485:SER:O	2:B:489:ASN:N	2.41	0.50
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.94	0.50
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.77	0.50
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	1.93	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.50
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.45	0.50
2:B:309:THR:O	2:B:313:SER:OG	2.30	0.50
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.77	0.50
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.93	0.50
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.45	0.50
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.94	0.50
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.94	0.50
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.43	0.50
2:B:940:GLY:O	2:B:1052:ASN:N	2.45	0.49
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	1.93	0.49
2:I:236:ALA:HA	2:I:242:ARG:HD2	1.93	0.49
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.49
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.94	0.49
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.94	0.49
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.93	0.49
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.44	0.49
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.95	0.49
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.94	0.49
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.94	0.49
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.77	0.49
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.94	0.49
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:41:GLY:O	2:I:45:ARG:NH1	2.45	0.49
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.94	0.49
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	1.93	0.49
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.94	0.49
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.94	0.49
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.94	0.49
2:E:41:GLY:O	2:E:45:ARG:NH1	2.45	0.49
2:G:236:ALA:HA	2:G:242:ARG:HD2	1.93	0.49
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.95	0.49
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.76	0.49
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	1.93	0.49
2:I:669:ASP:OD2	2:I:790:ARG:NH2	2.41	0.49
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	1.93	0.49
2:G:41:GLY:O	2:G:45:ARG:NH1	2.45	0.49
2:G:940:GLY:O	2:G:1052:ASN:N	2.45	0.49
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.44	0.49
2:G:2868:SER:O	2:G:2872:GLN:N	2.43	0.49
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.95	0.49
2:B:3842:LEU:O	2:B:3929:SER:OG	2.30	0.49
2:I:451:TYR:O	2:I:474:ARG:NH1	2.43	0.49
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.94	0.49
2:E:309:THR:O	2:E:313:SER:OG	2.30	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.45	0.49
2:E:3842:LEU:O	2:E:3929:SER:OG	2.30	0.49
2:G:451:TYR:O	2:G:474:ARG:NH1	2.43	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.46	0.49
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.46	0.49
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.95	0.49
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.94	0.49
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.94	0.49
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.95	0.49
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	1.93	0.49
2:E:290:TYR:O	2:E:302:VAL:N	2.46	0.49
2:E:940:GLY:O	2:E:1052:ASN:N	2.45	0.49
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.94	0.49
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	1.93	0.49
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.46	0.49
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.77	0.49
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	1.93	0.49
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.94	0.49
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:THR:HA	1:A:49:ARG:HA	1.95	0.49
2:B:41:GLY:O	2:B:45:ARG:NH1	2.45	0.49
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.45	0.49
2:E:451:TYR:O	2:E:474:ARG:NH1	2.43	0.49
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.46	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.94	0.49
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.95	0.49
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.94	0.49
2:G:309:THR:O	2:G:313:SER:OG	2.30	0.49
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.46	0.49
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.95	0.48
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.95	0.48
1:F:21:THR:HA	1:F:49:ARG:HA	1.95	0.48
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.95	0.48
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.95	0.48
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.46	0.48
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.95	0.48
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.46	0.48
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.95	0.48
2:I:2868:SER:O	2:I:2872:GLN:N	2.43	0.48
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.48
2:G:1991:THR:O	2:G:1995:THR:OG1	2.32	0.48
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.95	0.48
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.46	0.48
2:I:1991:THR:O	2:I:1995:THR:OG1	2.32	0.48
2:B:290:TYR:O	2:B:302:VAL:N	2.46	0.48
2:B:621:ILE:O	2:B:625:LEU:N	2.46	0.48
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.48
2:G:290:TYR:O	2:G:302:VAL:N	2.46	0.48
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.95	0.48
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.78	0.48
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.46	0.48
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.46	0.48
1:J:21:THR:HA	1:J:49:ARG:HA	1.95	0.48
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.95	0.48
2:B:4892:ARG:NH2	2:I:4898:GLY:O	2.47	0.48
2:B:4898:GLY:O	2:E:4892:ARG:NH2	2.47	0.48
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.96	0.48
2:I:940:GLY:O	2:I:1052:ASN:N	2.45	0.48
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.43	0.48
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.96	0.48
2:I:4973:HIS:ND1	2:G:4227:GLU:OE2	2.47	0.48
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.95	0.48
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.78	0.47
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.79	0.47
2:I:2742:THR:OG1	2:I:2811:GLU:OE1	2.31	0.47
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.95	0.47
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.78	0.47
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.95	0.47
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.79	0.47
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.95	0.47
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.95	0.47
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.96	0.47
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.95	0.47
2:B:451:TYR:O	2:B:474:ARG:NH1	2.43	0.47
2:B:4973:HIS:ND1	2:I:4227:GLU:OE2	2.47	0.47
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.47
2:I:1171:SER:OG	2:I:1175:SER:N	2.47	0.47
2:I:4892:ARG:NH2	2:G:4898:GLY:O	2.47	0.47
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.95	0.47
2:G:2758:PHE:O	2:G:2762:THR:N	2.45	0.47
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.96	0.47
2:E:2876:GLU:OE1	2:E:2920:ARG:NH2	2.48	0.47
1:H:21:THR:HA	1:H:49:ARG:HA	1.95	0.47
2:B:2876:GLU:OE1	2:B:2920:ARG:NH2	2.48	0.47
2:I:290:TYR:O	2:I:302:VAL:N	2.46	0.47
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.47	0.47
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.96	0.47
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.78	0.47
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.95	0.47
2:I:2876:GLU:OE1	2:I:2920:ARG:NH2	2.48	0.47
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.97	0.47
2:E:1171:SER:OG	2:E:1175:SER:N	2.47	0.47
2:E:1232:ARG:HH21	2:E:1701:ALA:HB1	1.80	0.47
2:G:1171:SER:OG	2:G:1175:SER:N	2.47	0.47
2:G:1232:ARG:HH21	2:G:1701:ALA:HB1	1.80	0.47
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.79	0.47
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.47	0.47
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.36	0.47
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.79	0.47
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.79	0.47
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.95	0.47
2:B:4227:GLU:OE2	2:E:4973:HIS:ND1	2.48	0.47
2:E:621:ILE:O	2:E:625:LEU:N	2.45	0.47
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.46	0.47
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.33	0.47
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.79	0.47
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.47
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.97	0.47
2:B:1991:THR:O	2:B:1995:THR:OG1	2.32	0.47
2:B:2868:SER:O	2:B:2872:GLN:N	2.43	0.47
2:E:4227:GLU:OE2	2:G:4973:HIS:ND1	2.48	0.47
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.97	0.47
2:B:1232:ARG:HH21	2:B:1701:ALA:HB1	1.80	0.47
2:I:485:SER:O	2:I:489:ASN:N	2.40	0.47
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.97	0.47
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.33	0.47
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.33	0.47
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.78	0.47
2:G:2876:GLU:OE1	2:G:2920:ARG:NH2	2.48	0.47
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.78	0.46
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.33	0.46
2:E:379:HIS:CD2	2:E:381:GLU:H	2.34	0.46
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.98	0.46
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.96	0.46
2:B:379:HIS:CD2	2:B:381:GLU:H	2.34	0.46
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.33	0.46
2:I:2758:PHE:O	2:I:2762:THR:N	2.45	0.46
2:G:621:ILE:O	2:G:625:LEU:N	2.45	0.46
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.33	0.46
2:B:1171:SER:OG	2:B:1175:SER:N	2.47	0.46
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.81	0.46
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.97	0.46
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.97	0.46
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.81	0.46
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.79	0.46
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.33	0.46
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.98	0.46
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.79	0.46
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.33	0.46
2:G:379:HIS:CD2	2:G:381:GLU:H	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.97	0.46
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	1.97	0.46
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.46
2:I:379:HIS:CD2	2:I:381:GLU:H	2.33	0.46
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	1.97	0.46
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.79	0.46
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.96	0.46
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.97	0.46
2:G:485:SER:O	2:G:489:ASN:N	2.40	0.46
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	1.98	0.46
2:B:4745:LEU:O	2:B:4749:GLU:N	2.46	0.46
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.79	0.46
2:E:4898:GLY:O	2:G:4892:ARG:NH2	2.48	0.46
2:E:4928:LEU:HD13	2:E:4931:ILE:HD12	1.98	0.46
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.97	0.46
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.98	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.97	0.46
2:I:2212:VAL:O	2:I:2216:GLY:N	2.48	0.46
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.98	0.46
2:G:2212:VAL:O	2:G:2216:GLY:N	2.48	0.46
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.47	0.46
1:F:34:LYS:NZ	1:F:35:LYS:O	2.44	0.46
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.43	0.46
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.98	0.46
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	1.98	0.46
2:E:2742:THR:OG1	2:E:2811:GLU:OE1	2.31	0.46
2:G:4928:LEU:HA	2:G:4931:ILE:HD12	1.97	0.46
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.98	0.46
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.46
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.97	0.46
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.97	0.46
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.49	0.46
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.98	0.46
2:E:4928:LEU:HA	2:E:4931:ILE:HD12	1.97	0.46
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.81	0.46
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.46	0.45
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.97	0.45
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.98	0.45
2:I:1232:ARG:HH21	2:I:1701:ALA:HB1	1.80	0.45
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.81	0.45
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.90	0.45
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.90	0.45
2:G:4928:LEU:HD13	2:G:4931:ILE:HD12	1.98	0.45
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.31	0.45
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.90	0.45
2:B:4239:GLU:OE2	2:B:5014:TYR:OH	2.30	0.45
2:E:649:PHE:HB3	2:E:776:LEU:HB3	1.99	0.45
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	1.97	0.45
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.97	0.45
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	1.98	0.45
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.99	0.45
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.98	0.45
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.98	0.45
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	1.98	0.45
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.98	0.45
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	1.98	0.45
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.35	0.45
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.81	0.45
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	1.98	0.45
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	1.97	0.45
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.97	0.45
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.98	0.45
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.97	0.45
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.98	0.45
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.43	0.45
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.90	0.45
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.49	0.45
2:B:649:PHE:HB3	2:B:776:LEU:HB3	1.99	0.45
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.34	0.45
2:I:621:ILE:O	2:I:625:LEU:N	2.45	0.45
2:I:4928:LEU:HD13	2:I:4931:ILE:HD12	1.98	0.45
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.49	0.45
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.98	0.45
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.49	0.45
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.99	0.45
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.35	0.45
2:I:4586:PRO:HA	2:I:4628:VAL:HG11	1.98	0.45
2:I:4928:LEU:HA	2:I:4931:ILE:HD12	1.97	0.45
2:I:4956:THR:O	2:I:4965:SER:N	2.50	0.45
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.97	0.45
2:E:4586:PRO:HA	2:E:4628:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.97	0.45
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.98	0.45
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.97	0.45
2:B:4928:LEU:HA	2:B:4931:ILE:HD12	1.97	0.45
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.81	0.45
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.47	0.45
2:E:4956:THR:O	2:E:4965:SER:N	2.50	0.45
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.98	0.45
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.98	0.45
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.52	0.45
2:G:134:ASP:OD1	2:G:134:ASP:N	2.50	0.45
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.99	0.45
2:B:1105:ALA:N	2:B:1189:LEU:O	2.50	0.45
2:I:495:ASN:HD21	2:I:550:LYS:HG3	1.82	0.45
2:I:649:PHE:HB3	2:I:776:LEU:HB3	1.99	0.45
2:G:4239:GLU:OE2	2:G:5014:TYR:OH	2.30	0.45
2:G:4982:GLU:HB3	2:G:4983:HIS:H	1.65	0.45
2:G:495:ASN:HD21	2:G:550:LYS:HG3	1.82	0.44
2:G:1516:UNK:N	2:G:1529:UNK:O	2.50	0.44
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.99	0.44
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.52	0.44
2:I:134:ASP:OD1	2:I:134:ASP:N	2.50	0.44
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.41	0.44
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	1.98	0.44
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.99	0.44
2:B:495:ASN:HD21	2:B:550:LYS:HG3	1.82	0.44
2:B:1516:UNK:N	2:B:1529:UNK:O	2.50	0.44
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.81	0.44
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.43	0.44
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.52	0.44
2:G:4586:PRO:HA	2:G:4628:VAL:HG11	1.98	0.44
2:B:1660:GLN:O	2:B:1664:SER:N	2.49	0.44
