



Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 03:18 AM EDT

PDB ID : 5TAL
EMDB ID : EMD-8378
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 1&2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

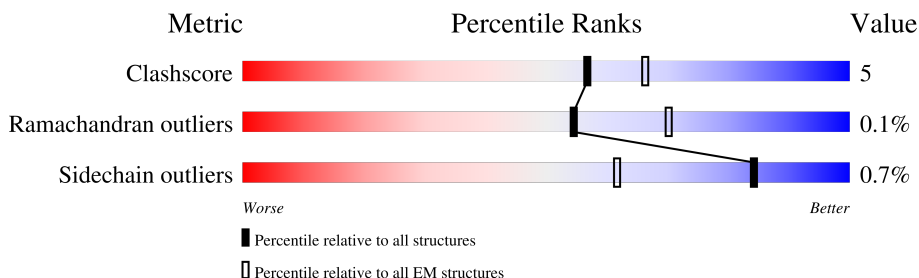
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	108	<div> <div>22%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	F	108	<div> <div>23%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	H	108	<div> <div>22%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	J	108	<div> <div>23%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	B	4416	<div> <div>37%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
2	E	4416	<div> <div>39%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
2	G	4416	<div> <div>38%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
2	I	4416	<div> <div>39%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 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.

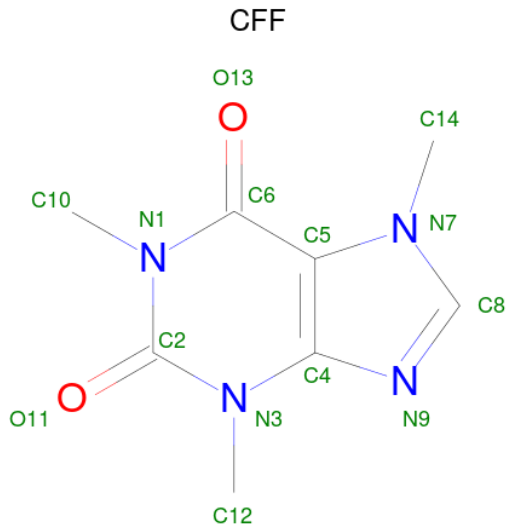
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0
3	I	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0

- 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	G	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	

- 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	G	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	

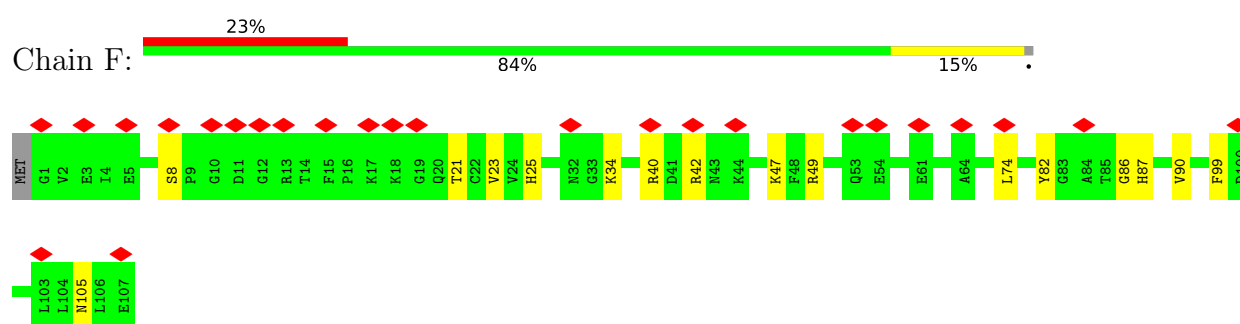
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

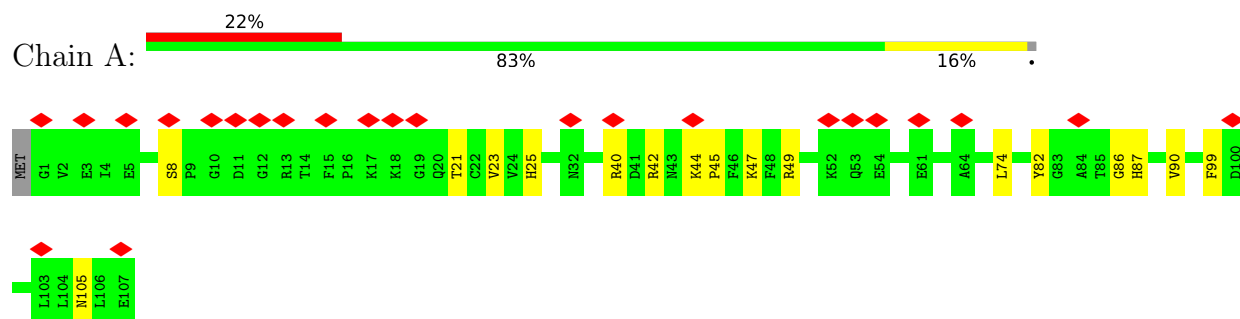
3 Residue-property plots [i](#)

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.

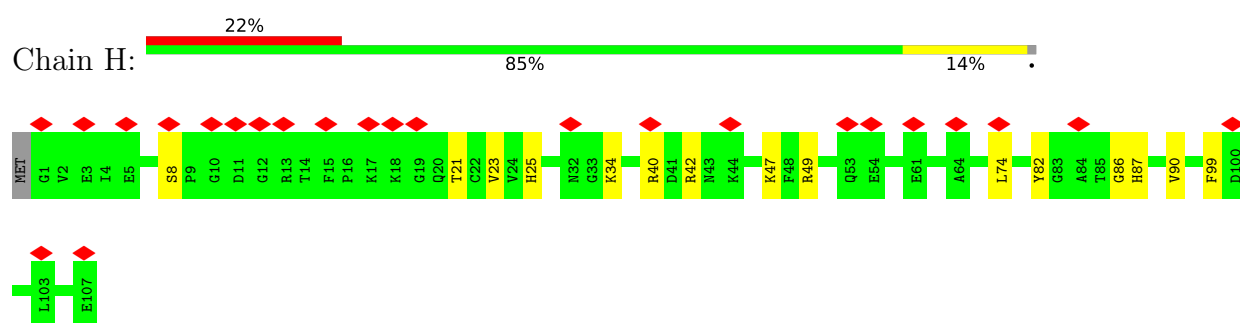
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



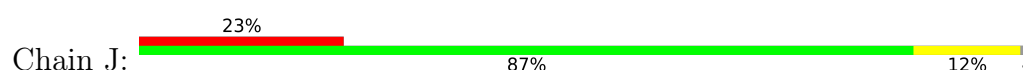
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

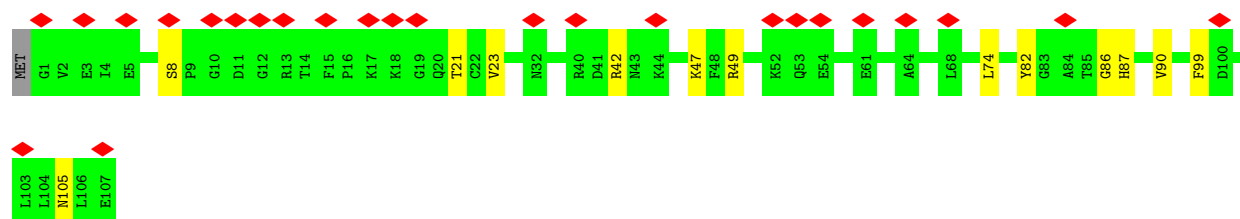


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



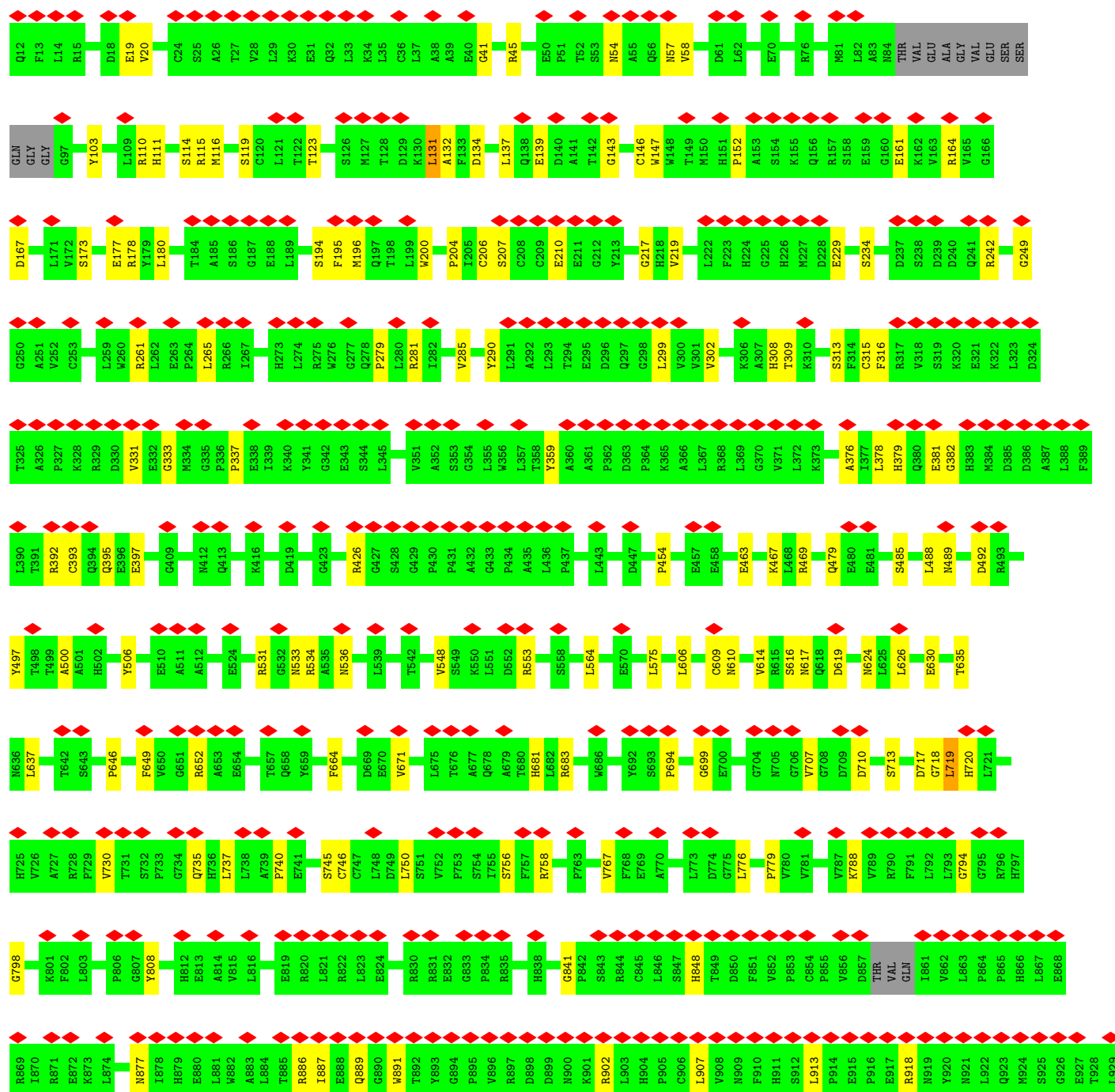
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





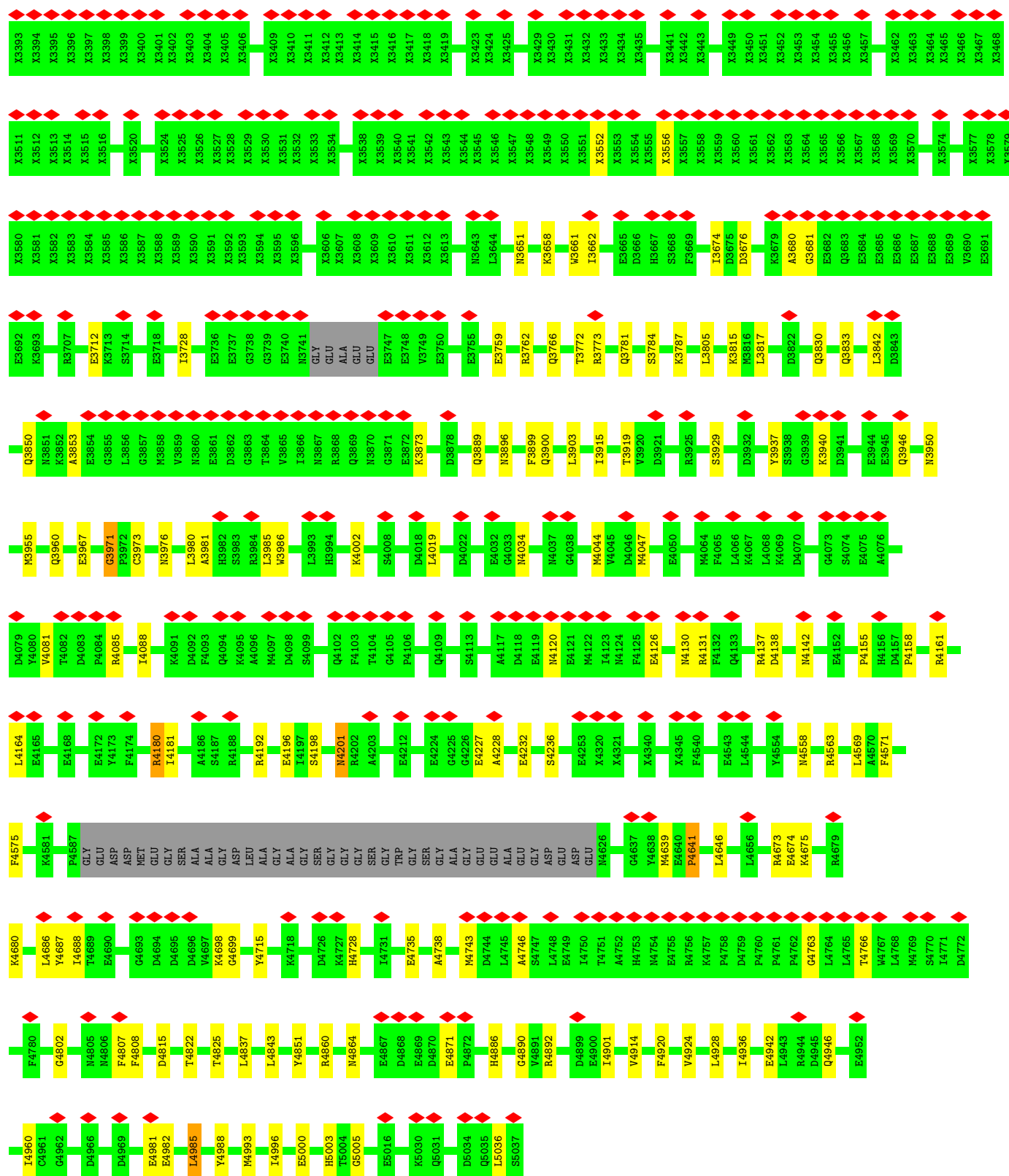
• Molecule 2: Ryanodine receptor 1

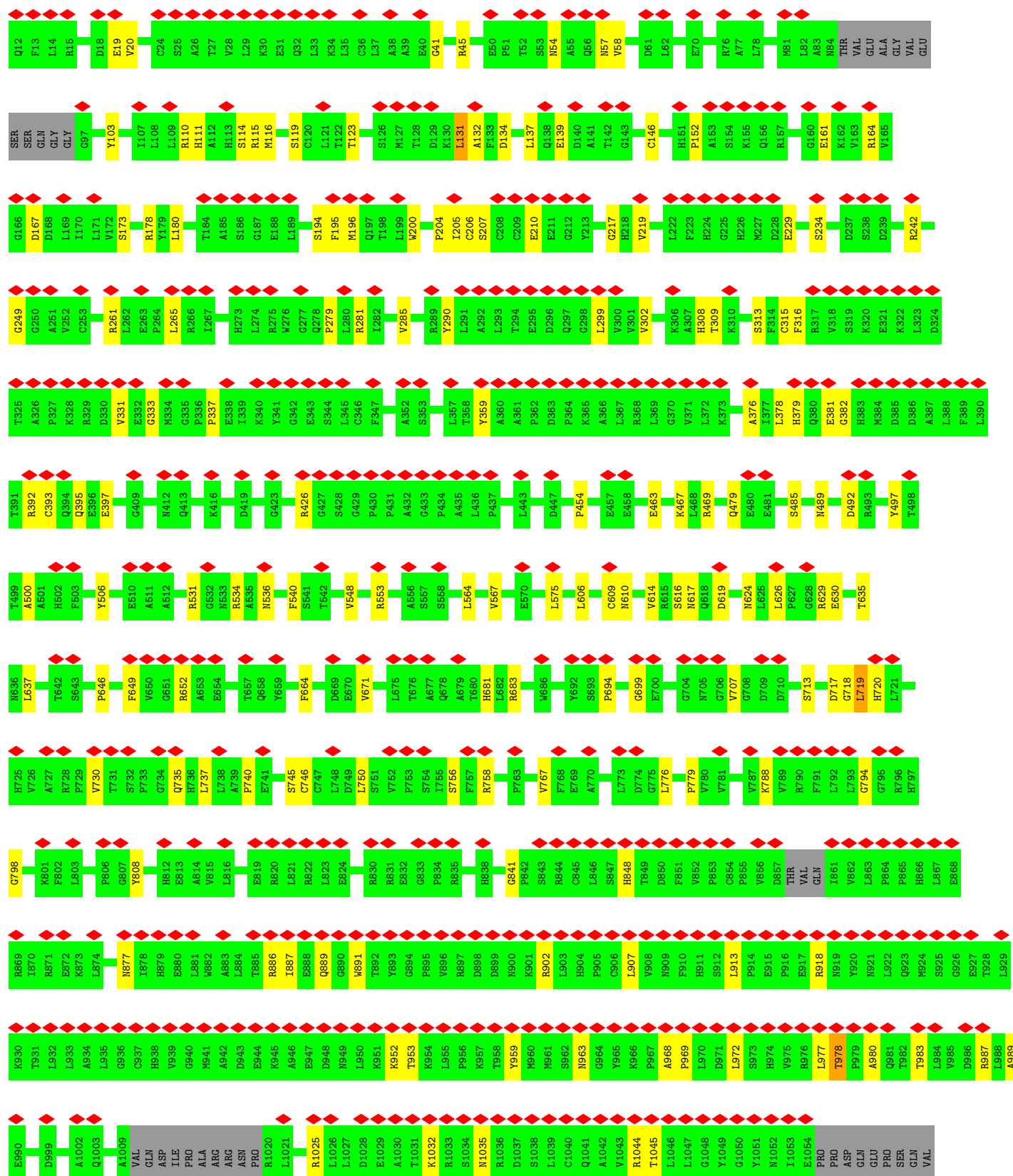
Chain B: 37% 83% 11% 5%





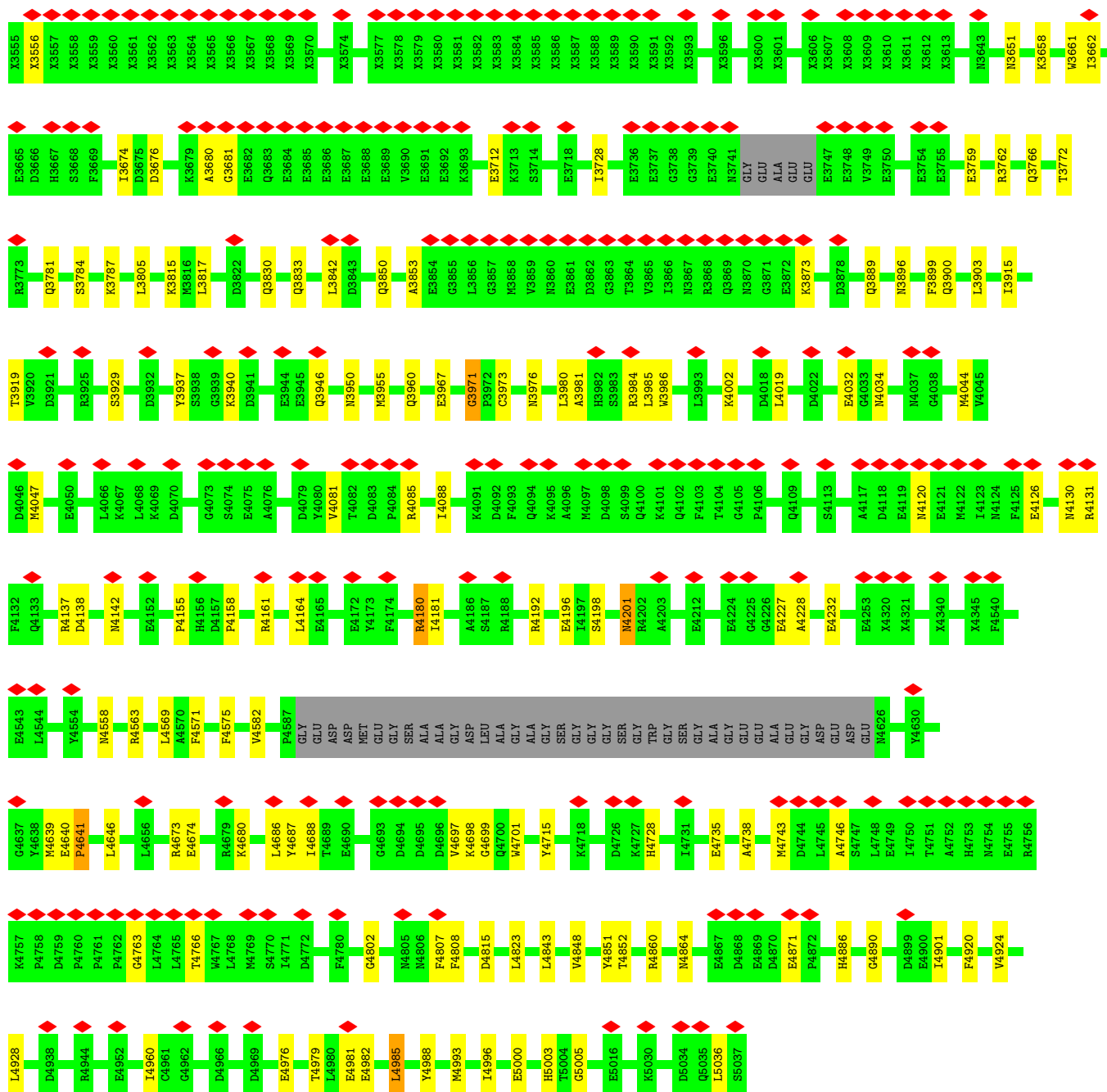
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X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331
X3199	X3200	X3201	X3202	X3205	X3206	X3207	X3208	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270			
X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3144	X3145	X3146	X3149	X3150	X3151	X3152	X3153	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3183	X3186	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3198				
X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3010	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3027	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3053	X3054	X3055	X3056	X3057	X3058	X3059					
E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	
X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3010	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3027	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3053	X3054	X3055	X3056	X3057	X3058	X3059					
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X3199	X3200	X3201	X3202	X3205	X3206	X3207	X3208	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270			
X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331		
X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392		





