



Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 04:19 AM EDT

PDB ID : 5TAQ
EMDB ID : EMD-8382
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 3&4)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.10 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

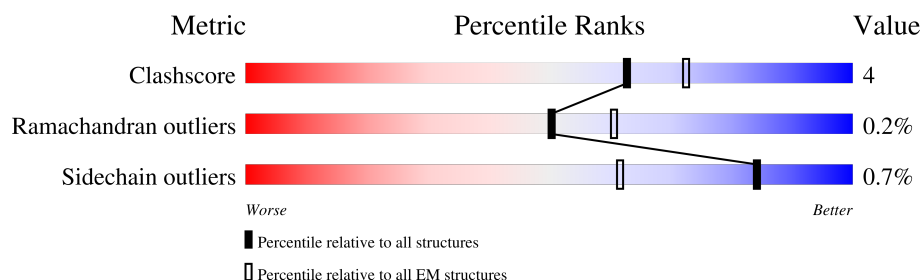
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




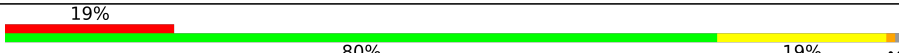
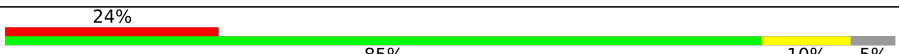

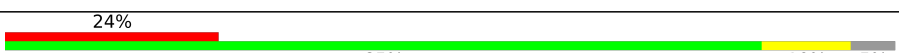
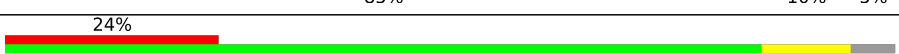
The reported resolution of this entry is 4.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition

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.

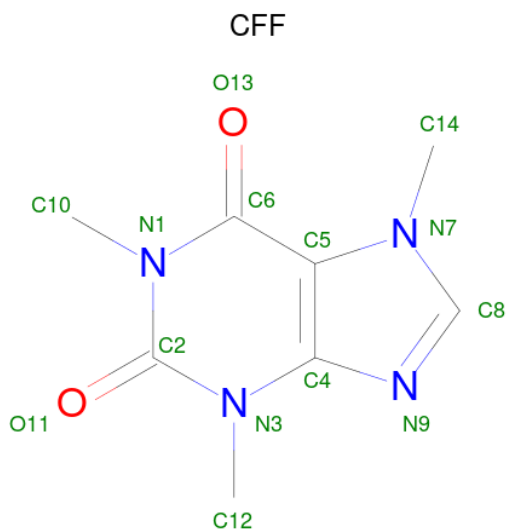
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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



Mol	Chain	Residues	Atoms					AltConf
3	B	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
3	I	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

- 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	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

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

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

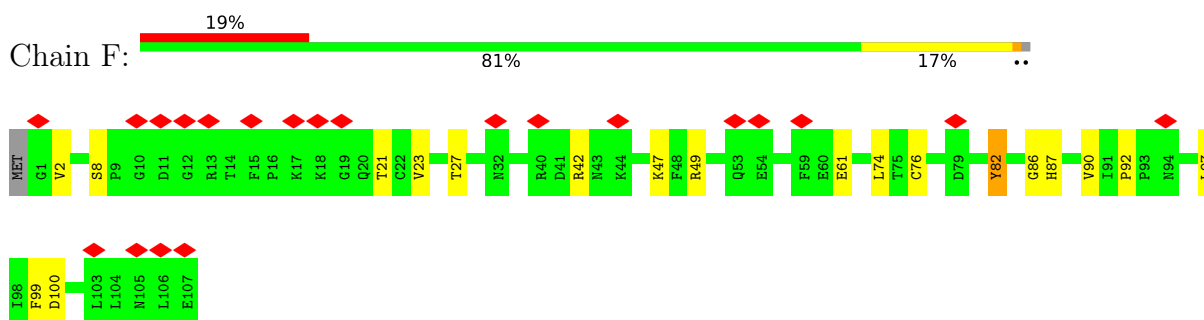
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

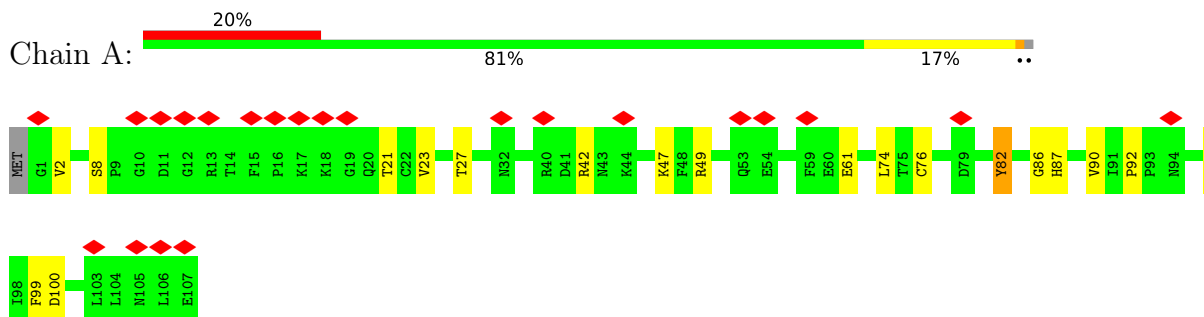
3 Residue-property plots [i](#)

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.

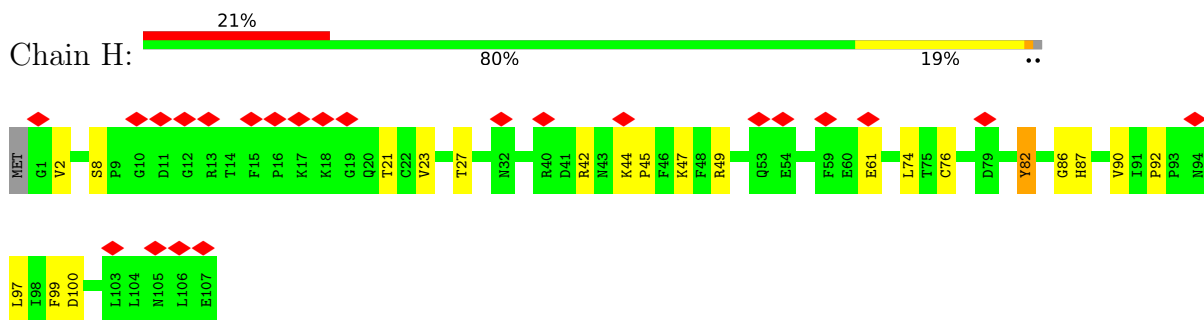
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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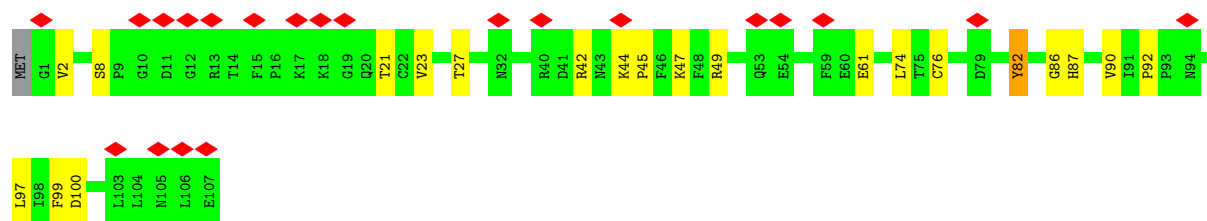


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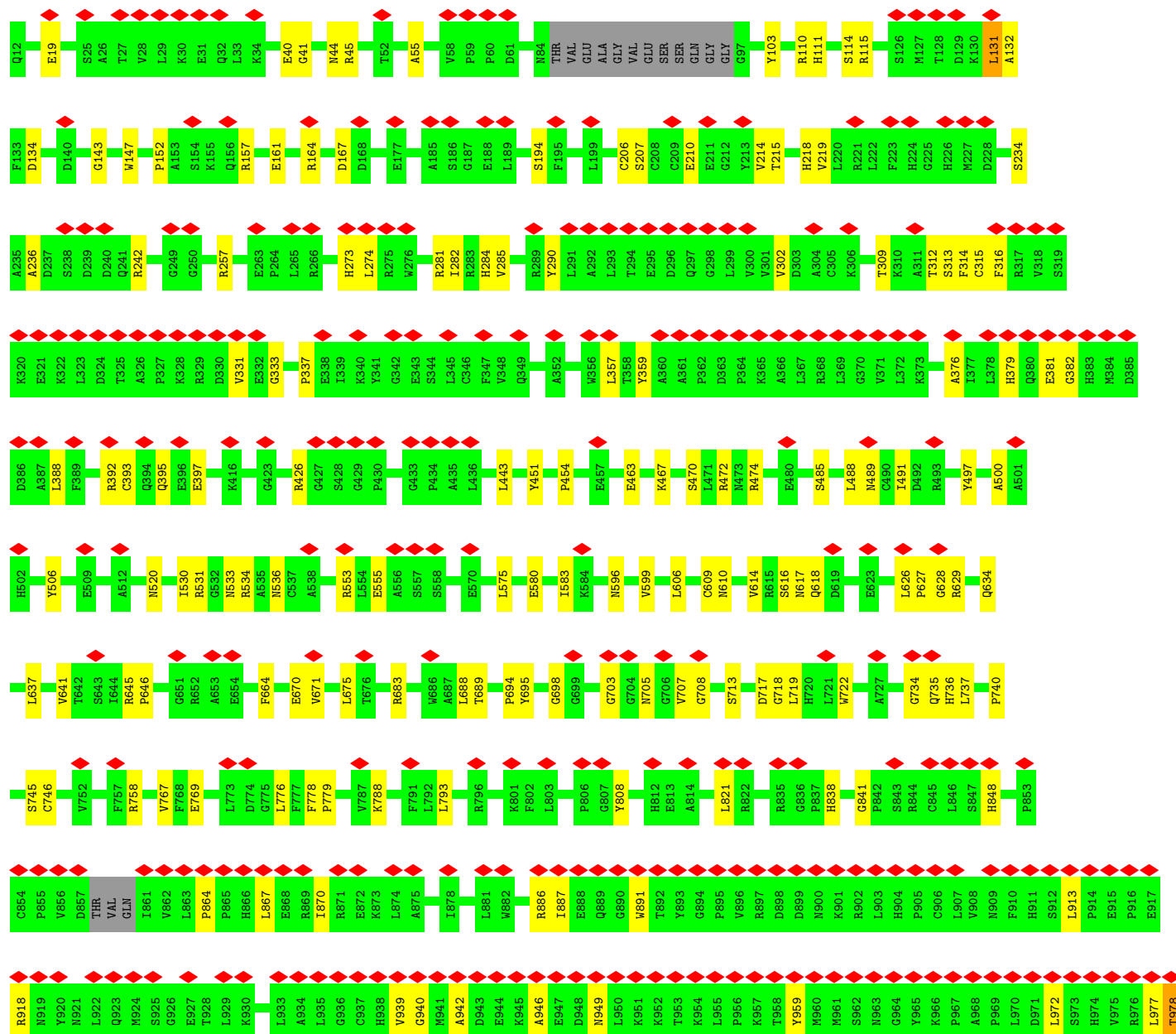
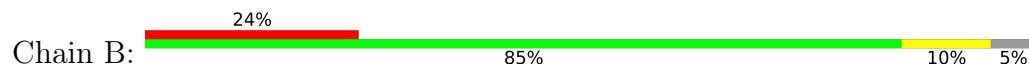


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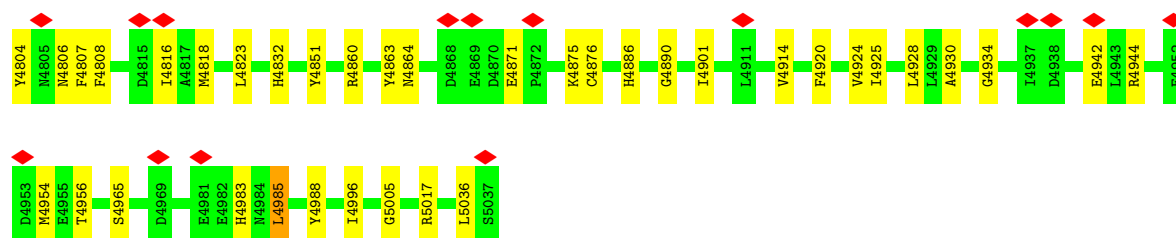


• Molecule 2: Ryanodine receptor 1

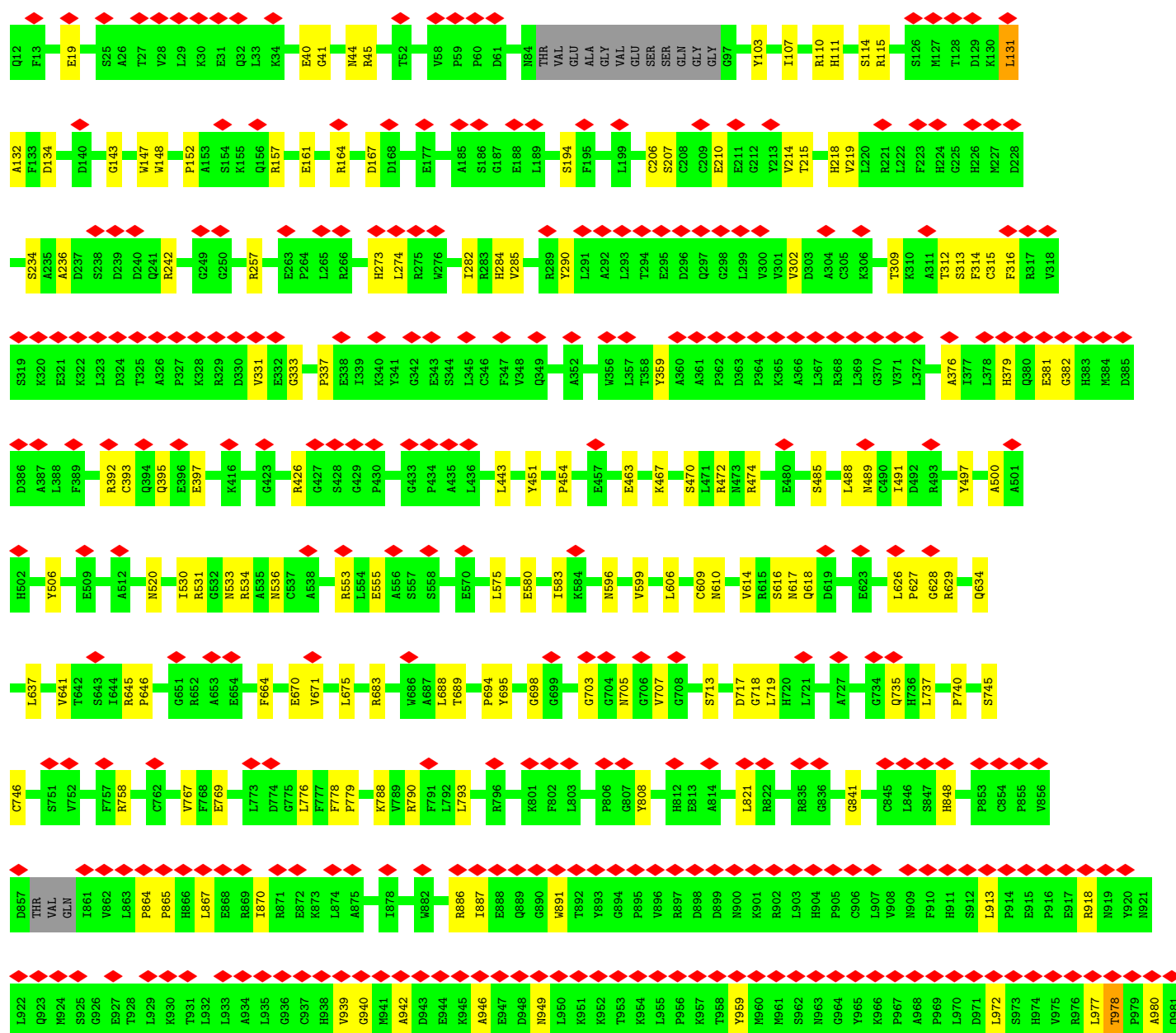
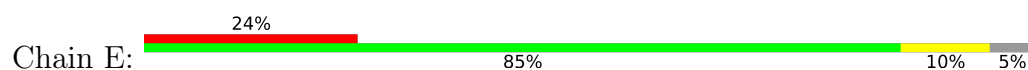






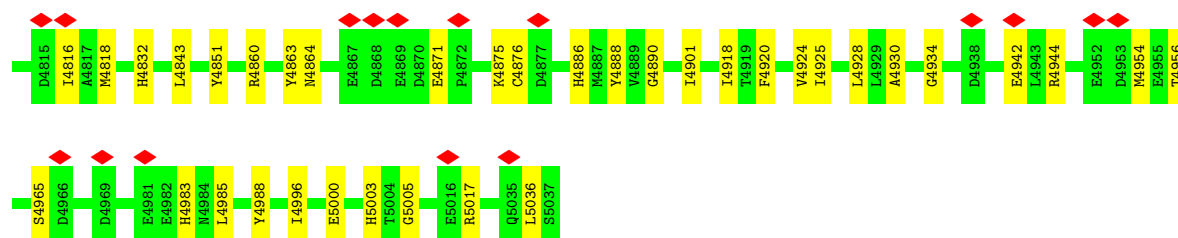


• Molecule 2: Ryanodine receptor 1

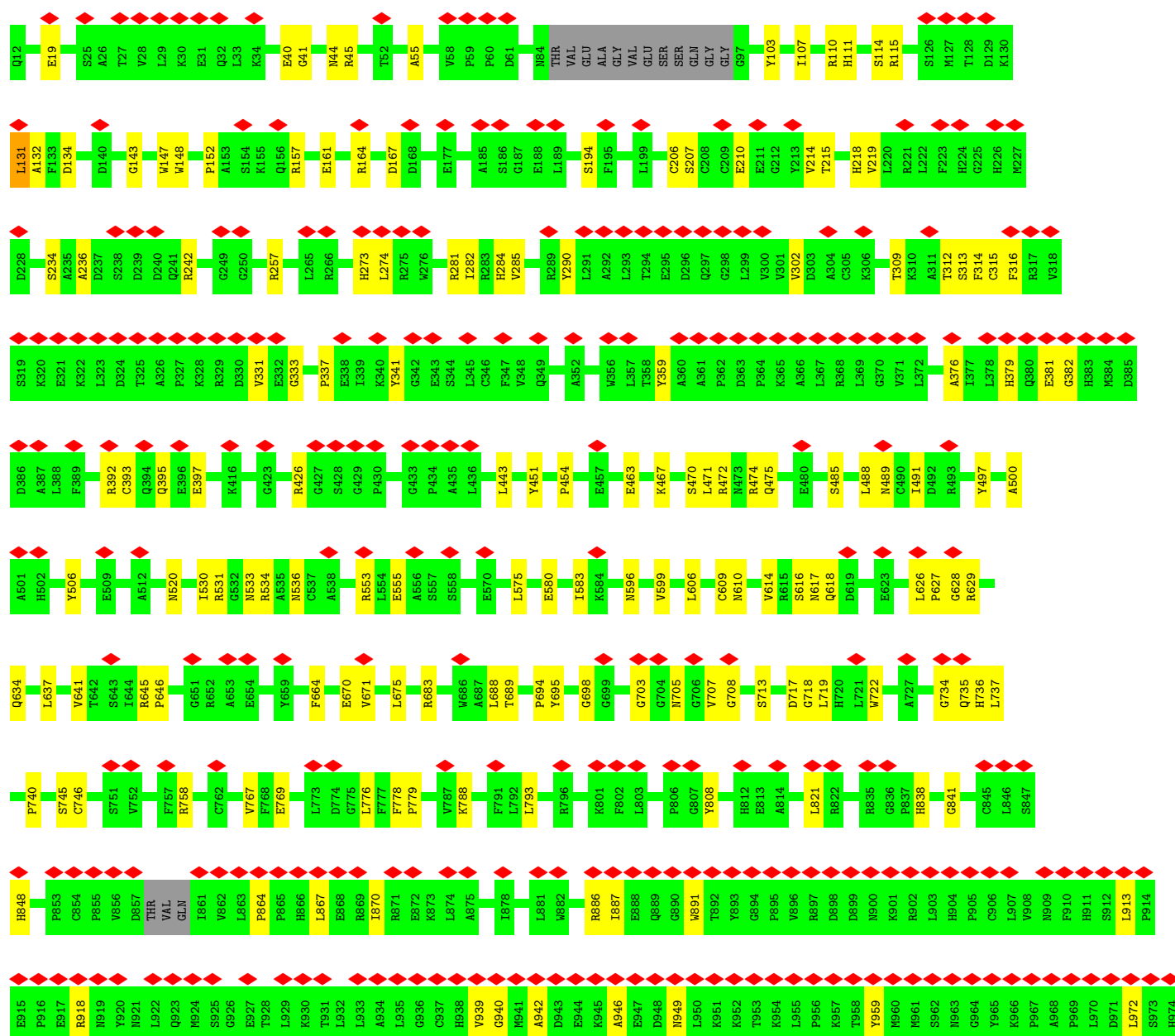
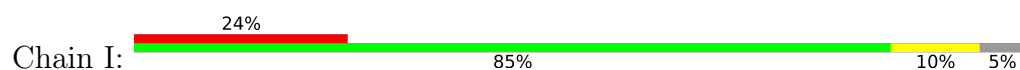