2:B:2758:PHE:O	2:B:2762:THR:N	2.45	0.44
2:B:4562:LEU:HD13	2:B:4656:LEU:HB3	2.00	0.44
2:B:4586:PRO:HA	2:B:4628:VAL:HG11	1.98	0.44
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.51	0.44
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.35	0.44
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.00	0.44
2:B:243:ARG:NH1	2:B:301:VAL:O	2.43	0.44
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	1.98	0.44
2:B:4928:LEU:HD13	2:B:4931:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1516:UNK:N	2:I:1529:UNK:O	2.50	0.44
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.52	0.44
2:E:134:ASP:N	2:E:134:ASP:OD1	2.50	0.44
2:E:1516:UNK:N	2:E:1529:UNK:O	2.50	0.44
2:G:649:PHE:HB3	2:G:776:LEU:HB3	1.99	0.44
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.98	0.44
2:G:1660:GLN:O	2:G:1664:SER:N	2.49	0.44
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.51	0.44
2:B:583:ILE:H	2:B:583:ILE:HG13	1.65	0.44
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.35	0.44
2:I:3842:LEU:O	2:I:3929:SER:OG	2.30	0.44
2:E:495:ASN:HD21	2:E:550:LYS:HG3	1.82	0.44
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.99	0.44
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.51	0.44
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.43	0.44
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.00	0.44
2:E:2758:PHE:O	2:E:2762:THR:N	2.45	0.44
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.99	0.44
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.83	0.44
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.99	0.44
2:B:3951:PHE:HD2	2:B:4012:LEU:HD11	1.83	0.44
2:E:3951:PHE:HD2	2:E:4012:LEU:HD11	1.83	0.44
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.83	0.44
2:G:4956:THR:O	2:G:4965:SER:N	2.50	0.44
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.83	0.44
2:B:4956:THR:O	2:B:4965:SER:N	2.50	0.44
2:I:4571:PHE:O	2:I:4575:PHE:N	2.51	0.44
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.43	0.44
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	2.00	0.44
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.43	0.44
2:G:395:GLN:HG3	2:G:397:GLU:H	1.83	0.44
2:G:4571:PHE:O	2:G:4575:PHE:N	2.51	0.44
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.99	0.43
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.83	0.43
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.83	0.43
2:E:4562:LEU:HD13	2:E:4656:LEU:HB3	2.00	0.43
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.43	0.43
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.99	0.43
2:B:395:GLN:HG3	2:B:397:GLU:H	1.83	0.43
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.41	0.43
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4562:LEU:HD13	2:I:4656:LEU:HB3	2.00	0.43
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.99	0.43
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.34	0.43
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.43	0.43
1:A:92:PRO:HD3	2:B:627:PRO:HB2	2.00	0.43
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.83	0.43
2:B:4913:ARG:O	2:B:4917:ASP:N	2.46	0.43
2:I:1105:ALA:N	2:I:1189:LEU:O	2.50	0.43
2:I:4982:GLU:HB3	2:I:4983:HIS:H	1.65	0.43
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.51	0.43
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.51	0.43
2:G:2863:SER:HG	2:G:2928:LYS:HZ3	1.63	0.43
2:G:3951:PHE:HD2	2:G:4012:LEU:HD11	1.83	0.43
2:B:1622:GLU:N	2:B:1627:ALA:O	2.51	0.43
2:I:1148:VAL:HB	2:I:1165:ASN:HA	2.01	0.43
2:I:1622:GLU:N	2:I:1627:ALA:O	2.51	0.43
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.01	0.43
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.01	0.43
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.84	0.43
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.01	0.43
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.83	0.43
2:B:4780:PHE:HD1	2:B:4783:ILE:HD12	1.84	0.43
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.84	0.43
2:G:3842:LEU:O	2:G:3929:SER:OG	2.30	0.43
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	2.01	0.43
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.51	0.43
2:E:2212:VAL:O	2:E:2216:GLY:N	2.48	0.43
2:G:1105:ALA:N	2:G:1189:LEU:O	2.50	0.43
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.31	0.43
2:G:4191:GLU:OE1	2:G:5006:GLN:NE2	2.51	0.43
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.99	0.43
1:H:21:THR:N	1:H:107:GLU:OE1	2.43	0.43
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.00	0.43
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.83	0.43
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.00	0.43
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.00	0.43
2:I:3951:PHE:HD2	2:I:4012:LEU:HD11	1.83	0.43
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.83	0.43
2:E:4780:PHE:HD1	2:E:4783:ILE:HD12	1.84	0.43
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.01	0.43
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:LYS:NZ	1:H:35:LYS:O	2.44	0.43
2:I:315:CYS:SG	2:I:316:PHE:N	2.92	0.43
2:I:395:GLN:HG3	2:I:397:GLU:H	1.83	0.43
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.83	0.43
2:E:1660:GLN:O	2:E:1664:SER:N	2.49	0.43
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.84	0.43
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.00	0.43
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.00	0.43
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.84	0.43
2:E:4191:GLU:OE1	2:E:5006:GLN:NE2	2.51	0.43
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.83	0.43
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.84	0.43
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.83	0.43
2:G:4562:LEU:HD13	2:G:4656:LEU:HB3	2.00	0.43
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.83	0.42
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.84	0.42
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	2.01	0.42
2:E:395:GLN:HG3	2:E:397:GLU:H	1.83	0.42
2:E:1105:ALA:N	2:E:1189:LEU:O	2.50	0.42
2:E:1622:GLU:N	2:E:1627:ALA:O	2.51	0.42
2:G:315:CYS:SG	2:G:316:PHE:N	2.92	0.42
2:B:2212:VAL:O	2:B:2216:GLY:N	2.48	0.42
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.84	0.42
2:B:4735:GLU:HA	2:B:4738:ALA:HB3	2.01	0.42
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.83	0.42
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.84	0.42
2:I:4191:GLU:OE1	2:I:5006:GLN:NE2	2.51	0.42
2:I:4780:PHE:HD1	2:I:4783:ILE:HD12	1.84	0.42
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.01	0.42
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.84	0.42
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.00	0.42
2:B:4191:GLU:OE1	2:B:5006:GLN:NE2	2.51	0.42
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.43	0.42
2:G:1148:VAL:HB	2:G:1165:ASN:HA	2.01	0.42
1:H:92:PRO:HD3	2:G:627:PRO:HB2	2.00	0.42
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	2.00	0.42
2:I:1189:LEU:HD12	2:I:1190:PRO:HD2	2.02	0.42
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.42	0.42
2:I:4735:GLU:HA	2:I:4738:ALA:HB3	2.01	0.42
2:G:1622:GLU:N	2:G:1627:ALA:O	2.51	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4913:ARG:O	2:G:4917:ASP:N	2.46	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.34	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.51	0.42
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.41	0.42
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.83	0.42
1:F:21:THR:N	1:F:107:GLU:OE1	2.43	0.42
2:B:164:ARG:N	2:B:167:ASP:OD2	2.53	0.42
2:B:315:CYS:SG	2:B:316:PHE:N	2.92	0.42
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.84	0.42
2:B:1148:VAL:HB	2:B:1165:ASN:HA	2.01	0.42
2:I:644:ILE:HA	2:I:825:PRO:HA	2.02	0.42
2:I:1660:GLN:O	2:I:1664:SER:N	2.49	0.42
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	2.02	0.42
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	2.01	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.42
2:G:4745:LEU:O	2:G:4749:GLU:N	2.46	0.42
2:I:1663:HIS:O	2:I:1667:LEU:N	2.52	0.42
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	2.00	0.42
2:E:1189:LEU:HD12	2:E:1190:PRO:HD2	2.02	0.42
2:G:164:ARG:N	2:G:167:ASP:OD2	2.53	0.42
2:G:583:ILE:H	2:G:583:ILE:HG13	1.66	0.42
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.84	0.42
2:G:4780:PHE:HD1	2:G:4783:ILE:HD12	1.84	0.42
2:B:1189:LEU:HD12	2:B:1190:PRO:HD2	2.02	0.42
2:E:315:CYS:SG	2:E:316:PHE:N	2.92	0.42
2:E:4713:SER:HA	2:E:4718:LYS:HE2	2.02	0.42
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	2.02	0.42
2:I:561:LEU:HD11	2:I:599:VAL:HG12	2.02	0.42
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.30	0.42
2:G:170:ILE:HD12	2:G:197:GLN:HB3	2.02	0.42
1:J:34:LYS:NZ	1:J:35:LYS:O	2.44	0.42
2:I:164:ARG:N	2:I:167:ASP:OD2	2.53	0.42
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.83	0.42
2:E:170:ILE:HD12	2:E:197:GLN:HB3	2.02	0.42
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.02	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:E:4735:GLU:HA	2:E:4738:ALA:HB3	2.01	0.42
2:G:644:ILE:HA	2:G:825:PRO:HA	2.02	0.42
2:G:1685:LEU:HD22	2:G:1718:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.42
2:G:4713:SER:HA	2:G:4718:LYS:HE2	2.02	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.41
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.84	0.41
2:E:561:LEU:HD11	2:E:599:VAL:HG12	2.02	0.41
2:E:1148:VAL:HB	2:E:1165:ASN:HA	2.01	0.41
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	2.02	0.41
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.51	0.41
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.84	0.41
2:B:644:ILE:HA	2:B:825:PRO:HA	2.02	0.41
2:B:3365:UNK:O	2:B:3369:UNK:N	2.53	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.84	0.41
2:E:164:ARG:N	2:E:167:ASP:OD2	2.53	0.41
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.02	0.41
2:E:2185:ILE:HA	2:E:2188:ASN:ND2	2.35	0.41
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	2.02	0.41
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.03	0.41
2:G:561:LEU:HD11	2:G:599:VAL:HG12	2.02	0.41
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.02	0.41
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	2.02	0.41
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	2.02	0.41
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	2.02	0.41
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	2.01	0.41
2:G:4735:GLU:HA	2:G:4738:ALA:HB3	2.01	0.41
1:A:21:THR:N	1:A:107:GLU:OE1	2.43	0.41
2:B:170:ILE:HD12	2:B:197:GLN:HB3	2.02	0.41
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.03	0.41
2:I:3552:UNK:O	2:I:3556:UNK:N	2.54	0.41
2:G:1189:LEU:HD12	2:G:1190:PRO:HD2	2.02	0.41
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.53	0.41
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.84	0.41
2:B:215:THR:HG22	2:B:273:HIS:HA	2.02	0.41
2:B:1973:GLN:O	2:B:1977:TYR:N	2.47	0.41
2:B:3552:UNK:O	2:B:3556:UNK:N	2.54	0.41
2:I:4172:GLU:HA	2:I:4175:ARG:HB2	2.02	0.41
2:E:644:ILE:HA	2:E:825:PRO:HA	2.02	0.41
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.84	0.41
2:B:561:LEU:HD11	2:B:599:VAL:HG12	2.02	0.41
2:B:637:LEU:HD23	2:B:1637:MET:HB3	2.02	0.41
2:B:939:VAL:HG22	2:B:1053:ILE:HG12	2.03	0.41
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	2.02	0.41
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	2.02	0.41
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	2.02	0.41
2:B:4713:SER:HA	2:B:4718:LYS:HE2	2.02	0.41
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.86	0.41
2:E:1663:HIS:O	2:E:1667:LEU:N	2.52	0.41
2:E:4745:LEU:O	2:E:4749:GLU:N	2.46	0.41
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.86	0.41
2:G:939:VAL:HG22	2:G:1053:ILE:HG12	2.02	0.41
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.03	0.41
2:G:3992:PHE:O	2:G:3996:PHE:N	2.44	0.41
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.02	0.41
2:I:2185:ILE:HA	2:I:2188:ASN:ND2	2.35	0.41
2:I:2869:ARG:HH12	2:I:2945:UNK:C	2.34	0.41
2:E:637:LEU:HD23	2:E:1637:MET:HB3	2.02	0.41
2:E:939:VAL:HG22	2:E:1053:ILE:HG12	2.03	0.41
2:E:1685:LEU:HD22	2:E:1718:ILE:HG21	2.02	0.41
2:E:3552:UNK:O	2:E:3556:UNK:N	2.54	0.41
2:G:470:SER:O	2:G:474:ARG:NE	2.53	0.41
2:G:2185:ILE:HA	2:G:2188:ASN:ND2	2.35	0.41
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	2.02	0.41
2:G:3696:ASP:O	2:G:3700:GLN:N	2.50	0.41
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.03	0.41
2:B:3658:LYS:HA	2:B:3661:TRP:CE2	2.56	0.41
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.54	0.41
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	2.02	0.41
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.03	0.41
2:I:4713:SER:HA	2:I:4718:LYS:HE2	2.02	0.41
2:I:4913:ARG:O	2:I:4917:ASP:N	2.46	0.41
2:E:3658:LYS:HA	2:E:3661:TRP:CE2	2.56	0.41
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	2.01	0.41
2:B:134:ASP:OD1	2:B:134:ASP:N	2.50	0.41
2:B:670:GLU:HG3	2:B:787:VAL:HG13	2.03	0.41
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	2.02	0.41
2:B:4172:GLU:HA	2:B:4175:ARG:HB2	2.02	0.41
2:I:470:SER:O	2:I:474:ARG:NE	2.53	0.41
2:I:583:ILE:H	2:I:583:ILE:HG13	1.65	0.41
2:I:864:PRO:HA	2:I:865:PRO:HD3	1.96	0.41
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.53	0.41
2:I:1685:LEU:HD22	2:I:1718:ILE:HG21	2.02	0.41
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.02	0.41
2:E:215:THR:HG22	2:E:273:HIS:HA	2.02	0.41
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.53	0.41
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	2.03	0.41
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.34	0.41
2:G:637:LEU:HD23	2:G:1637:MET:HB3	2.02	0.41
2:G:870:ILE:O	2:G:874:LEU:N	2.45	0.41
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	2.02	0.41
2:G:4172:GLU:HA	2:G:4175:ARG:HB2	2.02	0.41
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.53	0.41
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	2.01	0.41
2:I:170:ILE:HD12	2:I:197:GLN:HB3	2.02	0.41
2:I:637:LEU:HD23	2:I:1637:MET:HB3	2.02	0.41
2:I:2004:GLU:HA	2:I:2007:ASN:HB2	2.03	0.41
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.86	0.41
2:E:1089:TYR:N	2:E:1224:GLU:O	2.54	0.41
2:G:218:HIS:HB3	2:G:392:ARG:HE	1.86	0.41
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.04	0.41
2:G:670:GLU:HG3	2:G:787:VAL:HG13	2.03	0.41
2:B:1089:TYR:N	2:B:1224:GLU:O	2.54	0.40
2:B:1154:ASP:HB3	2:B:1157:GLU:HB3	2.03	0.40
2:B:2185:ILE:HA	2:B:2188:ASN:ND2	2.35	0.40
2:B:3696:ASP:O	2:B:3700:GLN:N	2.50	0.40
2:I:4239:GLU:OE2	2:I:5014:TYR:OH	2.30	0.40
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.03	0.40
2:E:1154:ASP:HB3	2:E:1157:GLU:HB3	2.03	0.40
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.03	0.40
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.85	0.40
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.86	0.40
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.03	0.40
2:I:1865:MET:SD	2:I:1865:MET:N	2.95	0.40
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.56	0.40
2:E:838:HIS:CE1	2:E:1201:HIS:HD2	2.40	0.40
2:E:4913:ARG:O	2:E:4917:ASP:N	2.46	0.40
2:G:215:THR:HG22	2:G:273:HIS:HA	2.02	0.40
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.03	0.40
2:G:1089:TYR:N	2:G:1224:GLU:O	2.54	0.40
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.53	0.40
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.03	0.40
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.03	0.40
2:B:2004:GLU:HA	2:B:2007:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:218:HIS:HB3	2:I:392:ARG:HE	1.86	0.40
2:I:1089:TYR:N	2:I:1224:GLU:O	2.54	0.40
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	2.02	0.40
2:I:4976:GLU:O	2:I:4979:THR:OG1	2.37	0.40
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.54	0.40
2:E:583:ILE:H	2:E:583:ILE:HG13	1.66	0.40
2:E:4172:GLU:HA	2:E:4175:ARG:HB2	2.02	0.40
2:E:4929:LEU:HD13	2:E:4929:LEU:HA	1.97	0.40
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.02	0.40
2:G:3658:LYS:HA	2:G:3661:TRP:CE2	2.56	0.40
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.42	0.40
2:I:939:VAL:HG22	2:I:1053:ILE:HG12	2.03	0.40
2:I:1154:ASP:HB3	2:I:1157:GLU:HB3	2.03	0.40
2:E:4571:PHE:O	2:E:4575:PHE:N	2.51	0.40
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.03	0.40
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.02	0.40
2:B:2950:UNK:O	2:B:2954:UNK:N	2.55	0.40
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.54	0.40
2:I:215:THR:HG22	2:I:273:HIS:HA	2.02	0.40
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.02	0.40
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.53	0.40
2:E:207:SER:OG	2:E:208:CYS:N	2.55	0.40
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.03	0.40
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.54	0.40
2:G:195:PHE:HB3	2:G:196:MET:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	2929 (90%)	304 (9%)	2 (0%)	48	83
2	E	3235/4416 (73%)	2931 (91%)	302 (9%)	2 (0%)	48	83
2	G	3235/4416 (73%)	2930 (91%)	303 (9%)	2 (0%)	48	83
2	I	3235/4416 (73%)	2930 (91%)	303 (9%)	2 (0%)	48	83
All	All	13360/18096 (74%)	12093 (90%)	1259 (9%)	8 (0%)	50	83