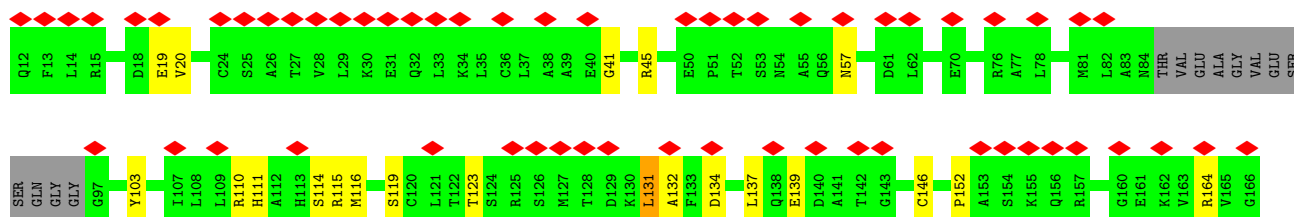


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H2902	P2903	L2904	L2905	L2906	P2907	P2908	D2909	T2910	L2911	T2912	A2913	A2914	E2915	K2916	A2917	D2918	D2919	R2920	E2921	A2922	A2923	Q2924	E2925	L2926	L2927	K2928	P2929	L2930	Q2931	M2932	N2933	Q2934	V2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	K2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963																																									
ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	Q2864	V2865	T2866	L2867	S2868	D2869	E2870	L2871	Q2872	M2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	V2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	D2897	G2898	G2899	Q2900	T2901																																										
D2762	E2763	E2764	L2765	L2766	T2767	H2768	P2769	M2770	L2791	R2792	P2793	T2794	K2795	L2796	P2797	S2798	E2799	K2800	D2801	L2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	P2753	Q2754	L2755	N2756	K2757	P2758	A2759	E2760	V2761	L2762	H2763	E2764	K2765	A2826	R2827	P2768	D2769	K2770	L2771	Q2772	N2773	V2774	W2775	S2776	V2777	E2778	P2779	N2780	V2781																																									
X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2632	X2633	X2634	X2638	X2639	X2640	X2643	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2658	X2662	X2663	X2664	X2665	X2666	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2682	X2683	X2686	X2687	X2688	X2689	X2690	X2691																																																
X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	P2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	P2753	Q2754	L2755	N2756	K2757	P2758	A2759	E2760	V2761	L2762	H2763	E2764	K2765	A2826	R2827	P2768	D2769	K2770	L2771	Q2772	N2773	V2774	W2775	S2776	V2777	E2778	P2779	N2780	V2781																																									
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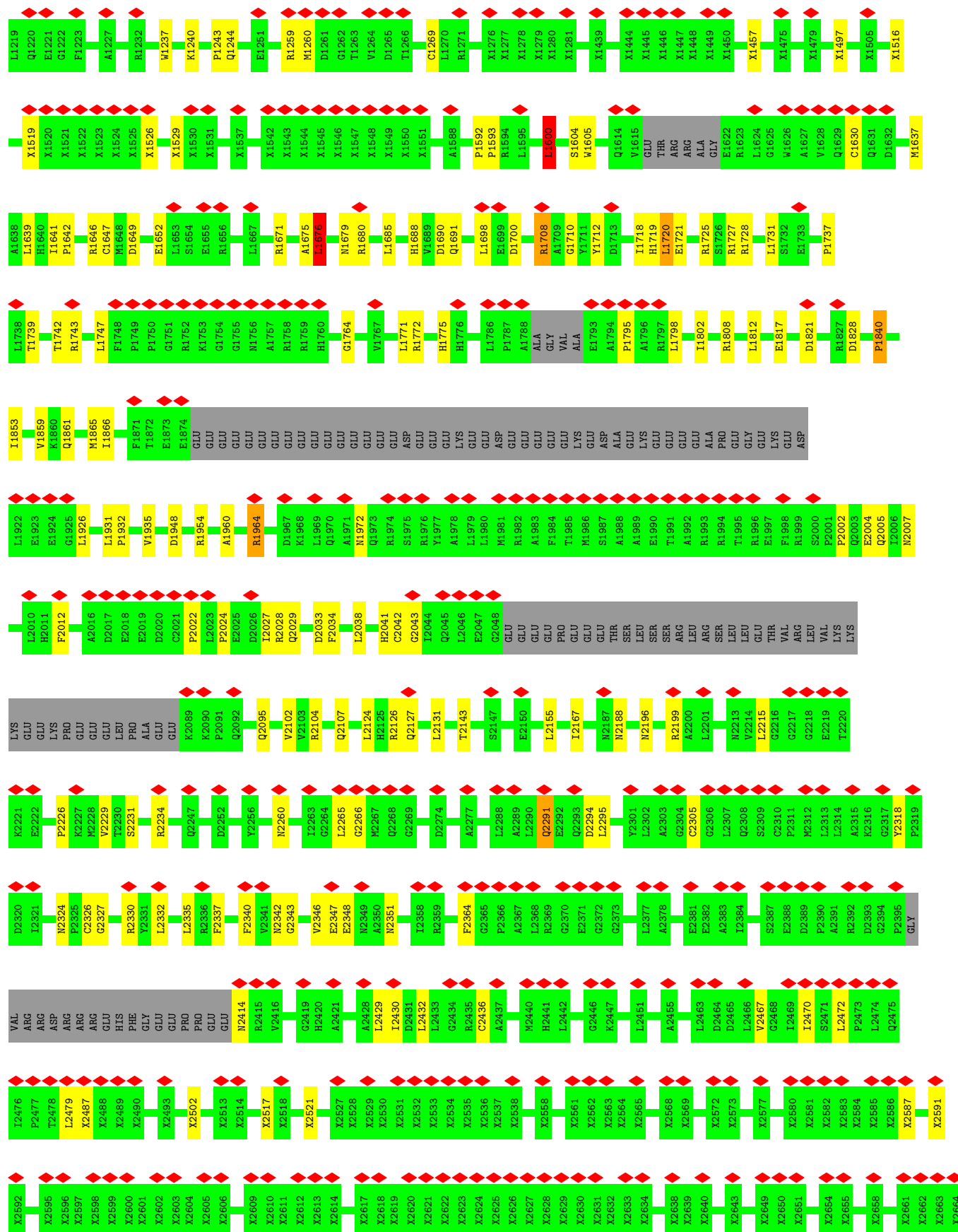


• Molecule 2: Ryanodine receptor 1

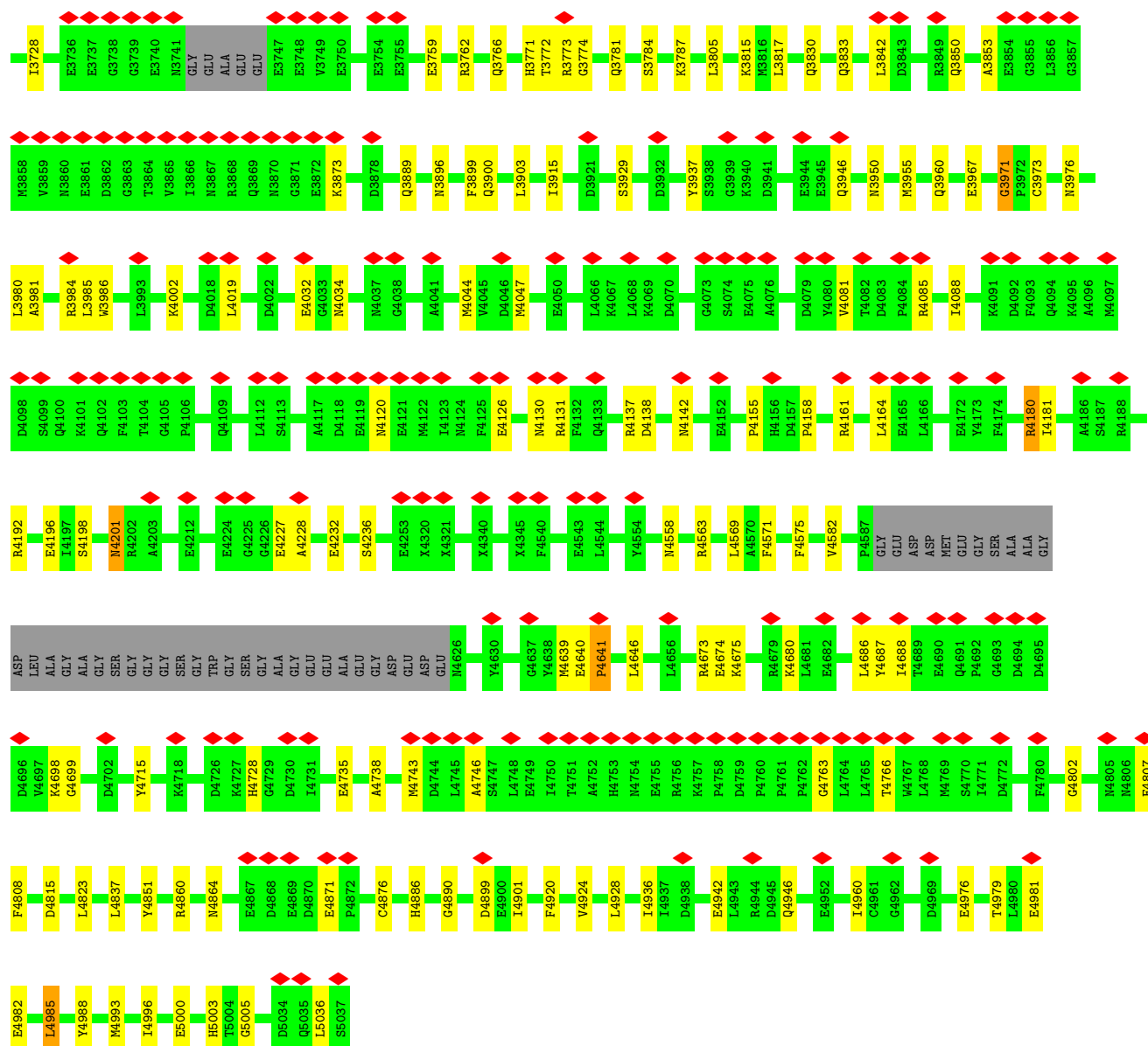
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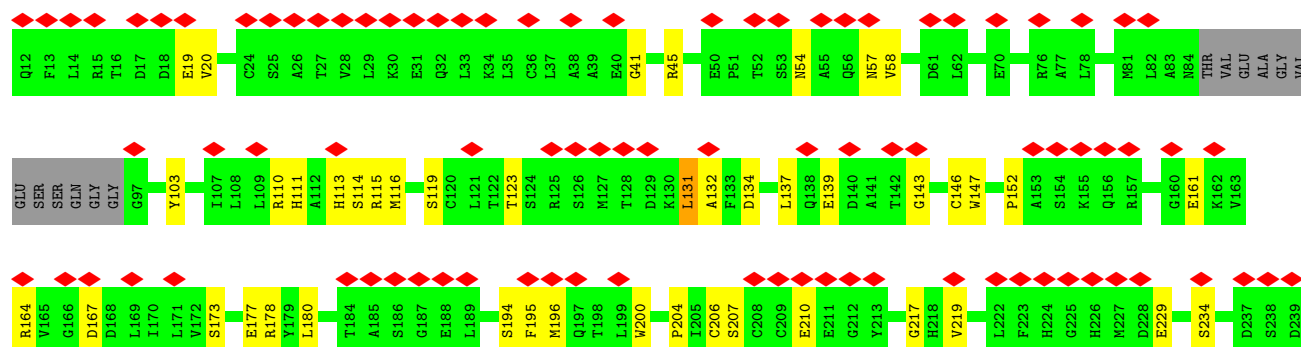
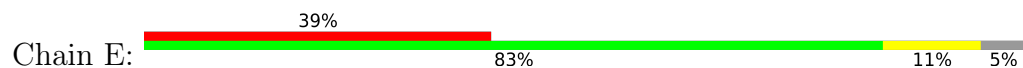