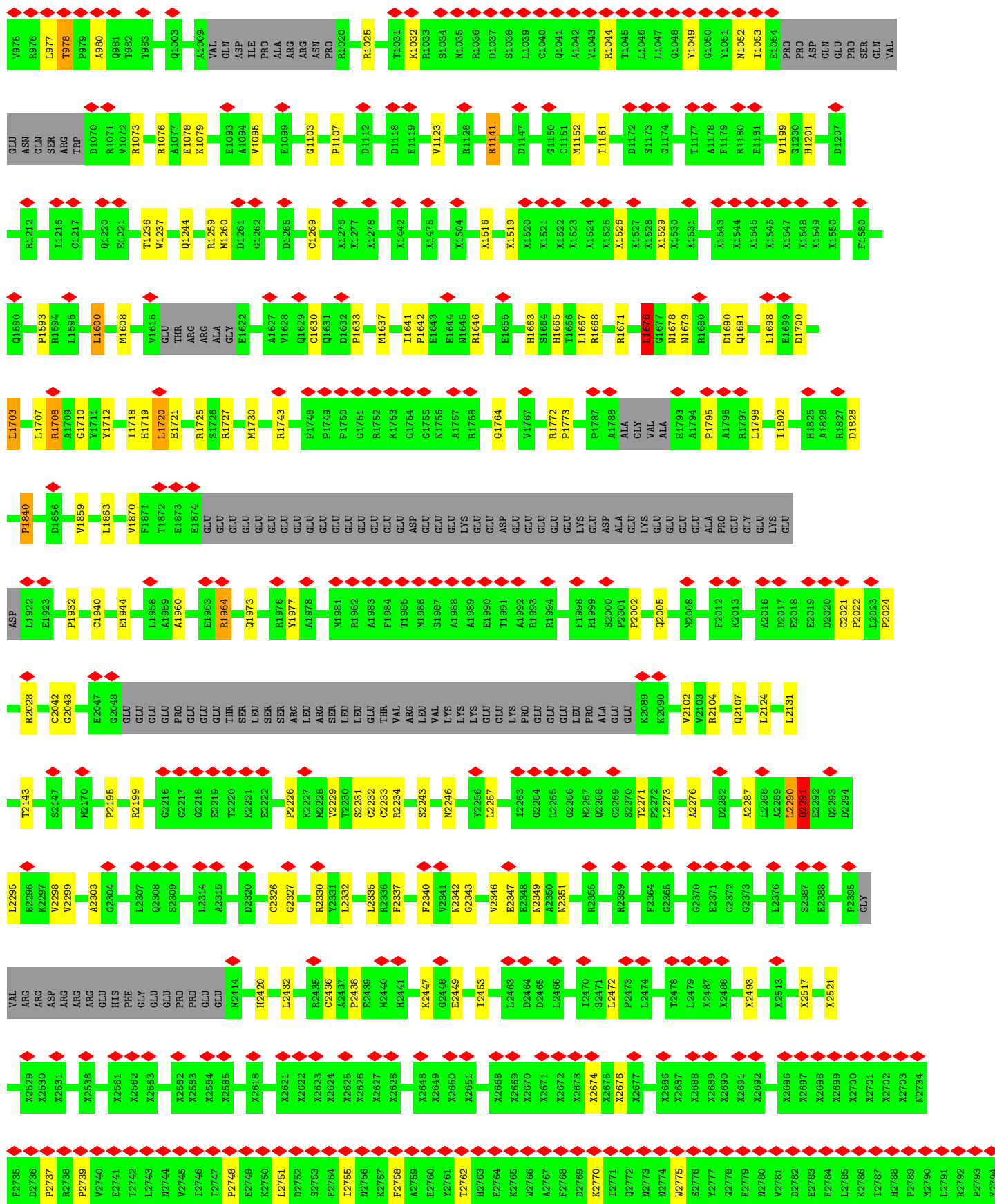
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E2292	Q2293	D2294	L2295	E2296	K2297	V2298	V2299	A2303	G2304	L2307	Q2308	S2309	L2314	A2315	D2320	C2326	G2327	R2330	Y2331	L2332	L2335	R2336	F2337	F2340	N2341	V2342	G2343	E2347	N2351	R2355	R2359	F2364	G2365	G2370	E2371	G2372	G2373	L2376	S2387	E2388	F2395	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
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P1840	D1856	V1859	L1863	V1870	F1871	T1872	E1873	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU



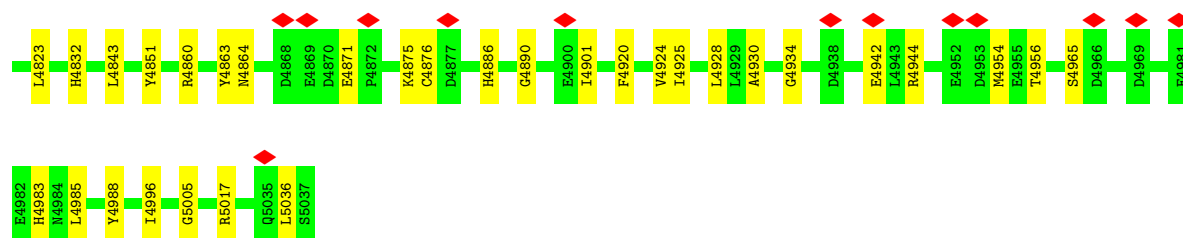


• Molecule 2: Ryanodine receptor 1

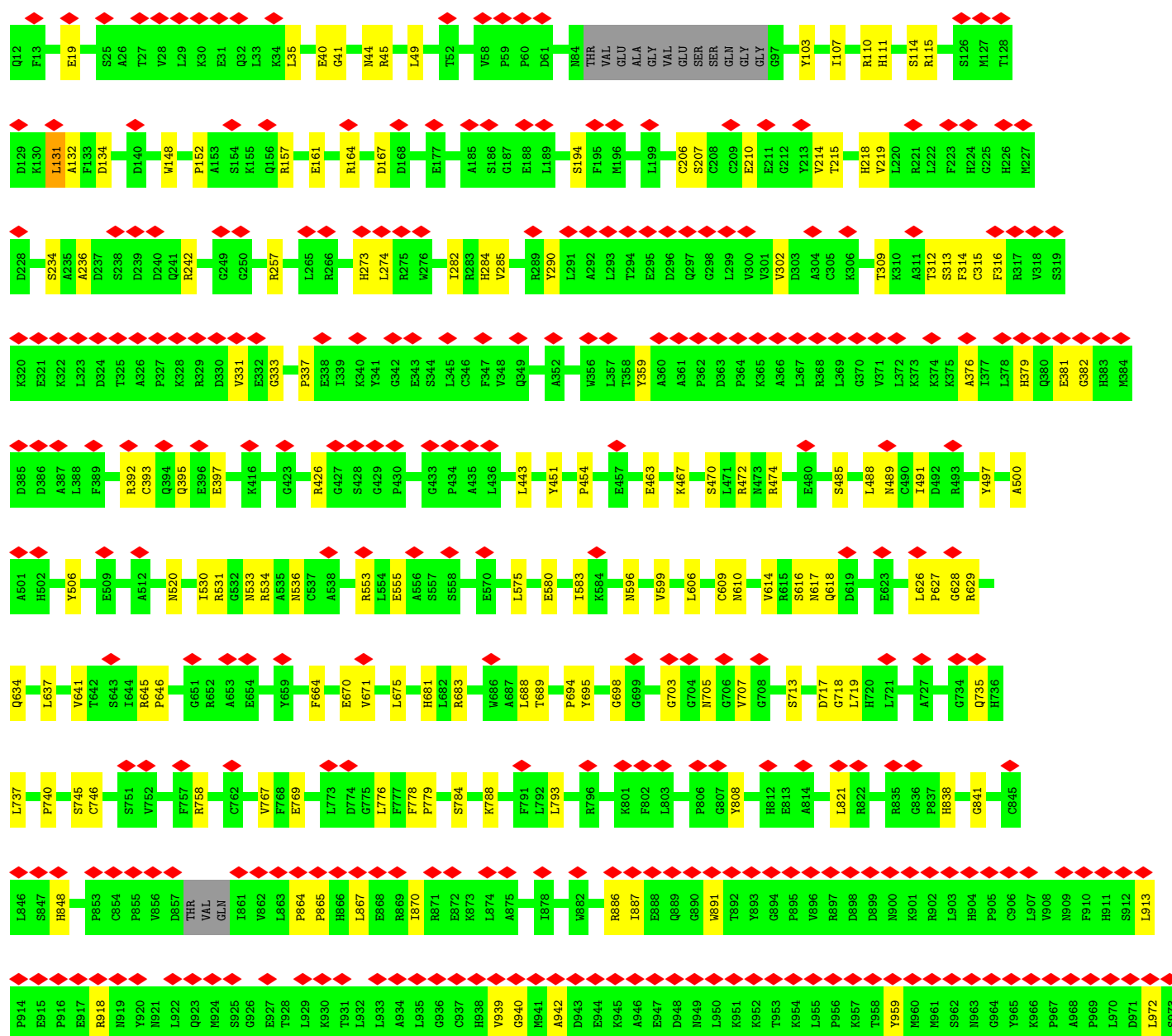
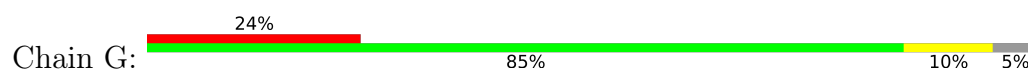




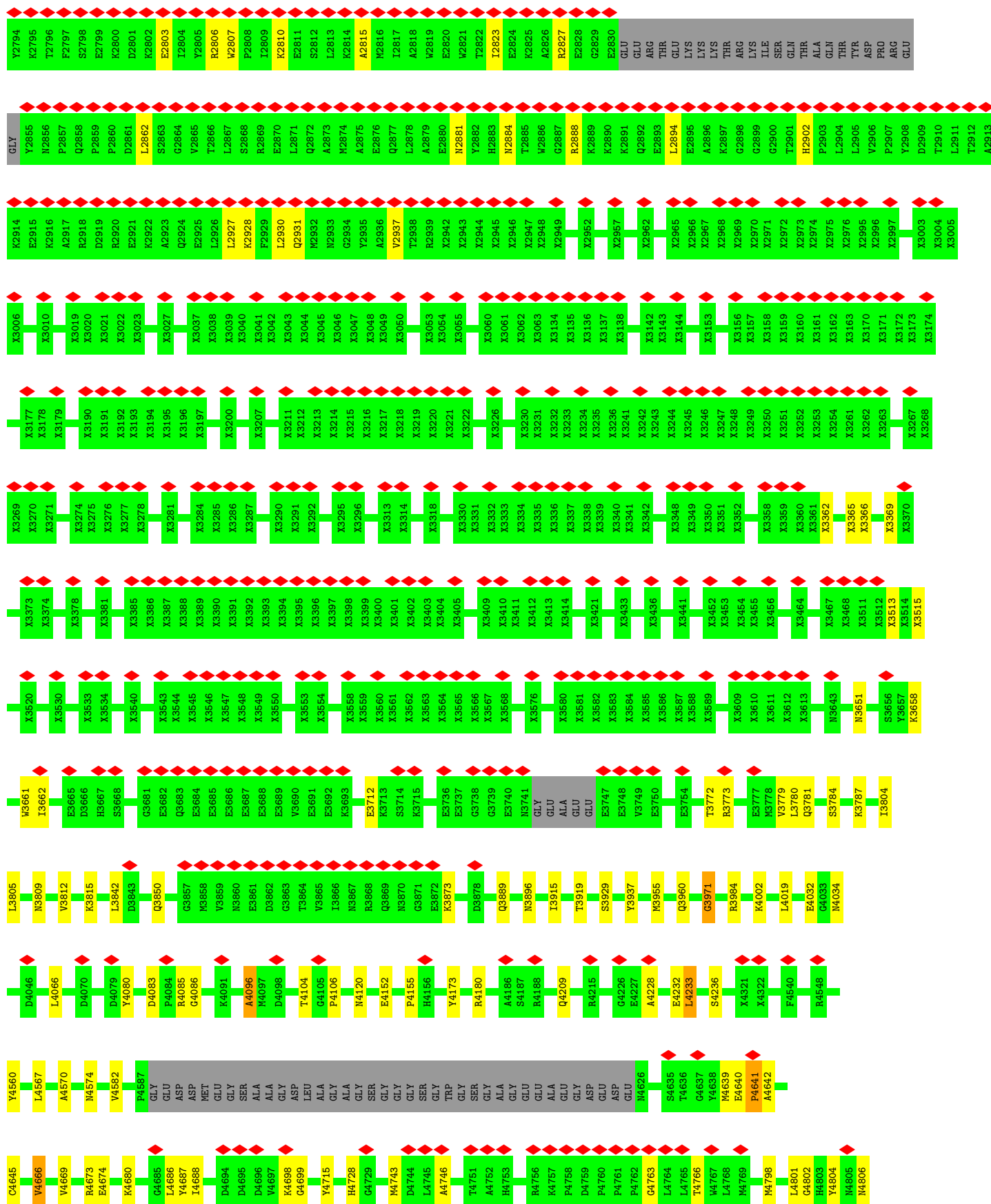
E4674	V4582	D4070	N3809	K3661	X3520	X3373	X3271	X3177	X3010	E2915	Y2855	K2795
K4680	P4587	D4079	K3815	L3662	X3530	X3374	X3274	X3178	X3019	K2916	N2856	T2796
L4686	GLU	D4080	L3942	E3665	X3533	X3375	X3275	X3179	X3020	A2917	P2857	F2797
I4688	ASP	P4083	D3943	D3666	X3534	X3376	X3276	X3190	X3021	R2918	Q2858	S2798
	ASP	R4085	Q3850	H3667	X3540	X3377	X3277	X3191	X3022	D2919	P2859	E2799
	MET	G4086		S3668	X3543	X3378	X3278	X3192	X3023	R2920	P2860	K2800
	GLY				X3544	X3386	X3280	X3193		E2921	D2861	D2801
	GLY	A4096		G3681	X3545	X3387	X3281	X3194	X3027	K2922	L2862	K2802
	GLY	M4097	G3857	Q3682	X3546	X3388	X3284	X3195	X3037	A2923	S2863	E2803
	ALA	D4098	M3858	Q3683	X3547	X3389	X3285	X3196	X3038	Q2924	G2864	T2804
	ASP		V3859	E3684	X3548	X3390	X3286	X3197	X3039	E2925	V2865	V2805
	LEU	T4104	N3860	E3685	X3549	X3391	X3287	X3200	X3040	L2926	T2866	R2806
	ALA	G4105	E3861	E3686	X3550	X3392	X3290	X3207	X3041	L2927	L2867	K2807
	ALA	P4106	D3862	E3687	X3553	X3393	X3291	X3211	X3042	K2928	S2868	P2808
	GLY		G3863	E3688	X3554	X3394	X3292	X3212	X3043	F2929	R2869	T2809
	GLY	N4120	T3864	E3689	X3558	X3395	X3293	X3213	X3044	L2930	E2870	K2810
	GLY	E4152	V3865	E3690	X3559	X3396	X3294	X3214	X3045	Q2931	L2871	E2811
	GLY	P4155	I3866	E3691	X3560	X3397	X3295	X3215	X3046	M2932	Q2872	S2812
	GLY	H4156	N3867	E3692	X3561	X3398	X3296	X3216	X3047	N2933	A2873	L2813
	SER		R3868	K3693	X3562	X3399	X3297	X3217	X3048	Q2934	M2874	K2814
	GLY	Y4173	Q3869		X3563	X3400	X3298	X3218	X3049	Y2935	A2875	A2815
	TRP		N3870	E3712	X3564	X3401	X3300	X3219	X3050	A2936	E2876	M2816
	GLY	R4180	G3871	S3714	X3565	X3402	X3301	X3220		V2937	Q2877	L2817
	GLY	A4186	E3872	K3715	X3566	X3403	X3302	X3221	X3053	T2938	A2878	A2818
	GLY	S4187	K3873		X3567	X3404	X3303	X3222	X3054	R2939	A2879	E2819
	GLY	R4188	D3878	E3736	X3568	X3405	X3304	X3223	X3055	Q2942	E2880	E2820
	GLU			E3737	X3576		X3305	X3224		K2943	N2881	K2821
	GLU	Q4209		G3738	X3580	X3409	X3306	X3225	X3060	Y2944	Y2882	T2822
	ALA		N3896	G3739	X3581	X3410	X3307	X3226	X3061	H2883	H2884	L2823
	GLY	R4215	M3896	E3740	X3582	X3411	X3308	X3227	X3062	E2884	T2885	E2824
	ASP		S3929	N3741	X3583	X3412	X3309	X3228	X3063	K2885	W2886	K2825
	ASP	G4226		GLY	X3584	X3413	X3310	X3229	X3134	G2886	G2887	A2826
	GLU	E4227		ALA	X3585	X3414	X3311	X3230	X3135	R2888	E2888	K2827
	GLU	A4228		GLU	X3586	X3415	X3312	X3231	X3136	K2889	K2889	E2828
	GLU		M3955	GLU	X3587	X3416	X3313	X3232	X3137	K2890	K2891	G2829
	GLU	E4232	Q3960	GLU	X3588	X3417	X3314	X3233	X3138	Q2892	Q2892	E2830
	GLU	L4233	E3967	E3747	X3589	X3418	X3315	X3234		E2893	E2893	GLU
	GLU	S4236		E3748	X3609	X3419	X3316	X3235	X3142	L2894	L2894	GLU
	GLU		G3971	V3749	X3610	X3420	X3317	X3236	X3143	E2895	E2895	ARG
	GLU	X4321	R3984	E3750	X3611	X3421	X3318	X3237	X3144	A2896	A2896	LYS
	GLU	X4322		E3754	X3612	X3422	X3319	X3238	X3153	K2897	K2897	LYS
	GLU	F4540	K4002	T3772	X3613	X3423	X3320	X3239	X3154	G2898	G2898	THR
	GLU	R4548	L4019	R3773	X3614	X3424	X3321	X3240	X3155	R2899	R2899	LYS
	GLU		E4032	E3777	X3615	X3425	X3322	X3241	X3156	G2900	G2900	ILE
	GLU	Y4560	C4033	M3778	X3616	X3426	X3323	X3242	X3157	X2901	X2901	SER
	GLU	L4567	M4034	V3779	X3617	X3427	X3324	X3243	X3158	H2902	H2902	GLN
	GLU	A4570	D4046	Q3781	X3618	X3428	X3325	X3244	X3159	P2903	P2903	THR
	GLU	N4574	L4066	S3784	X3619	X3429	X3326	X3245	X3160	L2904	L2904	ALA
	GLU			K3787	X3620	X3430	X3327	X3246	X3161	T2905	T2905	GLN
	GLU				X3621	X3431	X3328	X3247	X3162	L2906	L2906	TVR
	GLU				X3622	X3432	X3329	X3248	X3163	L2907	L2907	ASP
	GLU				X3623	X3433	X3330	X3249	X3164	P2908	P2908	PRO
	GLU				X3624	X3434	X3331	X3250	X3165	D2909	D2909	ARG
	GLU				X3625	X3435	X3332	X3251	X3166	T2910	T2910	GLY
	GLU				X3626	X3436	X3333	X3252	X3167	X3003	X3003	
	GLU				X3627	X3437	X3334	X3253	X3168	X3004	X3004	
	GLU				X3628	X3438	X3335	X3254	X3169	X3005	X3005	
	GLU				X3629	X3439	X3336	X3255	X3170	X3006	X3006	
	GLU				X3630	X3440	X3337	X3256	X3171			
	GLU				X3631	X3441	X3338	X3257	X3172			
	GLU				X3632	X3442	X3339	X3258	X3173			
	GLU				X3633	X3443	X3340	X3259	X3174			
	GLU				X3634	X3444	X3341	X3260				
	GLU				X3635	X3445	X3342	X3261				
	GLU				X3636	X3446	X3343	X3262				
	GLU				X3637	X3447	X3344	X3263				
	GLU				X3638	X3448	X3345	X3264				
	GLU				X3639	X3449	X3346	X3265				
	GLU				X3640	X3450	X3347	X3266				
	GLU				X3641	X3451	X3348	X3267				
	GLU				X3642	X3452	X3349	X3268				
	GLU				X3643	X3453	X3350	X3269				
	GLU				X3644	X3454	X3351	X3270				
	GLU				X3645	X3455	X3352	X3271				
	GLU				X3646	X3456	X3353	X3272				
	GLU				X3647	X3457	X3354	X3273				
	GLU				X3648	X3458	X3355	X3274				
	GLU				X3649	X3459	X3356	X3275				
	GLU				X3650	X3460	X3357	X3276				
	GLU				X3651	X3461	X3358	X3277				
	GLU				X3652	X3462	X3359	X3278				
	GLU				X3653	X3463	X3360	X3279				
	GLU				X3654	X3464	X3361	X3280				
	GLU				X3655	X3465	X3362	X3281				
	GLU				X3656	X3466	X3363	X3282				
	GLU				X3657	X3467	X3364	X3283				
	GLU				X3658	X3468	X3365	X3284				
	GLU				X3659	X3469	X3366	X3285				
	GLU				X3660	X3470	X3367	X3286				
	GLU				X3661	X3471	X3368	X3287				
	GLU				X3662	X3472	X3369	X3288				
	GLU				X3663	X3473	X3370	X3289				
	GLU				X3664	X3474	X3371	X3290				
	GLU				X3665	X3475	X3372	X3291				
	GLU				X3666	X3476	X3373	X3292				
	GLU				X3667	X3477	X3374	X3293				
	GLU				X3668	X3478	X3375	X3294				
	GLU				X3669	X3479	X3376	X3295				
	GLU				X3670	X3480	X3377	X3296				
	GLU				X3671	X3481	X3378	X3297				
	GLU				X3672	X3482	X3379	X3298				
	GLU				X3673	X3483	X3380	X3299				
	GLU				X3674	X3484	X3381	X3300				
	GLU				X3675	X3485	X3382	X3301				
	GLU				X3676	X3486	X3383	X3302				
	GLU				X3677	X3487	X3384	X3303				
	GLU				X3678	X3488	X3385	X3304				
	GLU				X3679	X3489	X3386	X3305				
	GLU				X3680	X3490	X3387	X3306				
	GLU				X3681	X3491	X3388	X3307				
	GLU				X3682	X3492	X3389	X3308				
	GLU				X3683	X3493	X3390	X3309				
	GLU				X3684	X3494	X3391	X3310				
	GLU				X3685	X3495	X3392	X3311				
	GLU				X3686	X3496	X3393	X3312				
	GLU				X3687	X3497	X3394	X3313				
	GLU				X3688	X3498	X3395	X3314				
	GLU				X3689	X3499	X3396	X3315				
	GLU				X3690	X3500	X3397	X3316				
	GLU				X3691	X3501	X3398	X3317				
	GLU				X3692	X3502	X3399	X3318				
	GLU				X3693	X3503	X3400	X3319				
	GLU				X3694	X3504	X3401	X3320				
	GLU				X3695	X3505	X3402	X3321				
	GLU				X3696	X3506	X3403	X3322				
	GLU				X3697	X3507	X3404	X3323				
	GLU				X3698	X3508	X3405	X3324				
	GLU				X3699	X3509	X3406	X3325				
	GLU				X3700	X3510	X3407	X3326				
	GLU				X3701	X3511	X3408	X3327				
	GLU				X3702	X3512	X3409	X3328				
	GLU				X3703	X3513	X3410	X3329				
	GLU				X3704	X3514	X3411	X3330				
	GLU											