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	B	4641	PRO
2	I	4641	PRO
2	E	4641	PRO
2	G	4641	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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%)	2476 (99%)	17 (1%)	81	87
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	81	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	81	87
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	81	87
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	80	87

All (68) 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	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4913	ARG
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3663	LEU
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4913	ARG

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Mol	Chain	Res	Type
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	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4913	ARG
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	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4913	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) 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

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Mol	Chain	Res	Type
2	B	57	ASN
2	B	71	GLN
2	B	111	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	413	GLN
2	B	495	ASN
2	B	582	HIS
2	B	838	HIS
2	B	1158	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2127	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	4034	ASN
2	B	4120	ASN
2	B	4728	HIS
2	B	4806	ASN
2	B	4946	GLN
2	B	5003	HIS
2	I	57	ASN
2	I	71	GLN
2	I	111	HIS
2	I	156	GLN
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	413	GLN
2	I	582	HIS
2	I	797	HIS
2	I	838	HIS

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Mol	Chain	Res	Type
2	I	1158	ASN
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2127	GLN
2	I	3809	ASN
2	I	3830	GLN
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	4034	ASN
2	I	4120	ASN
2	I	4728	HIS
2	I	4806	ASN
2	I	4946	GLN
2	I	5003	HIS
2	E	57	ASN
2	E	71	GLN
2	E	111	HIS
2	E	156	GLN
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	413	GLN
2	E	582	HIS
2	E	765	GLN
2	E	838	HIS
2	E	1158	ASN
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2127	GLN
2	E	3809	ASN

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Mol	Chain	Res	Type
2	E	3830	GLN
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	4034	ASN
2	E	4120	ASN
2	E	4553	ASN
2	E	4728	HIS
2	E	4806	ASN
2	E	4946	GLN
2	E	5003	HIS
2	G	57	ASN
2	G	71	GLN
2	G	111	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	413	GLN
2	G	582	HIS
2	G	797	HIS
2	G	838	HIS
2	G	1158	ASN
2	G	1598	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2127	GLN
2	G	3809	ASN
2	G	3830	GLN
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	4034	ASN
2	G	4120	ASN

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Mol	Chain	Res	Type
2	G	4553	ASN
2	G	4728	HIS
2	G	4806	ASN
2	G	4946	GLN
2	G	5003	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	B	5101	-	28,33,33	1.00	2 (7%)	34,52,52	1.10	2 (5%)
4	CFF	B	5102	-	8,15,15	2.05	3 (37%)	8,23,23	1.34	1 (12%)
4	CFF	E	5102	-	8,15,15	2.05	3 (37%)	8,23,23	1.32	1 (12%)
3	ATP	I	5101	-	28,33,33	1.00	2 (7%)	34,52,52	1.10	2 (5%)
4	CFF	I	5102	-	8,15,15	2.04	3 (37%)	8,23,23	1.32	1 (12%)
3	ATP	E	5101	-	28,33,33	1.01	2 (7%)	34,52,52	1.10	2 (5%)
3	ATP	G	5101	-	28,33,33	1.00	2 (7%)	34,52,52	1.10	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CFF	G	5102	-	8,15,15	2.06	3 (37%)	8,23,23	1.34	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	6/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	6/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	6/18/38/38	0/3/3/3
3	ATP	G	5101	-	-	6/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C5-C4	-3.39	1.33	1.39
4	G	5102	CFF	C5-C4	-3.39	1.33	1.39
4	I	5102	CFF	C5-C4	-3.39	1.33	1.39
4	B	5102	CFF	C5-C4	-3.34	1.33	1.39
4	B	5102	CFF	C6-N1	-3.28	1.32	1.38
4	G	5102	CFF	C6-N1	-3.28	1.32	1.38
4	E	5102	CFF	C6-N1	-3.25	1.32	1.38
4	I	5102	CFF	C6-N1	-3.19	1.32	1.38
4	B	5102	CFF	O13-C6	-2.49	1.18	1.24
4	I	5102	CFF	O13-C6	-2.48	1.18	1.24
4	E	5102	CFF	O13-C6	-2.48	1.18	1.24
4	G	5102	CFF	O13-C6	-2.44	1.18	1.24
3	G	5101	ATP	PB-O3A	2.17	1.61	1.59
3	B	5101	ATP	PB-O3A	2.14	1.61	1.59
3	E	5101	ATP	PB-O3A	2.14	1.61	1.59
3	I	5101	ATP	PB-O3A	2.13	1.61	1.59
3	B	5101	ATP	PA-O3A	2.12	1.61	1.59
3	I	5101	ATP	PA-O3A	2.12	1.61	1.59
3	E	5101	ATP	PA-O3A	2.12	1.61	1.59
3	G	5101	ATP	PA-O3A	2.09	1.61	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5101	ATP	N3-C2-N1	-3.49	123.93	128.67
3	G	5101	ATP	N3-C2-N1	-3.49	123.94	128.67
3	I	5101	ATP	N3-C2-N1	-3.47	123.96	128.67
3	B	5101	ATP	N3-C2-N1	-3.46	123.98	128.67
4	B	5102	CFF	C14-N7-C8	-2.87	111.63	125.43
4	G	5102	CFF	C14-N7-C8	-2.86	111.67	125.43
4	E	5102	CFF	C14-N7-C8	-2.85	111.70	125.43
4	I	5102	CFF	C14-N7-C8	-2.85	111.72	125.43
3	I	5101	ATP	C4-C5-N7	-2.12	107.10	109.34
3	B	5101	ATP	C4-C5-N7	-2.11	107.11	109.34
3	G	5101	ATP	C4-C5-N7	-2.10	107.11	109.34
3	E	5101	ATP	C4-C5-N7	-2.07	107.15	109.34

There are no chirality outliers.