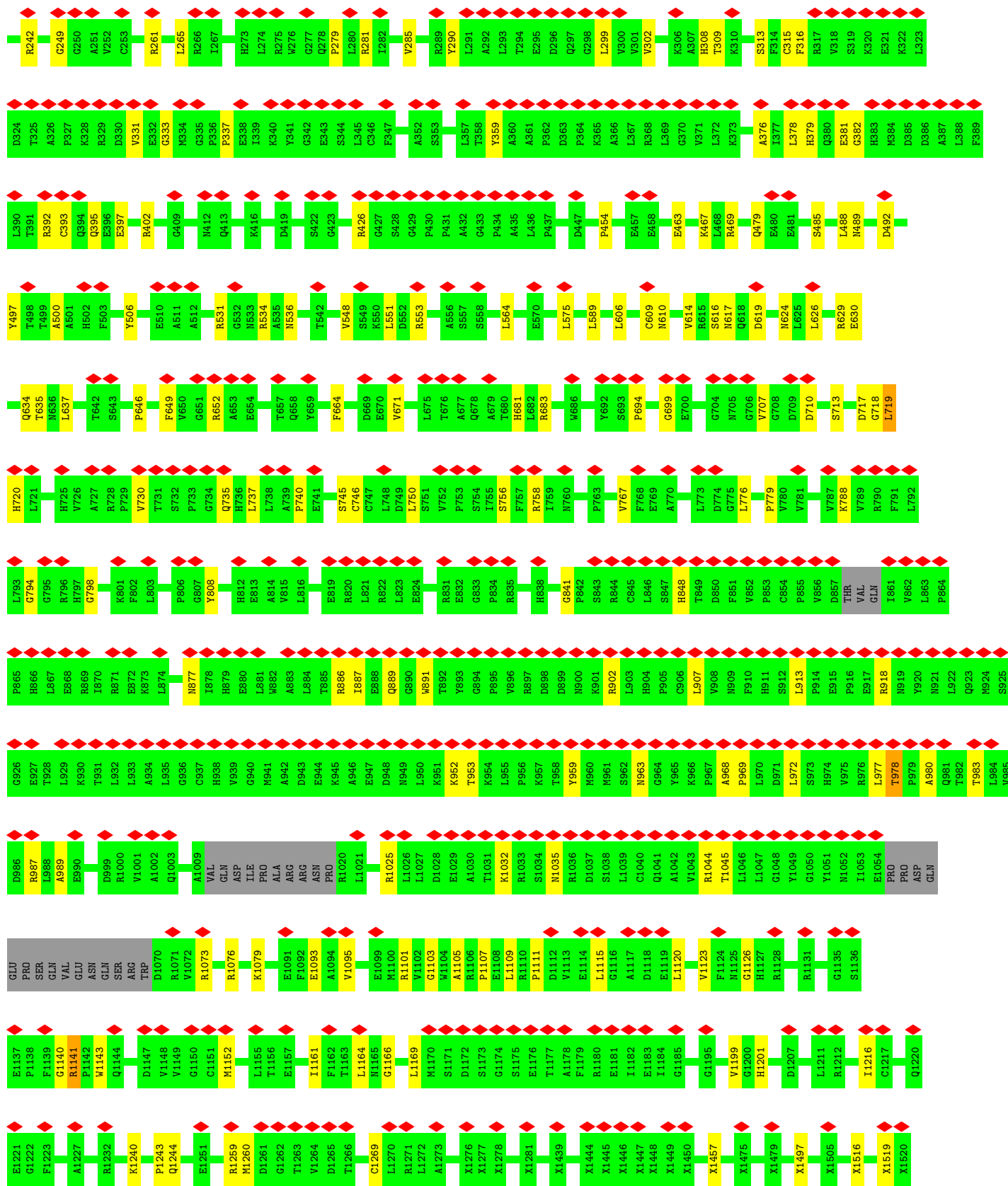






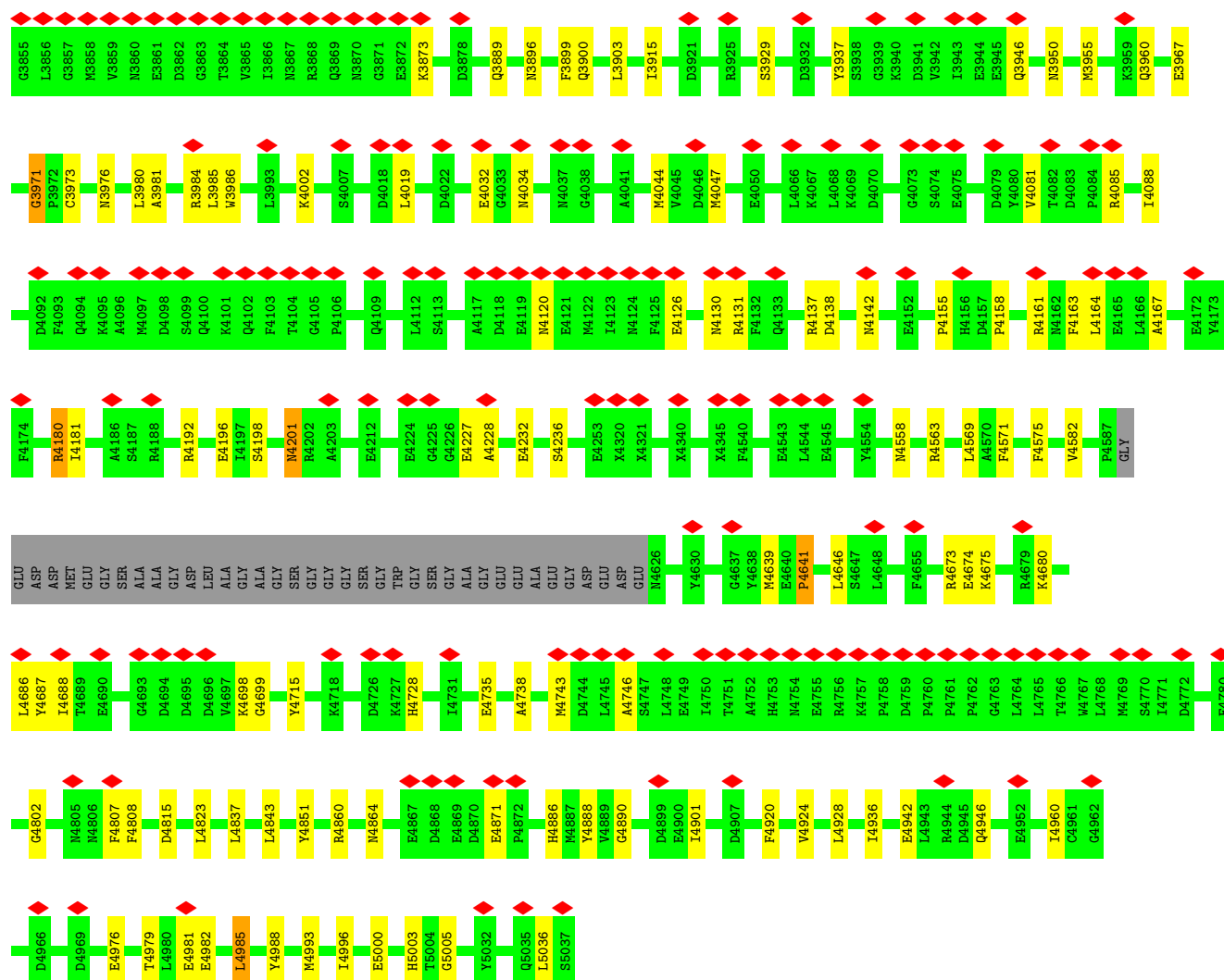
• Molecule 2: Ryanodine receptor 1







S3714	K3592	K3527	K3419	K3358	K3296	K3226	K3156	K3022	K2942	E2880	E2820	S3714	K3592	K3527	K3419	K3358	K3296	K3226	K3156	K3022	K2942	E2880	E2820
E3718	K3593	K3528	K3420	K3359	K3297	K3227	K3157	K3023	K2943	M2881	W2821	E3718	K3593	K3528	K3420	K3359	K3297	K3227	K3157	K3023	K2943	M2881	W2821
K3720	K3596	K3530	K3422	K3360	K3298	K3228	K3158	K3027	K2944	H2882	T2822	K3720	K3596	K3530	K3422	K3360	K3298	K3228	K3158	K3027	K2944	H2882	T2822
I3728	K3597	K3531	K3423	K3362	K3299	K3229	K3159	K3028	K2945	H2883	I2823	I3728	K3597	K3531	K3423	K3362	K3299	K3229	K3159	K3028	K2945	H2883	I2823
E3736	K3600	K3532	K3424	K3363	K3300	K3230	K3160	K3029	K2946	T2885	K2825	E3736	K3600	K3532	K3424	K3363	K3300	K3230	K3160	K3029	K2946	T2885	K2825
E3737	K3601	K3533	K3425	K3364	K3301	K3231	K3161	K3031	K2947	W2886	A2826	E3737	K3601	K3533	K3425	K3364	K3301	K3231	K3161	K3031	K2947	W2886	A2826
G3738	K3604	K3534	K3426	K3365	K3302	K3232	K3162	K3032	K2948	G2887	K2827	G3738	K3604	K3534	K3426	K3365	K3302	K3232	K3162	K3032	K2948	G2887	K2827
G3739	K3608	K3538	K3428	K3366	K3303	K3233	K3163	K3033	K2950	K2888	E2828	G3739	K3608	K3538	K3428	K3366	K3303	K3233	K3163	K3033	K2950	K2888	E2828
E3740	K3609	K3539	K3429	K3367	K3304	K3234	K3170	K3034	K2951	K2889	G2829	E3740	K3609	K3539	K3429	K3367	K3304	K3234	K3170	K3034	K2951	K2889	G2829
N3741	K3608	K3540	K3430	K3368	K3309	K3236	K3172	K3035	K2952	K2890	E2830	N3741	K3608	K3540	K3430	K3368	K3309	K3236	K3172	K3035	K2952	K2890	E2830
GLY	K3610	K3541	K3431	K3370	K3310	K3242	K3173	K3036	K2953	K2891	GLU	GLY	K3610	K3541	K3431	K3370	K3310	K3242	K3173	K3036	K2953	K2891	GLU
ALA	K3611	K3542	K3432	K3371	K3311	K3243	K3174	K3037	K2954	Q2892	ARG	ALA	K3611	K3542	K3432	K3371	K3311	K3243	K3174	K3037	K2954	Q2892	ARG
GLU	K3612	K3543	K3433	K3372	K3312	K3244	K3175	K3038	K2955	E2893	THR	GLU	K3612	K3543	K3433	K3372	K3312	K3244	K3175	K3038	K2955	E2893	THR
GLU	K3613	K3544	K3434	K3373	K3313	K3245	K3176	K3039	K2956	L2894	LYS	GLU	K3613	K3544	K3434	K3373	K3313	K3245	K3176	K3039	K2956	L2894	LYS
GLU	K3613	K3545	K3435	K3374	K3314	K3246	K3177	K3040	K2957	E2895	LYS	GLU	K3613	K3545	K3435	K3374	K3314	K3246	K3177	K3040	K2957	E2895	LYS
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E3748	L3644	K3547	K3439	K3378	K3316	K3247	K3179	K3042	K2961	K2897	THR	E3748	L3644	K3547	K3439	K3378	K3316	K3247	K3179	K3042	K2961	K2897	THR
V3749	K3609	K3548	K3440	K3379	K3317	K3248	K3180	K3043	K2962	G2898	LYS	V3749	K3609	K3548	K3440	K3379	K3317	K3248	K3180	K3043	K2962	G2898	LYS
E3750	N3651	K3549	K3441	K3380	K3318	K3249	K3181	K3044	K2963	G2899	ILE	E3750	N3651	K3549	K3441	K3380	K3318	K3249	K3181	K3044	K2963	G2899	ILE
K3662	K3652	K3550	K3442	K3381	K3319	K3250	K3182	K3045	K2964	G2900	SER	K3662	K3652	K3550	K3442	K3381	K3319	K3250	K3182	K3045	K2964	G2900	SER
F3662	F3653	K3551	K3442	K3381	K3319	K3250	K3182	K3046	K2965	T2901	GLN	F3662	F3653	K3551	K3442	K3381	K3319	K3250	K3182	K3046	K2965	T2901	GLN
K3658	K3658	K3552	K3443	K3382	K3320	K3251	K3183	K3047	K2966	H2902	THR	K3658	K3658	K3552	K3443	K3382	K3320	K3251	K3183	K3047	K2966	H2902	THR
W3661	I3662	K3553	K3443	K3382	K3321	K3252	K3184	K3048	K2967	K2903	ALA	W3661	I3662	K3553	K3443	K3382	K3321	K3252	K3184	K3048	K2967	K2903	ALA
E3759	K3661	K3554	K3444	K3383	K3322	K3253	K3185	K3049	K2968	L2904	GLN	E3759	K3661	K3554	K3444	K3383	K3322	K3253	K3185	K3049	K2968	L2904	GLN
R3762	K3662	K3555	K3445	K3384	K3323	K3254	K3186	K3050	K2969	K2905	LYS	R3762	K3662	K3555	K3445	K3384	K3323	K3254	K3186	K3050	K2969	K2905	LYS
Q3766	E3665	K3556	K3446	K3385	K3324	K3254	K3186	K3051	K2969	L2906	THR	Q3766	E3665	K3556	K3446	K3385	K3324	K3254	K3186	K3051	K2969	L2906	THR
T3772	D3666	K3557	K3449	K3386	K3325	K3256	K3187	K3052	K2970	V2906	ASP	T3772	D3666	K3557	K3449	K3386	K3325	K3256	K3187	K3052	K2970	V2906	ASP
R3773	H3667	K3559	K3450	K3387	K3326	K3256	K3187	K3053	K2971	P2907	K2786	R3773	H3667	K3559	K3450	K3387	K3326	K3256	K3187	K3053	K2971	P2907	K2786
S3784	S3668	K3560	K3453	K3388	K3327	K3256	K3187	K3054	K2972	Y2908	GLU	S3784	S3668	K3560	K3453	K3388	K3327	K3256	K3187	K3054	K2972	Y2908	GLU
K3787	F3669	K3561	K3454	K3389	K3328	K3256	K3187	K3055	K2973	D2909	GLY	K3787	F3669	K3561	K3454	K3389	K3328	K3256	K3187	K3055	K2973	D2909	GLY
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K3815	D3674	K3563	K3458	K3393	K3331	K3257	K3187	K3057	K2975	L2911	LYS	K3815	D3674	K3563	K3458	K3393	K3331	K3257	K3187	K3057	K2975	L2911	LYS
E3816	D3675	K3564	K3459	K3394	K3332	K3257	K3187	K3058	K2976	T2912	LYS	E3816	D3675	K3564	K3459	K3394	K3332	K3257	K3187	K3058	K2976	T2912	LYS
L3817	D3676	K3565	K3460	K3395	K3333	K3257	K3187	K3059	K2976	A2913	LYS	L3817	D3676	K3565	K3460	K3395	K3333	K3257	K3187	K3059	K2976	A2913	LYS
Q3830	K3679	K3566	K3463	K3396	K3334	K3257	K3187	K3060	K2976	K2859	LYS	Q3830	K3679	K3566	K3463	K3396	K3334	K3257	K3187	K3060	K2976	K2859	LYS
E3833	A3680	K3567	K3464	K3397	K3335	K3257	K3187	K3062	K2976	K2861	LYS	E3833	A3680	K3567	K3464	K3397	K3335	K3257	K3187	K3062	K2976	K2861	LYS
L3842	K3680	K3568	K3465	K3398	K3336	K3257	K3187	K3063	K2976	L2862	LYS	L3842	K3680	K3568	K3465	K3398	K3336	K3257	K3187	K3063	K2976	L2862	LYS
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		K3588	K3523	K3414	K3352	K3257	K3187	K3078	K2976	K2877	LYS			K3588	K3523	K3414	K3352	K3257	K3187	K3078	K2976	K2877	LYS
		K3589	K3524	K3415	K3353	K3257	K3187	K3079	K2976	L2878	LYS			K3589	K3524	K3415	K3353	K3257	K3187	K3079	K2976	L2878	LYS
		K3590	K3525	K3416	K3354	K3257	K3187	K3080	K2976	K2879	LYS			K3590	K3525	K3416	K3354	K3257	K3187	K3080	K2976	K2879	LYS
		K3591	K3526	K3417	K3355	K3257	K3187	K3081	K2976	K2879	LYS			K3591	K3526	K3417	K3355	K3257	K3187	K3081	K2976	K2879	LYS



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	0.088	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	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: ZN, CFF, CA, ATP

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	0.53	0/1123
1	F	0.32	0/834	0.53	0/1123
1	H	0.32	0/834	0.53	0/1123
1	J	0.32	0/834	0.53	0/1123
2	B	0.31	0/25428	0.55	8/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	32/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	17
2	E	0	17
2	G	0	17
2	I	0	17
All	All	0	72

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	131	LEU	CA-CB-CG	7.51	132.57	115.30
2	G	131	LEU	CA-CB-CG	7.51	132.56	115.30
2	I	131	LEU	CA-CB-CG	7.51	132.56	115.30
2	B	131	LEU	CA-CB-CG	7.49	132.53	115.30
2	B	1676	LEU	CA-CB-CG	6.38	129.96	115.30
2	E	1676	LEU	CA-CB-CG	6.37	129.95	115.30
2	G	1676	LEU	CA-CB-CG	6.35	129.91	115.30
2	I	1676	LEU	CA-CB-CG	6.35	129.91	115.30
2	G	1600	LEU	CA-CB-CG	6.08	129.29	115.30
2	B	1600	LEU	CA-CB-CG	6.07	129.26	115.30
2	E	1600	LEU	CA-CB-CG	6.07	129.26	115.30
2	I	1600	LEU	CA-CB-CG	6.06	129.25	115.30
2	B	4901	ILE	CG1-CB-CG2	-6.04	98.11	111.40
2	G	4901	ILE	CG1-CB-CG2	-6.03	98.12	111.40
2	I	4901	ILE	CG1-CB-CG2	-6.03	98.13	111.40
2	E	4901	ILE	CG1-CB-CG2	-6.02	98.15	111.40
2	I	977	LEU	CA-CB-CG	5.50	127.96	115.30
2	E	977	LEU	CA-CB-CG	5.50	127.95	115.30
2	B	977	LEU	CA-CB-CG	5.50	127.94	115.30
2	G	977	LEU	CA-CB-CG	5.48	127.90	115.30
2	B	4639	MET	C-N-CA	5.42	135.26	121.70
2	I	4639	MET	C-N-CA	5.41	135.22	121.70
2	G	4639	MET	C-N-CA	5.40	135.21	121.70
2	E	4639	MET	C-N-CA	5.39	135.19	121.70
2	I	1140	GLY	C-N-CA	5.23	134.77	121.70
2	B	1140	GLY	C-N-CA	5.22	134.75	121.70
2	G	1140	GLY	C-N-CA	5.20	134.70	121.70
2	E	1140	GLY	C-N-CA	5.20	134.70	121.70
2	B	4985	LEU	CA-CB-CG	5.18	127.21	115.30
2	I	4985	LEU	CA-CB-CG	5.18	127.21	115.30
2	E	4985	LEU	CA-CB-CG	5.17	127.19	115.30
2	G	4985	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1720	LEU	Peptide
2	B	1795	PRO	Peptide