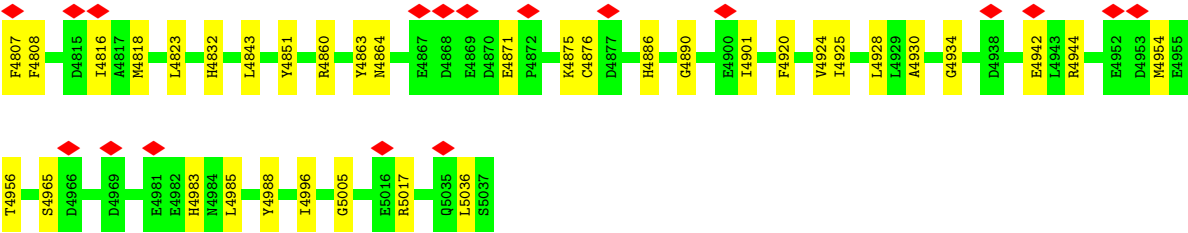


• Molecule 2: Ryanodine receptor 1









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	0.114	Depositor
Minimum map value	-0.070	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: CA, CFF, ZN, 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	0.32	0/834	0.54	0/1123
1	F	0.32	0/834	0.54	0/1123
1	H	0.32	0/834	0.54	0/1123
1	J	0.32	0/834	0.54	0/1123
2	B	0.32	0/25428	0.57	13/34534 (0.0%)
2	E	0.32	0/25428	0.57	13/34534 (0.0%)
2	G	0.32	0/25428	0.57	13/34534 (0.0%)
2	I	0.32	0/25428	0.57	13/34534 (0.0%)
All	All	0.32	0/105048	0.57	52/142628 (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	2
1	F	0	2
1	H	0	2
1	J	0	2
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	80

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	131	LEU	CA-CB-CG	8.14	134.03	115.30
2	B	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	E	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	I	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	E	4639	MET	C-N-CA	6.84	138.79	121.70
2	B	4639	MET	C-N-CA	6.82	138.75	121.70
2	E	1676	LEU	CA-CB-CG	6.81	130.97	115.30
2	I	4639	MET	C-N-CA	6.81	138.73	121.70
2	G	4639	MET	C-N-CA	6.81	138.72	121.70
2	B	1676	LEU	CA-CB-CG	6.81	130.95	115.30
2	I	1676	LEU	CA-CB-CG	6.80	130.94	115.30
2	G	1676	LEU	CA-CB-CG	6.80	130.94	115.30
2	G	1600	LEU	CA-CB-CG	6.27	129.73	115.30
2	E	1600	LEU	CA-CB-CG	6.26	129.71	115.30
2	B	1600	LEU	CA-CB-CG	6.25	129.69	115.30
2	I	1600	LEU	CA-CB-CG	6.25	129.68	115.30
2	B	2290	LEU	CA-CB-CG	6.02	129.15	115.30
2	E	2290	LEU	CA-CB-CG	6.01	129.13	115.30
2	I	2290	LEU	CA-CB-CG	6.00	129.11	115.30
2	G	2290	LEU	CA-CB-CG	6.00	129.09	115.30
2	G	1667	LEU	CA-CB-CG	5.85	128.75	115.30
2	E	1667	LEU	CA-CB-CG	5.85	128.75	115.30
2	B	1667	LEU	CA-CB-CG	5.84	128.74	115.30
2	I	1667	LEU	CA-CB-CG	5.83	128.71	115.30
2	B	4985	LEU	CA-CB-CG	5.66	128.31	115.30
2	I	4985	LEU	CA-CB-CG	5.65	128.29	115.30
2	E	4985	LEU	CA-CB-CG	5.65	128.29	115.30
2	G	4985	LEU	CA-CB-CG	5.62	128.23	115.30
2	B	2291	GLN	C-N-CA	5.47	135.38	121.70
2	E	2291	GLN	C-N-CA	5.45	135.34	121.70
2	G	2291	GLN	C-N-CA	5.44	135.29	121.70
2	I	2291	GLN	C-N-CA	5.42	135.25	121.70
2	B	977	LEU	CA-CB-CG	5.26	127.41	115.30
2	E	977	LEU	CA-CB-CG	5.26	127.39	115.30
2	I	977	LEU	CA-CB-CG	5.25	127.38	115.30
2	G	977	LEU	CA-CB-CG	5.24	127.36	115.30
2	E	688	LEU	CA-CB-CG	5.23	127.34	115.30
2	I	688	LEU	CA-CB-CG	5.23	127.33	115.30
2	G	688	LEU	CA-CB-CG	5.22	127.31	115.30
2	B	688	LEU	CA-CB-CG	5.22	127.30	115.30
2	G	1703	LEU	CA-CB-CG	5.19	127.24	115.30
2	B	4233	LEU	CA-CB-CG	5.19	127.23	115.30
2	E	1703	LEU	CA-CB-CG	5.19	127.23	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4233	LEU	CA-CB-CG	5.18	127.22	115.30
2	I	1703	LEU	CA-CB-CG	5.18	127.22	115.30
2	B	1703	LEU	CA-CB-CG	5.18	127.21	115.30
2	E	4233	LEU	CA-CB-CG	5.18	127.21	115.30
2	I	4233	LEU	CA-CB-CG	5.17	127.20	115.30
2	G	4901	ILE	CG1-CB-CG2	-5.04	100.32	111.40
2	B	4901	ILE	CG1-CB-CG2	-5.04	100.32	111.40
2	I	4901	ILE	CG1-CB-CG2	-5.02	100.36	111.40
2	E	4901	ILE	CG1-CB-CG2	-5.01	100.38	111.40

There are no chirality outliers.

All (80) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
1	A	82	TYR	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1720	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4096	ALA	Peptide
2	B	4641	PRO	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	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

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Mol	Chain	Res	Type	Group
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4096	ALA	Peptide
2	E	4641	PRO	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
1	F	82	TYR	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	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4096	ALA	Peptide
2	G	4641	PRO	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
1	H	82	TYR	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