All (24) torsion outliers are listed below:

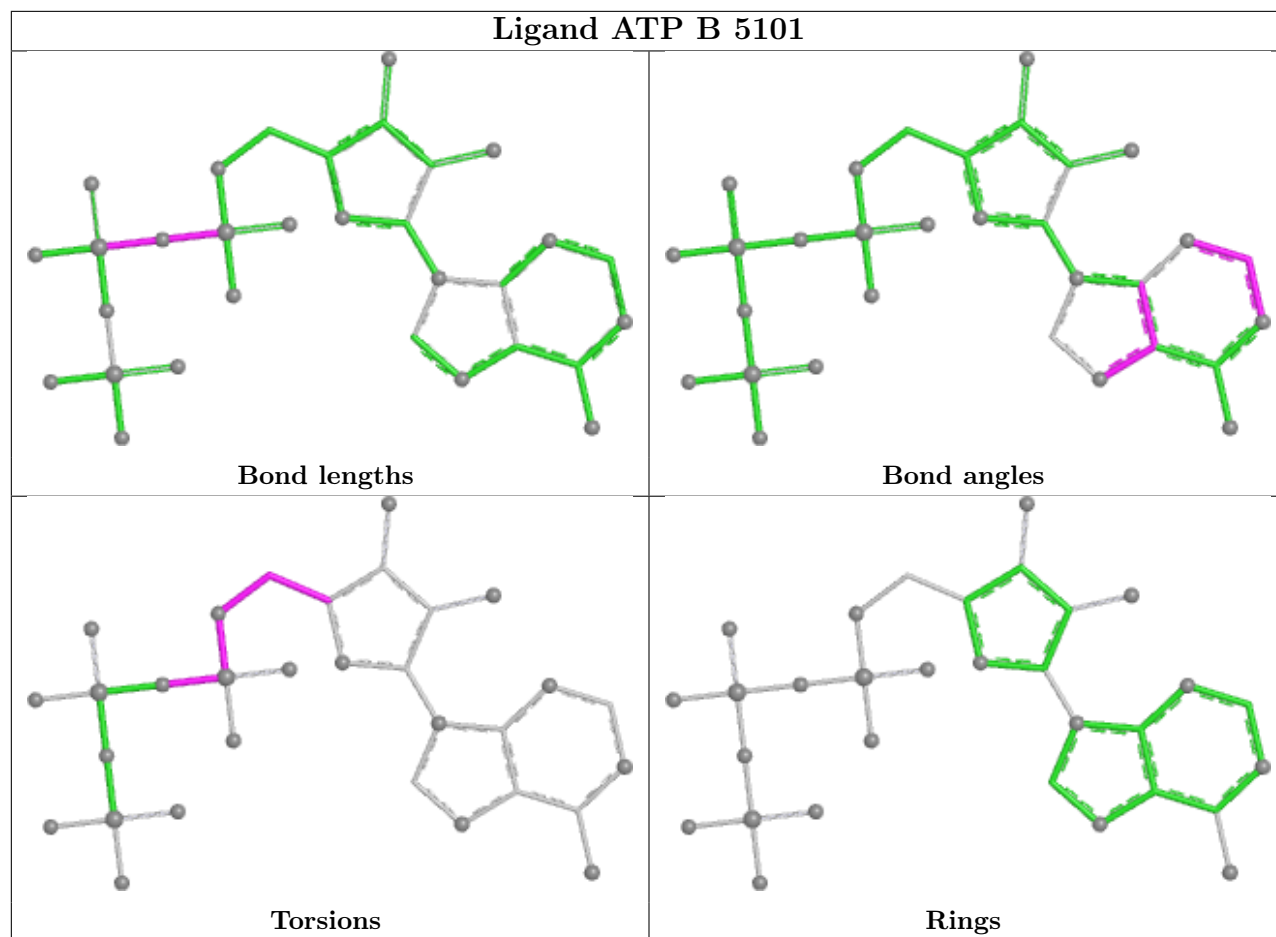
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O2A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O2A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	PB-O3A-PA-O5'
3	I	5101	ATP	PB-O3A-PA-O5'
3	E	5101	ATP	PB-O3A-PA-O5'
3	G	5101	ATP	PB-O3A-PA-O5'
3	B	5101	ATP	C4'-C5'-O5'-PA
3	I	5101	ATP	C4'-C5'-O5'-PA
3	E	5101	ATP	C4'-C5'-O5'-PA
3	G	5101	ATP	C4'-C5'-O5'-PA
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	E	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'

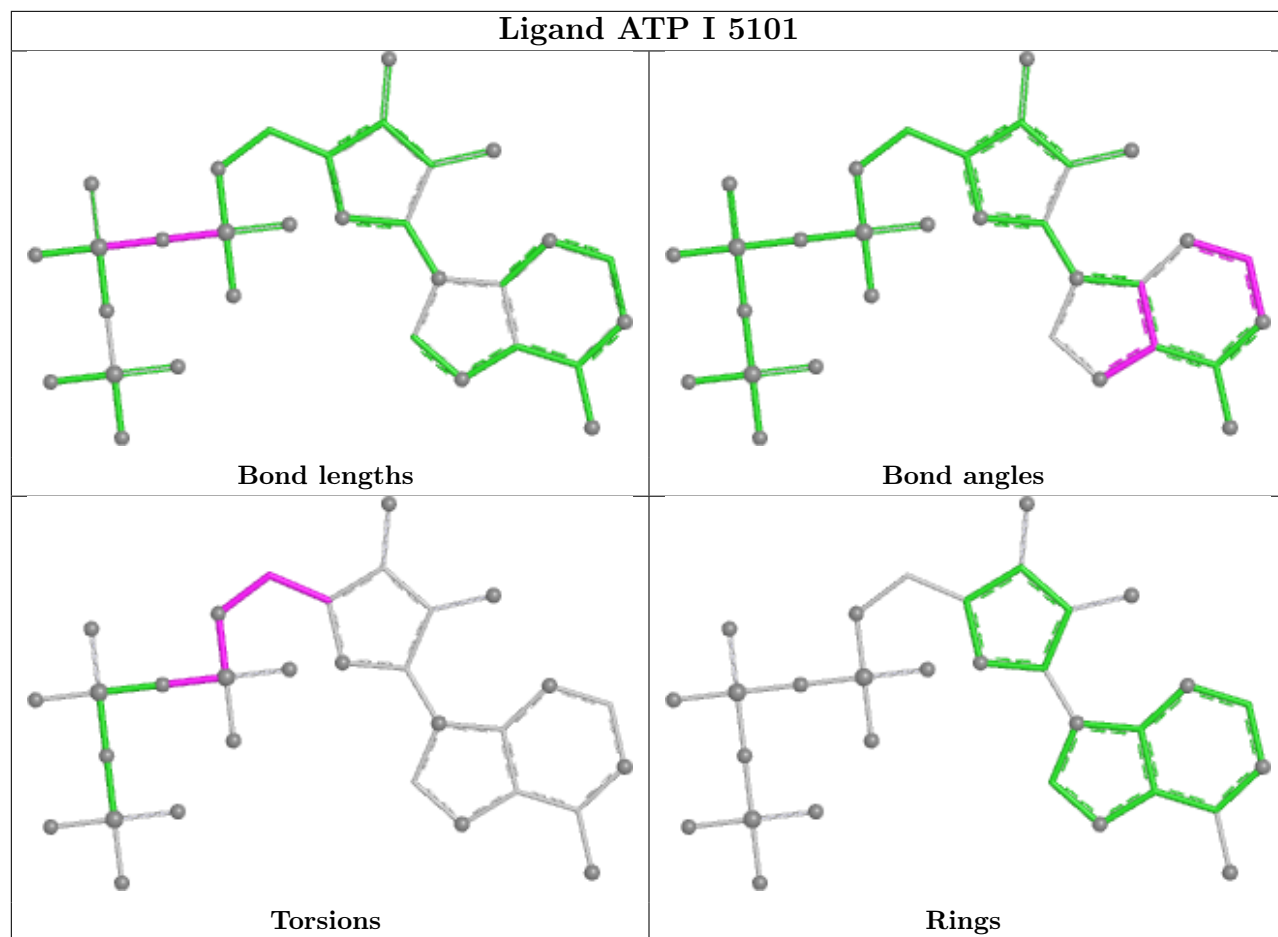
There are no ring outliers.

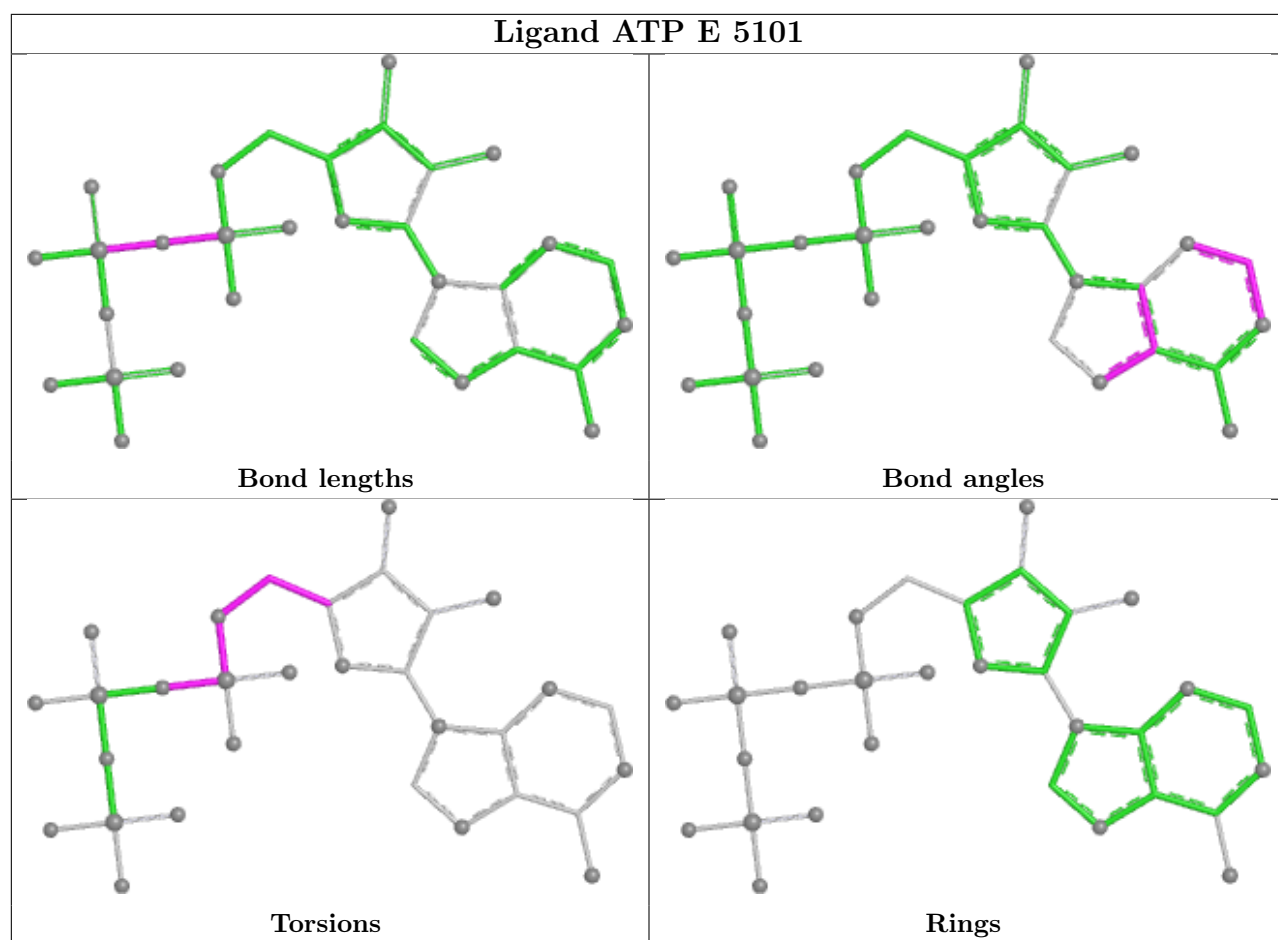
8 monomers are involved in 8 short contacts:

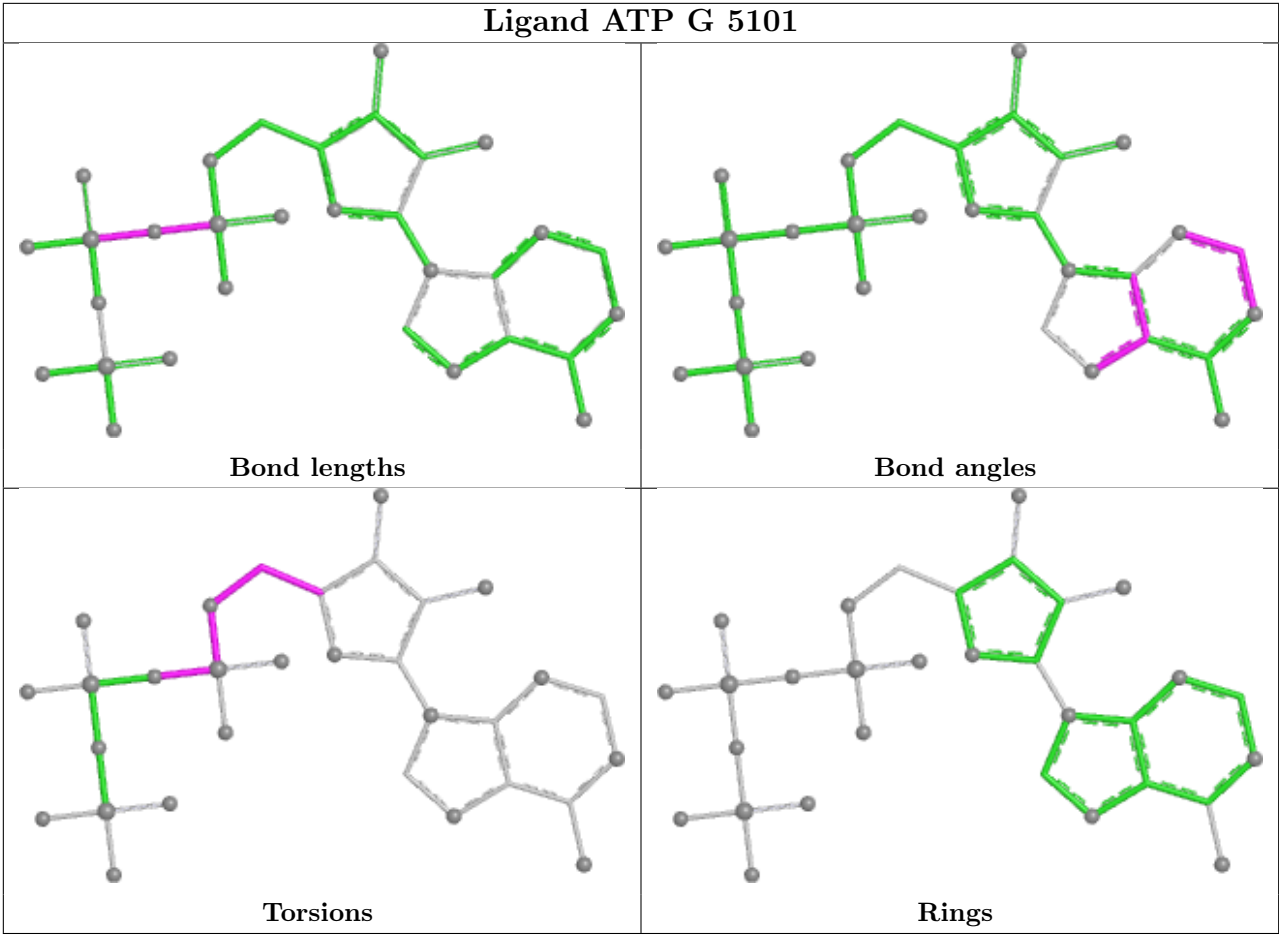
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
4	B	5102	CFF	1	0
4	E	5102	CFF	1	0
3	I	5101	ATP	1	0
4	I	5102	CFF	1	0
3	E	5101	ATP	1	0
3	G	5101	ATP	1	0
4	G	5102	CFF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	E	14
2	I	14
2	G	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	74.23
1	E	4345:UNK	C	4540:PHE	N	74.23

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	74.22
1	G	4345:UNK	C	4540:PHE	N	74.22
1	I	3613:UNK	C	3639:THR	N	43.91
1	B	3613:UNK	C	3639:THR	N	43.90
1	G	3613:UNK	C	3639:THR	N	43.90
1	E	3613:UNK	C	3639:THR	N	43.89
1	B	4253:GLU	C	4320:UNK	N	26.88
1	I	4253:GLU	C	4320:UNK	N	26.88
1	E	4253:GLU	C	4320:UNK	N	26.88
1	G	4253:GLU	C	4320:UNK	N	26.88
1	I	3163:UNK	C	3170:UNK	N	16.01
1	G	3163:UNK	C	3170:UNK	N	16.01
1	B	3163:UNK	C	3170:UNK	N	16.00
1	E	3163:UNK	C	3170:UNK	N	16.00
1	B	3063:UNK	C	3134:UNK	N	14.82
1	I	3063:UNK	C	3134:UNK	N	14.82
1	E	3063:UNK	C	3134:UNK	N	14.82
1	G	3063:UNK	C	3134:UNK	N	14.82
1	B	3468:UNK	C	3511:UNK	N	14.51
1	I	3468:UNK	C	3511:UNK	N	14.51
1	E	3468:UNK	C	3511:UNK	N	14.51
1	G	3468:UNK	C	3511:UNK	N	14.51
1	E	2703:UNK	C	2734:ASN	N	14.06
1	B	2703:UNK	C	2734:ASN	N	14.05
1	I	2703:UNK	C	2734:ASN	N	14.05
1	G	2703:UNK	C	2734:ASN	N	14.05
1	B	3236:UNK	C	3241:UNK	N	13.47
1	I	3236:UNK	C	3241:UNK	N	13.47
1	E	3236:UNK	C	3241:UNK	N	13.47
1	G	3236:UNK	C	3241:UNK	N	13.47
1	B	2976:UNK	C	2995:UNK	N	12.24
1	I	2976:UNK	C	2995:UNK	N	12.24
1	E	2976:UNK	C	2995:UNK	N	12.24
1	G	2976:UNK	C	2995:UNK	N	12.24
1	E	1564:UNK	C	1573:MET	N	12.12
1	G	1564:UNK	C	1573:MET	N	12.12
1	B	1564:UNK	C	1573:MET	N	12.11
1	I	1564:UNK	C	1573:MET	N	12.11
1	B	3254:UNK	C	3261:UNK	N	8.26
1	I	3254:UNK	C	3261:UNK	N	8.26
1	E	3254:UNK	C	3261:UNK	N	8.26
1	G	3254:UNK	C	3261:UNK	N	8.26

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	5.81
1	I	1297:UNK	C	1430:UNK	N	5.81
1	E	1297:UNK	C	1430:UNK	N	5.81
1	G	1297:UNK	C	1430:UNK	N	5.81
1	E	2939:ARG	C	2942:UNK	N	3.53
1	G	2939:ARG	C	2942:UNK	N	3.53
1	B	2939:ARG	C	2942:UNK	N	3.52
1	I	2939:ARG	C	2942:UNK	N	3.52
1	I	2479:LEU	C	2487:UNK	N	3.25
1	B	2479:LEU	C	2487:UNK	N	3.24
1	E	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24

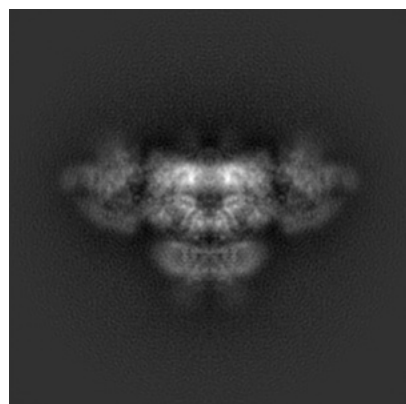
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8384. These allow visual inspection of the internal detail of the map and identification of artifacts.

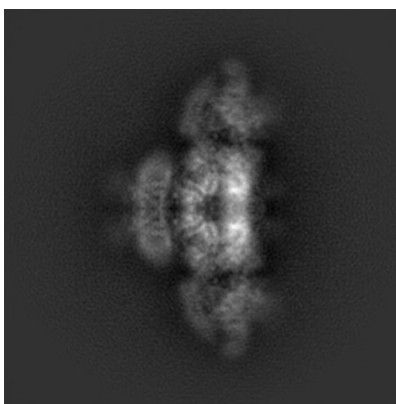
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

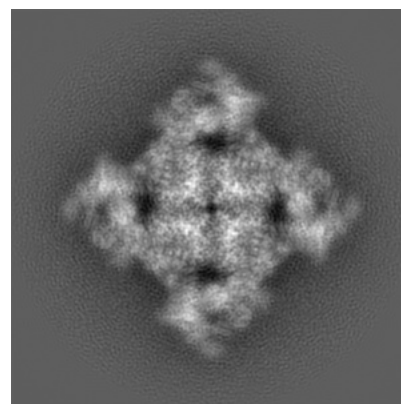
6.1.1 Primary map



X

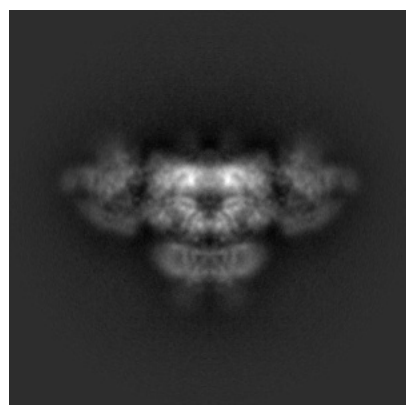


Y

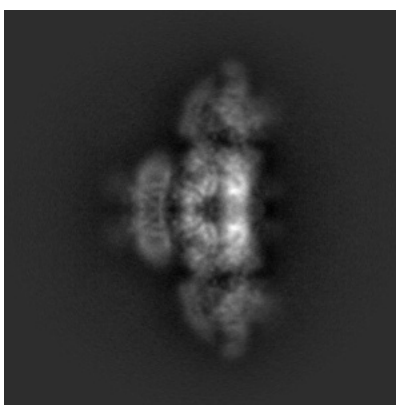


Z

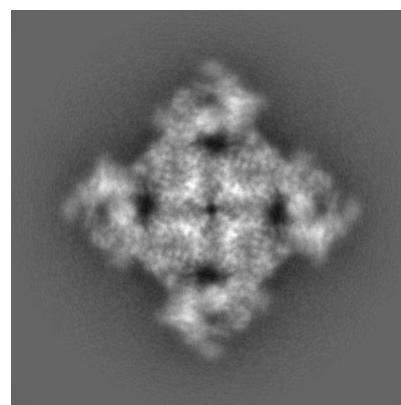
6.1.2 Raw map



X



Y

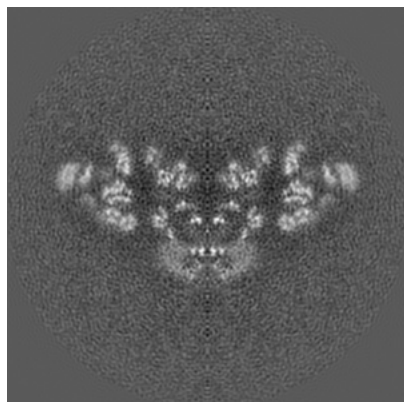


Z

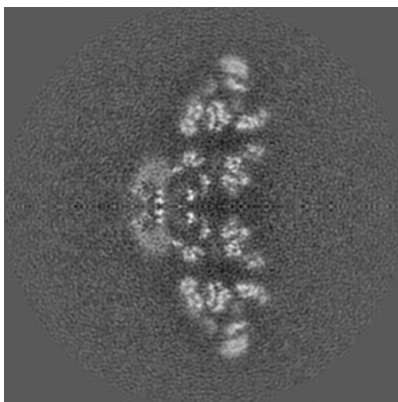
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