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Mol	Chain	Res	Type	Group
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	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	4807	PHE	Peptide
2	B	624	ASN	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1720	LEU	Peptide
2	E	1795	PRO	Peptide
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	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	4807	PHE	Peptide
2	E	624	ASN	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1720	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	3971	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	G	4641	PRO	Peptide
2	G	4807	PHE	Peptide
2	G	624	ASN	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1720	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	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4807	PHE	Peptide
2	I	624	ASN	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	10	0
1	F	818	0	824	11	0
1	H	818	0	824	8	0
1	J	818	0	824	7	0
2	B	29499	0	24746	286	0
2	E	29499	0	24747	282	0
2	G	29499	0	24747	279	0
2	I	29499	0	24747	284	0
3	B	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	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
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102371	1145	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 (1145) 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:2318:TYR:HH	2:E:2414:ASN:N	1.86	0.74
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.86	0.72
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.86	0.71
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.87	0.71
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.56	0.70
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.57	0.70
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.74	0.70
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.58	0.69
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.57	0.69
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.56	0.68
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.58	0.68
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.58	0.68
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.58	0.68
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.58	0.67
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.78	0.66
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.78	0.65
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.78	0.65
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.62	0.65
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.64
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.62	0.64
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.64
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.62	0.64
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.62	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.62	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.80	0.63
2:G:2266:GLY:O	2:G:2330:ARG:NH2	2.32	0.63
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.33	0.62
2:B:2266:GLY:O	2:B:2330:ARG:NH2	2.32	0.62
2:E:2266:GLY:O	2:E:2330:ARG:NH2	2.32	0.62
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.33	0.62
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.33	0.62
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.33	0.62
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.82	0.62
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.82	0.62
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.82	0.61
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.82	0.61
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.33	0.61
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.33	0.61
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.33	0.61
2:I:2266:GLY:O	2:I:2330:ARG:NH2	2.32	0.61
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.82	0.61
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.82	0.61
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.33	0.61
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.83	0.61
2:B:379:HIS:HD2	2:B:382:GLY:H	1.47	0.61
2:G:379:HIS:HD2	2:G:382:GLY:H	1.47	0.61
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.83	0.61
2:I:379:HIS:HD2	2:I:382:GLY:H	1.47	0.60
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.82	0.60
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.83	0.60
2:G:173:SER:HB3	2:G:178:ARG:H	1.66	0.60
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.66	0.60
2:I:173:SER:HB3	2:I:178:ARG:H	1.66	0.60
2:E:379:HIS:HD2	2:E:382:GLY:H	1.48	0.60
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.82	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.84	0.60
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.84	0.60
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.84	0.60
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.67	0.60
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.83	0.60
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.67	0.59
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.84	0.59
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.83	0.59
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.83	0.59
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.35	0.59
2:B:173:SER:HB3	2:B:178:ARG:H	1.66	0.59
2:G:132:ALA:HA	2:G:194:SER:HB2	1.85	0.59
2:I:132:ALA:HA	2:I:194:SER:HB2	1.85	0.59
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.84	0.59
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.83	0.59
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.59
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.59
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.35	0.59
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.59
2:E:173:SER:HB3	2:E:178:ARG:H	1.66	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.67	0.59
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.84	0.59
2:B:606:LEU:O	2:B:617:ASN:ND2	2.36	0.59
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.76	0.59
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.85	0.59
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.36	0.59
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.36	0.59
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.67	0.59
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.85	0.59
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.36	0.58
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.67	0.58
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.84	0.58
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.67	0.58
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.85	0.58
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.67	0.58
2:E:132:ALA:HA	2:E:194:SER:HB2	1.85	0.58
2:B:132:ALA:HA	2:B:194:SER:HB2	1.85	0.58
2:I:606:LEU:O	2:I:617:ASN:ND2	2.36	0.58
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.76	0.58
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.84	0.58
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.85	0.58
2:G:606:LEU:O	2:G:617:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.84	0.58
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.37	0.58
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.36	0.58
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.84	0.58
2:I:978:THR:HB	2:I:980:ALA:H	1.69	0.58
2:E:606:LEU:O	2:E:617:ASN:ND2	2.36	0.58
2:E:978:THR:HB	2:E:980:ALA:H	1.69	0.58
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.76	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.37	0.58
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.37	0.58
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.86	0.58
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.37	0.58
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.35	0.58
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.37	0.58
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.76	0.58
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.37	0.58
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.35	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.58
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.84	0.57
2:B:978:THR:HB	2:B:980:ALA:H	1.69	0.57
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.35	0.57
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.86	0.57
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.86	0.57
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.85	0.57
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.86	0.57
2:G:978:THR:HB	2:G:980:ALA:H	1.69	0.57
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.85	0.57
2:G:2107:GLN:HG3	2:G:3681:GLY:HA2	1.87	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.86	0.57
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.87	0.57
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.37	0.57
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.86	0.57
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.86	0.57
2:I:359:TYR:HA	2:I:376:ALA:HA	1.86	0.57
2:I:2107:GLN:HG3	2:I:3681:GLY:HA2	1.87	0.56
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.56
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.87	0.56
2:B:359:TYR:HA	2:B:376:ALA:HA	1.86	0.56
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.37	0.56
2:E:2107:GLN:HG3	2:E:3681:GLY:HA2	1.87	0.56
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.56
2:B:2107:GLN:HG3	2:B:3681:GLY:HA2	1.87	0.56
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.88	0.56
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.88	0.56
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.88	0.56
2:G:217:GLY:O	2:G:261:ARG:NH1	2.39	0.56
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.88	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.56
2:E:4192:ARG:NH1	2:E:4982:GLU:OE2	2.39	0.56
2:B:217:GLY:O	2:B:261:ARG:NH1	2.39	0.56
2:I:217:GLY:O	2:I:261:ARG:NH1	2.39	0.56
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.88	0.56
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.86	0.56
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.87	0.56
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.70	0.56
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.88	0.56
2:I:265:LEU:HD12	2:I:279:PRO:HB2	1.88	0.56
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.86	0.56
2:B:265:LEU:HD12	2:B:279:PRO:HB2	1.88	0.56
2:G:359:TYR:HA	2:G:376:ALA:HA	1.86	0.56
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.86	0.56
2:E:359:TYR:HA	2:E:376:ALA:HA	1.86	0.55
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.88	0.55
2:B:4192:ARG:NH1	2:B:4982:GLU:OE2	2.39	0.55
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.39	0.55
2:G:4192:ARG:NH1	2:G:4982:GLU:OE2	2.39	0.55
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.37	0.55
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.86	0.55
2:G:614:VAL:HG22	2:G:616:SER:H	1.71	0.55
2:G:2347:GLU:O	2:G:2351:ASN:N	2.38	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.38	0.55
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.89	0.55
2:G:265:LEU:HD12	2:G:279:PRO:HB2	1.88	0.55
2:I:4192:ARG:NH1	2:I:4982:GLU:OE2	2.39	0.55
2:E:265:LEU:HD12	2:E:279:PRO:HB2	1.88	0.55
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.89	0.55
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.89	0.55
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.70	0.55
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.89	0.55
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:217:GLY:O	2:E:261:ARG:NH1	2.39	0.55
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.89	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.89	0.55
2:I:614:VAL:HG22	2:I:616:SER:H	1.71	0.55
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.88	0.55
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.89	0.55
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.70	0.55
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.89	0.55
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.89	0.55
2:I:180:LEU:O	2:I:200:TRP:NE1	2.36	0.55
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.72	0.55
2:I:315:CYS:SG	2:I:316:PHE:N	2.80	0.55
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.89	0.55
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.40	0.55
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.40	0.55
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.89	0.55
2:E:315:CYS:SG	2:E:316:PHE:N	2.80	0.55
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.40	0.55
2:E:2347:GLU:O	2:E:2351:ASN:N	2.38	0.55
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.89	0.55
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.89	0.55
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.39	0.55
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.40	0.55
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.89	0.54
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.88	0.54
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.89	0.54
2:B:614:VAL:HG22	2:B:616:SER:H	1.71	0.54
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.72	0.54
2:G:315:CYS:SG	2:G:316:PHE:N	2.80	0.54
2:B:315:CYS:SG	2:B:316:PHE:N	2.80	0.54
2:G:180:LEU:O	2:G:200:TRP:NE1	2.36	0.54
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.90	0.54
2:B:2347:GLU:O	2:B:2351:ASN:N	2.38	0.54
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.40	0.54
2:I:2347:GLU:O	2:I:2351:ASN:N	2.38	0.54
2:E:111:HIS:HD2	2:E:114:SER:H	1.54	0.54
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.40	0.54
2:B:4914:VAL:HG23	2:E:4888:TYR:HD1	1.72	0.54
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.89	0.54
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.37	0.54
2:E:683:ARG:NH1	2:E:707:VAL:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.40	0.54
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.89	0.54
2:E:614:VAL:HG22	2:E:616:SER:H	1.71	0.54
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.89	0.54
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.89	0.54
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.90	0.54
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.89	0.54
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.37	0.54
2:I:111:HIS:HD2	2:I:114:SER:H	1.54	0.54
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.54
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.89	0.54
2:E:1948:ASP:OD1	2:E:2126:ARG:NH2	2.39	0.54
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.90	0.53
2:B:111:HIS:HD2	2:B:114:SER:H	1.54	0.53
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.41	0.53
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.41	0.53
2:B:309:THR:O	2:B:313:SER:OG	2.27	0.53
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.90	0.53
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.90	0.53
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.40	0.53
2:B:4161:ARG:HD3	2:B:4164:LEU:HD12	1.90	0.53
2:G:111:HIS:HD2	2:G:114:SER:H	1.54	0.53
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.72	0.53
2:E:4161:ARG:HD3	2:E:4164:LEU:HD12	1.91	0.53
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.42	0.53
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.41	0.53
2:I:309:THR:O	2:I:313:SER:OG	2.27	0.53
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.53
2:G:309:THR:O	2:G:313:SER:OG	2.27	0.53
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.41	0.53
2:E:652:ARG:HB2	2:E:750:LEU:HD13	1.91	0.53
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.89	0.53
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.91	0.53
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.91	0.53
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.91	0.53
2:B:4236:SER:OG	2:B:4675:LYS:NZ	2.38	0.53
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.90	0.53
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.53
2:I:331:VAL:HG12	2:I:333:GLY:H	1.74	0.53
2:E:309:THR:O	2:E:313:SER:OG	2.27	0.53
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.91	0.52
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.89	0.52
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.42	0.52
2:I:652:ARG:HB2	2:I:750:LEU:HD13	1.91	0.52
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.41	0.52
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.43	0.52
2:G:2107:GLN:NE2	2:G:3680:ALA:O	2.43	0.52
2:I:4161:ARG:HD3	2:I:4164:LEU:HD12	1.90	0.52
2:E:219:VAL:O	2:E:392:ARG:NH1	2.43	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.52
2:G:331:VAL:HG12	2:G:333:GLY:H	1.74	0.52
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.92	0.52
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.37	0.52
2:B:652:ARG:HB2	2:B:750:LEU:HD13	1.91	0.52
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.42	0.52
2:G:219:VAL:O	2:G:392:ARG:NH1	2.43	0.52
2:B:180:LEU:O	2:B:200:TRP:NE1	2.36	0.52
2:B:331:VAL:HG12	2:B:333:GLY:H	1.74	0.52
2:E:331:VAL:HG12	2:E:333:GLY:H	1.74	0.52
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.43	0.52
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.91	0.52
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.43	0.52
2:I:2107:GLN:NE2	2:I:3680:ALA:O	2.43	0.52
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.90	0.52
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.92	0.52
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.52
2:G:652:ARG:HB2	2:G:750:LEU:HD13	1.91	0.52
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.91	0.52
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.43	0.52
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.43	0.52
2:G:4161:ARG:HD3	2:G:4164:LEU:HD12	1.90	0.51
2:B:683:ARG:NH1	2:B:707:VAL:O	2.38	0.51
2:I:219:VAL:O	2:I:392:ARG:NH1	2.43	0.51
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.43	0.51
2:E:889:GLN:O	2:E:902:ARG:NH1	2.44	0.51
1:A:82:TYR:O	1:A:86:GLY:N	2.43	0.51
2:B:219:VAL:O	2:B:392:ARG:NH1	2.43	0.51
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.43	0.51
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.93	0.51
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.93	0.51
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:41:GLY:O	2:G:45:ARG:NH1	2.44	0.51
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.41	0.51
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.91	0.51
2:E:2107:GLN:NE2	2:E:3680:ALA:O	2.43	0.51
1:F:82:TYR:O	1:F:86:GLY:N	2.43	0.51
2:B:2107:GLN:NE2	2:B:3680:ALA:O	2.43	0.51
1:J:82:TYR:O	1:J:86:GLY:N	2.43	0.51
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.91	0.51
2:G:161:GLU:HA	2:I:3984:ARG:HH22	1.75	0.51
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.42	0.51
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.92	0.51
2:E:776:LEU:HG	2:E:848:HIS:HA	1.93	0.51
2:B:889:GLN:O	2:B:902:ARG:NH1	2.44	0.51
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.91	0.51
2:E:4198:SER:HB3	2:E:4201:ASN:HB2	1.93	0.51
2:E:4563:ARG:NH1	2:E:4815:ASP:OD1	2.44	0.51
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.93	0.51
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.43	0.51
2:G:889:GLN:O	2:G:902:ARG:NH1	2.44	0.51
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.51
2:E:3900:GLN:NE2	2:E:3967:GLU:O	2.44	0.51
2:B:776:LEU:HG	2:B:848:HIS:HA	1.93	0.50
2:G:683:ARG:NH1	2:G:707:VAL:O	2.38	0.50
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.92	0.50
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.93	0.50
2:B:1516:UNK:N	2:B:1529:UNK:O	2.44	0.50
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.44	0.50
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.44	0.50
2:I:889:GLN:O	2:I:902:ARG:NH1	2.44	0.50
2:I:4198:SER:HB3	2:I:4201:ASN:HB2	1.93	0.50
2:E:3773:ARG:HG3	2:E:3815:LYS:HZ3	1.75	0.50
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.94	0.50
2:B:4563:ARG:NH1	2:B:4815:ASP:OD1	2.44	0.50
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.76	0.50
2:I:41:GLY:O	2:I:45:ARG:NH1	2.44	0.50
2:I:776:LEU:HG	2:I:848:HIS:HA	1.93	0.50
2:E:180:LEU:O	2:E:200:TRP:NE1	2.36	0.50
1:H:82:TYR:O	1:H:86:GLY:N	2.43	0.50
2:B:3900:GLN:NE2	2:B:3967:GLU:O	2.44	0.50
2:G:3900:GLN:NE2	2:G:3967:GLU:O	2.44	0.50
2:I:1516:UNK:N	2:I:1529:UNK:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.93	0.50
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.42	0.50
2:E:907:LEU:O	2:E:963:ASN:ND2	2.38	0.50
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.44	0.50
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.44	0.50
2:G:776:LEU:HG	2:G:848:HIS:HA	1.93	0.50
2:G:1516:UNK:N	2:G:1529:UNK:O	2.45	0.50
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.93	0.50
2:B:41:GLY:O	2:B:45:ARG:NH1	2.44	0.50
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.44	0.50
2:G:4563:ARG:NH1	2:G:4815:ASP:OD1	2.44	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.45	0.50
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.38	0.50
2:B:4198:SER:HB3	2:B:4201:ASN:HB2	1.93	0.50
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.94	0.50
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.47	0.50
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.94	0.50
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.44	0.50
2:G:4198:SER:HB3	2:G:4201:ASN:HB2	1.93	0.50
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.93	0.50
2:I:4563:ARG:NH1	2:I:4815:ASP:OD1	2.44	0.50
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.44	0.50
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.47	0.49
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.45	0.49
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.45	0.49
2:G:3759:GLU:HB3	2:G:3762:ARG:HH21	1.77	0.49
2:I:3900:GLN:NE2	2:I:3967:GLU:O	2.44	0.49
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.93	0.49
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.76	0.49
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.42	0.49
2:E:2332:LEU:HD13	2:E:2335:LEU:HD12	1.94	0.49
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.47	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.49
2:B:3759:GLU:HB3	2:B:3762:ARG:HH21	1.77	0.49
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.47	0.49
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.45	0.49
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.76	0.49
2:G:907:LEU:O	2:G:963:ASN:ND2	2.38	0.49
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.76	0.49
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.94	0.49
2:G:2318:TYR:OH	2:G:2414:ASN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1457:UNK:N	2:B:1497:UNK:O	2.46	0.49
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.93	0.49
2:I:3759:GLU:HB3	2:I:3762:ARG:HH21	1.77	0.49
2:E:41:GLY:O	2:E:45:ARG:NH1	2.44	0.49
2:E:2318:TYR:OH	2:E:2414:ASN:N	2.46	0.49
2:B:2332:LEU:HD13	2:B:2335:LEU:HD12	1.94	0.49
2:G:164:ARG:N	2:G:167:ASP:OD2	2.43	0.49
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.95	0.49
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.44	0.49
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.48	0.49
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.95	0.49
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.94	0.49
2:I:1457:UNK:N	2:I:1497:UNK:O	2.46	0.49
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.41	0.49
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.42	0.49
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.48	0.49
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.41	0.49
2:B:907:LEU:O	2:B:963:ASN:ND2	2.38	0.49
2:B:2318:TYR:OH	2:B:2414:ASN:N	2.46	0.49
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.93	0.49
2:E:164:ARG:N	2:E:167:ASP:OD2	2.43	0.49
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.78	0.49
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.78	0.48
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.95	0.48
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.95	0.48
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.45	0.48
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.95	0.48
2:G:2305:CYS:HA	2:G:2324:ASN:HD22	1.79	0.48
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.95	0.48
2:E:3842:LEU:O	2:E:3929:SER:OG	2.32	0.48
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.78	0.48
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.37	0.48
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.96	0.48
2:I:1166:GLY:HA3	2:I:1216:ILE:HD13	1.96	0.48
2:B:234:SER:O	2:B:242:ARG:NE	2.46	0.48
2:B:1166:GLY:HA3	2:B:1216:ILE:HD13	1.96	0.48
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.79	0.48
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.48	0.48
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.78	0.48
2:G:1166:GLY:HA3	2:G:1216:ILE:HD13	1.96	0.48
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:730:VAL:O	2:E:735:GLN:NE2	2.47	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.94	0.48
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.96	0.48
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.96	0.48
2:I:2332:LEU:HD13	2:I:2335:LEU:HD12	1.94	0.48
2:E:234:SER:O	2:E:242:ARG:NE	2.46	0.48
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.78	0.48
2:B:730:VAL:O	2:B:735:GLN:NE2	2.47	0.48
2:B:3842:LEU:O	2:B:3929:SER:OG	2.32	0.48
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.79	0.48
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.96	0.48
2:E:3759:GLU:HB3	2:E:3762:ARG:HH21	1.77	0.48
2:B:2950:UNK:O	2:B:2954:UNK:N	2.47	0.48
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.32	0.48
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.47	0.48
2:G:116:MET:HB2	2:G:137:LEU:HD12	1.96	0.48
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.42	0.48
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.79	0.48
2:E:1457:UNK:N	2:E:1497:UNK:O	2.46	0.48
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.79	0.48
2:B:116:MET:HB2	2:B:137:LEU:HD12	1.96	0.48
2:B:119:SER:HA	2:B:146:CYS:HA	1.96	0.48
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.79	0.48
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.48	0.48
2:I:2004:GLU:HA	2:I:2007:ASN:HB2	1.96	0.48
2:I:2318:TYR:OH	2:I:2414:ASN:N	2.45	0.48
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.37	0.48
2:E:2305:CYS:HA	2:E:2324:ASN:HD22	1.79	0.48
2:B:2004:GLU:HA	2:B:2007:ASN:HB2	1.96	0.48
2:G:2332:LEU:HD13	2:G:2335:LEU:HD12	1.94	0.48
2:G:3842:LEU:O	2:G:3929:SER:OG	2.32	0.48
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.37	0.48
2:I:3903:LEU:HG	2:I:3915:ILE:HD12	1.96	0.48
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.96	0.48
2:E:1166:GLY:HA3	2:E:1216:ILE:HD13	1.96	0.48
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.95	0.48
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.79	0.48
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.32	0.48
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.96	0.48
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.96	0.48
2:G:3940:LYS:O	2:G:4002:LYS:NZ	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.96	0.48
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.96	0.47
2:B:2305:CYS:HA	2:B:2324:ASN:HD22	1.79	0.47
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.96	0.47
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.79	0.47
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.97	0.47
2:G:1457:UNK:N	2:G:1497:UNK:O	2.46	0.47
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.96	0.47
2:G:2868:SER:O	2:G:2872:GLN:N	2.47	0.47
2:G:4843:LEU:HD12	2:I:4823:LEU:HD23	1.96	0.47
2:I:164:ARG:N	2:I:167:ASP:OD2	2.43	0.47
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.95	0.47
2:G:119:SER:HA	2:G:146:CYS:HA	1.96	0.47
2:G:730:VAL:O	2:G:735:GLN:NE2	2.47	0.47
2:I:730:VAL:O	2:I:735:GLN:NE2	2.47	0.47
2:I:4137:ARG:NH2	2:I:4196:GLU:OE2	2.48	0.47
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.96	0.47
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.79	0.47
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.78	0.47
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.48	0.47
2:E:2868:SER:O	2:E:2872:GLN:N	2.47	0.47
2:G:2950:UNK:O	2:G:2954:UNK:N	2.47	0.47
2:G:3903:LEU:HG	2:G:3915:ILE:HD12	1.96	0.47
2:E:4851:TYR:HD2	2:E:4920:PHE:HD1	1.62	0.47
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.97	0.47
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.78	0.47
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.97	0.47
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.78	0.47
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.95	0.47
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.96	0.47
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.96	0.47
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.97	0.47
2:B:123:THR:OG1	2:B:134:ASP:OD1	2.33	0.47
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.88	0.47
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.97	0.47
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.88	0.47
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.96	0.47
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.46	0.47
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.48	0.47
2:G:4137:ARG:NH2	2:G:4196:GLU:OE2	2.48	0.47
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.96	0.47
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.96	0.47
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.95	0.47
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.80	0.47
2:E:4976:GLU:O	2:E:4979:THR:OG1	2.29	0.47
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.96	0.47
2:G:234:SER:O	2:G:242:ARG:NE	2.46	0.47
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.97	0.47
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.42	0.47
2:G:2004:GLU:HA	2:G:2007:ASN:HB2	1.96	0.47
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.79	0.47
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.97	0.47
2:I:119:SER:HA	2:I:146:CYS:HA	1.96	0.47
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.80	0.47
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.97	0.47
2:E:116:MET:HB2	2:E:137:LEU:HD12	1.96	0.47
2:E:123:THR:OG1	2:E:134:ASP:OD1	2.33	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.97	0.47
2:E:2950:UNK:O	2:E:2954:UNK:N	2.48	0.47
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.95	0.47
2:G:1817:GLU:O	2:G:1821:ASP:N	2.45	0.47
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.79	0.47
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.96	0.47
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.97	0.47
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.88	0.47
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.42	0.47
2:I:2305:CYS:HA	2:I:2324:ASN:HD22	1.79	0.47
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.48	0.47
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.79	0.47
2:E:3903:LEU:HG	2:E:3915:ILE:HD12	1.96	0.47
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.97	0.47
2:B:1747:LEU:HD21	2:B:2041:HIS:HB2	1.97	0.47
2:G:2452:ARG:HH12	2:E:177:GLU:HG3	1.79	0.47
2:G:4851:TYR:HD2	2:G:4920:PHE:HD1	1.62	0.47
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.88	0.47
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.97	0.47
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.97	0.47
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.46	0.46
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.48	0.46
2:I:234:SER:O	2:I:242:ARG:NE	2.46	0.46
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4236:SER:OG	2:I:4675:LYS:NZ	2.38	0.46