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Mol	Chain	Res	Type	Group
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4096	ALA	Peptide
2	I	4641	PRO	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide
1	J	82	TYR	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	10	0
1	H	818	0	824	11	0
1	J	818	0	824	11	0
2	B	29499	0	24752	242	0
2	E	29499	0	24752	242	0
2	G	29499	0	24752	241	0
2	I	29499	0	24752	243	0
3	B	31	0	12	1	0
3	E	31	0	12	0	0
3	G	31	0	12	0	0
3	I	31	0	12	0	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	1	0	0	0	0
All	All	121456	0	102392	986	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (986) 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:G:646:PRO:HD2	2:G:779:PRO:HB2	1.73	0.70
2:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.69
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.73	0.69
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.75	0.69
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.75	0.69
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.74	0.68
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.73	0.68
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.76	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.76	0.67
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.76	0.67
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.75	0.67
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.76	0.67
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.67
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.75	0.67
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.60	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.66
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.78	0.66
2:B:3984:ARG:HH22	2:I:161:GLU:HA	1.59	0.66
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.78	0.66
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.61	0.65
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.60	0.65
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.60	0.64
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.78	0.64
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.78	0.64
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.31	0.64
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.31	0.63
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.31	0.63
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.81	0.62
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.31	0.62
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.81	0.62
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.64	0.62
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.64	0.61
2:B:1703:LEU:HD12	2:B:1708:ARG:HB2	1.83	0.61
2:I:1703:LEU:HD12	2:I:1708:ARG:HB2	1.83	0.61
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.81	0.61
2:E:1703:LEU:HD12	2:E:1708:ARG:HB2	1.83	0.61
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.81	0.61
2:G:1703:LEU:HD12	2:G:1708:ARG:HB2	1.82	0.60
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.64	0.60
2:B:2347:GLU:O	2:B:2351:ASN:N	2.31	0.60
2:I:331:VAL:HG12	2:I:333:GLY:H	1.66	0.60
2:G:331:VAL:HG12	2:G:333:GLY:H	1.66	0.60
2:B:331:VAL:HG12	2:B:333:GLY:H	1.67	0.60
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.84	0.59
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.68	0.59
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.84	0.59
2:E:331:VAL:HG12	2:E:333:GLY:H	1.67	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.76	0.59
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.68	0.59
2:G:2347:GLU:O	2:G:2351:ASN:N	2.31	0.59
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.36	0.59
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.68	0.58
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.85	0.58
2:G:609:CYS:SG	2:G:610:ASN:N	2.76	0.58
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.84	0.58
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.85	0.58
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.85	0.58
2:G:309:THR:O	2:G:313:SER:OG	2.22	0.58
2:B:626:LEU:HG	2:B:628:GLY:H	1.68	0.58
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.37	0.58
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.85	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.85	0.58
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.58
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.85	0.58
2:E:309:THR:O	2:E:313:SER:OG	2.22	0.58
2:I:609:CYS:SG	2:I:610:ASN:N	2.76	0.58
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.84	0.58
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.76	0.58
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.37	0.58
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.58
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.85	0.58
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.86	0.58
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.86	0.58
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.36	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.37	0.58
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.85	0.58
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.86	0.57
2:I:626:LEU:HG	2:I:628:GLY:H	1.69	0.57
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.86	0.57
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.36	0.57
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.84	0.57
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.36	0.57
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.87	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.85	0.57
2:I:2347:GLU:O	2:I:2351:ASN:N	2.31	0.57
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.68	0.57
2:B:309:THR:O	2:B:313:SER:OG	2.22	0.57
2:E:2347:GLU:O	2:E:2351:ASN:N	2.31	0.57
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.38	0.57
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.38	0.57
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.86	0.57
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.38	0.57
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.38	0.57
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.87	0.57
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.57
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.38	0.57
2:I:309:THR:O	2:I:313:SER:OG	2.22	0.57
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.38	0.57
2:G:257:ARG:O	2:G:284:HIS:NE2	2.38	0.57
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.38	0.57
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.86	0.57
2:B:257:ARG:O	2:B:284:HIS:NE2	2.37	0.56
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.38	0.56
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.85	0.56
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.38	0.56
2:G:626:LEU:HG	2:G:628:GLY:H	1.68	0.56
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.38	0.56
2:E:626:LEU:HG	2:E:628:GLY:H	1.69	0.56
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.38	0.56
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.38	0.56
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.39	0.56
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.88	0.56
2:I:257:ARG:O	2:I:284:HIS:NE2	2.38	0.56
2:I:315:CYS:SG	2:I:316:PHE:N	2.79	0.56
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.88	0.56
2:G:614:VAL:HG22	2:G:616:SER:H	1.70	0.56
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.38	0.56
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.79	0.56
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.88	0.56
2:G:315:CYS:SG	2:G:316:PHE:N	2.79	0.56
2:B:4996:ILE:HG12	4:B:5102:CFF:H123	1.87	0.56
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.87	0.56
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.79	0.56
1:H:27:THR:HB	1:H:100:ASP:HB3	1.88	0.56
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.86	0.56
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.86	0.56
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.88	0.56
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.88	0.56
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.88	0.56
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.87	0.56
2:I:614:VAL:HG22	2:I:616:SER:H	1.70	0.56
2:G:132:ALA:HA	2:G:194:SER:HB2	1.88	0.56
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.38	0.56
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.71	0.56
2:E:4996:ILE:HG12	4:E:5102:CFF:H123	1.88	0.56
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.38	0.56
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.71	0.56
1:A:27:THR:HB	1:A:100:ASP:HB3	1.88	0.55
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.79	0.55
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.38	0.55
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.38	0.55
2:E:315:CYS:SG	2:E:316:PHE:N	2.79	0.55
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.71	0.55
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.38	0.55
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.79	0.55
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.72	0.55
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.71	0.55
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.88	0.55
2:E:161:GLU:HA	2:G:3984:ARG:HH22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.38	0.55
2:I:132:ALA:HA	2:I:194:SER:HB2	1.88	0.55
2:I:4996:ILE:HG12	4:I:5102:CFF:H123	1.89	0.55
2:G:4996:ILE:HG12	4:G:5102:CFF:H123	1.88	0.55
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.89	0.55
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.71	0.55
2:E:257:ARG:O	2:E:284:HIS:NE2	2.38	0.55
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.89	0.55
2:E:3773:ARG:HG3	2:E:3815:LYS:HZ3	1.71	0.55
2:B:315:CYS:SG	2:B:316:PHE:N	2.79	0.55
2:E:2827:ARG:HH21	2:E:2931:GLN:HG3	1.72	0.55
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.72	0.55
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.38	0.55
2:G:2827:ARG:HH21	2:G:2931:GLN:HG3	1.72	0.55
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.89	0.55
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.89	0.55
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.71	0.55
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.88	0.55
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.89	0.55
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.40	0.55
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.89	0.55
2:B:614:VAL:HG22	2:B:616:SER:H	1.71	0.55
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.88	0.55
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.88	0.55
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.88	0.55
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.89	0.55
1:F:27:THR:HB	1:F:100:ASP:HB3	1.88	0.54
2:E:132:ALA:HA	2:E:194:SER:HB2	1.88	0.54
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.71	0.54
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.40	0.54
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.73	0.54
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.88	0.54
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.40	0.54
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.40	0.54
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.88	0.54
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.88	0.54
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.54
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.89	0.54
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.54
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.89	0.54
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:27:THR:HB	1:J:100:ASP:HB3	1.88	0.54
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.90	0.54
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.89	0.54
2:E:614:VAL:HG22	2:E:616:SER:H	1.71	0.54
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	1.90	0.54
2:B:132:ALA:HA	2:B:194:SER:HB2	1.88	0.54
2:E:111:HIS:HD2	2:E:114:SER:H	1.56	0.54
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.54
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	1.90	0.54
2:B:111:HIS:HD2	2:B:114:SER:H	1.56	0.54
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.38	0.54
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.89	0.54
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.71	0.54
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.90	0.53
2:E:359:TYR:HA	2:E:376:ALA:HA	1.90	0.53
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.90	0.53
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	1.90	0.53
2:I:111:HIS:HD2	2:I:114:SER:H	1.56	0.53
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	1.90	0.53
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.53
2:G:359:TYR:HA	2:G:376:ALA:HA	1.90	0.53
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.38	0.53
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.91	0.53
2:B:1663:HIS:HD2	2:B:1707:LEU:HD11	1.74	0.53
2:G:111:HIS:HD2	2:G:114:SER:H	1.56	0.53
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.91	0.53
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.42	0.53
2:E:776:LEU:HG	2:E:848:HIS:HA	1.91	0.53
2:I:470:SER:O	2:I:474:ARG:NE	2.38	0.53
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.91	0.53
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.38	0.53
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.89	0.53
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.91	0.53
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.91	0.53
2:B:4944:ARG:HH12	2:I:4942:GLU:HB2	1.74	0.53
2:E:1663:HIS:HD2	2:E:1707:LEU:HD11	1.74	0.53
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.89	0.53
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.90	0.53
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.42	0.53
2:I:1663:HIS:HD2	2:I:1707:LEU:HD11	1.74	0.53
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.74	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.42	0.52
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.91	0.52
2:B:776:LEU:HG	2:B:848:HIS:HA	1.91	0.52
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.38	0.52
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.91	0.52
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.91	0.52
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.74	0.52
2:B:359:TYR:HA	2:B:376:ALA:HA	1.90	0.52
2:G:1663:HIS:HD2	2:G:1707:LEU:HD11	1.74	0.52
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.42	0.52
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.91	0.52
2:I:359:TYR:HA	2:I:376:ALA:HA	1.90	0.52
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.91	0.52
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.91	0.52
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.91	0.52
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.91	0.52
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.91	0.52
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.91	0.52
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.92	0.52
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.43	0.52
2:I:776:LEU:HG	2:I:848:HIS:HA	1.91	0.52
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.93	0.51
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.92	0.51
2:I:1707:LEU:HG	2:I:1708:ARG:HG3	1.92	0.51
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.93	0.51
2:I:282:ILE:HD12	2:I:314:PHE:HD2	1.76	0.51
2:G:1707:LEU:HG	2:G:1708:ARG:HG3	1.92	0.51
2:G:282:ILE:HD12	2:G:314:PHE:HD2	1.76	0.51
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.92	0.51
2:G:776:LEU:HG	2:G:848:HIS:HA	1.91	0.51
2:E:282:ILE:HD12	2:E:314:PHE:HD2	1.76	0.51
2:E:4843:LEU:HD12	2:G:4823:LEU:HD23	1.92	0.51
2:I:1078:GLU:HG3	2:I:1237:TRP:HE1	1.76	0.51
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.76	0.51
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.93	0.51
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.91	0.51
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.93	0.51
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.76	0.51
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.76	0.51
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.51
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.43	0.51
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.51
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.76	0.51
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.93	0.51
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.74	0.51
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.92	0.51
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.91	0.51
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.74	0.51
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.76	0.51
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.92	0.51
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.93	0.51
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.93	0.51
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.92	0.50
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.92	0.50
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.92	0.50
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.93	0.50
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.50
2:B:282:ILE:HD12	2:B:314:PHE:HD2	1.76	0.50
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.94	0.50
2:B:1078:GLU:HG3	2:B:1237:TRP:HE1	1.76	0.50
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.93	0.50
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.93	0.50
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.94	0.50
2:B:1707:LEU:HG	2:B:1708:ARG:HG3	1.92	0.50
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.93	0.50
2:B:470:SER:O	2:B:474:ARG:NE	2.38	0.50
2:B:520:ASN:ND2	2:B:555:GLU:OE2	2.45	0.50
2:E:520:ASN:ND2	2:E:555:GLU:OE2	2.45	0.50
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.92	0.50
2:G:520:ASN:ND2	2:G:555:GLU:OE2	2.45	0.50
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.94	0.50
2:E:1078:GLU:HG3	2:E:1237:TRP:HE1	1.76	0.50
2:E:1707:LEU:HG	2:E:1708:ARG:HG3	1.92	0.50
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.94	0.50
2:I:4228:ALA:O	2:I:4232:GLU:N	2.43	0.50
2:G:1078:GLU:HG3	2:G:1237:TRP:HE1	1.76	0.50
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.93	0.50
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.93	0.50
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.43	0.50
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.94	0.50
2:I:451:TYR:O	2:I:474:ARG:NH1	2.39	0.50
2:I:520:ASN:ND2	2:I:555:GLU:OE2	2.45	0.50
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.93	0.50
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.36	0.50
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.46	0.50
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.93	0.50
2:B:485:SER:O	2:B:489:ASN:N	2.37	0.50
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.50
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.93	0.50
2:E:698:GLY:HA2	2:E:703:GLY:HA2	1.94	0.50
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.36	0.50
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.46	0.50
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.76	0.50
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.94	0.50
2:I:4886:HIS:O	2:I:4890:GLY:N	2.45	0.50
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.92	0.50
2:B:698:GLY:HA2	2:B:703:GLY:HA2	1.94	0.49
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.36	0.49
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.49
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.94	0.49
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.45	0.49
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.94	0.49
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.94	0.49
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.93	0.49
2:E:219:VAL:O	2:E:392:ARG:NH1	2.45	0.49
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.46	0.49
2:I:219:VAL:O	2:I:392:ARG:NH1	2.45	0.49
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.38	0.49
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.76	0.49
2:E:4798:MET:HA	2:E:4801:LEU:HB2	1.95	0.49
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.45	0.49
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.94	0.49
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.76	0.49
1:J:21:THR:HA	1:J:49:ARG:HA	1.94	0.49
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.93	0.49
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.45	0.49
2:B:2758:PHE:O	2:B:2762:THR:N	2.44	0.49
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.95	0.49
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.94	0.49
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.94	0.49
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.95	0.49
2:I:4823:LEU:HD23	2:G:4843:LEU:HD12	1.95	0.49
2:G:1516:UNK:N	2:G:1529:UNK:O	2.46	0.49
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.94	0.49
2:B:978:THR:HB	2:B:980:ALA:H	1.77	0.49
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.95	0.49
2:G:219:VAL:O	2:G:392:ARG:NH1	2.45	0.49
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.95	0.49
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.94	0.49
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.43	0.49
2:G:4228:ALA:O	2:G:4232:GLU:N	2.43	0.49
2:B:1516:UNK:N	2:B:1529:UNK:O	2.46	0.49
2:E:3842:LEU:O	2:E:3929:SER:OG	2.30	0.49
1:F:21:THR:HA	1:F:49:ARG:HA	1.94	0.49
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.95	0.49
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.95	0.49
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.95	0.49
2:E:1516:UNK:N	2:E:1529:UNK:O	2.46	0.49
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.93	0.49
2:G:4798:MET:HA	2:G:4801:LEU:HB2	1.95	0.49
1:H:21:THR:HA	1:H:49:ARG:HA	1.94	0.49
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.95	0.49
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.45	0.49
2:I:1516:UNK:N	2:I:1529:UNK:O	2.46	0.49
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.94	0.49
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.94	0.48
2:B:219:VAL:O	2:B:392:ARG:NH1	2.45	0.48
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.38	0.48
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.94	0.48
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.95	0.48
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.94	0.48
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.95	0.48
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.94	0.48
2:I:4152:GLU:OE2	2:I:4180:ARG:NH1	2.46	0.48
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.95	0.48
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.95	0.48
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.93	0.48
2:B:4228:ALA:O	2:B:4232:GLU:N	2.43	0.48
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.94	0.48
1:A:21:THR:HA	1:A:49:ARG:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1973:GLN:O	2:B:1977:TYR:N	2.44	0.48
2:B:4798:MET:HA	2:B:4801:LEU:HB2	1.95	0.48
2:I:698:GLY:HA2	2:I:703:GLY:HA2	1.94	0.48
2:G:395:GLN:HG3	2:G:397:GLU:H	1.79	0.48
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.95	0.48
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.95	0.48
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.62	0.48
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.43	0.48
2:B:3842:LEU:O	2:B:3929:SER:OG	2.30	0.48
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.46	0.48
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.43	0.48
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.62	0.48
2:G:164:ARG:N	2:G:167:ASP:OD2	2.42	0.48
2:G:698:GLY:HA2	2:G:703:GLY:HA2	1.94	0.48
2:G:1973:GLN:O	2:G:1977:TYR:N	2.44	0.48
2:B:3365:UNK:O	2:B:3369:UNK:N	2.47	0.48
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.95	0.48
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.95	0.48
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.95	0.48
2:I:3365:UNK:O	2:I:3369:UNK:N	2.47	0.48
2:E:3365:UNK:O	2:E:3369:UNK:N	2.47	0.48
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.95	0.48
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.47	0.48
2:B:395:GLN:HG3	2:B:397:GLU:H	1.78	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.46	0.48
2:E:451:TYR:O	2:E:474:ARG:NH1	2.39	0.48
2:E:978:THR:HB	2:E:980:ALA:H	1.77	0.48
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.46	0.48
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.46	0.48
2:I:978:THR:HB	2:I:980:ALA:H	1.77	0.48
2:I:4798:MET:HA	2:I:4801:LEU:HB2	1.95	0.48
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.96	0.48
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.46	0.48
2:G:978:THR:HB	2:G:980:ALA:H	1.77	0.48
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.96	0.47
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.46	0.47
2:B:451:TYR:O	2:B:474:ARG:NH1	2.39	0.47
2:E:395:GLN:HG3	2:E:397:GLU:H	1.78	0.47
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.62	0.47
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.47	0.47
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1973:GLN:O	2:E:1977:TYR:N	2.44	0.47
2:E:4930:ALA:O	2:E:4934:GLY:N	2.47	0.47
2:G:4886:HIS:O	2:G:4890:GLY:N	2.45	0.47
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.95	0.47
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.47	0.47
2:I:1973:GLN:O	2:I:1977:TYR:N	2.44	0.47
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.62	0.47
2:G:3365:UNK:O	2:G:3369:UNK:N	2.47	0.47
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.46	0.47
1:J:82:TYR:O	1:J:86:GLY:N	2.45	0.47
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.97	0.47
2:I:606:LEU:O	2:I:617:ASN:ND2	2.48	0.47
2:G:606:LEU:O	2:G:617:ASN:ND2	2.48	0.47
2:G:4930:ALA:O	2:G:4934:GLY:N	2.47	0.47
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.95	0.47
2:B:4930:ALA:O	2:B:4934:GLY:N	2.47	0.47
2:E:3362:UNK:O	2:E:3366:UNK:N	2.48	0.47
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.48	0.47
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.96	0.47
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.96	0.47
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.46	0.47
2:G:3842:LEU:O	2:G:3929:SER:OG	2.30	0.47
2:G:4152:GLU:OE2	2:G:4180:ARG:NH1	2.47	0.47
2:E:606:LEU:O	2:E:617:ASN:ND2	2.48	0.47
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.38	0.47
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.47
2:I:395:GLN:HG3	2:I:397:GLU:H	1.78	0.47
2:I:3842:LEU:O	2:I:3929:SER:OG	2.30	0.47
2:I:4930:ALA:O	2:I:4934:GLY:N	2.47	0.47
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.96	0.47
2:B:606:LEU:O	2:B:617:ASN:ND2	2.48	0.47
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.96	0.47
2:G:3362:UNK:O	2:G:3366:UNK:N	2.48	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.47
2:G:3773:ARG:HG3	2:G:3815:LYS:HZ3	1.80	0.47
2:B:290:TYR:O	2:B:302:VAL:N	2.48	0.47
2:E:4152:GLU:OE2	2:E:4180:ARG:NH1	2.47	0.47
2:E:4236:SER:HG	2:E:4675:LYS:HZ1	1.58	0.47
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.97	0.47
2:G:157:ARG:HH21	2:G:164:ARG:HD2	1.80	0.47
2:G:913:LEU:O	2:G:918:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.96	0.47
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.96	0.47
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.47	0.47
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.97	0.47
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.96	0.47
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.47
2:E:913:LEU:O	2:E:918:ARG:NH2	2.48	0.47
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.96	0.47
2:I:157:ARG:HH21	2:I:164:ARG:HD2	1.80	0.47
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.47	0.47
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.45	0.47
2:I:3362:UNK:O	2:I:3366:UNK:N	2.48	0.47
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.48	0.47
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.80	0.47
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.97	0.47
2:E:290:TYR:O	2:E:302:VAL:N	2.48	0.46
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.97	0.46
2:E:4209:GLN:HE22	2:E:4560:TYR:HE2	1.63	0.46
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.98	0.46
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.46	0.46
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.47	0.46
2:G:4209:GLN:HE22	2:G:4560:TYR:HE2	1.63	0.46
2:B:164:ARG:N	2:B:167:ASP:OD2	2.42	0.46
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.47	0.46
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.46
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.97	0.46
2:E:4228:ALA:O	2:E:4232:GLU:N	2.43	0.46
2:I:290:TYR:O	2:I:302:VAL:N	2.48	0.46
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.97	0.46
1:H:82:TYR:O	1:H:86:GLY:N	2.45	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.97	0.46
2:E:164:ARG:N	2:E:167:ASP:OD2	2.42	0.46
2:E:236:ALA:HA	2:E:242:ARG:HD2	1.98	0.46
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.45	0.46
2:E:2299:VAL:O	2:E:2303:ALA:N	2.48	0.46
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.97	0.46
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.47	0.46
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.42	0.46
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.48	0.46
2:B:3362:UNK:O	2:B:3366:UNK:N	2.48	0.46
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4886:HIS:O	2:E:4890:GLY:N	2.45	0.46
2:I:913:LEU:O	2:I:918:ARG:NH2	2.48	0.46
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.46	0.46
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.48	0.46
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.33	0.46
2:B:157:ARG:HH21	2:B:164:ARG:HD2	1.80	0.46
2:B:2295:LEU:HA	2:B:2298:VAL:HG22	1.97	0.46
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.48	0.46
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.46	0.46
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.33	0.46
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.48	0.46
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.98	0.46
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.97	0.46
2:B:913:LEU:O	2:B:918:ARG:NH2	2.48	0.46
2:B:4832:HIS:NE2	2:B:4942:GLU:OE2	2.48	0.46
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.48	0.46
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.97	0.46
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.98	0.46
2:E:157:ARG:HH21	2:E:164:ARG:HD2	1.80	0.46
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.96	0.46
2:I:2758:PHE:O	2:I:2762:THR:N	2.44	0.46
2:G:4832:HIS:NE2	2:G:4942:GLU:OE2	2.48	0.46
2:B:236:ALA:HA	2:B:242:ARG:HD2	1.98	0.46
2:B:2432:LEU:O	2:B:2436:CYS:N	2.49	0.46
2:E:689:THR:H	2:E:778:PHE:HE2	1.64	0.46
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.96	0.46
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.46
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.97	0.46
2:B:4080:TYR:CZ	2:B:4096:ALA:HB3	2.51	0.46
2:E:4832:HIS:NE2	2:E:4942:GLU:OE2	2.48	0.46
2:I:485:SER:O	2:I:489:ASN:N	2.37	0.46
2:I:670:GLU:HG3	2:I:788:LYS:H	1.81	0.46
2:I:2432:LEU:O	2:I:2436:CYS:N	2.49	0.46
2:B:689:THR:H	2:B:778:PHE:HE2	1.64	0.46
2:B:2299:VAL:O	2:B:2303:ALA:N	2.49	0.46
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.49	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.44	0.46
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.97	0.46
2:G:290:TYR:O	2:G:302:VAL:N	2.48	0.46
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.99	0.45
2:B:4209:GLN:HE22	2:B:4560:TYR:HE2	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2295:LEU:HA	2:E:2298:VAL:HG22	1.97	0.45
2:I:236:ALA:HA	2:I:242:ARG:HD2	1.98	0.45
2:I:4209:GLN:HE22	2:I:4560:TYR:HE2	1.63	0.45
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.49	0.45
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.45	0.45
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.98	0.45
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.97	0.45
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.36	0.45
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.97	0.45
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.97	0.45
2:B:670:GLU:HG3	2:B:788:LYS:H	1.81	0.45
2:E:670:GLU:HG3	2:E:788:LYS:H	1.81	0.45
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.98	0.45
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.98	0.45
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.97	0.45
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.98	0.45
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.45
2:G:215:THR:HG22	2:G:273:HIS:HA	1.98	0.45
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.97	0.45
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.82	0.45
2:G:4863:TYR:HD2	2:G:4875:LYS:HB2	1.82	0.45
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.45	0.45
2:B:4642:ALA:HA	2:B:4645:CYS:HB2	1.98	0.45
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.97	0.45
2:G:670:GLU:HG3	2:G:788:LYS:H	1.81	0.45
2:B:4886:HIS:O	2:B:4890:GLY:N	2.45	0.45
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.98	0.45
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.97	0.45
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.82	0.45
2:I:4863:TYR:HD2	2:I:4875:LYS:HB2	1.82	0.45
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.99	0.45
2:G:2295:LEU:HA	2:G:2298:VAL:HG22	1.97	0.45
2:B:215:THR:HG22	2:B:273:HIS:HA	1.98	0.45
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.50	0.45
2:B:4863:TYR:HD2	2:B:4875:LYS:HB2	1.82	0.45
2:I:2295:LEU:HA	2:I:2298:VAL:HG22	1.97	0.45
2:I:2299:VAL:O	2:I:2303:ALA:N	2.49	0.45
2:I:4642:ALA:HA	2:I:4645:CYS:HB2	1.98	0.45
2:G:2290:LEU:HG	2:G:2291:GLN:H	1.82	0.45
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.33	0.45
2:B:2290:LEU:HG	2:B:2291:GLN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4863:TYR:HD2	2:E:4875:LYS:HB2	1.82	0.45
2:I:2290:LEU:HG	2:I:2291:GLN:H	1.82	0.45
2:G:236:ALA:HA	2:G:242:ARG:HD2	1.98	0.45
2:I:939:VAL:HG22	2:I:1053:ILE:HG23	1.99	0.45
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	1.99	0.45
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.97	0.45
2:B:4942:GLU:HB2	2:E:4944:ARG:HH12	1.81	0.45
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.97	0.45
2:I:689:THR:H	2:I:778:PHE:HE2	1.64	0.45
2:I:4851:TYR:HD2	2:I:4920:PHE:HD1	1.65	0.45
2:G:2758:PHE:O	2:G:2762:THR:N	2.44	0.45
2:G:4642:ALA:HA	2:G:4645:CYS:HB2	1.98	0.45
1:A:82:TYR:O	1:A:86:GLY:N	2.45	0.44
2:E:2290:LEU:HG	2:E:2291:GLN:H	1.82	0.44
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.50	0.44
2:E:4080:TYR:CZ	2:E:4096:ALA:HB3	2.51	0.44
2:I:210:GLU:H	2:I:273:HIS:HE1	1.66	0.44
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.99	0.44
2:G:470:SER:O	2:G:474:ARG:NE	2.38	0.44
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	1.99	0.44
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.49	0.44
2:I:618:GLN:OE1	2:I:1678:ASN:ND2	2.51	0.44
2:I:4080:TYR:CZ	2:I:4096:ALA:HB3	2.51	0.44
2:G:45:ARG:HG2	2:G:443:LEU:HD21	2.00	0.44
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.51	0.44
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.33	0.44
2:E:4642:ALA:HA	2:E:4645:CYS:HB2	1.98	0.44
2:G:485:SER:O	2:G:489:ASN:N	2.37	0.44
2:G:618:GLN:OE1	2:G:1678:ASN:ND2	2.51	0.44
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	1.99	0.44
2:G:4080:TYR:CZ	2:G:4096:ALA:HB3	2.51	0.44
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.50	0.44
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.00	0.44
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	2.00	0.44
2:B:4851:TYR:HD2	2:B:4920:PHE:HD1	1.65	0.44
2:E:210:GLU:H	2:E:273:HIS:HE1	1.66	0.44
2:E:215:THR:HG22	2:E:273:HIS:HA	1.98	0.44
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.99	0.44
2:G:451:TYR:O	2:G:474:ARG:NH1	2.39	0.44
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.99	0.44
2:I:2243:SER:HB3	2:I:2246:ASN:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:GLU:H	2:B:273:HIS:HE1	1.66	0.44
2:B:939:VAL:HG22	2:B:1053:ILE:HG23	1.99	0.44
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.00	0.44
2:E:41:GLY:O	2:E:45:ARG:NH1	2.51	0.44
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.46	0.44
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	2.00	0.44
2:E:4942:GLU:HB2	2:G:4944:ARG:HH12	1.82	0.44
2:I:41:GLY:O	2:I:45:ARG:NH1	2.51	0.44
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	2.00	0.44
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.46	0.44
2:E:580:GLU:HG2	2:E:583:ILE:HD11	2.00	0.44
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.50	0.44
2:I:45:ARG:HG2	2:I:443:LEU:HD21	2.00	0.44
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	1.99	0.44
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.46	0.44
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.83	0.44
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.00	0.44
2:B:4914:VAL:HG23	2:E:4888:TYR:HD1	1.83	0.44
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.83	0.44
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	2.00	0.44
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.50	0.44
1:F:82:TYR:O	1:F:86:GLY:N	2.45	0.44
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	1.99	0.44
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.00	0.44
2:I:215:THR:HG22	2:I:273:HIS:HA	1.98	0.44
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.50	0.44
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.00	0.44
2:G:210:GLU:H	2:G:273:HIS:HE1	1.66	0.44
2:B:41:GLY:O	2:B:45:ARG:NH1	2.51	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.82	0.43
2:G:689:THR:H	2:G:778:PHE:HE2	1.64	0.43
2:G:4851:TYR:HD2	2:G:4920:PHE:HD1	1.65	0.43
2:I:575:LEU:HD22	2:I:609:CYS:HB3	2.01	0.43
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.51	0.43
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	2.00	0.43
2:G:41:GLY:O	2:G:45:ARG:NH1	2.51	0.43
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.83	0.43
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.51	0.43
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.76	0.43
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.99	0.43
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4832:HIS:NE2	2:I:4942:GLU:OE2	2.48	0.43
2:G:4066:LEU:HD11	2:G:4173:TYR:HB2	2.00	0.43
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	1.99	0.43
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.83	0.43
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.00	0.43
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.51	0.43
2:G:2243:SER:HB3	2:G:2246:ASN:H	1.83	0.43
1:A:74:LEU:HB2	1:A:99:PHE:HB2	2.00	0.43
2:E:218:HIS:HB3	2:E:392:ARG:HD3	2.01	0.43
2:E:939:VAL:HG22	2:E:1053:ILE:HG23	1.99	0.43
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.00	0.43
2:G:206:CYS:SG	2:G:207:SER:N	2.92	0.43
2:G:575:LEU:HD22	2:G:609:CYS:HB3	2.01	0.43
2:G:939:VAL:HG22	2:G:1053:ILE:HG23	1.99	0.43
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	2.00	0.43
2:B:580:GLU:HG2	2:B:583:ILE:HD11	2.00	0.43
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.51	0.43
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.52	0.43
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	2.00	0.43
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.00	0.43
2:E:4851:TYR:HD2	2:E:4920:PHE:HD1	1.65	0.43
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.00	0.43
2:I:4944:ARG:HH12	2:G:4942:GLU:HB2	1.82	0.43
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.76	0.43
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.83	0.43
1:F:74:LEU:HB2	1:F:99:PHE:HB2	2.00	0.43
2:B:45:ARG:HG2	2:B:443:LEU:HD21	2.00	0.43
2:B:2243:SER:HB3	2:B:2246:ASN:H	1.83	0.43
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.84	0.43
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.82	0.43
2:E:1641:ILE:HA	2:E:1642:PRO:HD3	1.89	0.43
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.00	0.43
2:I:3773:ARG:HG3	2:I:3815:LYS:HZ3	1.83	0.43
2:I:4066:LEU:HD11	2:I:4173:TYR:HB2	2.00	0.43
2:G:864:PRO:HD2	2:G:867:LEU:HD12	2.01	0.43
2:G:2332:LEU:HD13	2:G:2335:LEU:HD12	2.01	0.43
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.52	0.43
2:I:767:VAL:HG12	2:I:769:GLU:HG3	2.01	0.43
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.46	0.43
2:G:767:VAL:HG12	2:G:769:GLU:HG3	2.01	0.43
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:793:LEU:HD22	2:B:821:LEU:HD13	2.00	0.43
2:B:864:PRO:HD2	2:B:867:LEU:HD12	2.01	0.43
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.00	0.43
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.50	0.43
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.00	0.43
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.51	0.43
2:E:2243:SER:HB3	2:E:2246:ASN:H	1.83	0.43
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.84	0.43
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.52	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.92	0.43
2:B:4066:LEU:HD11	2:B:4173:TYR:HB2	2.00	0.43
2:B:4570:ALA:O	2:B:4574:ASN:ND2	2.52	0.43
2:E:4066:LEU:HD11	2:E:4173:TYR:HB2	2.00	0.43
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.50	0.43
2:G:580:GLU:HG2	2:G:583:ILE:HD11	2.00	0.43
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.00	0.42
2:I:164:ARG:N	2:I:167:ASP:OD2	2.41	0.42
2:I:580:GLU:HG2	2:I:583:ILE:HD11	2.00	0.42
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.84	0.42
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	2.00	0.42
1:J:74:LEU:HB2	1:J:99:PHE:HB2	2.00	0.42
2:B:575:LEU:HD22	2:B:609:CYS:HB3	2.01	0.42
2:B:767:VAL:HG12	2:B:769:GLU:HG3	2.01	0.42
2:B:2332:LEU:HD13	2:B:2335:LEU:HD12	2.01	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	1.99	0.42
2:E:575:LEU:HD22	2:E:609:CYS:HB3	2.01	0.42
2:E:4956:THR:O	2:E:4965:SER:N	2.52	0.42
2:I:206:CYS:SG	2:I:207:SER:N	2.92	0.42
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.84	0.42
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.00	0.42
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.00	0.42
2:E:485:SER:O	2:E:489:ASN:N	2.37	0.42
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.84	0.42
2:I:1641:ILE:HA	2:I:1642:PRO:HD3	1.89	0.42
2:I:4570:ALA:O	2:I:4574:ASN:ND2	2.52	0.42
2:I:4956:THR:O	2:I:4965:SER:N	2.52	0.42
1:H:74:LEU:HB2	1:H:99:PHE:HB2	2.00	0.42
2:B:218:HIS:HB3	2:B:392:ARG:HD3	2.01	0.42
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.84	0.42
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.51	0.42
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:629:ARG:HD3	2:E:634:GLN:HG2	2.01	0.42
2:E:767:VAL:HG12	2:E:769:GLU:HG3	2.01	0.42
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.76	0.42
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.52	0.42
2:G:218:HIS:HB3	2:G:392:ARG:HD3	2.01	0.42
2:G:2432:LEU:O	2:G:2436:CYS:N	2.49	0.42
2:B:734:GLY:O	2:B:736:HIS:ND1	2.53	0.42
2:B:940:GLY:O	2:B:1052:ASN:N	2.53	0.42
2:B:1720:LEU:HD23	2:B:1721:GLU:HA	2.02	0.42
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.84	0.42
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.55	0.42
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.84	0.42
2:G:530:ILE:HD13	2:G:536:ASN:HB3	2.02	0.42
2:B:379:HIS:CD2	2:B:381:GLU:H	2.37	0.42
2:B:2423:MET:O	2:B:2427:ALA:N	2.48	0.42
2:E:45:ARG:HG2	2:E:443:LEU:HD21	2.00	0.42
2:E:530:ILE:HD13	2:E:536:ASN:HB3	2.02	0.42
2:E:793:LEU:HD22	2:E:821:LEU:HD13	2.00	0.42
2:I:218:HIS:HB3	2:I:392:ARG:HD3	2.01	0.42
2:I:793:LEU:HD22	2:I:821:LEU:HD13	2.00	0.42
2:I:1720:LEU:HD23	2:I:1721:GLU:HA	2.02	0.42
2:G:2299:VAL:O	2:G:2303:ALA:N	2.48	0.42
2:G:4570:ALA:O	2:G:4574:ASN:ND2	2.52	0.42
2:B:134:ASP:OD1	2:B:134:ASP:N	2.53	0.42
2:B:4956:THR:O	2:B:4965:SER:N	2.52	0.42
2:E:4570:ALA:O	2:E:4574:ASN:ND2	2.52	0.42
2:G:793:LEU:HD22	2:G:821:LEU:HD13	2.00	0.42
2:B:629:ARG:HD3	2:B:634:GLN:HG2	2.01	0.42
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.84	0.42
2:B:2195:PRO:HB3	2:B:2246:ASN:HD21	1.84	0.42
2:B:2517:UNK:O	2:B:2521:UNK:N	2.53	0.42
2:E:134:ASP:N	2:E:134:ASP:OD1	2.53	0.42
2:E:2195:PRO:HB3	2:E:2246:ASN:HD21	1.84	0.42
2:E:2517:UNK:O	2:E:2521:UNK:N	2.53	0.42
2:I:629:ARG:HB3	2:I:634:GLN:NE2	2.35	0.42
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	2.01	0.42
2:G:940:GLY:O	2:G:1052:ASN:N	2.53	0.42
2:G:1641:ILE:HA	2:G:1642:PRO:HD3	1.89	0.42
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.30	0.42
2:B:4083:ASP:HB3	2:B:4086:GLY:H	1.85	0.42
2:I:103:TYR:HB3	2:I:152:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:379:HIS:CD2	2:I:381:GLU:H	2.37	0.42
2:I:4083:ASP:HB3	2:I:4086:GLY:H	1.85	0.42
2:G:629:ARG:HD3	2:G:634:GLN:HG2	2.01	0.42
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.02	0.42
2:B:4641:PRO:O	2:B:4645:CYS:N	2.52	0.42
2:E:206:CYS:SG	2:E:207:SER:N	2.92	0.42
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.00	0.42
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	2.01	0.42
2:I:864:PRO:HD2	2:I:867:LEU:HD12	2.01	0.42
2:I:1940:CYS:O	2:I:1944:GLU:N	2.53	0.42
2:I:2517:UNK:O	2:I:2521:UNK:N	2.53	0.42
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.55	0.42
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	2.02	0.41
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.01	0.41
2:B:3915:ILE:O	2:B:3919:THR:N	2.52	0.41
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.93	0.41
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.55	0.41
2:E:2332:LEU:HD13	2:E:2335:LEU:HD12	2.01	0.41
2:E:2432:LEU:O	2:E:2436:CYS:N	2.49	0.41
2:I:40:GLU:HB3	2:I:44:ASN:HB3	2.02	0.41
2:G:234:SER:O	2:G:242:ARG:NE	2.52	0.41
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.84	0.41
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.85	0.41
2:E:103:TYR:HB3	2:E:152:PRO:HD3	2.02	0.41
2:I:234:SER:O	2:I:242:ARG:NE	2.52	0.41
2:I:530:ILE:HD13	2:I:536:ASN:HB3	2.02	0.41
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	2.02	0.41
2:G:4956:THR:O	2:G:4965:SER:N	2.52	0.41
1:H:44:LYS:HA	1:H:45:PRO:HD3	1.88	0.41
2:E:40:GLU:HB3	2:E:44:ASN:HB3	2.03	0.41
2:E:234:SER:O	2:E:242:ARG:NE	2.52	0.41
2:E:379:HIS:CD2	2:E:381:GLU:H	2.37	0.41
2:E:940:GLY:O	2:E:1052:ASN:N	2.53	0.41
2:E:1720:LEU:HD23	2:E:1721:GLU:HA	2.02	0.41
2:I:734:GLY:O	2:I:736:HIS:ND1	2.53	0.41
2:G:107:ILE:HG22	2:G:148:TRP:HB2	2.03	0.41
2:G:379:HIS:CD2	2:G:381:GLU:H	2.37	0.41
2:G:2517:UNK:O	2:G:2521:UNK:N	2.53	0.41
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.93	0.41
2:B:870:ILE:HD11	2:B:1049:TYR:CG	2.55	0.41
2:E:107:ILE:HG22	2:E:148:TRP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	2.02	0.41
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.02	0.41
2:E:4233:LEU:HA	2:E:4236:SER:HB3	2.03	0.41
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.54	0.41
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	2.03	0.41
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.85	0.41
2:G:134:ASP:OD1	2:G:134:ASP:N	2.53	0.41
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.93	0.41
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.35	0.41
2:G:1720:LEU:HD23	2:G:1721:GLU:HA	2.02	0.41
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	2.01	0.41
2:B:530:ILE:HD13	2:B:536:ASN:HB3	2.02	0.41
2:B:4233:LEU:HA	2:B:4236:SER:HB3	2.03	0.41
2:E:864:PRO:HD2	2:E:867:LEU:HD12	2.01	0.41
2:E:946:ALA:HA	2:E:949:ASN:HB2	2.03	0.41
2:I:629:ARG:HD3	2:I:634:GLN:HG2	2.01	0.41
2:I:940:GLY:O	2:I:1052:ASN:N	2.53	0.41
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.54	0.41
2:G:2195:PRO:HB3	2:G:2246:ASN:HD21	1.85	0.41
2:G:2423:MET:O	2:G:2427:ALA:N	2.48	0.41
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.02	0.41
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.85	0.41
2:B:40:GLU:HB3	2:B:44:ASN:HB3	2.02	0.41
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.35	0.41
2:B:4804:TYR:HB3	2:B:4806:ASN:HD22	1.85	0.41
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.86	0.41
2:I:4804:TYR:HB3	2:I:4806:ASN:HD22	1.85	0.41
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.41
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	2.03	0.41
2:B:357:LEU:HD12	2:B:388:LEU:HD11	2.03	0.41
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.86	0.41
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	2.02	0.41
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.35	0.41
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.94	0.41
2:E:1940:CYS:O	2:E:1944:GLU:N	2.53	0.41
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	2.03	0.41
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.93	0.41
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.02	0.41
2:I:2674:UNK:O	2:I:2676:UNK:N	2.54	0.41
2:G:2674:UNK:O	2:G:2676:UNK:N	2.54	0.41
2:G:4804:TYR:HB3	2:G:4806:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TYR:HB3	2:B:152:PRO:HD3	2.02	0.41
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.86	0.41
2:B:2232:CYS:SG	2:B:2233:CYS:N	2.94	0.41
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	2.03	0.41
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.54	0.41
2:E:2143:THR:N	2:E:3651:ASN:OD1	2.54	0.41
2:I:946:ALA:HA	2:I:949:ASN:HB2	2.03	0.41
2:I:2332:LEU:HD13	2:I:2335:LEU:HD12	2.01	0.41
2:I:3513:UNK:O	2:I:3515:UNK:N	2.54	0.41
2:I:3889:GLN:HG3	2:I:3967:GLU:HG3	2.03	0.41
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	2.03	0.41
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	2.03	0.41
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	2.02	0.41
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	2.03	0.41
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	2.03	0.41
1:F:92:PRO:HD3	2:E:627:PRO:HB2	2.02	0.41
2:B:55:ALA:O	2:B:281:ARG:NH2	2.54	0.41
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.41
2:E:2674:UNK:O	2:E:2676:UNK:N	2.54	0.41
2:E:4083:ASP:HB3	2:E:4086:GLY:H	1.85	0.41
2:E:4142:ASN:HA	2:E:4145:VAL:HG12	2.02	0.41
2:E:4641:PRO:O	2:E:4645:CYS:N	2.52	0.41
2:I:134:ASP:OD1	2:I:134:ASP:N	2.53	0.41
2:I:2143:THR:N	2:I:3651:ASN:OD1	2.54	0.41
2:I:2195:PRO:HB3	2:I:2246:ASN:HD21	1.84	0.41
2:I:2232:CYS:SG	2:I:2233:CYS:N	2.94	0.41
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	2.03	0.41
2:G:40:GLU:HB3	2:G:44:ASN:HB3	2.03	0.41
2:G:103:TYR:HB3	2:G:152:PRO:HD3	2.02	0.41
2:G:4083:ASP:HB3	2:G:4086:GLY:H	1.85	0.41
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	2.02	0.41
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	2.03	0.41
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	2.03	0.41
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	2.03	0.41
2:E:4918:ILE:HD13	2:E:4918:ILE:HA	1.93	0.41
2:I:2346:VAL:HG13	2:I:2349:ASN:H	1.86	0.41
2:G:3513:UNK:O	2:G:3515:UNK:N	2.54	0.41
2:G:4233:LEU:HA	2:G:4236:SER:HB3	2.02	0.41
1:J:44:LYS:HA	1:J:45:PRO:HD3	1.88	0.40
2:B:2346:VAL:HG13	2:B:2349:ASN:H	1.86	0.40
2:B:3513:UNK:O	2:B:3515:UNK:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:214:VAL:HG22	2:I:341:TYR:CE1	2.56	0.40
2:I:4983:HIS:HB2	2:I:4988:TYR:HE2	1.86	0.40
2:G:35:LEU:HD13	2:G:49:LEU:HD13	2.03	0.40
2:G:3915:ILE:O	2:G:3919:THR:N	2.52	0.40
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.53	0.40
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	2.03	0.40
2:G:4983:HIS:HB2	2:G:4988:TYR:HE2	1.86	0.40
2:B:234:SER:O	2:B:242:ARG:NE	2.52	0.40
2:B:1641:ILE:HA	2:B:1642:PRO:HD3	1.89	0.40
2:B:1940:CYS:O	2:B:1944:GLU:N	2.53	0.40
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	2.03	0.40
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	2.03	0.40
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.03	0.40
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.85	0.40
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.86	0.40
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	2.03	0.40
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.03	0.40
2:G:838:HIS:HA	2:G:1201:HIS:HB3	2.04	0.40
2:G:2143:THR:N	2:G:3651:ASN:OD1	2.54	0.40
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.86	0.40
2:E:2232:CYS:SG	2:E:2233:CYS:N	2.94	0.40
2:E:3513:UNK:O	2:E:3515:UNK:N	2.54	0.40
2:E:4763:GLY:H	2:E:4767:TRP:HE1	1.69	0.40
2:E:4804:TYR:HB3	2:E:4806:ASN:HD22	1.85	0.40
2:I:4233:LEU:HA	2:I:4236:SER:HB3	2.03	0.40
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.03	0.40
2:B:614:VAL:HA	2:B:2169:GLN:HB3	2.03	0.40
2:B:708:GLY:HA3	2:B:722:TRP:HB3	2.03	0.40
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.76	0.40
2:B:4763:GLY:H	2:B:4767:TRP:HE1	1.69	0.40
2:B:4983:HIS:HB2	2:B:4988:TYR:HE2	1.86	0.40
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.03	0.40
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.39	0.40
2:E:4983:HIS:HB2	2:E:4988:TYR:HE2	1.86	0.40
2:E:5000:GLU:HA	2:E:5003:HIS:CD2	2.57	0.40
2:I:55:ALA:O	2:I:281:ARG:NH2	2.54	0.40
2:I:107:ILE:HG22	2:I:148:TRP:HB2	2.03	0.40
2:I:838:HIS:HA	2:I:1201:HIS:HB3	2.03	0.40
2:I:2021:CYS:HA	2:I:2022:PRO:HD3	1.96	0.40
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.86	0.40
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:838:HIS:HA	2:B:1201:HIS:HB3	2.04	0.40
2:B:946:ALA:HA	2:B:949:ASN:HB2	2.03	0.40
2:E:2034:PHE:O	2:E:2038:LEU:N	2.55	0.40
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.53	0.40
2:I:471:LEU:O	2:I:475:GLN:N	2.53	0.40
2:I:708:GLY:HA3	2:I:722:TRP:HB3	2.03	0.40
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.53	0.40
2:G:864:PRO:HA	2:G:865:PRO:HD3	1.94	0.40
2:G:1940:CYS:O	2:G:1944:GLU:N	2.53	0.40
2:G:2437:ALA:HA	2:G:2438:PRO:HD3	1.96	0.40
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2877 (89%)	352 (11%)	6 (0%)	47	80
2	E	3235/4416 (73%)	2878 (89%)	351 (11%)	6 (0%)	47	80
2	G	3235/4416 (73%)	2877 (89%)	352 (11%)	6 (0%)	47	80
2	I	3235/4416 (73%)	2878 (89%)	351 (11%)	6 (0%)	47	80
All	All	13360/18096 (74%)	11884 (89%)	1452 (11%)	24 (0%)	50	80