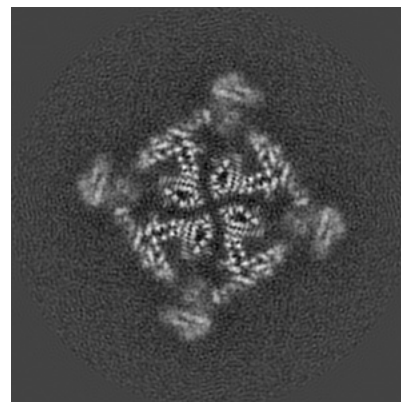
6.2.1 Primary map



X Index: 200

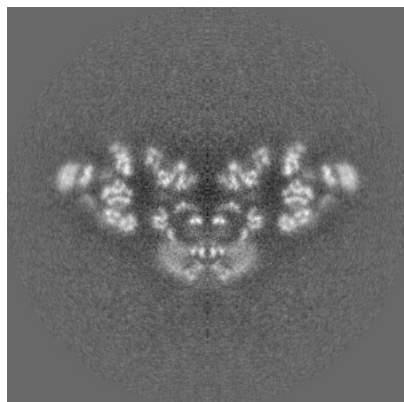


Y Index: 200

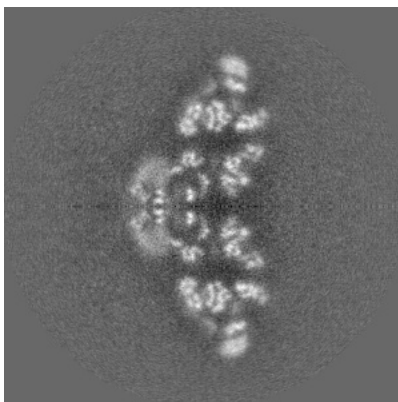


Z Index: 200

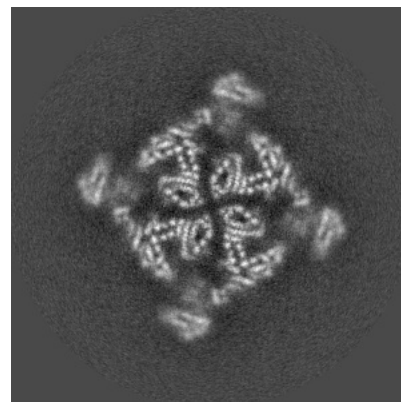
6.2.2 Raw map



X Index: 200



Y Index: 200

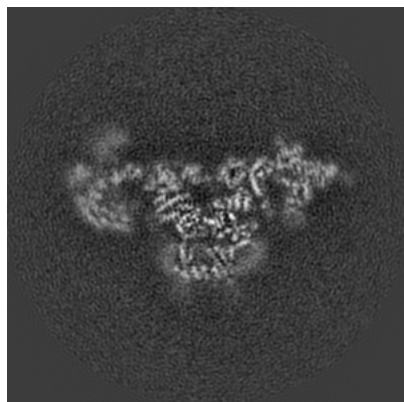


Z Index: 200

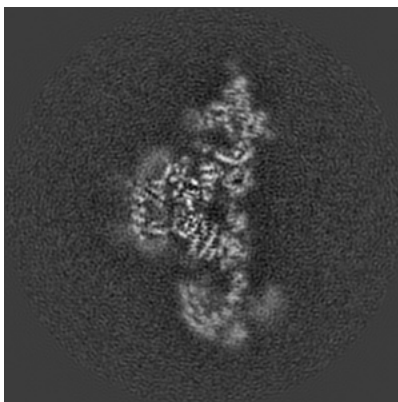
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

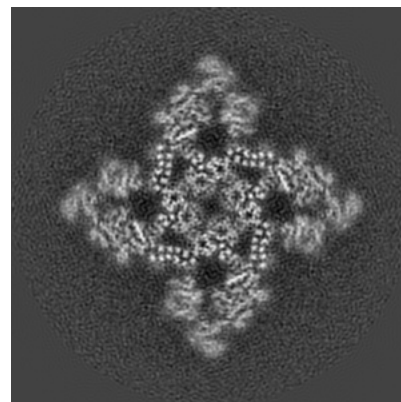
6.3.1 Primary map



X Index: 184

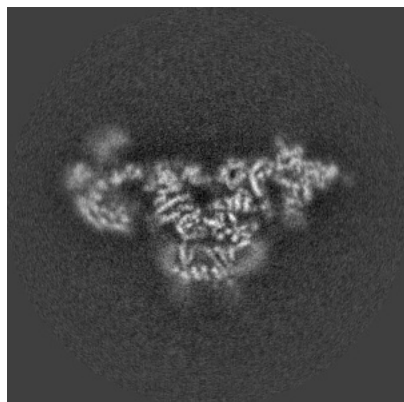


Y Index: 216

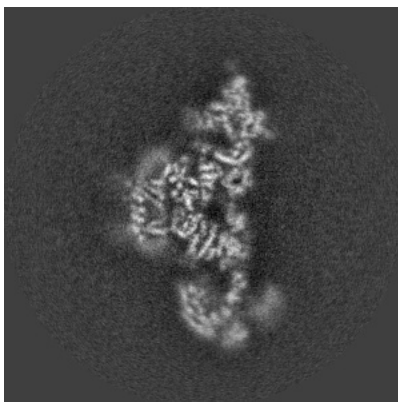


Z Index: 227

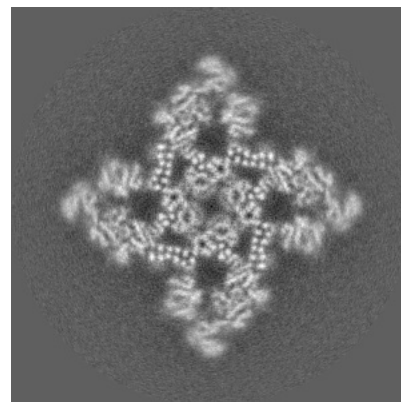
6.3.2 Raw map



X Index: 184



Y Index: 216

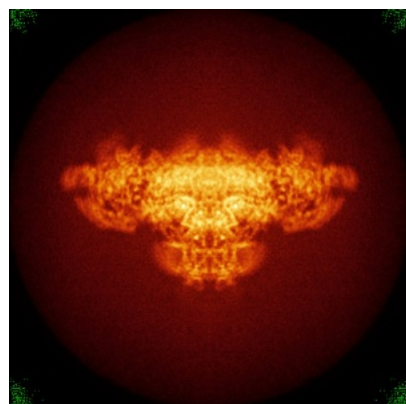


Z Index: 227

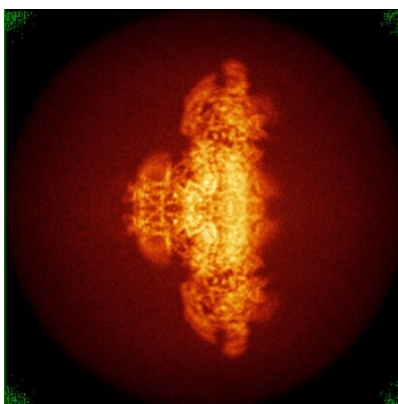
The images above show the largest variance slices of the map in three orthogonal directions.

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

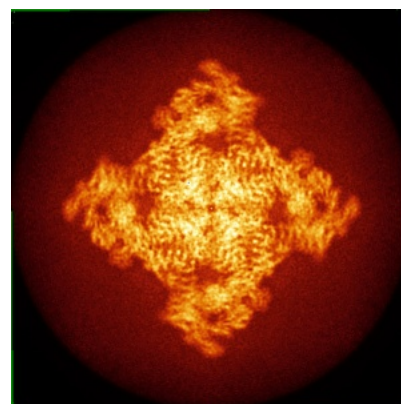
6.4.1 Primary map



X

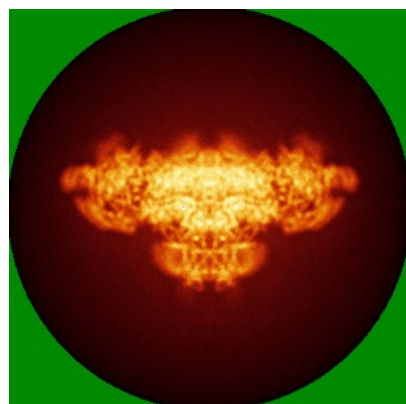


Y

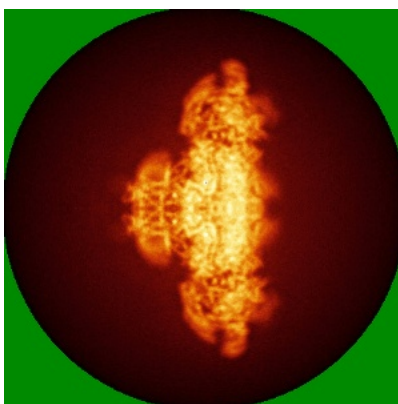


Z

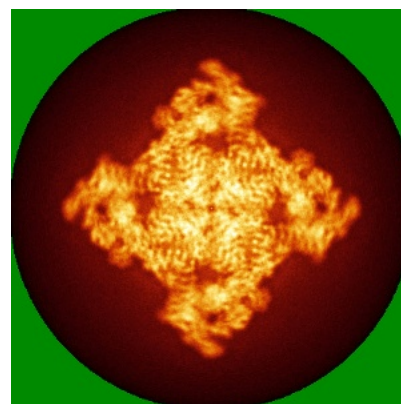
6.4.2 Raw map



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 0.035. 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.