2:I:907:LEU:O	2:I:963:ASN:ND2	2.38	0.46
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.97	0.46
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.97	0.46
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.96	0.46
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.78	0.46
2:B:4137:ARG:NH2	2:B:4196:GLU:OE2	2.48	0.46
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.48	0.46
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.32	0.46
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.38	0.46
2:E:1747:LEU:HD21	2:E:2041:HIS:HB2	1.97	0.46
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.98	0.46
2:G:206:CYS:SG	2:G:207:SER:N	2.88	0.46
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.97	0.46
2:I:116:MET:HB2	2:I:137:LEU:HD12	1.96	0.46
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.48	0.46
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.46	0.46
2:B:3903:LEU:HG	2:B:3915:ILE:HD12	1.96	0.46
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.81	0.46
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.98	0.46
2:G:3361:UNK:O	2:G:3365:UNK:N	2.49	0.46
2:I:2868:SER:O	2:I:2872:GLN:N	2.47	0.46
2:I:3842:LEU:O	2:I:3929:SER:OG	2.32	0.46
2:E:4886:HIS:O	2:E:4890:GLY:N	2.44	0.46
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.98	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.98	0.46
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.97	0.46
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.97	0.46
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.97	0.46
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.97	0.46
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.97	0.46
2:I:123:THR:OG1	2:I:134:ASP:OD1	2.33	0.46
2:I:2950:UNK:O	2:I:2954:UNK:N	2.48	0.46
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.51	0.46
2:B:1954:ARG:HE	2:B:2041:HIS:HD2	1.63	0.46
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.51	0.46
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.98	0.46
2:I:4851:TYR:HD2	2:I:4920:PHE:HD1	1.62	0.46
2:E:206:CYS:SG	2:E:207:SER:N	2.88	0.46
2:E:2004:GLU:HA	2:E:2007:ASN:HB2	1.96	0.46
2:E:4137:ARG:NH2	2:E:4196:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.38	0.46
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.51	0.46
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.80	0.46
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.88	0.46
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.80	0.46
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.51	0.46
2:I:3361:UNK:O	2:I:3365:UNK:N	2.48	0.46
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.97	0.46
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.97	0.46
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.46	0.46
2:E:3361:UNK:O	2:E:3365:UNK:N	2.48	0.46
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.97	0.46
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.48	0.46
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.98	0.46
2:G:123:THR:OG1	2:G:134:ASP:OD1	2.33	0.46
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.98	0.46
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.98	0.46
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.48	0.46
2:B:2024:PRO:O	2:B:2028:ARG:NE	2.45	0.46
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.97	0.46
2:I:2479:LEU:O	2:I:2487:UNK:N	2.49	0.46
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.32	0.46
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.99	0.45
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.81	0.45
2:G:626:LEU:HD23	2:G:630:GLU:H	1.82	0.45
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.81	0.45
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.97	0.45
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.81	0.45
2:E:290:TYR:O	2:E:302:VAL:N	2.49	0.45
2:B:2868:SER:O	2:B:2872:GLN:N	2.47	0.45
2:G:290:TYR:O	2:G:302:VAL:N	2.49	0.45
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.81	0.45
2:E:119:SER:HA	2:E:146:CYS:HA	1.96	0.45
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.97	0.45
2:E:3552:UNK:O	2:E:3556:UNK:N	2.49	0.45
2:B:206:CYS:SG	2:B:207:SER:N	2.88	0.45
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.50	0.45
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.98	0.45
2:G:1707:LEU:O	2:G:1710:GLY:N	2.33	0.45
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.99	0.45
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:626:LEU:HD23	2:E:630:GLU:H	1.82	0.45
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.88	0.45
1:J:21:THR:HA	1:J:49:ARG:HA	1.99	0.45
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.99	0.45
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.98	0.45
2:E:1954:ARG:HE	2:E:2041:HIS:HD2	1.63	0.45
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.50	0.45
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.99	0.45
2:B:2874:MET:O	2:B:2878:LEU:N	2.44	0.45
2:B:4851:TYR:HD2	2:B:4920:PHE:HD1	1.62	0.45
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.82	0.45
2:I:1747:LEU:HD21	2:I:2041:HIS:HB2	1.97	0.45
2:I:3552:UNK:O	2:I:3556:UNK:N	2.50	0.45
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.81	0.45
2:B:626:LEU:HD23	2:B:630:GLU:H	1.82	0.45
2:B:2012:PHE:CG	2:B:2022:PRO:HD3	2.52	0.45
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.99	0.45
2:G:1747:LEU:HD21	2:G:2041:HIS:HB2	1.97	0.45
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.97	0.45
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.98	0.45
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.50	0.45
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.97	0.45
2:G:3552:UNK:O	2:G:3556:UNK:N	2.50	0.45
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.98	0.45
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.99	0.45
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.50	0.45
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.98	0.45
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.99	0.45
2:I:206:CYS:SG	2:I:207:SER:N	2.88	0.45
2:I:2029:GLN:O	2:I:2033:ASP:N	2.48	0.45
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.99	0.45
1:F:21:THR:HA	1:F:49:ARG:HA	1.99	0.45
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.46	0.45
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.82	0.45
2:B:3552:UNK:O	2:B:3556:UNK:N	2.50	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
2:G:2012:PHE:CG	2:G:2022:PRO:HD3	2.52	0.45
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.45
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.97	0.45
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.50	0.45
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.99	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.45
2:B:290:TYR:O	2:B:302:VAL:N	2.49	0.44
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.50	0.44
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.98	0.44
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.82	0.44
2:I:1954:ARG:HE	2:I:2041:HIS:HD2	1.63	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.50	0.44
2:E:2012:PHE:CG	2:E:2022:PRO:HD3	2.52	0.44
2:B:161:GLU:HG2	2:E:3984:ARG:HH12	1.82	0.44
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.44
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.50	0.44
2:G:1675:ALA:HB1	2:G:1676:LEU:HD13	1.99	0.44
2:G:1954:ARG:HE	2:G:2041:HIS:HD2	1.63	0.44
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.98	0.44
2:G:4976:GLU:O	2:G:4979:THR:OG1	2.29	0.44
2:I:290:TYR:O	2:I:302:VAL:N	2.49	0.44
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.46	0.44
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.50	0.44
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.50	0.44
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	2.00	0.44
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.81	0.44
2:E:4942:GLU:O	2:E:4946:GLN:N	2.47	0.44
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.00	0.44
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	2.00	0.44
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.81	0.44
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	2.00	0.44
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.83	0.44
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.00	0.44
2:I:2012:PHE:CG	2:I:2022:PRO:HD3	2.52	0.44
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.30	0.44
1:H:21:THR:HA	1:H:49:ARG:HA	1.99	0.44
2:B:1101:ARG:HH21	2:B:1115:LEU:H	1.65	0.44
2:B:1720:LEU:HD23	2:B:1721:GLU:HA	2.00	0.44
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.83	0.44
2:G:4823:LEU:HD23	2:E:4843:LEU:HD12	1.98	0.44
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.83	0.44
2:I:626:LEU:HD23	2:I:630:GLU:H	1.82	0.44
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.50	0.44
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.44
2:G:1720:LEU:HD23	2:G:1721:GLU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1675:ALA:HB1	2:I:1676:LEU:HD13	1.99	0.44
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.99	0.44
2:B:3361:UNK:O	2:B:3365:UNK:N	2.50	0.44
2:B:4044:MET:HA	2:B:4047:MET:HG2	2.00	0.44
2:I:548:VAL:HG12	2:I:564:LEU:HD22	2.00	0.44
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.50	0.44
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.82	0.44
2:E:1720:LEU:HD23	2:E:1721:GLU:HA	2.00	0.44
2:E:2479:LEU:O	2:E:2487:UNK:N	2.50	0.44
2:B:983:THR:O	2:B:987:ARG:N	2.49	0.44
2:B:3781:GLN:HA	2:B:3784:SER:HB3	2.00	0.44
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.83	0.44
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.00	0.44
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.88	0.44
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	2.00	0.44
2:E:1675:ALA:HB1	2:E:1676:LEU:HD13	1.99	0.44
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.38	0.44
2:B:164:ARG:N	2:B:167:ASP:OD2	2.43	0.44
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.50	0.44
2:B:719:LEU:HD22	2:B:735:GLN:HG2	2.00	0.44
2:B:794:GLY:H	2:B:798:GLY:HA3	1.83	0.44
2:B:2034:PHE:O	2:B:2038:LEU:N	2.51	0.44
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.98	0.44
2:B:4886:HIS:O	2:B:4890:GLY:N	2.44	0.44
2:G:1101:ARG:HH21	2:G:1115:LEU:H	1.65	0.44
2:G:4044:MET:HA	2:G:4047:MET:HG2	2.00	0.44
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.50	0.44
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.99	0.44
2:B:1865:MET:SD	2:B:1865:MET:N	2.91	0.44
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	1.99	0.44
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	2.00	0.44
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	2.00	0.44
2:G:2034:PHE:O	2:G:2038:LEU:N	2.51	0.44
2:I:1720:LEU:HD23	2:I:1721:GLU:HA	2.00	0.44
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.00	0.44
2:I:1737:PRO:HD3	2:I:1771:LEU:HD21	2.00	0.44
2:I:2034:PHE:O	2:I:2038:LEU:N	2.51	0.44
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.00	0.44
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.83	0.44
2:E:1865:MET:SD	2:E:1865:MET:N	2.91	0.44
2:G:1695:LEU:HB3	2:G:1810:LYS:HZ2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	2.00	0.43
2:G:2874:MET:O	2:G:2878:LEU:N	2.44	0.43
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	2.00	0.43
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.50	0.43
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.98	0.43
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.99	0.43
2:I:4976:GLU:O	2:I:4979:THR:OG1	2.29	0.43
2:E:548:VAL:HG12	2:E:564:LEU:HD22	2.00	0.43
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.50	0.43
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	1.99	0.43
2:E:4802:GLY:HA2	2:E:4808:PHE:HB2	2.00	0.43
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.82	0.43
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.83	0.43
2:B:1737:PRO:HD3	2:B:1771:LEU:HD21	2.00	0.43
2:B:2432:LEU:O	2:B:2436:CYS:N	2.50	0.43
2:G:1737:PRO:HD3	2:G:1771:LEU:HD21	2.00	0.43
2:G:3365:UNK:O	2:G:3369:UNK:N	2.51	0.43
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.99	0.43
2:E:195:PHE:HB3	2:E:196:MET:HG2	2.00	0.43
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.00	0.43
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.00	0.43
1:A:21:THR:HA	1:A:49:ARG:HA	1.99	0.43
2:B:195:PHE:HB3	2:B:196:MET:HG2	2.00	0.43
2:B:886:ARG:HB3	2:B:891:TRP:HB2	2.01	0.43
2:B:2029:GLN:O	2:B:2033:ASP:N	2.48	0.43
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.92	0.43
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.00	0.43
2:I:485:SER:O	2:I:489:ASN:N	2.38	0.43
2:I:4044:MET:HA	2:I:4047:MET:HG2	2.00	0.43
2:E:794:GLY:H	2:E:798:GLY:HA3	1.83	0.43
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.99	0.43
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.92	0.43
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.00	0.43
2:I:699:GLY:O	2:I:1647:CYS:N	2.50	0.43
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	2.00	0.43
2:E:54:ASN:O	2:E:58:VAL:N	2.46	0.43
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.01	0.43
2:B:2364:PHE:HD1	2:B:2429:LEU:HD21	1.83	0.43
2:B:4843:LEU:HD12	2:E:4823:LEU:HD23	2.01	0.43
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.00	0.43
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:134:ASP:OD1	2:I:134:ASP:N	2.52	0.43
2:I:195:PHE:HB3	2:I:196:MET:HG2	2.01	0.43
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.00	0.43
2:E:4044:MET:HA	2:E:4047:MET:HG2	2.00	0.43
2:E:4163:PHE:O	2:E:4167:ALA:N	2.45	0.43
2:B:548:VAL:HG12	2:B:564:LEU:HD22	2.00	0.43
2:B:1675:ALA:HB1	2:B:1676:LEU:HD13	1.99	0.43
2:B:1695:LEU:HB3	2:B:1810:LYS:HZ2	1.83	0.43
2:G:719:LEU:HD22	2:G:735:GLN:HG2	2.00	0.43
2:G:794:GLY:H	2:G:798:GLY:HA3	1.83	0.43
2:I:794:GLY:H	2:I:798:GLY:HA3	1.83	0.43
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	2.01	0.43
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.01	0.43
2:I:2364:PHE:HD1	2:I:2429:LEU:HD21	1.84	0.43
2:I:2432:LEU:O	2:I:2436:CYS:N	2.50	0.43
2:B:489:ASN:HA	2:B:492:ASP:HB2	2.00	0.43
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	2.00	0.43
2:I:489:ASN:HA	2:I:492:ASP:HB2	2.00	0.43
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	2.01	0.43
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	1.99	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	2.00	0.43
2:E:719:LEU:HD22	2:E:735:GLN:HG2	2.00	0.43
2:E:1101:ARG:HH21	2:E:1115:LEU:H	1.65	0.43
2:E:1817:GLU:O	2:E:1821:ASP:N	2.45	0.43
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.92	0.43
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.52	0.43
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.00	0.43
2:B:2587:UNK:O	2:B:2591:UNK:N	2.52	0.43
2:G:548:VAL:HG12	2:G:564:LEU:HD22	2.00	0.43
2:G:886:ARG:HB3	2:G:891:TRP:HB2	2.01	0.43
2:G:2029:GLN:O	2:G:2033:ASP:N	2.48	0.43
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.01	0.43
2:G:2364:PHE:HD1	2:G:2429:LEU:HD21	1.84	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.84	0.43
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.00	0.43
2:I:2587:UNK:O	2:I:2591:UNK:N	2.52	0.43
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.99	0.43
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.00	0.43
2:E:2587:UNK:O	2:E:2591:UNK:N	2.52	0.43
2:E:4558:ASN:OD1	2:E:4558:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.00	0.43
2:B:2479:LEU:O	2:B:2487:UNK:N	2.52	0.43
2:G:134:ASP:OD1	2:G:134:ASP:N	2.52	0.43
2:G:681:HIS:HE2	2:G:683:ARG:NE	2.17	0.43
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.49	0.43
2:I:1101:ARG:HH21	2:I:1115:LEU:H	1.65	0.43
2:I:1866:ILE:HG13	2:I:1926:LEU:HB3	2.01	0.43
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.00	0.43
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.82	0.43
2:E:681:HIS:HE2	2:E:683:ARG:NE	2.17	0.43
2:E:3781:GLN:HA	2:E:3784:SER:HB3	2.00	0.43
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.01	0.43
2:B:4138:ASP:O	2:B:4142:ASN:ND2	2.52	0.43
2:G:2215:LEU:HD23	2:G:2260:ASN:HB3	2.01	0.43
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	1.99	0.43
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.52	0.43
2:I:1865:MET:SD	2:I:1865:MET:N	2.91	0.43
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.84	0.43
2:E:699:GLY:O	2:E:1647:CYS:N	2.50	0.43
2:E:1737:PRO:HD3	2:E:1771:LEU:HD21	2.00	0.43
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.00	0.43
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.92	0.43
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.84	0.43
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.84	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.42
2:G:299:LEU:HD13	2:G:378:LEU:HG	2.01	0.42
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	2.01	0.42
2:I:719:LEU:HD22	2:I:735:GLN:HG2	2.00	0.42
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.92	0.42
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	2.01	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.42
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.01	0.42
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.52	0.42
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.30	0.42
2:G:195:PHE:HB3	2:G:196:MET:HG2	2.00	0.42
2:G:699:GLY:O	2:G:1647:CYS:N	2.50	0.42
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	2.01	0.42
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.84	0.42
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.52	0.42
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.52	0.42
2:E:2364:PHE:HD1	2:E:2429:LEU:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:681:HIS:HE2	2:B:683:ARG:NE	2.17	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.53	0.42
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.52	0.42
2:G:1865:MET:SD	2:G:1865:MET:N	2.91	0.42
2:G:2479:LEU:O	2:G:2487:UNK:N	2.52	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.42
2:G:3984:ARG:HH22	2:E:161:GLU:HA	1.83	0.42
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.99	0.42
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.84	0.42
2:I:2215:LEU:HD23	2:I:2260:ASN:HB3	2.01	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.52	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:E:1695:LEU:HB3	2:E:1810:LYS:HZ2	1.84	0.42
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.52	0.42
2:E:4138:ASP:O	2:E:4142:ASN:ND2	2.52	0.42
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.42
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	2.01	0.42
2:B:1641:ILE:HA	2:B:1642:PRO:HD3	1.89	0.42
2:B:3365:UNK:O	2:B:3369:UNK:N	2.52	0.42
2:B:4942:GLU:O	2:B:4946:GLN:N	2.47	0.42
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.84	0.42
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.52	0.42
2:G:4138:ASP:O	2:G:4142:ASN:ND2	2.52	0.42
2:G:4571:PHE:O	2:G:4575:PHE:N	2.53	0.42
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.00	0.42
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.52	0.42
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.92	0.42
2:I:4571:PHE:O	2:I:4575:PHE:N	2.53	0.42
2:E:489:ASN:HA	2:E:492:ASP:HB2	2.00	0.42
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.84	0.42
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.01	0.42
2:B:54:ASN:O	2:B:58:VAL:N	2.46	0.42
2:B:299:LEU:HD13	2:B:378:LEU:HG	2.01	0.42
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.37	0.42
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.00	0.42
2:G:1240:LYS:HB3	2:G:1604:SER:H	1.84	0.42
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.92	0.42
2:I:1817:GLU:O	2:I:1821:ASP:N	2.45	0.42
2:I:2024:PRO:O	2:I:2028:ARG:NE	2.45	0.42
2:I:4942:GLU:O	2:I:4946:GLN:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:LYS:HE3	2:E:634:GLN:HB3	2.02	0.42
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.52	0.42
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.00	0.42
2:G:4697:VAL:O	2:G:4701:TRP:N	2.52	0.42
2:I:886:ARG:HB3	2:I:891:TRP:HB2	2.01	0.42
2:I:2902:HIS:HE1	2:I:2904:LEU:HD12	1.85	0.42
2:E:913:LEU:O	2:E:918:ARG:NH2	2.53	0.42
2:E:983:THR:O	2:E:987:ARG:N	2.49	0.42
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	2.00	0.42
2:B:1866:ILE:HG13	2:B:1926:LEU:HB3	2.01	0.42
2:B:2902:HIS:HE1	2:B:2904:LEU:HD12	1.85	0.42
2:B:4236:SER:HG	2:B:4675:LYS:HZ1	1.61	0.42
2:G:913:LEU:O	2:G:918:ARG:NH2	2.53	0.42
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.46	0.42
2:G:1866:ILE:HG13	2:G:1926:LEU:HB3	2.01	0.42
2:I:1641:ILE:HA	2:I:1642:PRO:HD3	1.90	0.42
2:I:4138:ASP:O	2:I:4142:ASN:ND2	2.52	0.42
2:I:4158:PRO:HA	2:I:4161:ARG:HB2	2.01	0.42
2:E:134:ASP:OD1	2:E:134:ASP:N	2.52	0.42
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	2.02	0.42
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.52	0.42
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.84	0.42
2:G:489:ASN:HA	2:G:492:ASP:HB2	2.00	0.42
2:I:756:SER:HB3	2:I:767:VAL:HG22	2.01	0.42
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.00	0.42
2:E:395:GLN:HG3	2:E:397:GLU:H	1.85	0.42
2:B:4558:ASN:OD1	2:B:4558:ASN:N	2.52	0.42
2:G:2587:UNK:O	2:G:2591:UNK:N	2.52	0.42
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.84	0.42
2:I:681:HIS:HE2	2:I:683:ARG:NE	2.17	0.42
2:I:913:LEU:O	2:I:918:ARG:NH2	2.53	0.42
2:I:2874:MET:O	2:I:2878:LEU:N	2.44	0.42
2:I:3771:HIS:O	2:I:3774:GLY:N	2.43	0.42
2:E:299:LEU:HD13	2:E:378:LEU:HG	2.01	0.42
2:B:913:LEU:O	2:B:918:ARG:NH2	2.53	0.42
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.92	0.42
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.85	0.42
2:I:299:LEU:HD13	2:I:378:LEU:HG	2.01	0.42
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.85	0.42
2:I:4181:ILE:HD11	2:I:4988:TYR:CD1	2.55	0.42
2:E:756:SER:HB3	2:E:767:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:953:THR:HB	2:E:969:PRO:HD2	2.02	0.42
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	2.01	0.42
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.85	0.42
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.45	0.42
2:E:4158:PRO:HA	2:E:4161:ARG:HB2	2.01	0.42
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	2.01	0.41
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.85	0.41
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.88	0.41
2:G:395:GLN:HG3	2:G:397:GLU:H	1.85	0.41
2:G:983:THR:O	2:G:987:ARG:N	2.50	0.41
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	2.02	0.41
2:G:4569:LEU:HD11	2:G:4646:LEU:HD22	2.02	0.41
2:I:1240:LYS:HB3	2:I:1604:SER:H	1.84	0.41
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	2.02	0.41
2:I:4138:ASP:N	2:I:4138:ASP:OD1	2.53	0.41
2:I:4886:HIS:O	2:I:4890:GLY:N	2.44	0.41
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.18	0.41
2:E:1866:ILE:HG13	2:E:1926:LEU:HB3	2.01	0.41
2:E:2215:LEU:HD23	2:E:2260:ASN:HB3	2.01	0.41
2:E:4181:ILE:HD11	2:E:4988:TYR:CD1	2.55	0.41
1:F:25:HIS:HB3	1:F:40:ARG:HD3	2.03	0.41
2:B:756:SER:HB3	2:B:767:VAL:HG22	2.01	0.41
2:B:1240:LYS:HB3	2:B:1604:SER:H	1.85	0.41
2:B:2215:LEU:HD23	2:B:2260:ASN:HB3	2.01	0.41
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.84	0.41
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	2.02	0.41
2:G:4735:GLU:HA	2:G:4738:ALA:HB3	2.02	0.41
2:I:4228:ALA:O	2:I:4232:GLU:N	2.52	0.41
2:I:5000:GLU:HA	2:I:5003:HIS:CD2	2.55	0.41
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	2.01	0.41
2:B:395:GLN:HG3	2:B:397:GLU:H	1.85	0.41
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.18	0.41
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.18	0.41
2:G:2024:PRO:O	2:G:2028:ARG:NE	2.45	0.41
2:G:4158:PRO:HA	2:G:4161:ARG:HB2	2.01	0.41
2:G:4558:ASN:OD1	2:G:4558:ASN:N	2.52	0.41
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.24	0.41
2:I:395:GLN:HG3	2:I:397:GLU:H	1.85	0.41
2:I:710:ASP:OD1	2:I:710:ASP:N	2.54	0.41
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	2.02	0.41
2:E:4228:ALA:O	2:E:4232:GLU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.84	0.41
2:B:1707:LEU:O	2:B:1710:GLY:N	2.33	0.41
2:G:54:ASN:O	2:G:58:VAL:N	2.46	0.41
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.41
2:I:953:THR:HB	2:I:969:PRO:HD2	2.02	0.41
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	2.01	0.41
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.49	0.41
2:E:4735:GLU:HA	2:E:4738:ALA:HB3	2.02	0.41
2:B:710:ASP:OD1	2:B:710:ASP:N	2.54	0.41
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.00	0.41
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	2.02	0.41
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.02	0.41
2:B:5000:GLU:HA	2:B:5003:HIS:CD2	2.56	0.41
2:G:205:ILE:HD12	2:G:205:ILE:HA	1.95	0.41
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.02	0.41
2:G:2959:UNK:O	2:G:2963:UNK:N	2.54	0.41
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	2.01	0.41
2:I:4558:ASN:OD1	2:I:4558:ASN:N	2.52	0.41
1:F:23:VAL:H	1:F:105:ASN:HB3	1.86	0.41
2:B:485:SER:HA	2:B:488:LEU:HB2	2.03	0.41
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.03	0.41
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	2.02	0.41
2:B:2467:VAL:HA	2:B:2470:ILE:HD12	2.03	0.41
2:B:2959:UNK:O	2:B:2963:UNK:N	2.53	0.41
2:B:4928:LEU:HD13	2:B:4928:LEU:HA	1.92	0.41
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	2.02	0.41
2:I:983:THR:O	2:I:987:ARG:N	2.50	0.41
2:E:710:ASP:OD1	2:E:710:ASP:N	2.54	0.41
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	2.01	0.41
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.02	0.41
2:E:4569:LEU:HD11	2:E:4646:LEU:HD22	2.02	0.41
1:A:25:HIS:HB3	1:A:40:ARG:HD3	2.02	0.41
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.86	0.41
2:B:4181:ILE:HD11	2:B:4988:TYR:CD1	2.55	0.41
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.38	0.41
2:G:4138:ASP:N	2:G:4138:ASP:OD1	2.53	0.41
2:G:4228:ALA:O	2:G:4232:GLU:N	2.52	0.41
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.03	0.41
2:I:2517:UNK:O	2:I:2521:UNK:N	2.53	0.41
2:I:3773:ARG:HG3	2:I:3815:LYS:HZ3	1.85	0.41
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2467:VAL:HA	2:E:2470:ILE:HD12	2.03	0.41
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.03	0.41
2:B:4158:PRO:HA	2:B:4161:ARG:HB2	2.01	0.41
2:B:4228:ALA:O	2:B:4232:GLU:N	2.52	0.41
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	2.01	0.41
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.03	0.41
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.84	0.41
2:G:2902:HIS:HE1	2:G:2904:LEU:HD12	1.85	0.41
2:G:4181:ILE:HD11	2:G:4988:TYR:CD1	2.55	0.41
1:F:23:VAL:HB	1:F:105:ASN:HA	2.03	0.41
1:A:23:VAL:H	1:A:105:ASN:HB3	1.86	0.41
1:H:25:HIS:HB3	1:H:40:ARG:HD3	2.03	0.41
1:J:23:VAL:H	1:J:105:ASN:HB3	1.86	0.41
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	2.02	0.41
2:B:4569:LEU:HD11	2:B:4646:LEU:HD22	2.02	0.41
2:G:756:SER:HB3	2:G:767:VAL:HG22	2.01	0.41
2:G:953:THR:HB	2:G:969:PRO:HD2	2.02	0.41
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.03	0.41
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.41
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	2.02	0.41
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.03	0.41
2:G:5000:GLU:HA	2:G:5003:HIS:CD2	2.56	0.41
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.18	0.41
2:I:485:SER:HA	2:I:488:LEU:HB2	2.03	0.41
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.42	0.41
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.03	0.41
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.46	0.41
2:E:1240:LYS:HB3	2:E:1604:SER:H	1.84	0.41
2:E:2432:LEU:O	2:E:2436:CYS:N	2.50	0.41
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.03	0.41
2:E:5000:GLU:HA	2:E:5003:HIS:CD2	2.56	0.41
1:A:23:VAL:HB	1:A:105:ASN:HA	2.03	0.41
2:B:953:THR:HB	2:B:969:PRO:HD2	2.02	0.41
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.42	0.41
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.32	0.41
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.86	0.41
2:B:4837:LEU:HD22	2:B:4936:ILE:HD11	2.02	0.41
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.86	0.41
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	2.02	0.41
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.03	0.41
2:I:4837:LEU:HD22	2:I:4936:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.86	0.41
2:E:2365:GLY:HA3	2:E:2426:TYR:HE1	1.86	0.41
2:B:699:GLY:O	2:B:1647:CYS:N	2.50	0.40
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.03	0.40
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	2.02	0.40
2:B:4735:GLU:HA	2:B:4738:ALA:HB3	2.02	0.40
2:G:485:SER:O	2:G:489:ASN:N	2.38	0.40
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.02	0.40
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.86	0.40
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.86	0.40
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	2.02	0.40
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.86	0.40
2:I:1592:PRO:HA	2:I:1593:PRO:HD3	1.96	0.40
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.03	0.40
2:I:2467:VAL:HA	2:I:2470:ILE:HD12	2.03	0.40
2:I:2959:UNK:O	2:I:2963:UNK:N	2.54	0.40
2:I:4569:LEU:HD11	2:I:4646:LEU:HD22	2.02	0.40
2:I:4735:GLU:HA	2:I:4738:ALA:HB3	2.02	0.40
2:E:485:SER:HA	2:E:488:LEU:HB2	2.03	0.40
2:E:2034:PHE:O	2:E:2038:LEU:N	2.51	0.40
2:G:2467:VAL:HA	2:G:2470:ILE:HD12	2.03	0.40
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.03	0.40
2:E:1739:THR:H	2:E:1742:THR:HB	1.86	0.40
2:E:2517:UNK:O	2:E:2521:UNK:N	2.54	0.40
2:E:2902:HIS:HE1	2:E:2904:LEU:HD12	1.85	0.40
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.86	0.40
1:A:44:LYS:HA	1:A:45:PRO:HD3	1.89	0.40
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.42	0.40
2:B:1817:GLU:O	2:B:1821:ASP:N	2.45	0.40
2:B:2365:GLY:HA3	2:B:2426:TYR:HE1	1.87	0.40
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.86	0.40
2:B:3915:ILE:O	2:B:3919:THR:N	2.52	0.40
2:G:1641:ILE:HA	2:G:1642:PRO:HD3	1.89	0.40
2:G:3915:ILE:O	2:G:3919:THR:N	2.52	0.40
2:G:4886:HIS:O	2:G:4890:GLY:N	2.44	0.40
2:I:540:PHE:HD2	2:I:567:VAL:HG11	1.87	0.40
2:I:1739:THR:H	2:I:1742:THR:HB	1.87	0.40
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.02	0.40
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.86	0.40
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	2.03	0.40
2:E:4837:LEU:HD22	2:E:4936:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.86	0.40
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.86	0.40
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.03	0.40
2:B:3940:LYS:O	2:B:4002:LYS:NZ	2.42	0.40
2:B:4822:THR:O	2:B:4825:THR:OG1	2.33	0.40
2:G:540:PHE:HD2	2:G:567:VAL:HG11	1.87	0.40
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.86	0.40
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	2.02	0.40
2:E:551:LEU:HD21	2:E:589:LEU:HD13	2.03	0.40
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.04	0.40
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.86	0.40
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.53	0.40
2:B:4571:PHE:O	2:B:4575:PHE:N	2.53	0.40
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.30	0.40
2:I:1092:PHE:N	2:I:1149:VAL:O	2.43	0.40
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.39	0.40
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.86	0.40
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.49	0.40
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.57	0.40
2:E:4571:PHE:O	2:E:4575:PHE:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	3235/4416 (73%)	2886 (89%)	345 (11%)	4 (0%)	51	85
2	E	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	51	85
2	G	3235/4416 (73%)	2889 (89%)	341 (10%)	5 (0%)	47	81
2	I	3235/4416 (73%)	2888 (89%)	342 (11%)	5 (0%)	47	81
All	All	13360/18096 (74%)	11935 (89%)	1407 (10%)	18 (0%)	54	85