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1840	PRO
2	B	1932	PRO
2	B	4641	PRO
2	E	1708	ARG
2	E	1840	PRO
2	E	1932	PRO
2	E	4641	PRO
2	I	1708	ARG
2	I	1840	PRO
2	I	1932	PRO
2	I	4641	PRO
2	G	1708	ARG
2	G	1840	PRO
2	G	1932	PRO
2	G	4641	PRO
2	B	2291	GLN
2	B	4640	GLU
2	E	2291	GLN
2	E	4640	GLU
2	I	2291	GLN
2	I	4640	GLU
2	G	2291	GLN
2	G	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
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	84	90

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	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	4818	MET
2	B	4954	MET
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
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
2	E	4085	ARG
2	E	4120	ASN
2	E	4818	MET
2	E	4954	MET

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Mol	Chain	Res	Type
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
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	4818	MET
2	I	4954	MET
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
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	4818	MET
2	G	4954	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS

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Mol	Chain	Res	Type
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	405	HIS
2	B	413	GLN
2	B	479	GLN
2	B	520	ASN
2	B	725	HIS
2	B	949	ASN
2	B	1598	GLN
2	B	1663	HIS
2	B	1679	ASN
2	B	1691	GLN
2	B	1693	GLN
2	B	1702	HIS
2	B	1719	HIS
2	B	1775	HIS
2	B	1972	ASN
2	B	2005	GLN
2	B	2127	GLN
2	B	2291	GLN
2	B	3771	HIS
2	B	3781	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4209	GLN
2	B	4691	GLN
2	B	4806	ASN
2	B	5003	HIS
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	273	HIS

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Mol	Chain	Res	Type
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	405	HIS
2	E	413	GLN
2	E	479	GLN
2	E	520	ASN
2	E	725	HIS
2	E	949	ASN
2	E	1598	GLN
2	E	1663	HIS
2	E	1679	ASN
2	E	1691	GLN
2	E	1693	GLN
2	E	1702	HIS
2	E	1719	HIS
2	E	1775	HIS
2	E	1972	ASN
2	E	2005	GLN
2	E	2127	GLN
2	E	2291	GLN
2	E	3771	HIS
2	E	3781	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4209	GLN
2	E	4691	GLN
2	E	4806	ASN
2	E	5003	HIS
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	405	HIS

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Mol	Chain	Res	Type
2	I	413	GLN
2	I	479	GLN
2	I	520	ASN
2	I	725	HIS
2	I	949	ASN
2	I	1598	GLN
2	I	1663	HIS
2	I	1679	ASN
2	I	1691	GLN
2	I	1693	GLN
2	I	1702	HIS
2	I	1719	HIS
2	I	1775	HIS
2	I	1972	ASN
2	I	2005	GLN
2	I	2127	GLN
2	I	2291	GLN
2	I	3771	HIS
2	I	3781	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4209	GLN
2	I	4691	GLN
2	I	4806	ASN
2	I	5003	HIS
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	405	HIS
2	G	413	GLN
2	G	479	GLN
2	G	520	ASN
2	G	725	HIS