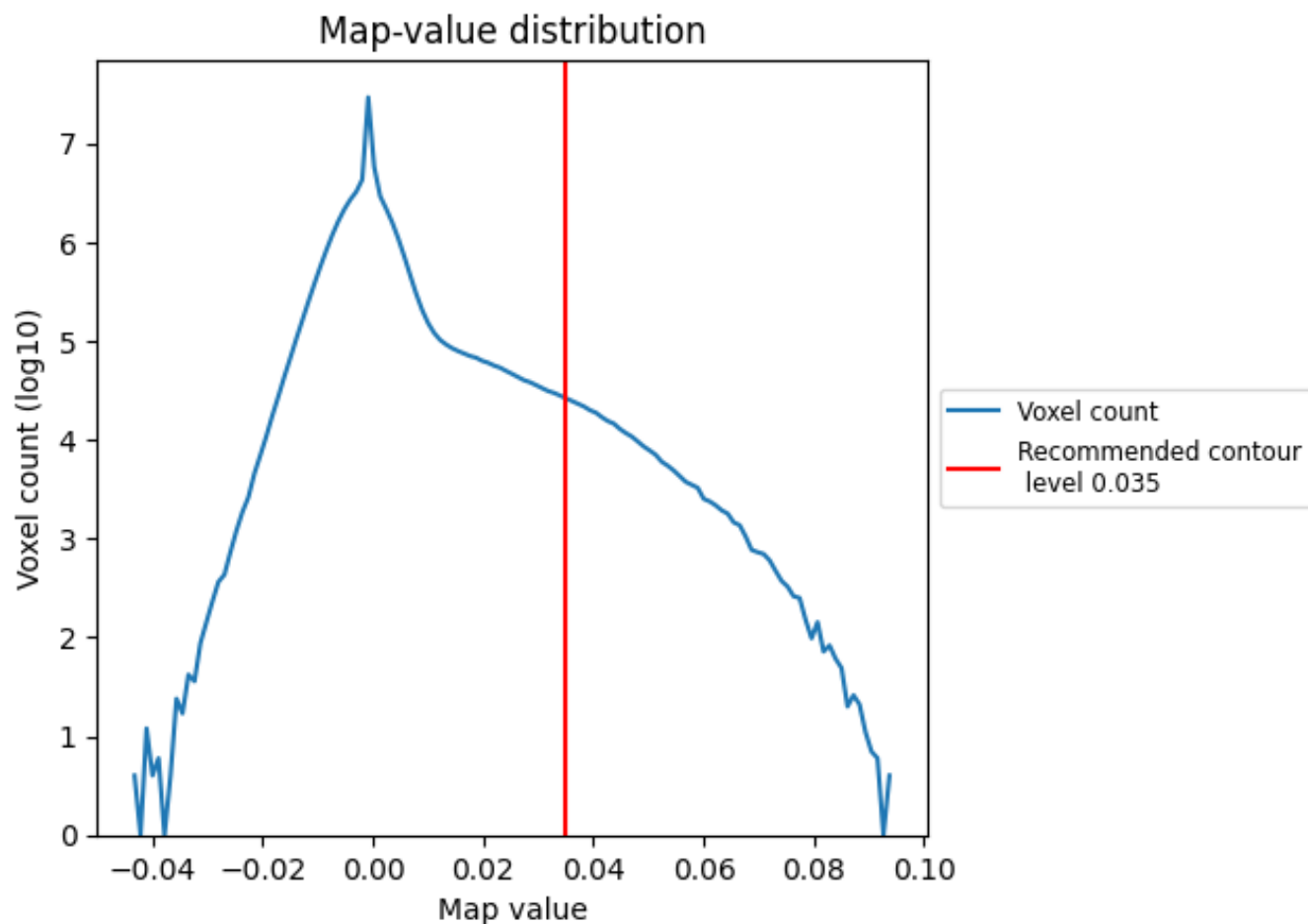
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

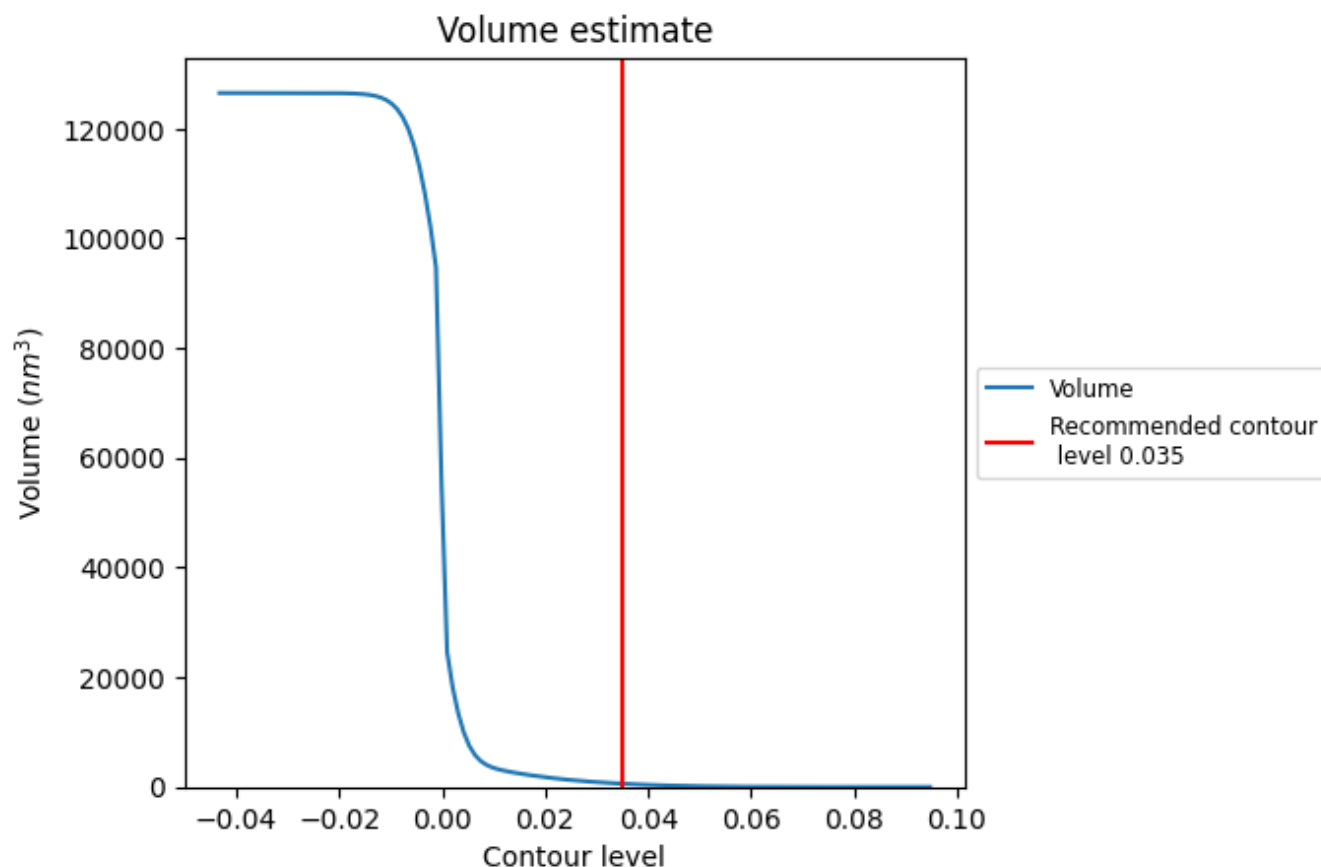
This section contains the results of statistical analysis of the map.

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.

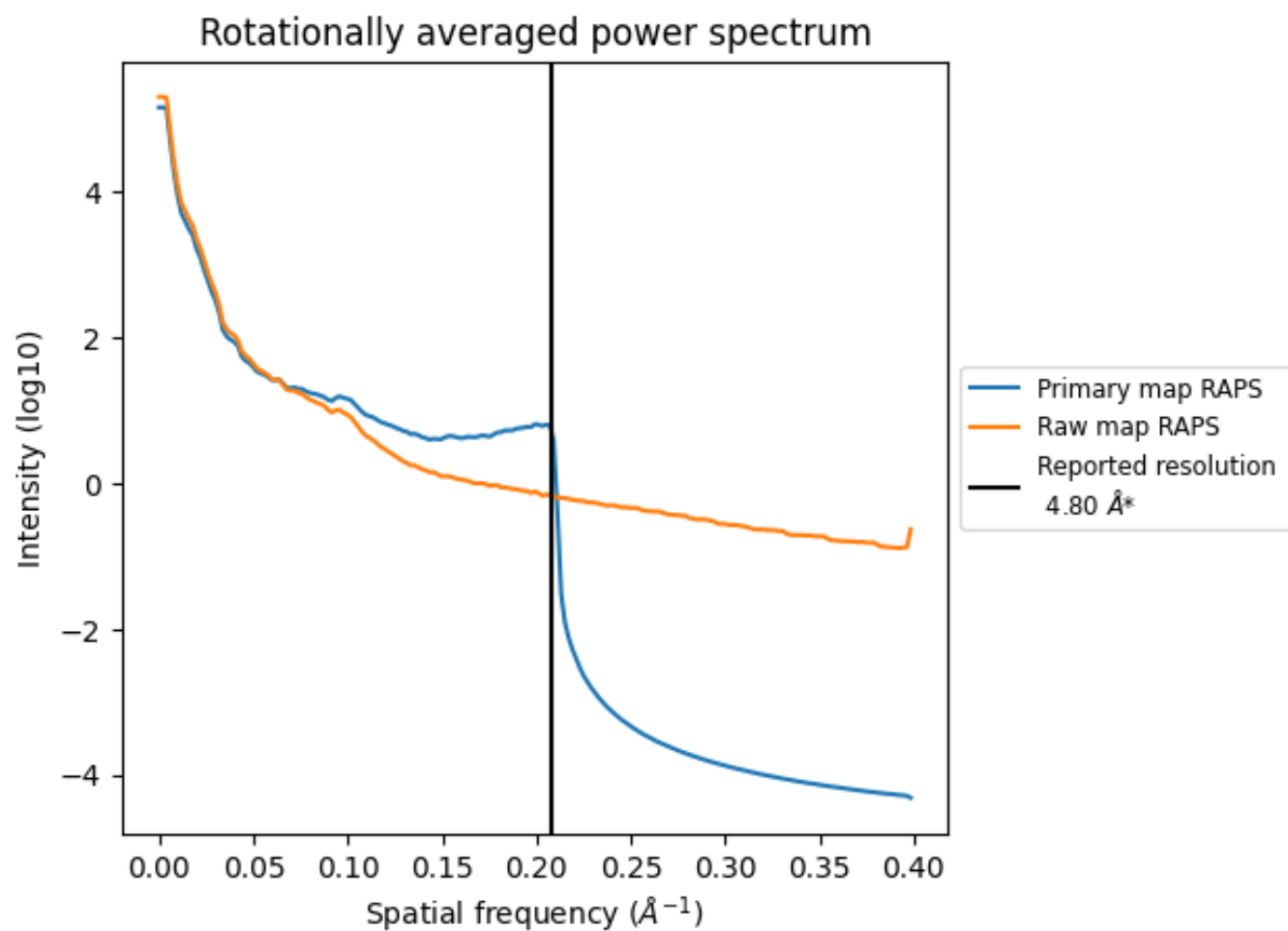
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 596 nm^3 ; this corresponds to an approximate mass of 539 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 ⓘ