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	4641	PRO
2	G	1708	ARG
2	G	4641	PRO
2	I	1708	ARG
2	I	4641	PRO
2	E	1708	ARG
2	E	4641	PRO
2	B	1840	PRO
2	B	1932	PRO
2	G	1840	PRO
2	G	1932	PRO
2	I	1840	PRO
2	I	1932	PRO
2	E	1840	PRO
2	E	1932	PRO
2	G	4640	GLU
2	I	4640	GLU

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

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

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

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	719	LEU
2	B	978	THR
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
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	4180	ARG
2	B	4201	ASN
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	719	LEU
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG

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Mol	Chain	Res	Type
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	4180	ARG
2	G	4201	ASN
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	719	LEU
2	I	978	THR
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
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	4180	ARG
2	I	4201	ASN
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	719	LEU
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN

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Mol	Chain	Res	Type
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4180	ARG
2	E	4201	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	151	HIS
2	B	273	HIS
2	B	379	HIS
2	B	395	GLN
2	B	479	GLN
2	B	520	ASN
2	B	582	HIS
2	B	725	HIS
2	B	921	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1952	GLN
2	B	1972	ASN
2	B	2041	HIS
2	B	2127	GLN
2	B	2291	GLN
2	B	3781	GLN
2	B	3809	ASN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3976	ASN
2	B	4034	ASN

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Mol	Chain	Res	Type
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4806	ASN
2	B	5003	HIS
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	151	HIS
2	G	273	HIS
2	G	379	HIS
2	G	395	GLN
2	G	479	GLN
2	G	520	ASN
2	G	582	HIS
2	G	725	HIS
2	G	921	ASN
2	G	1598	GLN
2	G	1679	ASN
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1972	ASN
2	G	2041	HIS
2	G	2127	GLN
2	G	2291	GLN
2	G	3781	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4142	ASN
2	G	4806	ASN
2	G	5003	HIS
2	I	57	ASN
2	I	111	HIS

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Mol	Chain	Res	Type
2	I	113	HIS
2	I	151	HIS
2	I	273	HIS
2	I	379	HIS
2	I	395	GLN
2	I	479	GLN
2	I	520	ASN
2	I	582	HIS
2	I	725	HIS
2	I	921	ASN
2	I	1598	GLN
2	I	1679	ASN
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2041	HIS
2	I	2127	GLN
2	I	2291	GLN
2	I	3781	GLN
2	I	3809	ASN
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	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4806	ASN
2	I	5003	HIS
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	151	HIS
2	E	273	HIS
2	E	379	HIS
2	E	395	GLN
2	E	479	GLN
2	E	520	ASN
2	E	582	HIS
2	E	725	HIS

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Mol	Chain	Res	Type
2	E	921	ASN
2	E	1598	GLN
2	E	1679	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1972	ASN
2	E	2041	HIS
2	E	2127	GLN
2	E	2291	GLN
2	E	3781	GLN
2	E	3809	ASN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3976	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4806	ASN
2	E	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 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	E	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.63	5 (16%)
3	ATP	B	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.64	5 (16%)
4	CFF	I	5102	-	8,15,15	2.54	3 (37%)	8,23,23	1.26	1 (12%)
3	ATP	I	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.64	5 (16%)
3	ATP	G	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.64	5 (16%)
4	CFF	B	5102	-	8,15,15	2.53	3 (37%)	8,23,23	1.26	1 (12%)
4	CFF	E	5102	-	8,15,15	2.55	3 (37%)	8,23,23	1.24	1 (12%)
4	CFF	G	5102	-	8,15,15	2.53	3 (37%)	8,23,23	1.25	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	E	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	B	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	G	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C5-C4	-4.60	1.33	1.39
4	B	5102	CFF	C5-C4	-4.57	1.33	1.39
4	I	5102	CFF	C5-C4	-4.55	1.33	1.39
4	G	5102	CFF	C5-C4	-4.54	1.33	1.39
4	G	5102	CFF	C6-N1	-4.23	1.32	1.38
4	I	5102	CFF	C6-N1	-4.23	1.32	1.38
4	E	5102	CFF	C6-N1	-4.21	1.32	1.38
4	B	5102	CFF	C6-N1	-4.18	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5102	CFF	O13-C6	-2.36	1.18	1.24
4	E	5102	CFF	O13-C6	-2.35	1.18	1.24
3	I	5101	ATP	C5-C4	2.34	1.47	1.40
4	B	5102	CFF	O13-C6	-2.33	1.18	1.24
3	B	5101	ATP	C5-C4	2.32	1.47	1.40
4	I	5102	CFF	O13-C6	-2.31	1.18	1.24
3	E	5101	ATP	C5-C4	2.30	1.47	1.40
3	G	5101	ATP	C5-C4	2.30	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5101	ATP	PB-O3B-PG	-3.66	120.26	132.83
3	E	5101	ATP	PB-O3B-PG	-3.66	120.27	132.83
3	G	5101	ATP	PB-O3B-PG	-3.64	120.32	132.83
3	B	5101	ATP	PB-O3B-PG	-3.63	120.36	132.83
3	I	5101	ATP	PA-O3A-PB	-3.50	120.80	132.83
3	G	5101	ATP	PA-O3A-PB	-3.50	120.82	132.83
3	B	5101	ATP	PA-O3A-PB	-3.49	120.84	132.83
3	E	5101	ATP	PA-O3A-PB	-3.49	120.85	132.83
3	E	5101	ATP	C3'-C2'-C1'	3.49	106.23	100.98
3	G	5101	ATP	C3'-C2'-C1'	3.46	106.19	100.98
3	I	5101	ATP	C3'-C2'-C1'	3.46	106.19	100.98
3	B	5101	ATP	C3'-C2'-C1'	3.44	106.16	100.98
3	G	5101	ATP	N3-C2-N1	-3.28	123.56	128.68
3	B	5101	ATP	N3-C2-N1	-3.25	123.60	128.68
3	I	5101	ATP	N3-C2-N1	-3.24	123.61	128.68
3	E	5101	ATP	N3-C2-N1	-3.18	123.70	128.68
4	B	5102	CFF	C14-N7-C8	-2.83	111.82	125.43
4	G	5102	CFF	C14-N7-C8	-2.81	111.90	125.43
4	I	5102	CFF	C14-N7-C8	-2.81	111.91	125.43
4	E	5102	CFF	C14-N7-C8	-2.81	111.93	125.43
3	I	5101	ATP	C4-C5-N7	-2.69	106.60	109.40
3	B	5101	ATP	C4-C5-N7	-2.68	106.60	109.40
3	E	5101	ATP	C4-C5-N7	-2.65	106.64	109.40
3	G	5101	ATP	C4-C5-N7	-2.62	106.67	109.40

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O2A

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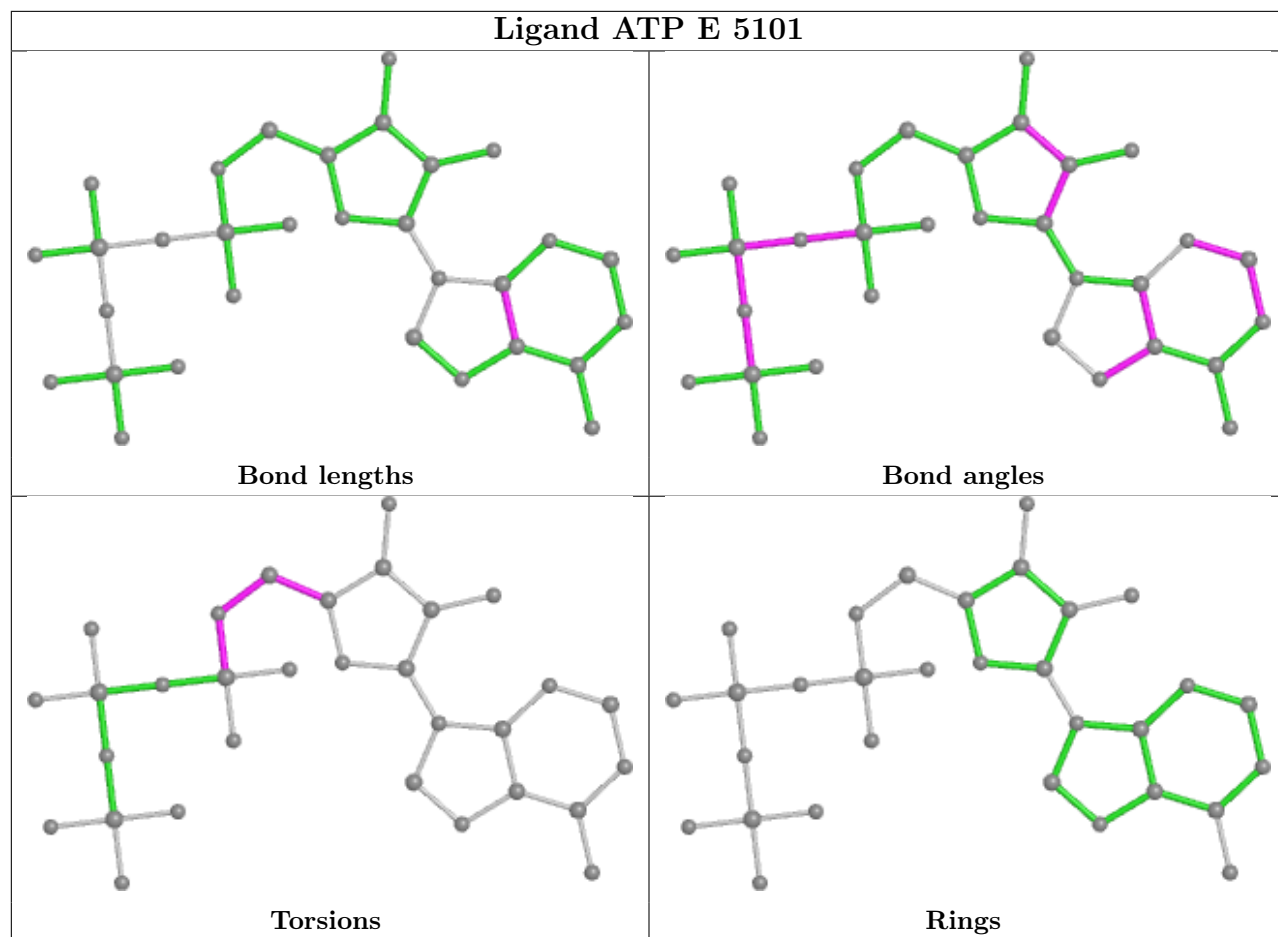
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O2A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O2A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C4'-C5'-O5'-PA
3	I	5101	ATP	C4'-C5'-O5'-PA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

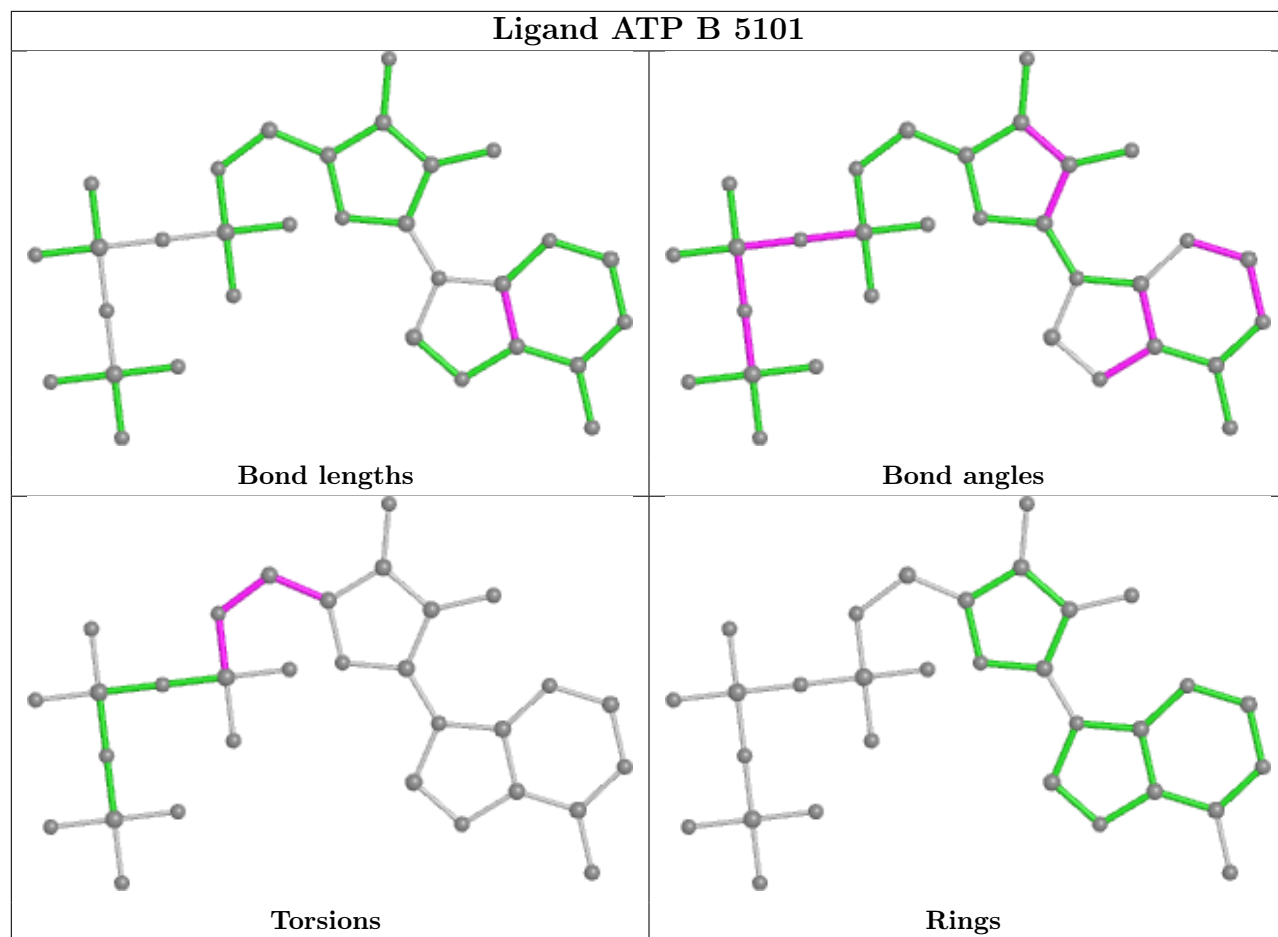
There are no ring outliers.

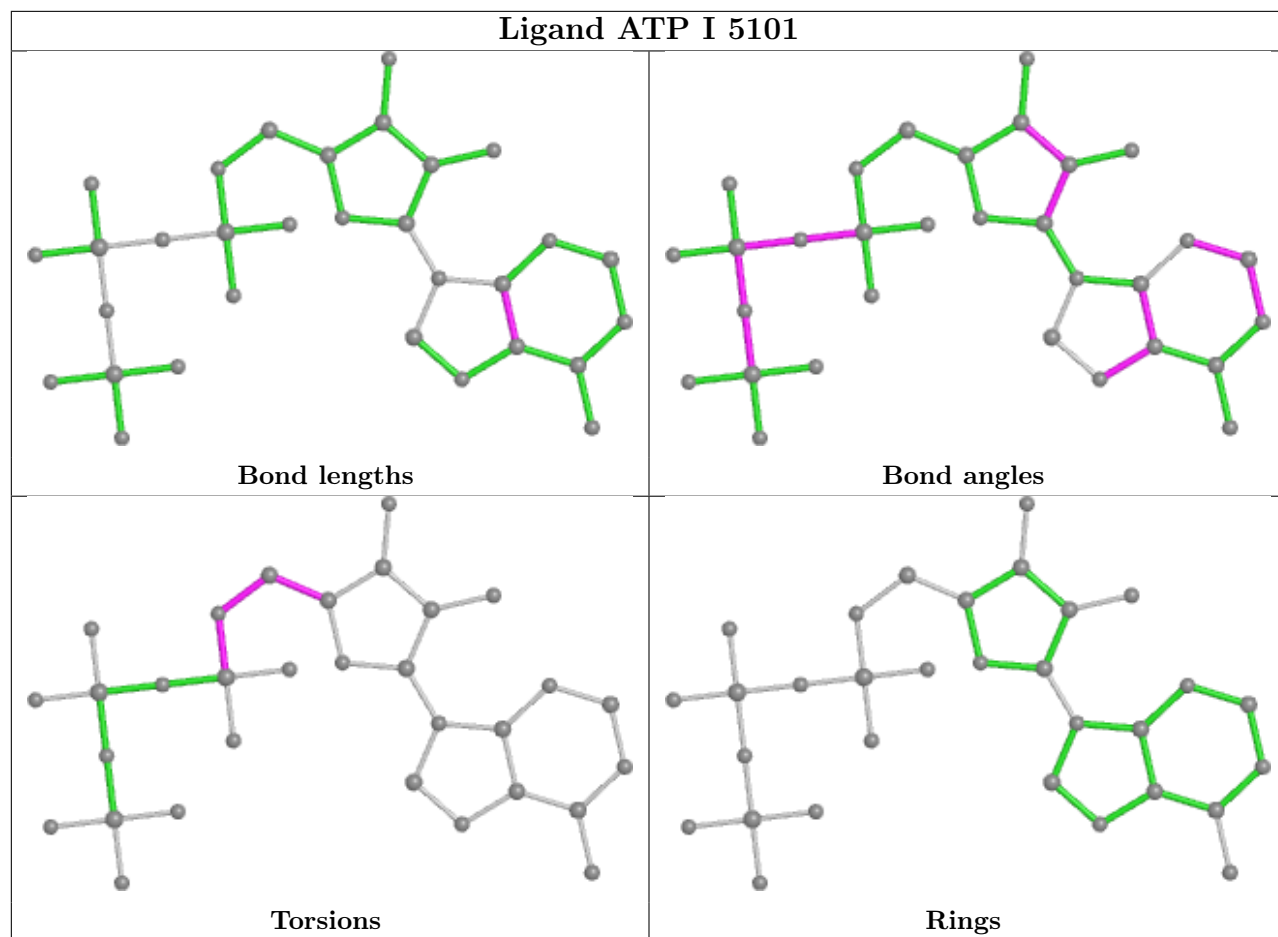
4 monomers are involved in 4 short contacts:

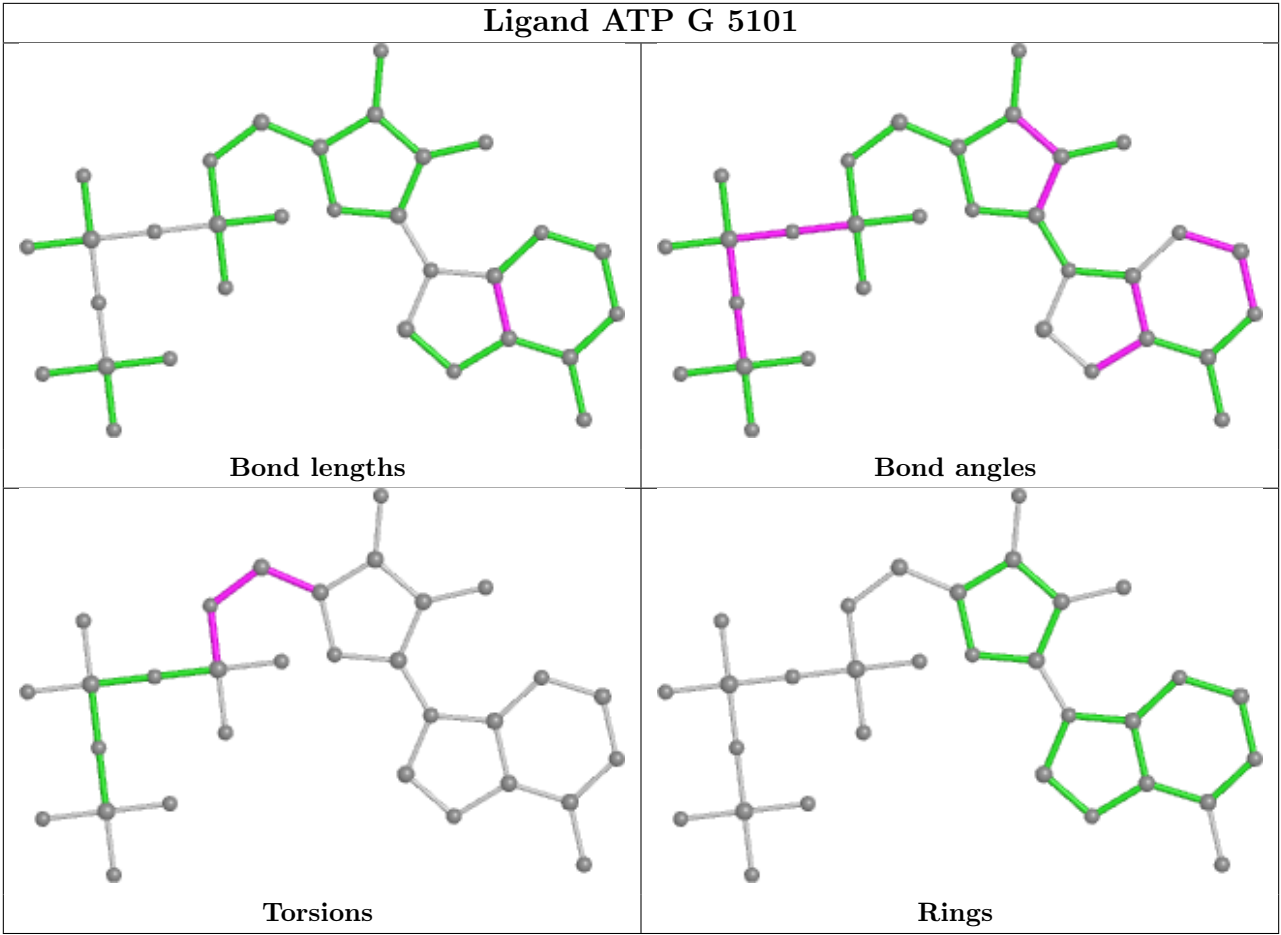
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	1	0
3	B	5101	ATP	1	0
3	I	5101	ATP	1	0
3	G	5101	ATP	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	G	14
2	I	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.32
1	G	4345:UNK	C	4540:PHE	N	73.24

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	73.23
1	E	4345:UNK	C	4540:PHE	N	73.22
1	E	3613:UNK	C	3639:THR	N	45.34
1	B	3613:UNK	C	3639:THR	N	45.33
1	G	3613:UNK	C	3639:THR	N	45.33
1	I	3613:UNK	C	3639:THR	N	45.32
1	B	4253:GLU	C	4320:UNK	N	28.10
1	G	4253:GLU	C	4320:UNK	N	28.05
1	E	4253:GLU	C	4320:UNK	N	28.05
1	I	4253:GLU	C	4320:UNK	N	28.04
1	B	3163:UNK	C	3170:UNK	N	16.08
1	G	3163:UNK	C	3170:UNK	N	16.07
1	I	3163:UNK	C	3170:UNK	N	16.06
1	E	3163:UNK	C	3170:UNK	N	16.06
1	B	3063:UNK	C	3134:UNK	N	14.99
1	G	3063:UNK	C	3134:UNK	N	14.99
1	I	3063:UNK	C	3134:UNK	N	14.99
1	E	3063:UNK	C	3134:UNK	N	14.98
1	I	3468:UNK	C	3511:UNK	N	14.52
1	E	3468:UNK	C	3511:UNK	N	14.52
1	G	3468:UNK	C	3511:UNK	N	14.49
1	B	3468:UNK	C	3511:UNK	N	14.46
1	I	2703:UNK	C	2734:ASN	N	13.80
1	E	2703:UNK	C	2734:ASN	N	13.79
1	G	2703:UNK	C	2734:ASN	N	13.75
1	B	2703:UNK	C	2734:ASN	N	13.73
1	I	3236:UNK	C	3241:UNK	N	12.95
1	E	3236:UNK	C	3241:UNK	N	12.95
1	G	3236:UNK	C	3241:UNK	N	12.92
1	B	3236:UNK	C	3241:UNK	N	12.90
1	E	1564:UNK	C	1573:MET	N	12.63
1	I	1564:UNK	C	1573:MET	N	12.60
1	G	1564:UNK	C	1573:MET	N	12.57
1	B	1564:UNK	C	1573:MET	N	12.51
1	I	2976:UNK	C	2995:UNK	N	12.40
1	E	2976:UNK	C	2995:UNK	N	12.40
1	G	2976:UNK	C	2995:UNK	N	12.39
1	B	2976:UNK	C	2995:UNK	N	12.37
1	B	3254:UNK	C	3261:UNK	N	8.55
1	G	3254:UNK	C	3261:UNK	N	8.53
1	I	3254:UNK	C	3261:UNK	N	8.52
1	E	3254:UNK	C	3261:UNK	N	8.52

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	6.03
1	I	1297:UNK	C	1430:UNK	N	6.03
1	G	1297:UNK	C	1430:UNK	N	6.02
1	E	1297:UNK	C	1430:UNK	N	5.99
1	E	2939:ARG	C	2942:UNK	N	3.40
1	G	2939:ARG	C	2942:UNK	N	3.35
1	I	2939:ARG	C	2942:UNK	N	3.35
1	B	2939:ARG	C	2942:UNK	N	3.33
1	B	2479:LEU	C	2487:UNK	N	3.32
1	G	2479:LEU	C	2487:UNK	N	3.32
1	I	2479:LEU	C	2487:UNK	N	3.30
1	E	2479:LEU	C	2487:UNK	N	3.30

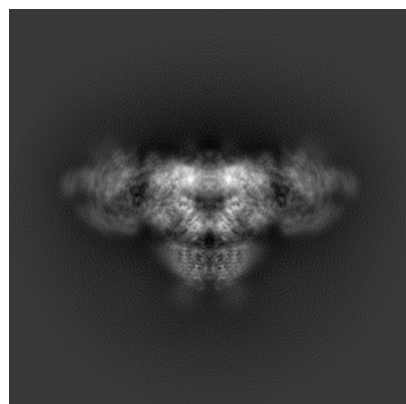
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8378. These allow visual inspection of the internal detail of the map and identification of artifacts.

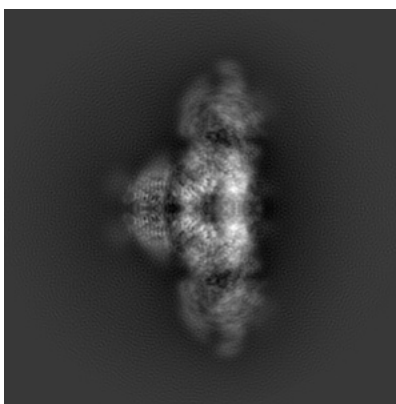
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

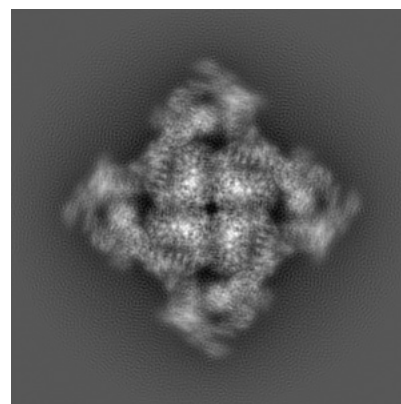
6.1.1 Primary map



X

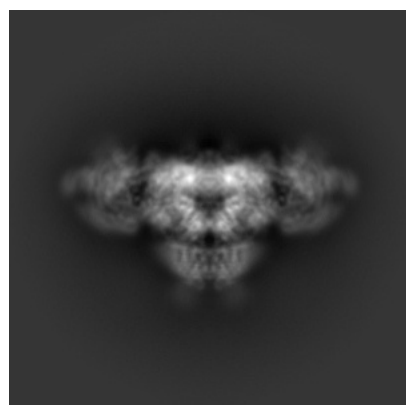


Y

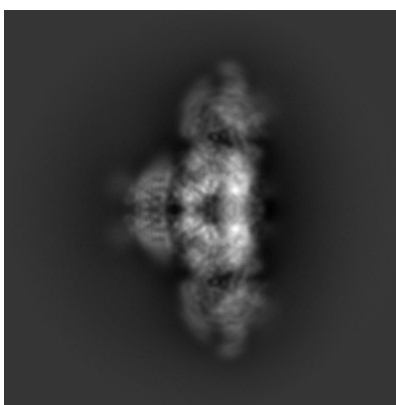


Z

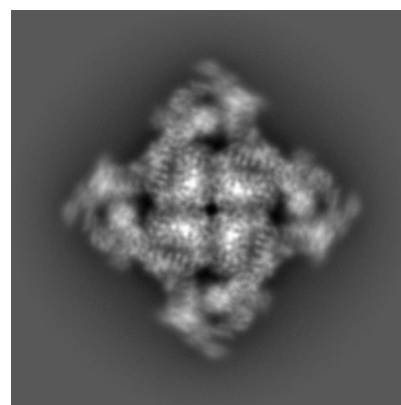
6.1.2 Raw map



X



Y

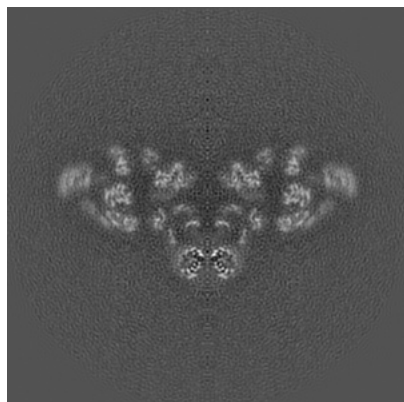


Z

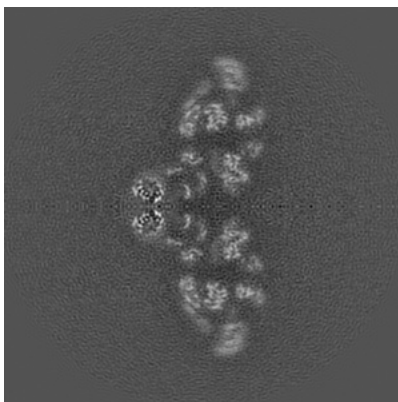
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

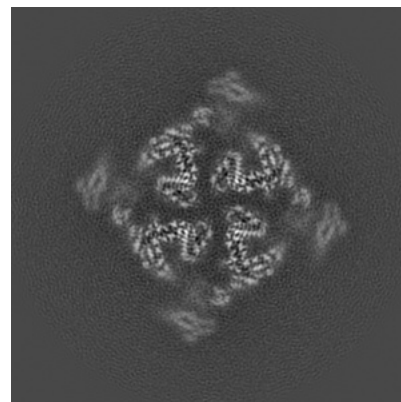
6.2.1 Primary map



X Index: 200

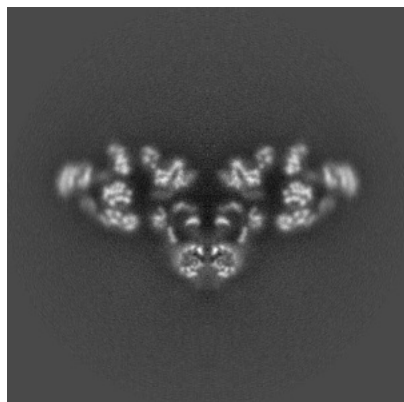


Y Index: 200

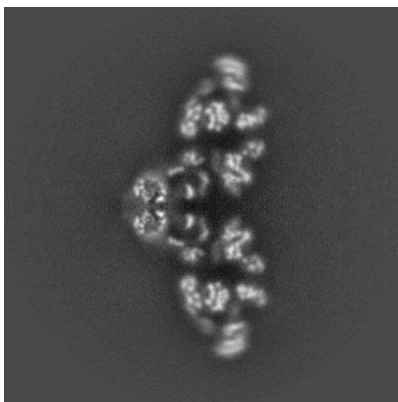


Z Index: 200

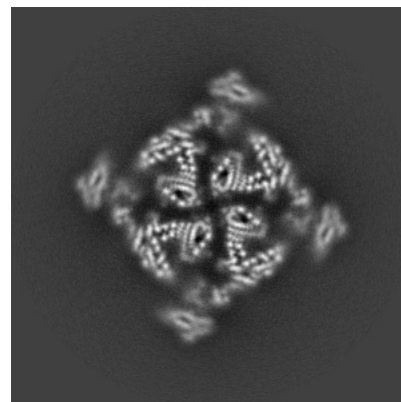
6.2.2 Raw map



X Index: 200



Y Index: 200

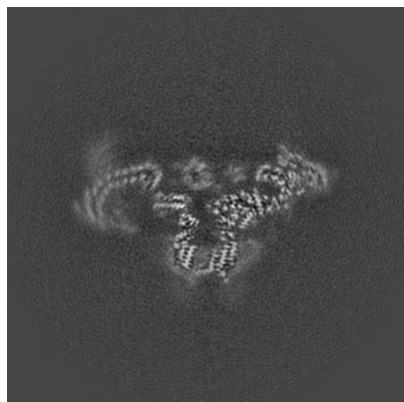


Z Index: 200

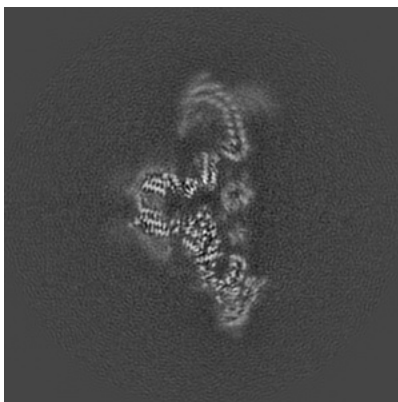
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

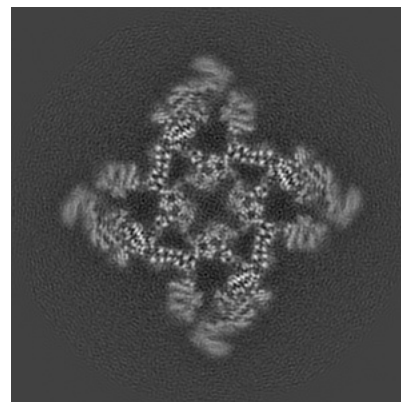
6.3.1 Primary map



X Index: 175

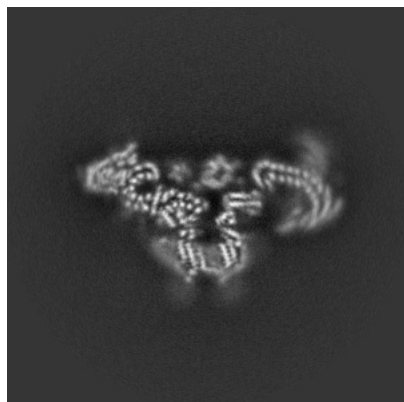


Y Index: 175

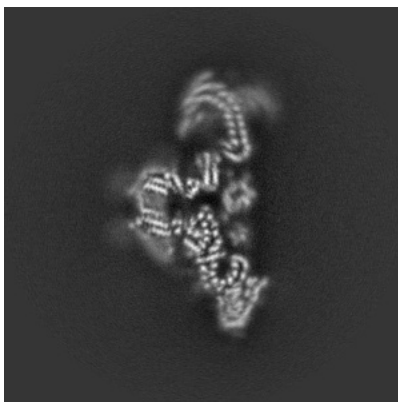


Z Index: 225

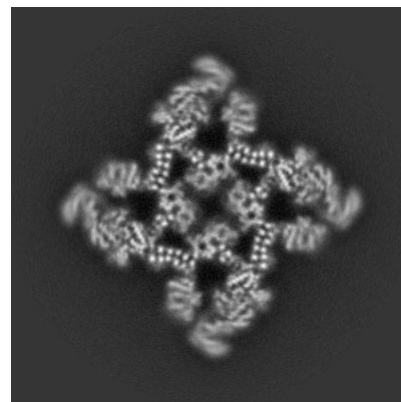
6.3.2 Raw map



X Index: 225



Y Index: 175

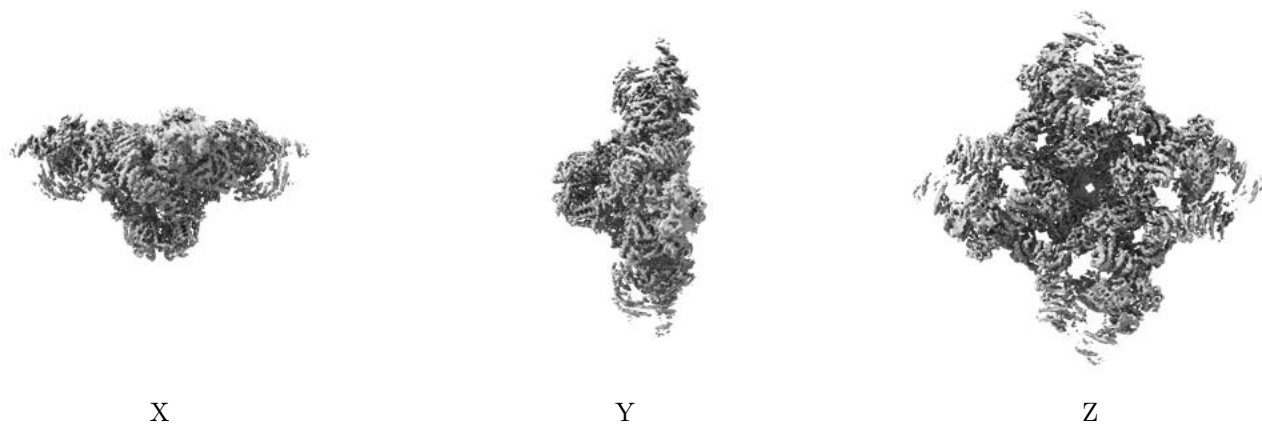


Z Index: 227

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

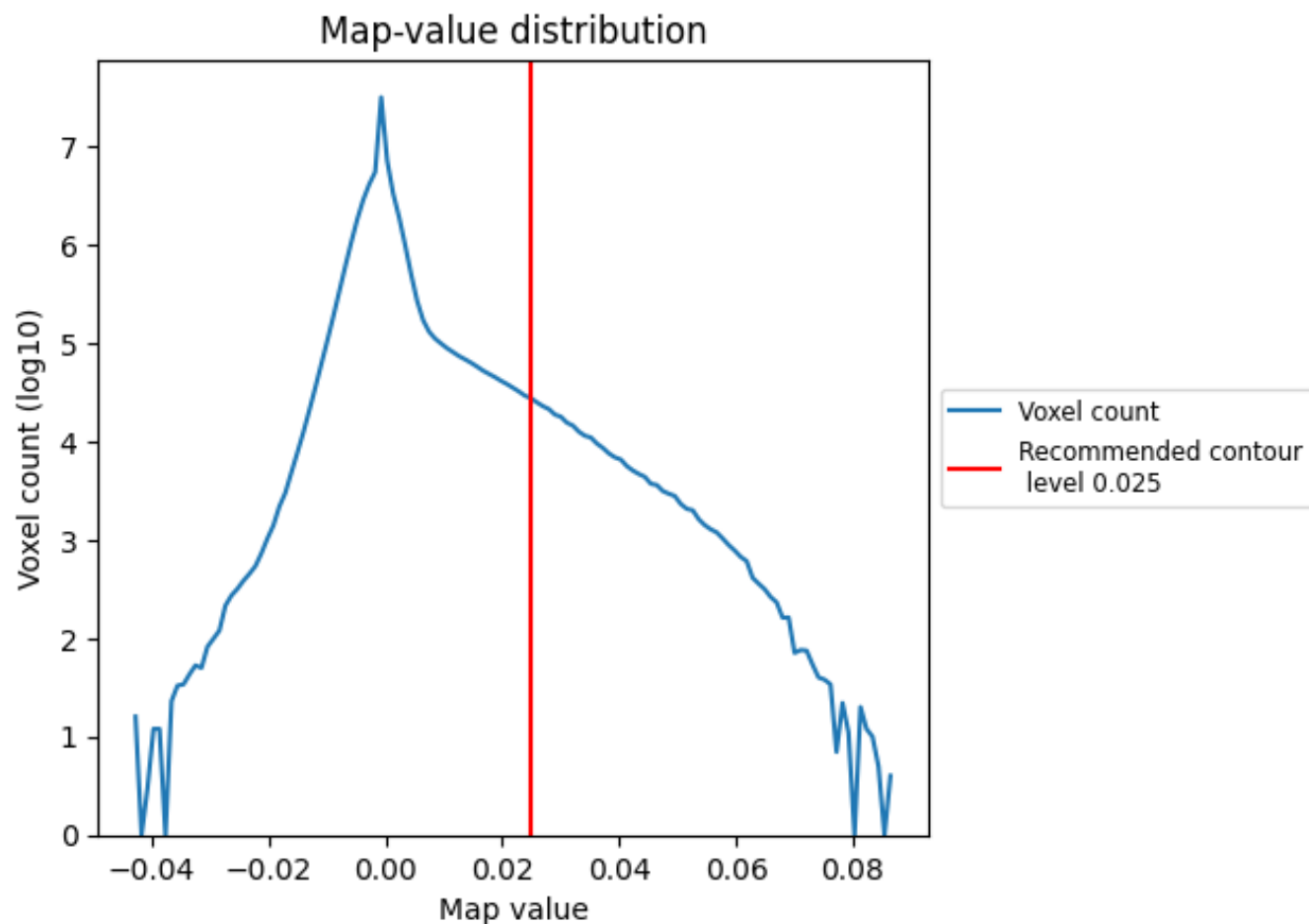
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