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Mol	Chain	Res	Type
2	G	949	ASN
2	G	1598	GLN
2	G	1663	HIS
2	G	1679	ASN
2	G	1691	GLN
2	G	1693	GLN
2	G	1702	HIS
2	G	1719	HIS
2	G	1775	HIS
2	G	1972	ASN
2	G	2005	GLN
2	G	2127	GLN
2	G	2291	GLN
2	G	3771	HIS
2	G	3781	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4142	ASN
2	G	4209	GLN
2	G	4691	GLN
2	G	4806	ASN
2	G	5003	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	0.87	1 (3%)	31,52,52	1.54	5 (16%)
3	ATP	I	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.55	5 (16%)
3	ATP	B	5101	-	26,33,33	0.87	1 (3%)	31,52,52	1.57	5 (16%)
4	CFF	E	5102	-	8,15,15	2.53	3 (37%)	8,23,23	1.20	1 (12%)
4	CFF	G	5102	-	8,15,15	2.53	4 (50%)	8,23,23	1.19	1 (12%)
3	ATP	G	5101	-	26,33,33	0.87	1 (3%)	31,52,52	1.54	5 (16%)
4	CFF	I	5102	-	8,15,15	2.53	3 (37%)	8,23,23	1.19	1 (12%)
4	CFF	B	5102	-	8,15,15	2.52	3 (37%)	8,23,23	1.19	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	-	-	4/18/38/38	0/3/3/3
3	ATP	I	5101	-	-	4/18/38/38	0/3/3/3
3	ATP	B	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	B	5102	-	-	-	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C6-N1	-4.46	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	C6-N1	-4.46	1.31	1.38
4	G	5102	CFF	C6-N1	-4.44	1.31	1.38
4	B	5102	CFF	C6-N1	-4.43	1.31	1.38
4	E	5102	CFF	C5-C4	-4.41	1.33	1.39
4	G	5102	CFF	C5-C4	-4.39	1.33	1.39
4	B	5102	CFF	C5-C4	-4.39	1.33	1.39
4	I	5102	CFF	C5-C4	-4.39	1.33	1.39
4	E	5102	CFF	O13-C6	-2.31	1.18	1.24
4	G	5102	CFF	O13-C6	-2.31	1.18	1.24
4	I	5102	CFF	O13-C6	-2.30	1.18	1.24
4	B	5102	CFF	O13-C6	-2.29	1.18	1.24
3	I	5101	ATP	C5-C4	2.20	1.46	1.40
3	E	5101	ATP	C5-C4	2.20	1.46	1.40
3	G	5101	ATP	C5-C4	2.19	1.46	1.40
3	B	5101	ATP	C5-C4	2.19	1.46	1.40
4	G	5102	CFF	C5-C6	-2.00	1.37	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5101	ATP	PB-O3B-PG	-3.54	120.69	132.83
3	E	5101	ATP	PB-O3B-PG	-3.53	120.71	132.83
3	G	5101	ATP	PB-O3B-PG	-3.51	120.77	132.83
3	B	5101	ATP	PB-O3B-PG	-3.51	120.80	132.83
3	E	5101	ATP	PA-O3A-PB	-3.35	121.34	132.83
3	G	5101	ATP	PA-O3A-PB	-3.34	121.36	132.83
3	B	5101	ATP	PA-O3A-PB	-3.34	121.38	132.83
3	I	5101	ATP	PA-O3A-PB	-3.33	121.38	132.83
3	B	5101	ATP	N3-C2-N1	-3.23	123.64	128.68
3	G	5101	ATP	N3-C2-N1	-3.14	123.77	128.68
3	E	5101	ATP	N3-C2-N1	-3.12	123.80	128.68
3	I	5101	ATP	N3-C2-N1	-3.10	123.83	128.68
4	B	5102	CFF	C14-N7-C8	-2.81	111.89	125.43
4	G	5102	CFF	C14-N7-C8	-2.81	111.91	125.43
4	E	5102	CFF	C14-N7-C8	-2.80	111.93	125.43
4	I	5102	CFF	C14-N7-C8	-2.80	111.94	125.43
3	B	5101	ATP	C4-C5-N7	-2.75	106.53	109.40
3	E	5101	ATP	C4-C5-N7	-2.74	106.55	109.40
3	G	5101	ATP	C4-C5-N7	-2.72	106.57	109.40
3	I	5101	ATP	C4-C5-N7	-2.71	106.58	109.40
3	I	5101	ATP	C3'-C2'-C1'	2.57	104.85	100.98
3	B	5101	ATP	C3'-C2'-C1'	2.57	104.85	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5101	ATP	C3'-C2'-C1'	2.57	104.84	100.98
3	E	5101	ATP	C3'-C2'-C1'	2.56	104.83	100.98

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	PA-O3A-PB-O1B
3	E	5101	ATP	PA-O3A-PB-O1B
3	I	5101	ATP	PA-O3A-PB-O1B
3	G	5101	ATP	PA-O3A-PB-O1B
3	E	5101	ATP	PA-O3A-PB-O2B
3	I	5101	ATP	PA-O3A-PB-O2B
3	G	5101	ATP	PA-O3A-PB-O2B
3	B	5101	ATP	PA-O3A-PB-O2B
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	E	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'

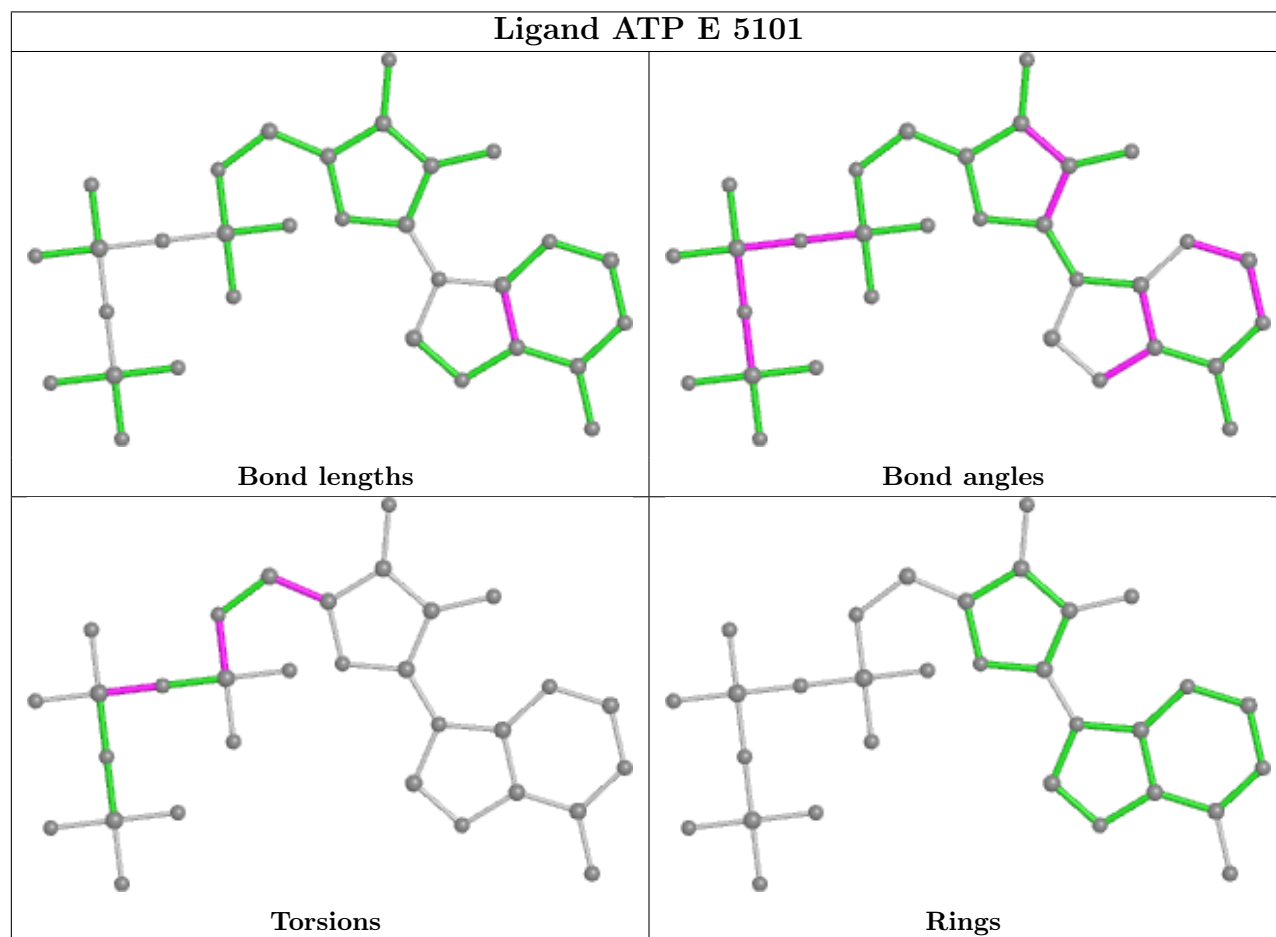
There are no ring outliers.

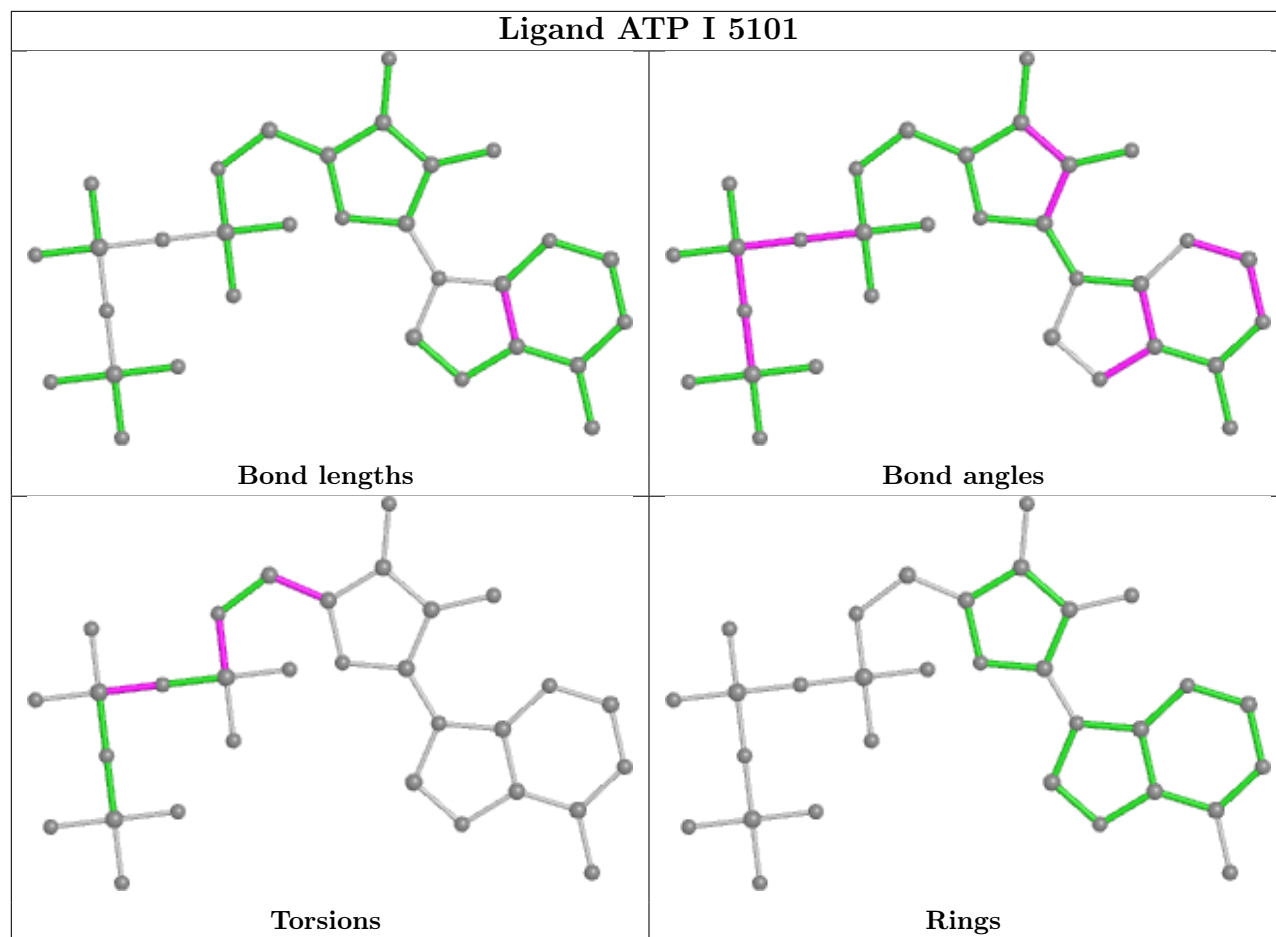
5 monomers are involved in 5 short contacts:

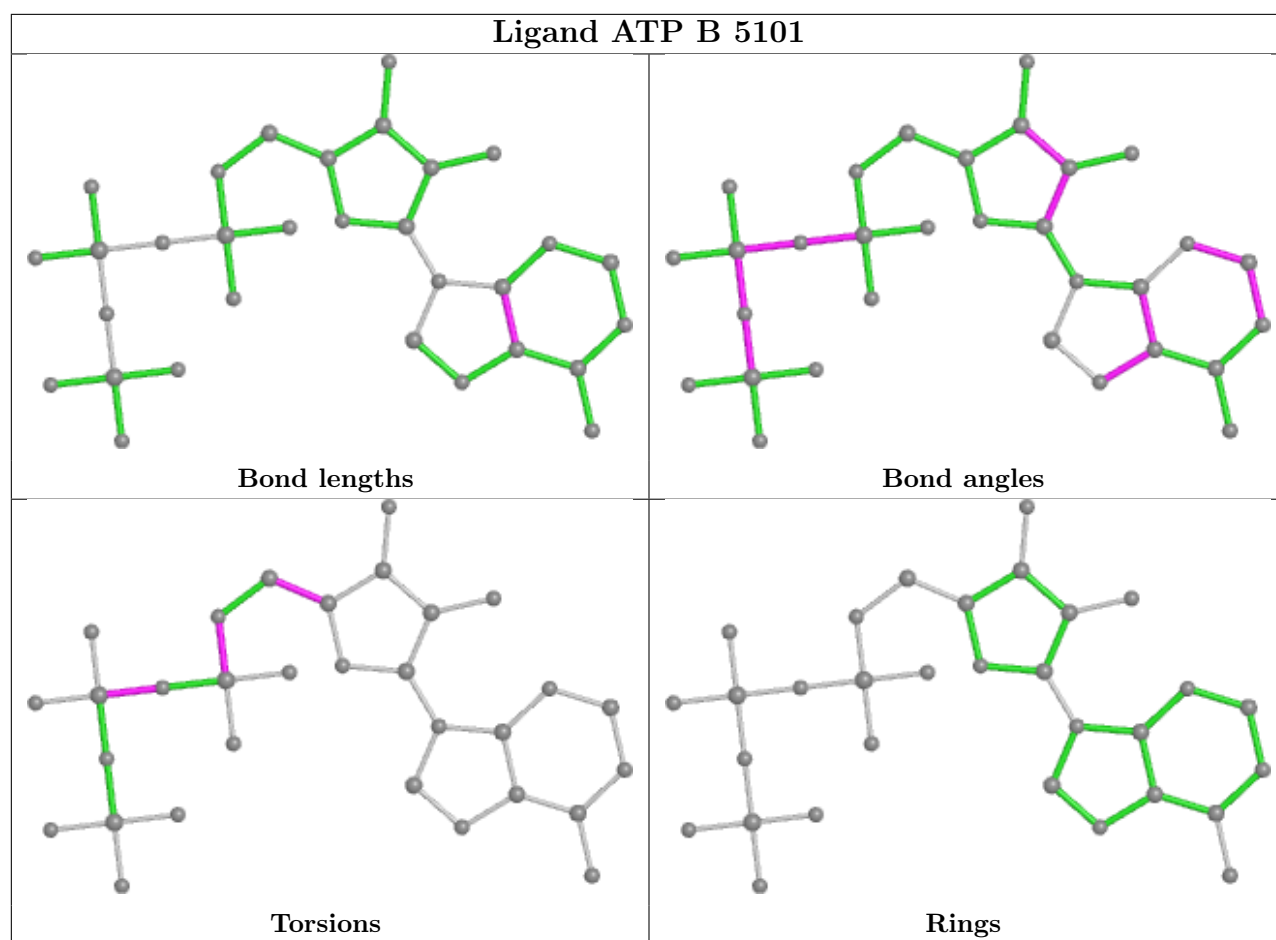
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
4	E	5102	CFF	1	0
4	G	5102	CFF	1	0
4	I	5102	CFF	1	0
4	B	5102	CFF	1	0

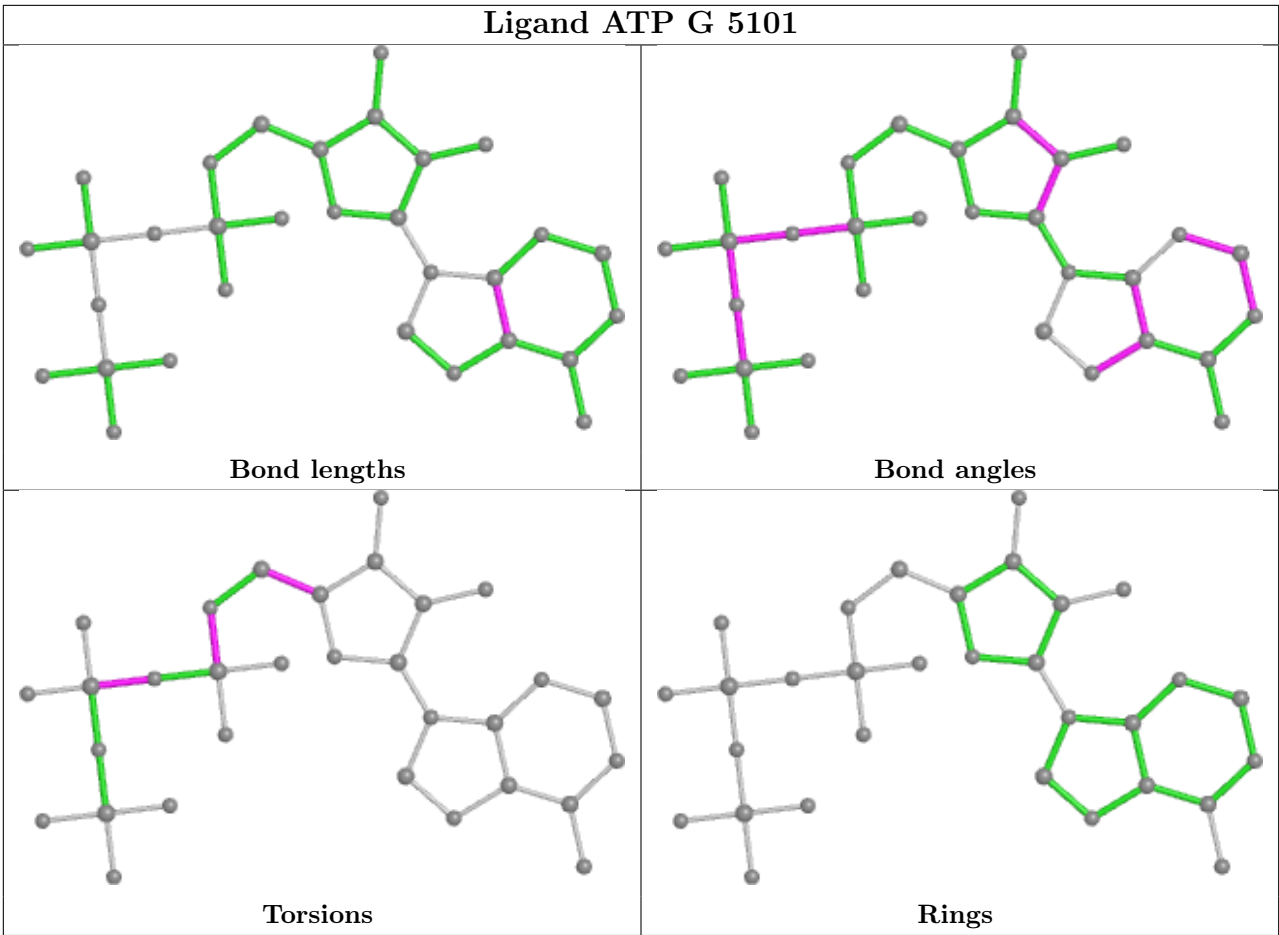
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4345:UNK	C	4540:PHE	N	72.62
1	B	4345:UNK	C	4540:PHE	N	72.61