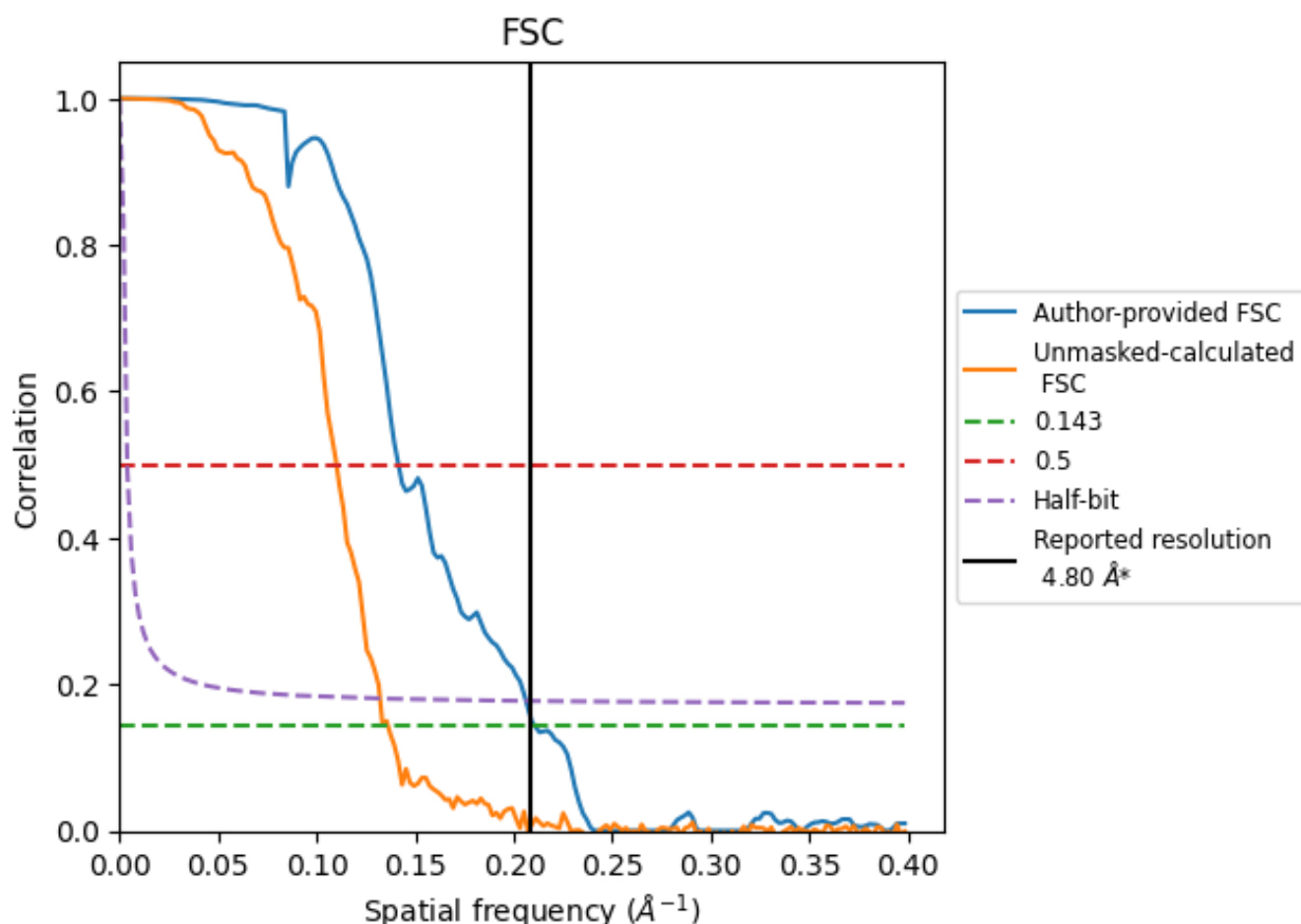


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 0.208 Å⁻¹

8.2 Resolution estimates [i](#)

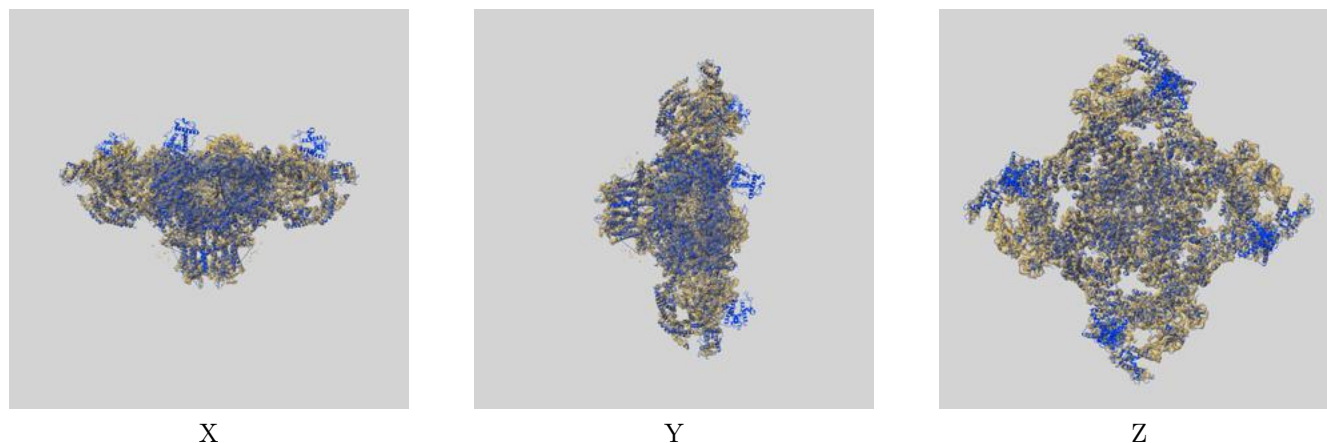
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.75	7.07	4.85
Unmasked-calculated*	7.34	9.09	7.57

*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 7.34 differs from the reported value 4.8 by more than 10 %

9 Map-model fit [i](#)

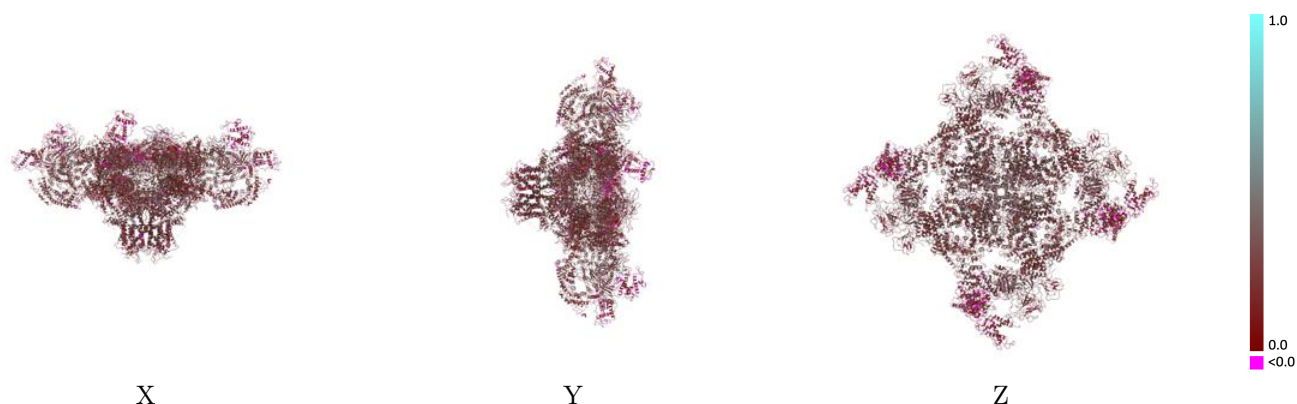
This section contains information regarding the fit between EMDB map EMD-8384 and PDB model 5TAT. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



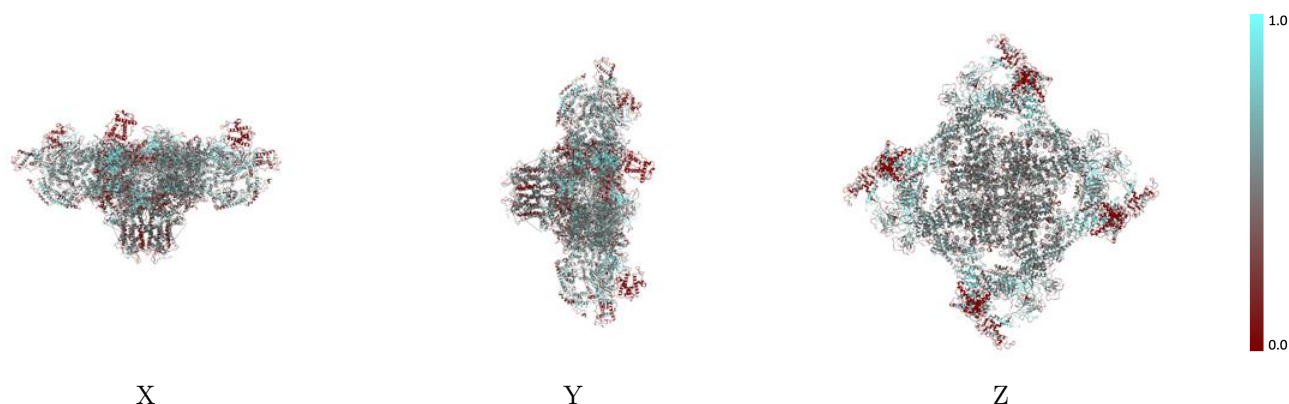
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



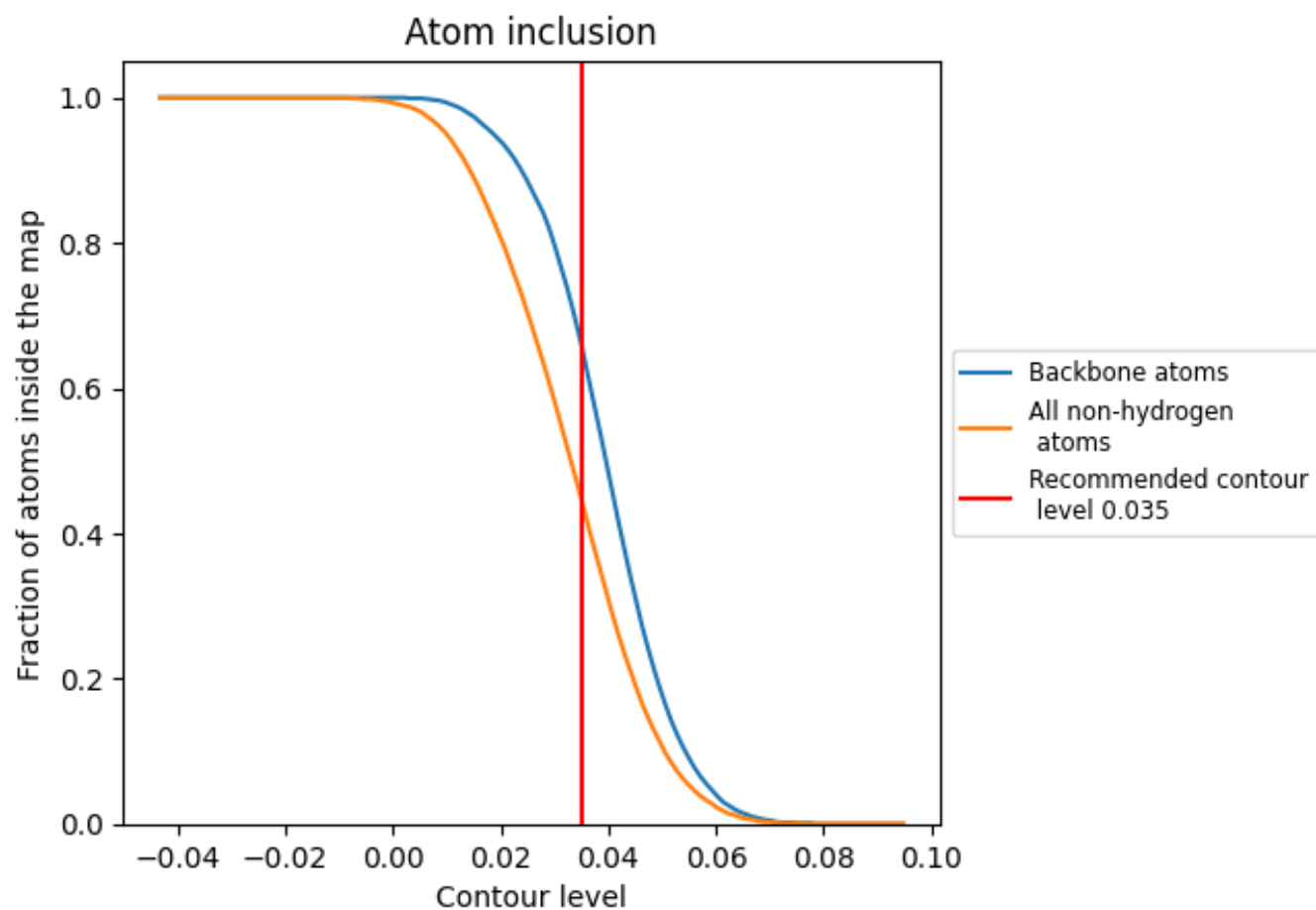
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 45% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4470	<div></div> 0.2510
A	<div></div> 0.4490	<div></div> 0.2490
B	<div></div> 0.4470	<div></div> 0.2510
E	<div></div> 0.4470	<div></div> 0.2510
F	<div></div> 0.4490	<div></div> 0.2530
G	<div></div> 0.4470	<div></div> 0.2510
H	<div></div> 0.4450	<div></div> 0.2510
I	<div></div> 0.4480	<div></div> 0.2520
J	<div></div> 0.4440	<div></div> 0.2510

1.0

0.0

<0.0