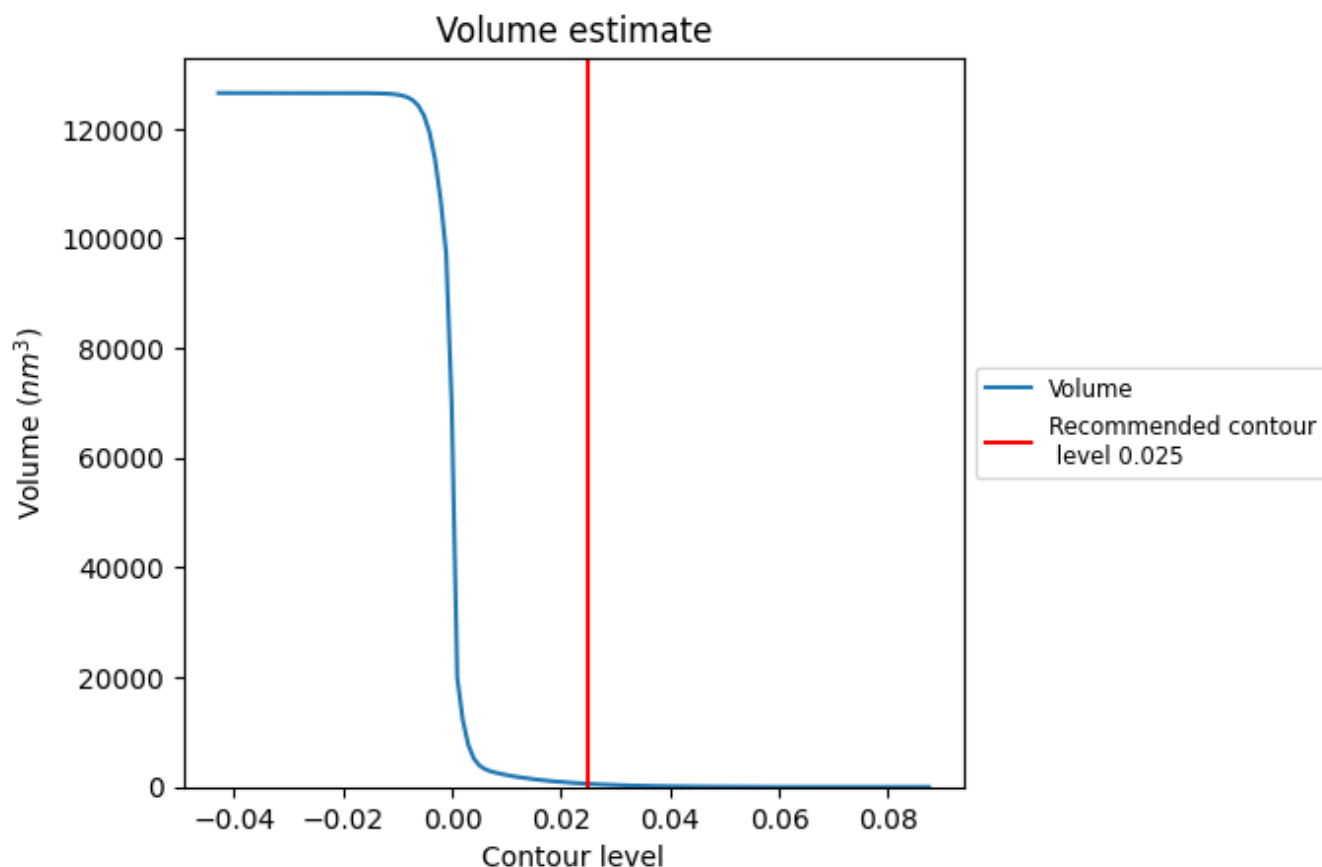
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

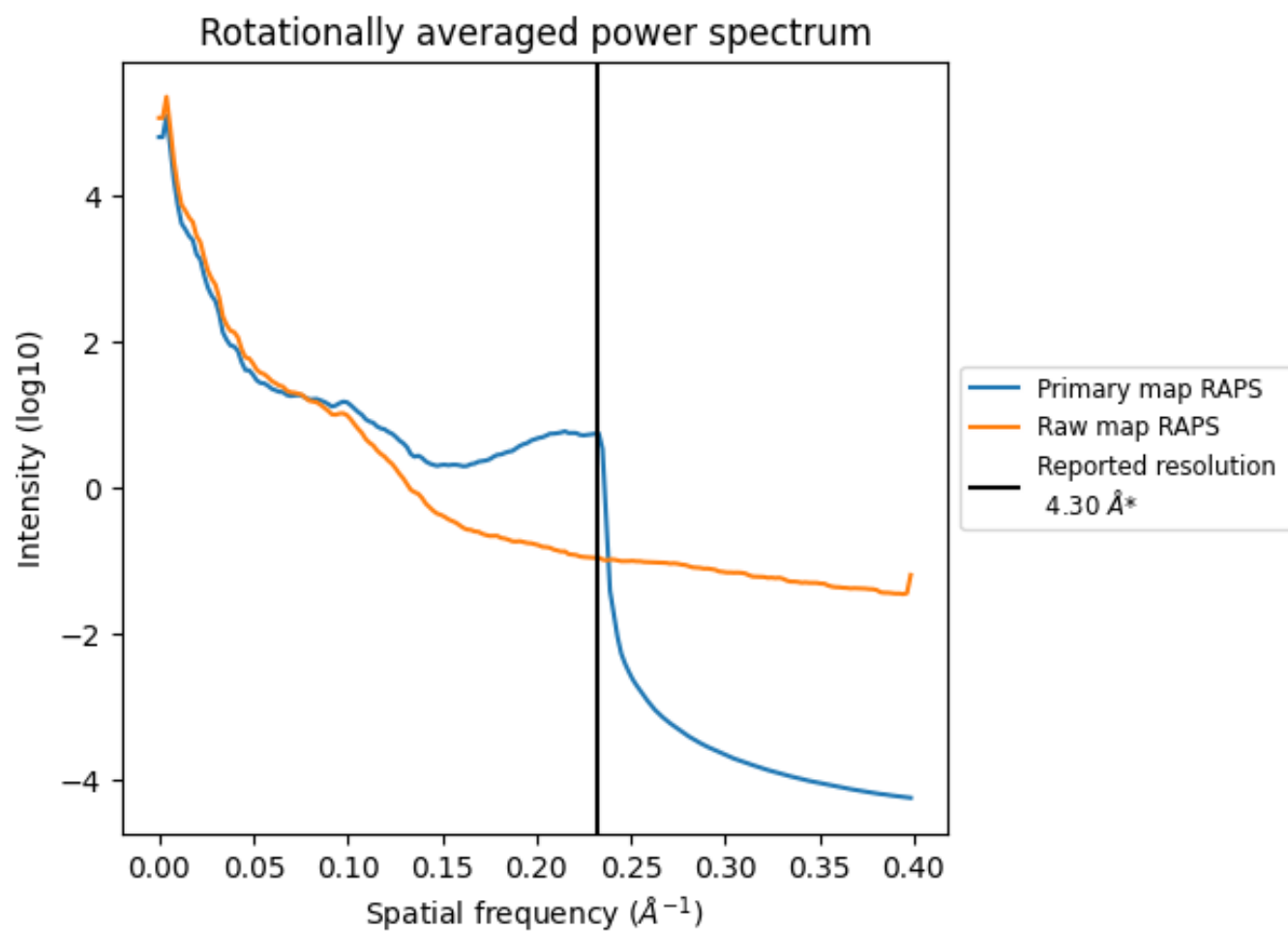
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 572 nm³; this corresponds to an approximate mass of 517 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

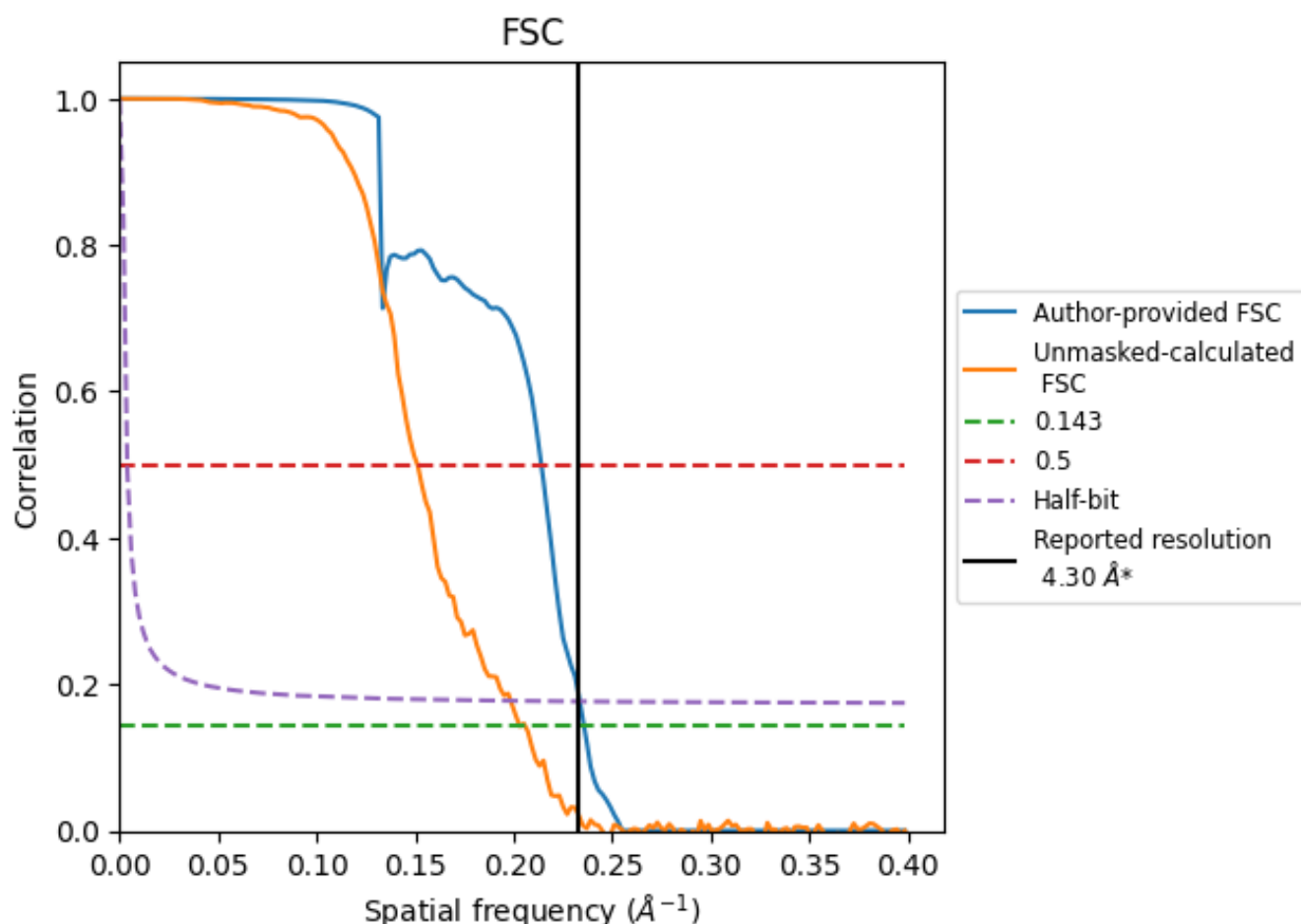


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 \AA^{-1}

8.2 Resolution estimates [i](#)

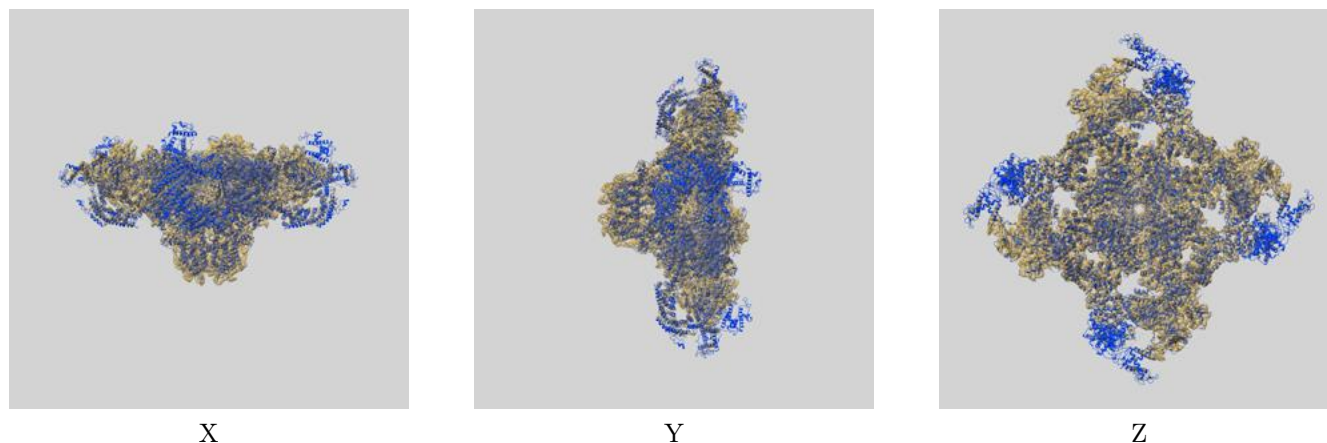
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.24	4.67	4.28
Unmasked-calculated*	4.92	6.61	5.04

*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 4.92 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

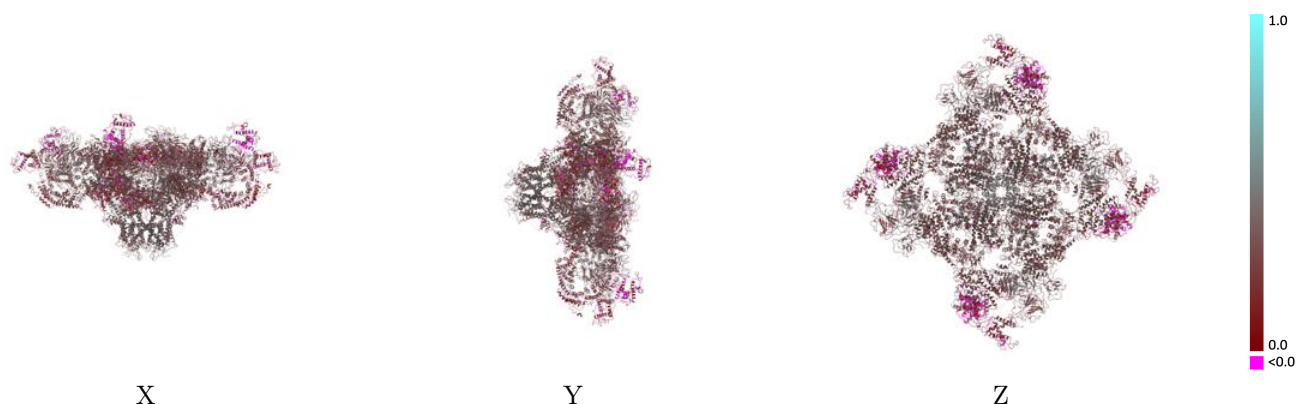
This section contains information regarding the fit between EMDB map EMD-8378 and PDB model 5TAL. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



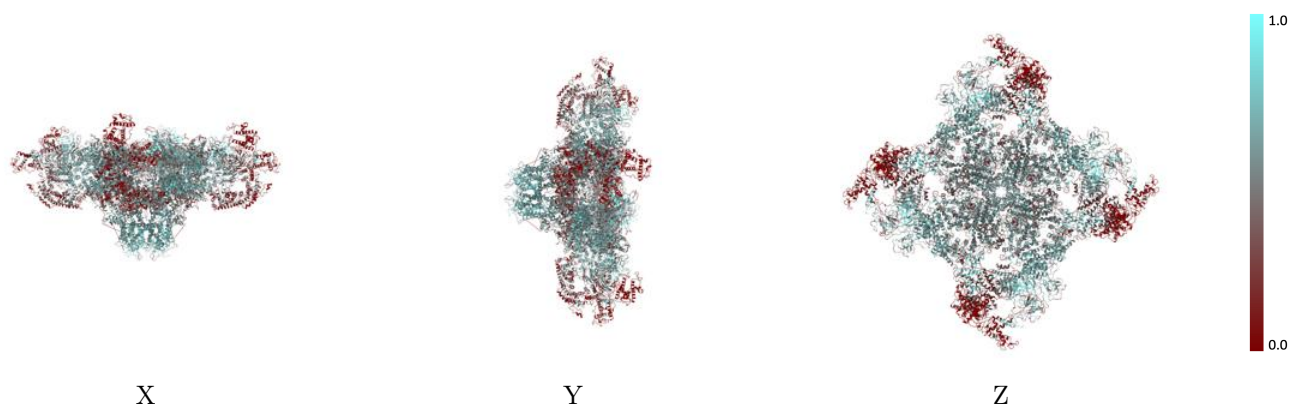
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



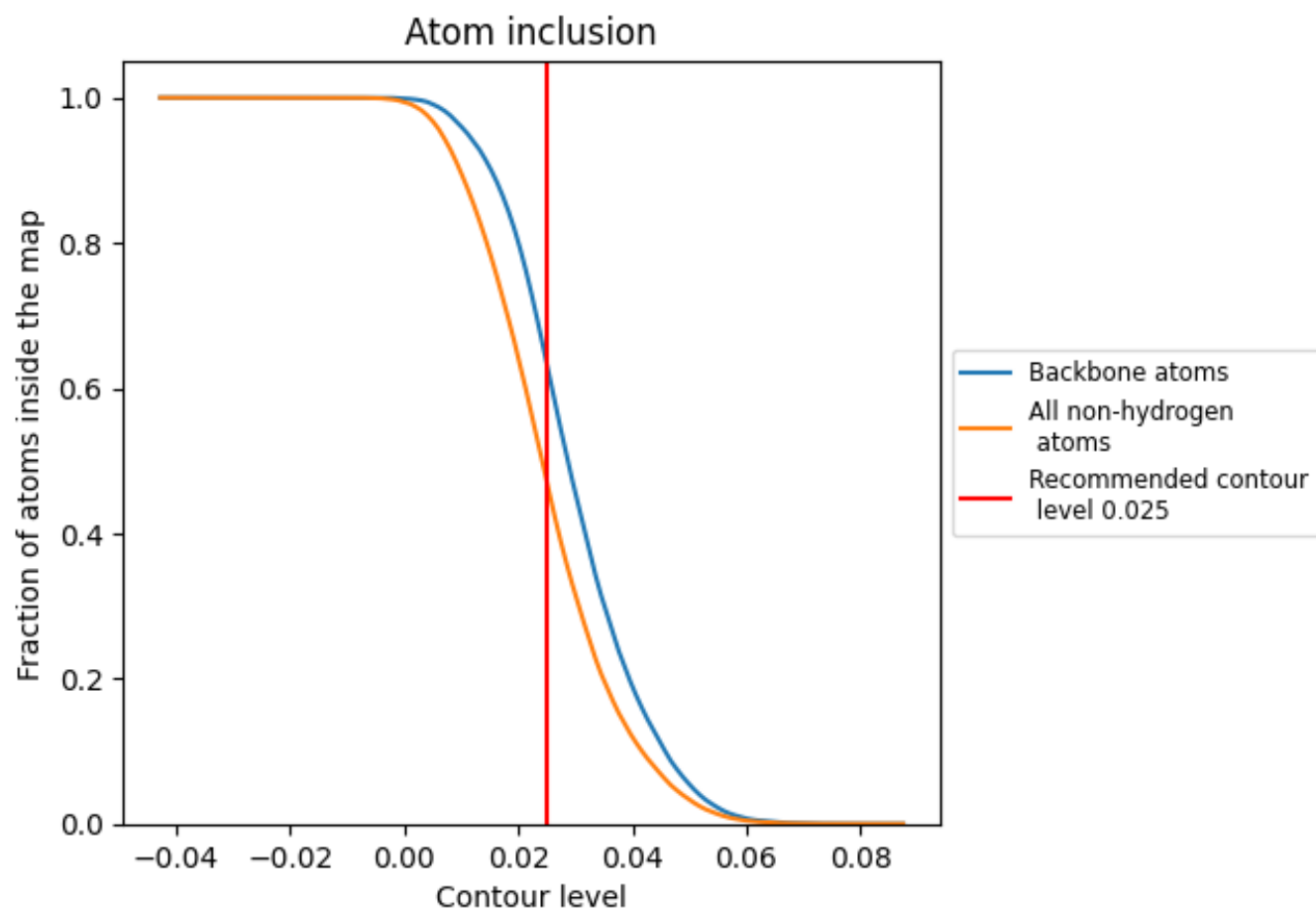
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 47% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4705	<div></div> 0.3030
A	<div></div> 0.5385	<div></div> 0.3550
B	<div></div> 0.4725	<div></div> 0.3050
E	<div></div> 0.4660	<div></div> 0.2980
F	<div></div> 0.5434	<div></div> 0.3580
G	<div></div> 0.4697	<div></div> 0.3030
H	<div></div> 0.5360	<div></div> 0.3570
I	<div></div> 0.4663	<div></div> 0.2990
J	<div></div> 0.5360	<div></div> 0.3550