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.60
1	G	4345:UNK	C	4540:PHE	N	72.60
1	E	3613:UNK	C	3639:THR	N	43.07
1	B	3613:UNK	C	3639:THR	N	43.04
1	I	3613:UNK	C	3639:THR	N	43.03
1	G	3613:UNK	C	3639:THR	N	43.03
1	B	4253:GLU	C	4320:UNK	N	27.32
1	E	4253:GLU	C	4320:UNK	N	27.31
1	I	4253:GLU	C	4320:UNK	N	27.29
1	G	4253:GLU	C	4320:UNK	N	27.28
1	B	3163:UNK	C	3170:UNK	N	16.19
1	E	3163:UNK	C	3170:UNK	N	16.19
1	I	3163:UNK	C	3170:UNK	N	16.19
1	G	3163:UNK	C	3170:UNK	N	16.19
1	B	3063:UNK	C	3134:UNK	N	14.97
1	E	3063:UNK	C	3134:UNK	N	14.96
1	I	3063:UNK	C	3134:UNK	N	14.96
1	G	3063:UNK	C	3134:UNK	N	14.96
1	E	3468:UNK	C	3511:UNK	N	14.60
1	G	3468:UNK	C	3511:UNK	N	14.60
1	B	3468:UNK	C	3511:UNK	N	14.59
1	I	3468:UNK	C	3511:UNK	N	14.59
1	B	2703:UNK	C	2734:ASN	N	14.53
1	G	2703:UNK	C	2734:ASN	N	14.49
1	E	2703:UNK	C	2734:ASN	N	14.48
1	I	2703:UNK	C	2734:ASN	N	14.48
1	E	3236:UNK	C	3241:UNK	N	13.44
1	B	3236:UNK	C	3241:UNK	N	13.43
1	I	3236:UNK	C	3241:UNK	N	13.43
1	G	3236:UNK	C	3241:UNK	N	13.43
1	E	2976:UNK	C	2995:UNK	N	12.55
1	B	2976:UNK	C	2995:UNK	N	12.54
1	I	2976:UNK	C	2995:UNK	N	12.54
1	G	2976:UNK	C	2995:UNK	N	12.54
1	B	1564:UNK	C	1573:MET	N	12.29
1	E	1564:UNK	C	1573:MET	N	12.29
1	I	1564:UNK	C	1573:MET	N	12.27
1	G	1564:UNK	C	1573:MET	N	12.27
1	B	3254:UNK	C	3261:UNK	N	8.31
1	E	3254:UNK	C	3261:UNK	N	8.31
1	I	3254:UNK	C	3261:UNK	N	8.31
1	G	3254:UNK	C	3261:UNK	N	8.31

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	1297:UNK	C	1430:UNK	N	6.25
1	I	1297:UNK	C	1430:UNK	N	6.25
1	G	1297:UNK	C	1430:UNK	N	6.25
1	B	1297:UNK	C	1430:UNK	N	6.24
1	B	2939:ARG	C	2942:UNK	N	3.30
1	E	2939:ARG	C	2942:UNK	N	3.27
1	G	2939:ARG	C	2942:UNK	N	3.27
1	I	2939:ARG	C	2942:UNK	N	3.26
1	I	2479:LEU	C	2487:UNK	N	3.25
1	E	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24
1	B	2479:LEU	C	2487:UNK	N	3.23

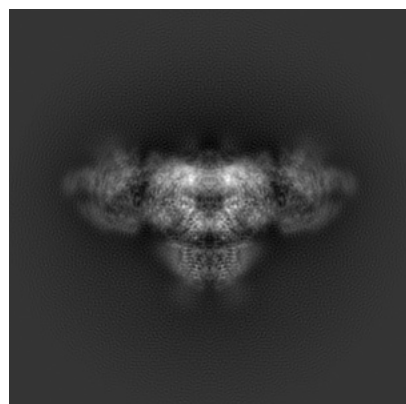
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8382. These allow visual inspection of the internal detail of the map and identification of artifacts.

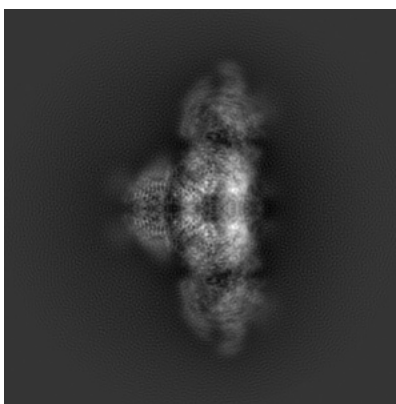
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

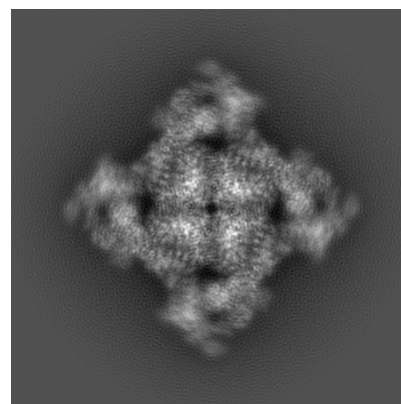
6.1.1 Primary map



X

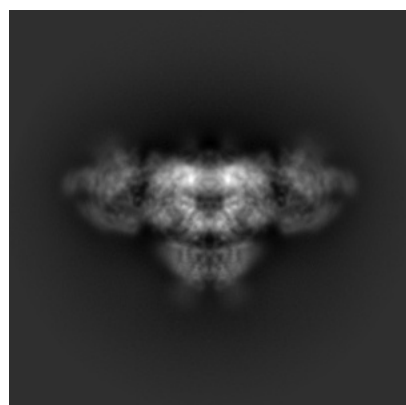


Y

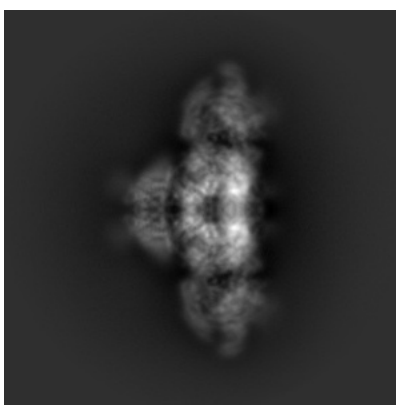


Z

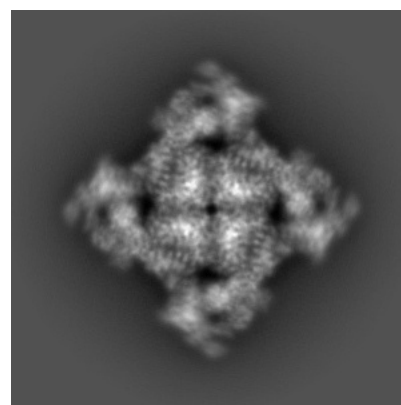
6.1.2 Raw map



X



Y

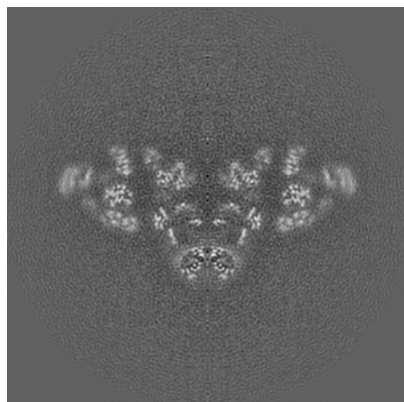


Z

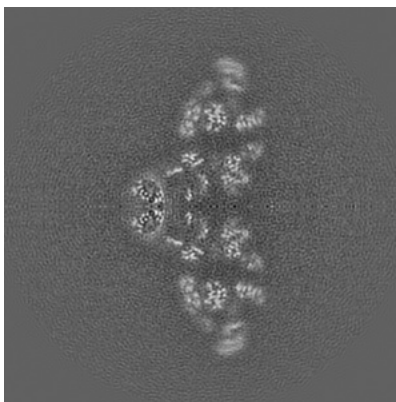
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

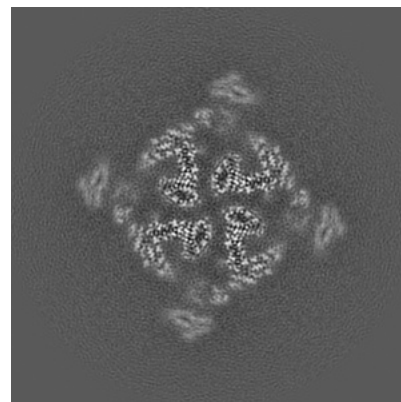
6.2.1 Primary map



X Index: 200

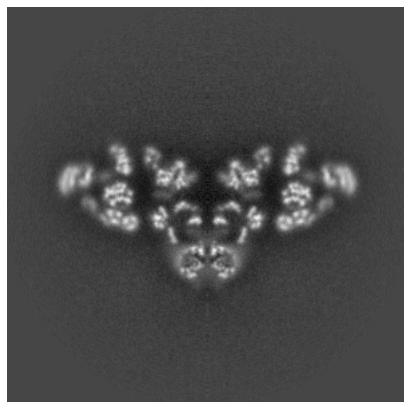


Y Index: 200

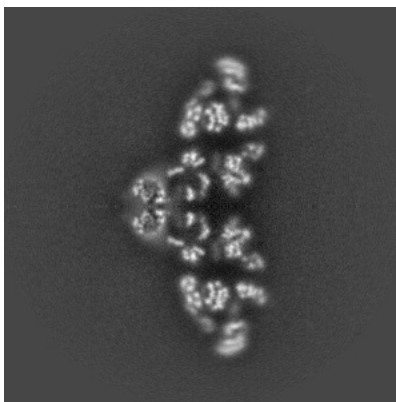


Z Index: 200

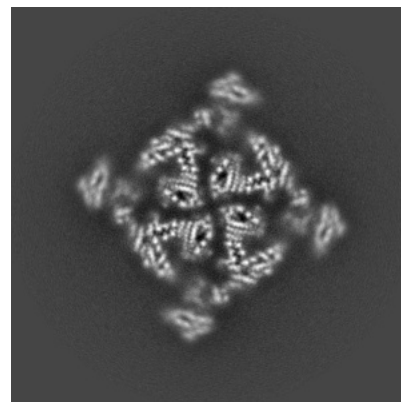
6.2.2 Raw map



X Index: 200



Y Index: 200

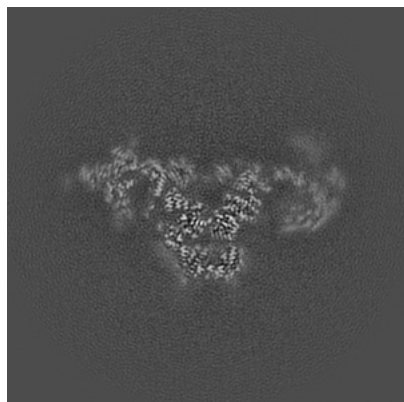


Z Index: 200

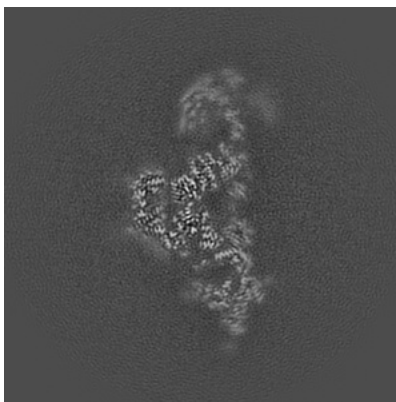
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

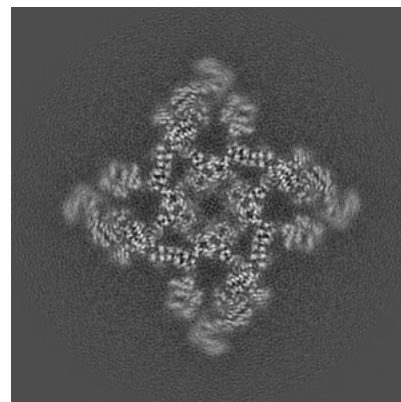
6.3.1 Primary map



X Index: 216

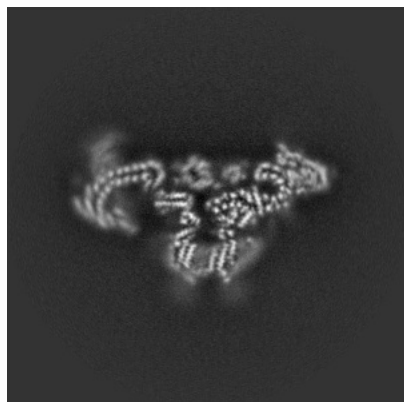


Y Index: 184

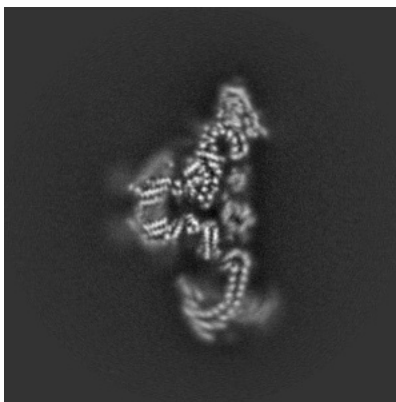


Z Index: 226

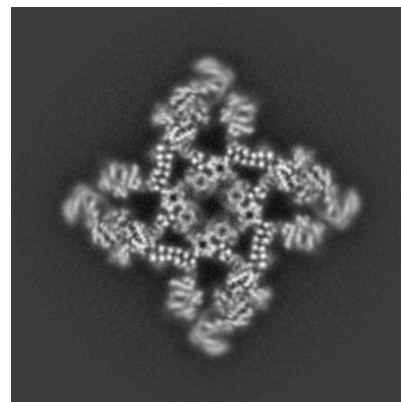
6.3.2 Raw map



X Index: 176



Y Index: 224

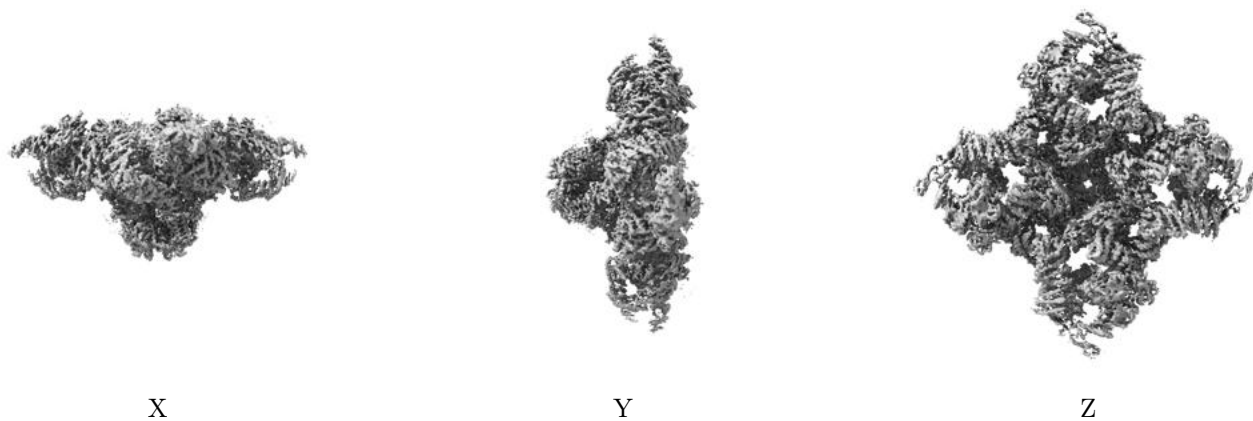


Z Index: 227

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.

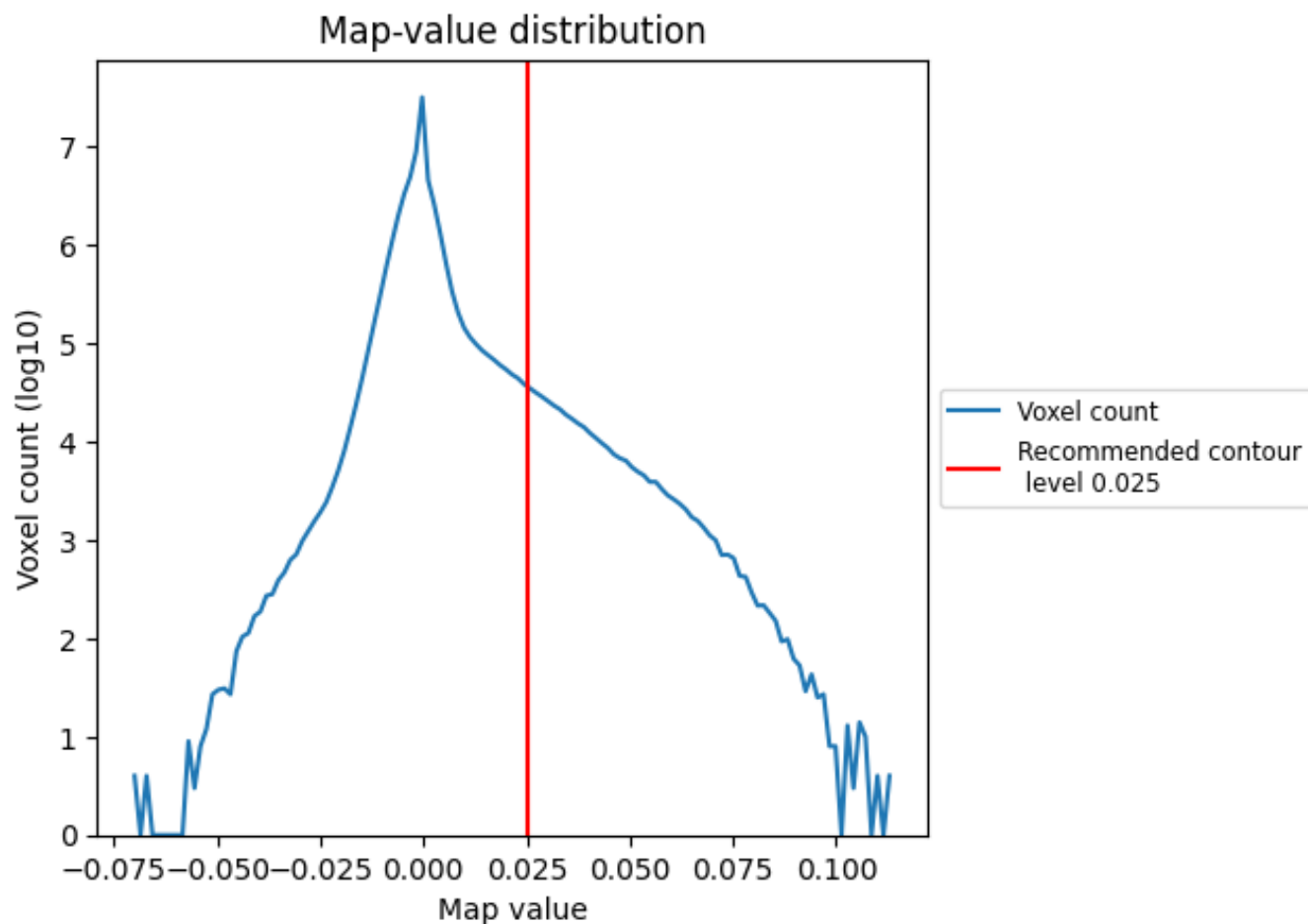
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

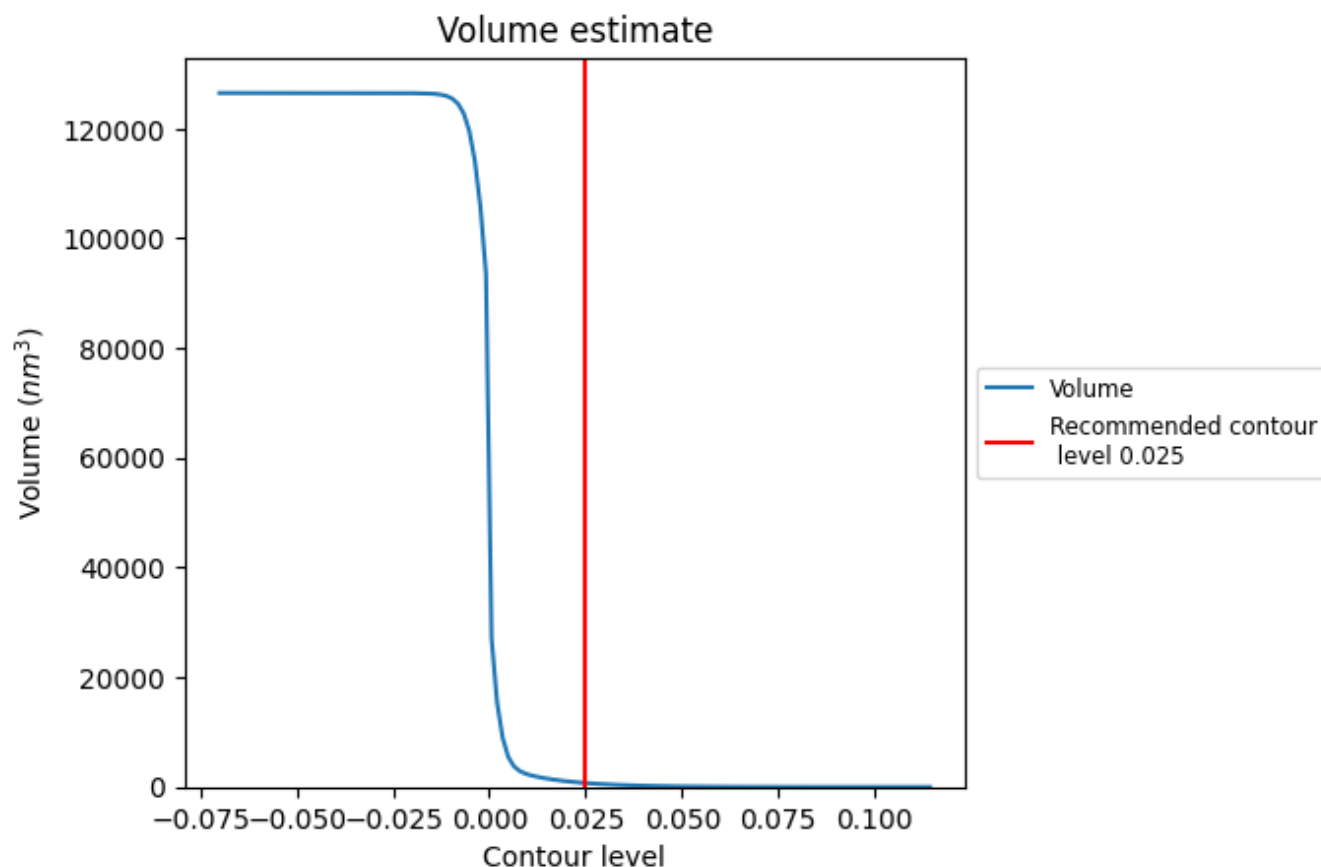
This section contains the results of statistical analysis of the map.

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.

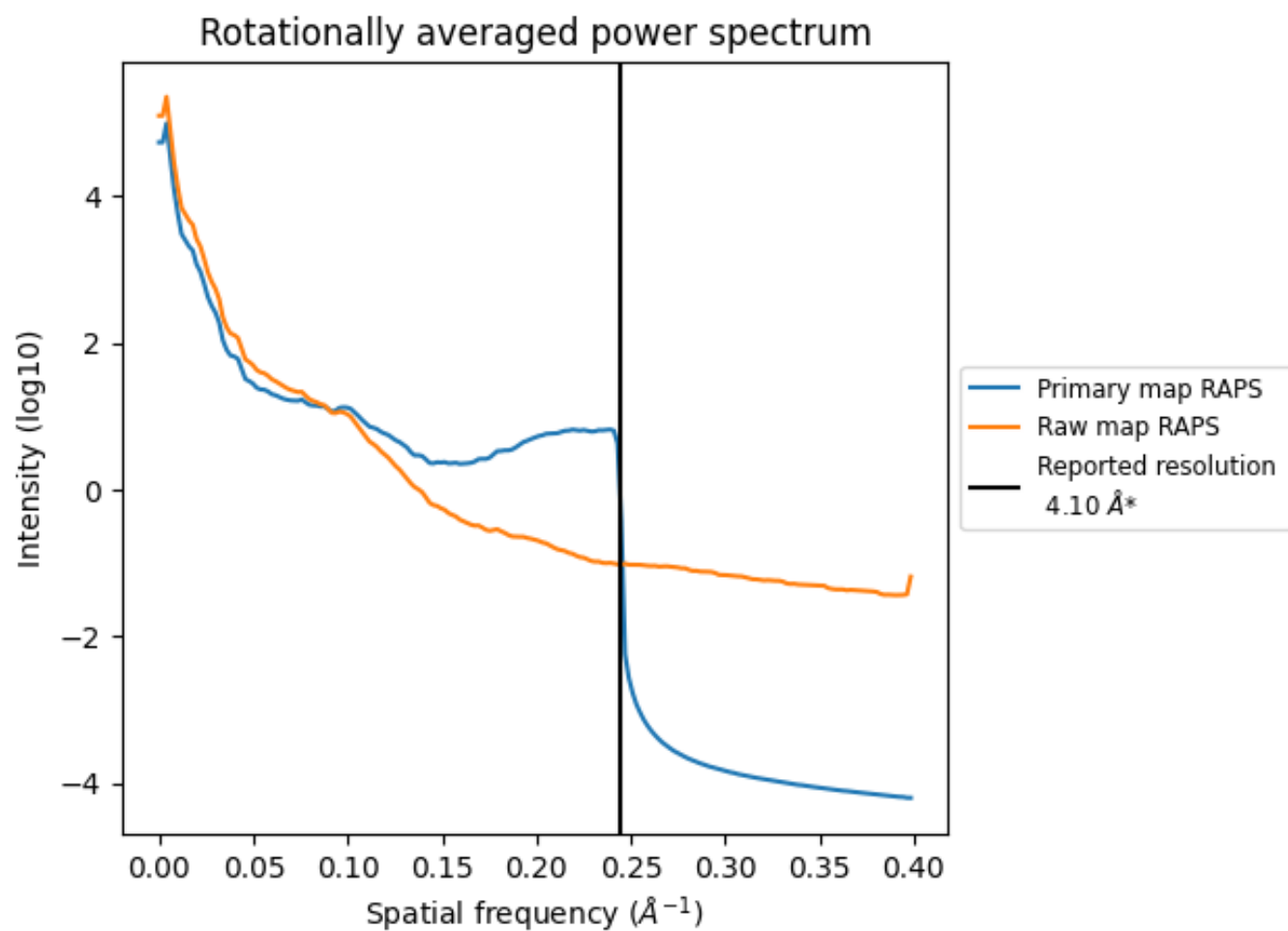
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 713 nm³; this corresponds to an approximate mass of 644 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

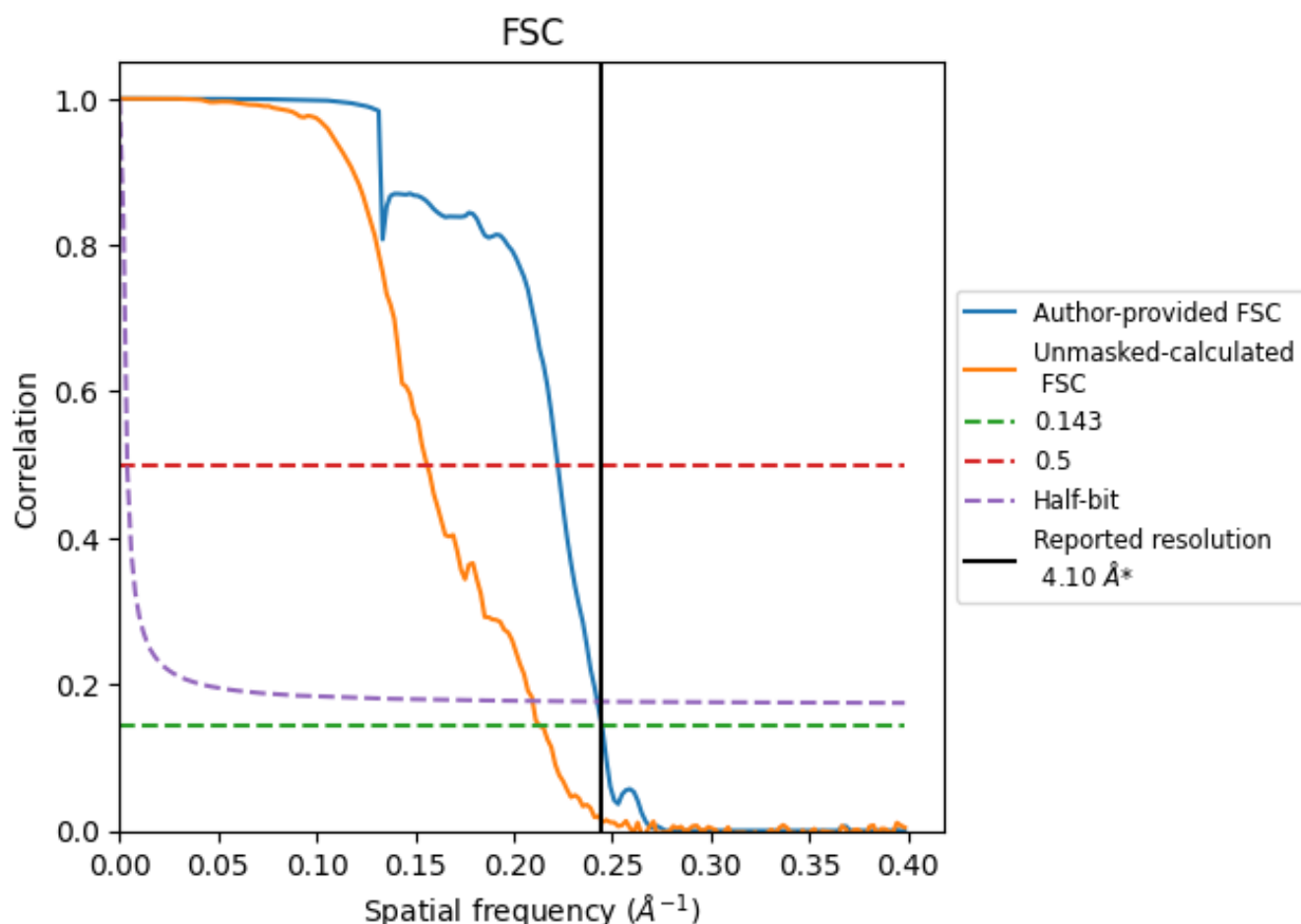


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 \AA^{-1}

8.2 Resolution estimates [i](#)

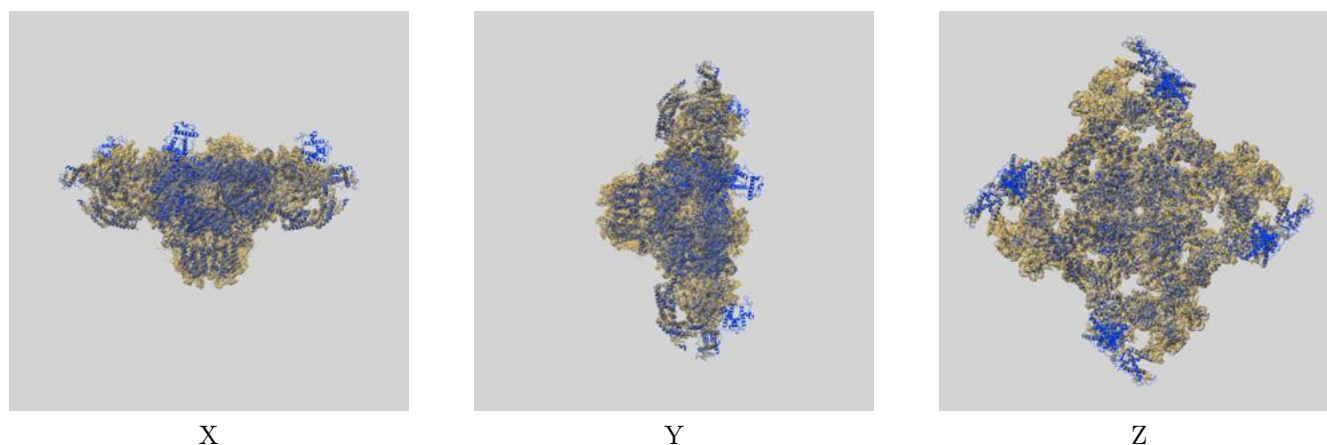
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.08	4.50	4.13
Unmasked-calculated*	4.69	6.41	4.77

*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 4.69 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

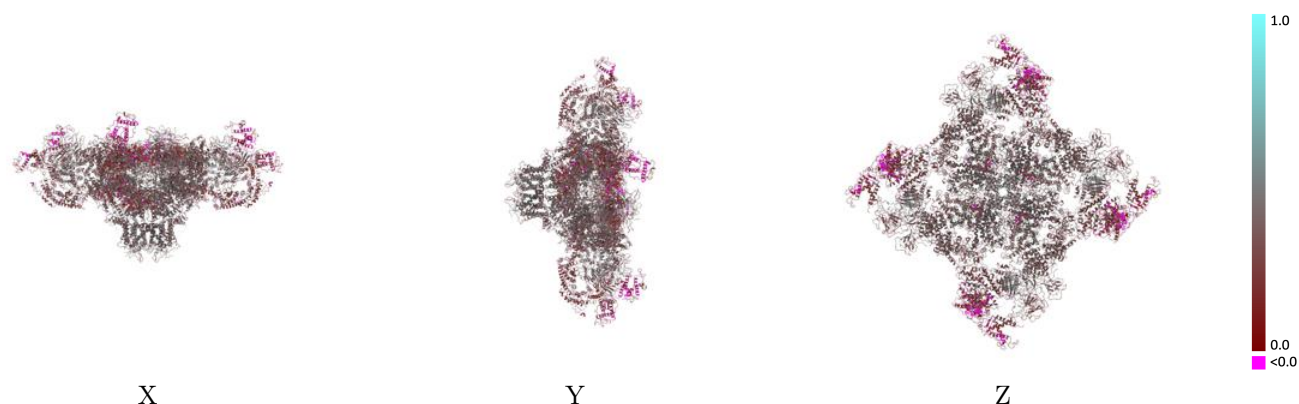
This section contains information regarding the fit between EMDB map EMD-8382 and PDB model 5TAQ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



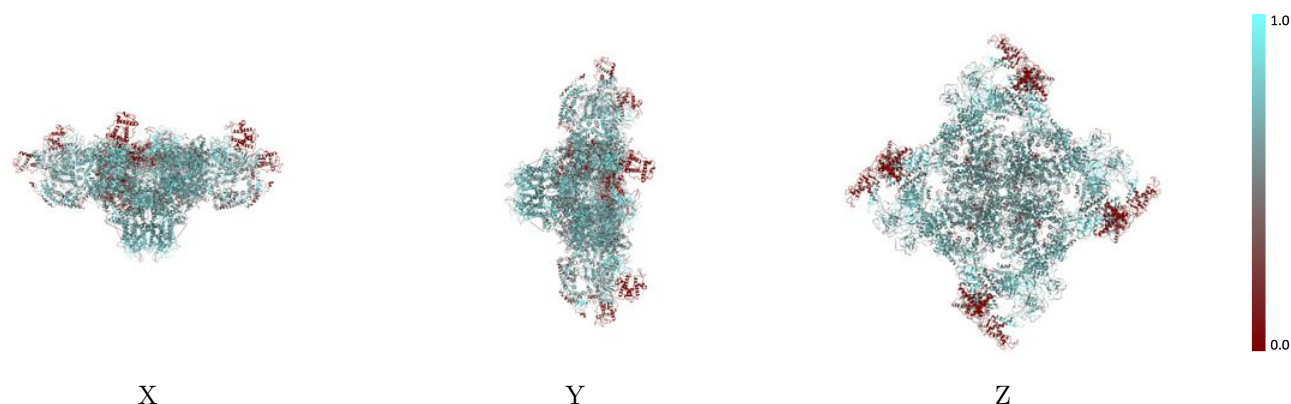
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



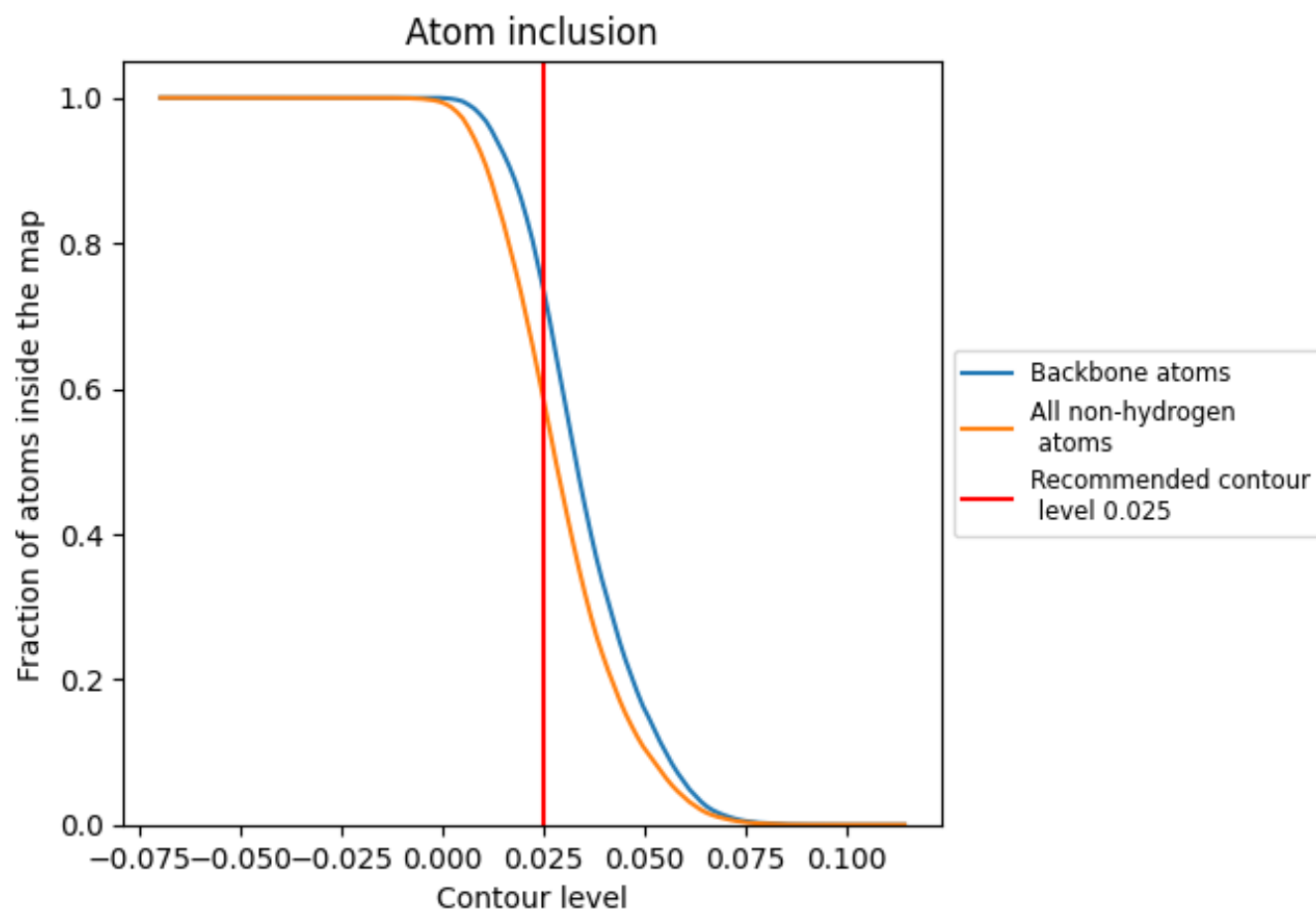
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 73% of all backbone atoms, 58% 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></div></div> 0.5829	<div><div></div></div> 0.3350
A	<div><div></div></div> 0.5571	<div><div></div></div> 0.3500
B	<div><div></div></div> 0.5830	<div><div></div></div> 0.3340
E	<div><div></div></div> 0.5836	<div><div></div></div> 0.3340
F	<div><div></div></div> 0.5596	<div><div></div></div> 0.3560
G	<div><div></div></div> 0.5841	<div><div></div></div> 0.3350
H	<div><div></div></div> 0.5558	<div><div></div></div> 0.3530
I	<div><div></div></div> 0.5838	<div><div></div></div> 0.3350
J	<div><div></div></div> 0.5620	<div><div></div></div> 0.3490

1.0

0.0

<0.0