



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:56 PM UTC

PDB ID : 5TAS / pdb_00005tas
EMDB ID : EMD-8383
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 6.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

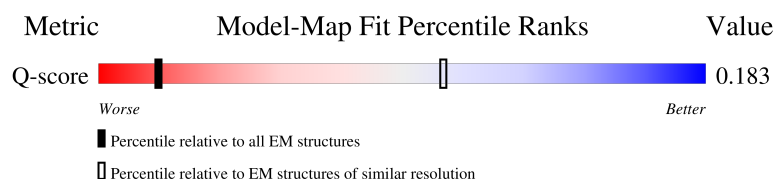
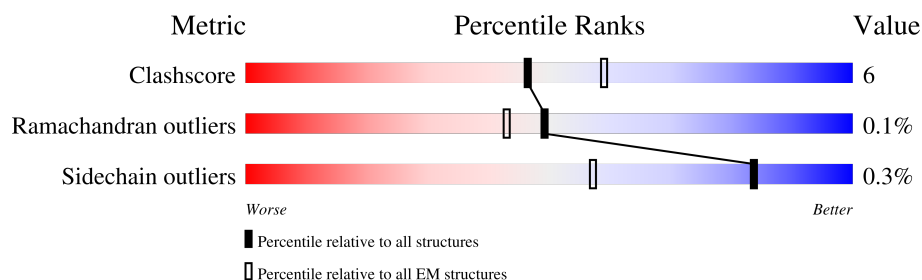
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	537 (5.70 - 6.70)

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

Mol	Chain	Length	Quality of chain
1	A	108	25% 69% 31%
1	F	108	24% 69% 31%
1	H	108	22% 71% 28%
1	J	108	22% 72% 27%

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Mol	Chain	Length	Quality of chain
2	B	4416	33% 82% 13% 5%
2	E	4416	33% 82% 13% 5%
2	G	4416	32% 82% 13% 5%
2	I	4416	33% 82% 13% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Ryanodine receptor 1.

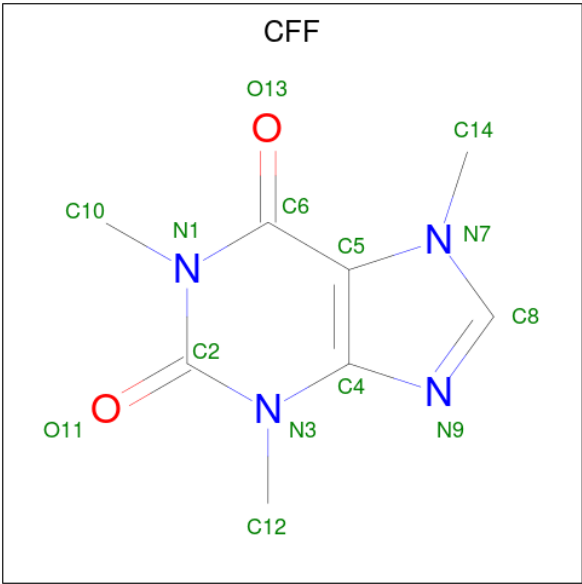
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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



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

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



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

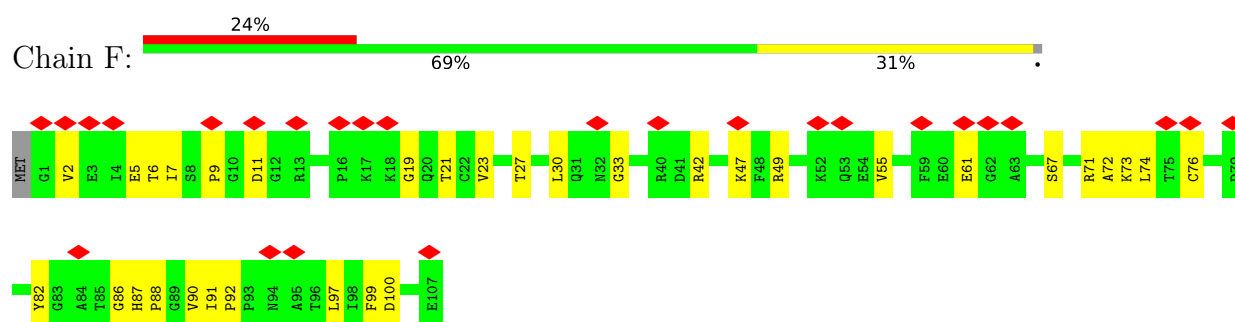
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

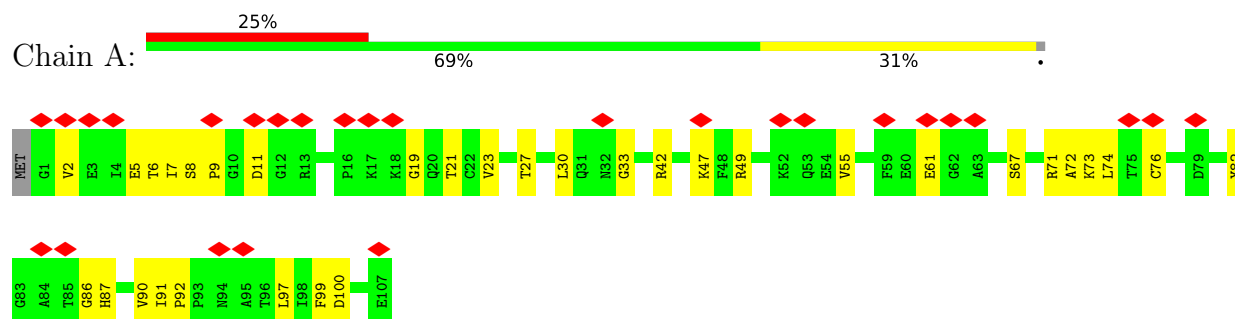
3 Residue-property plots [i](#)

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

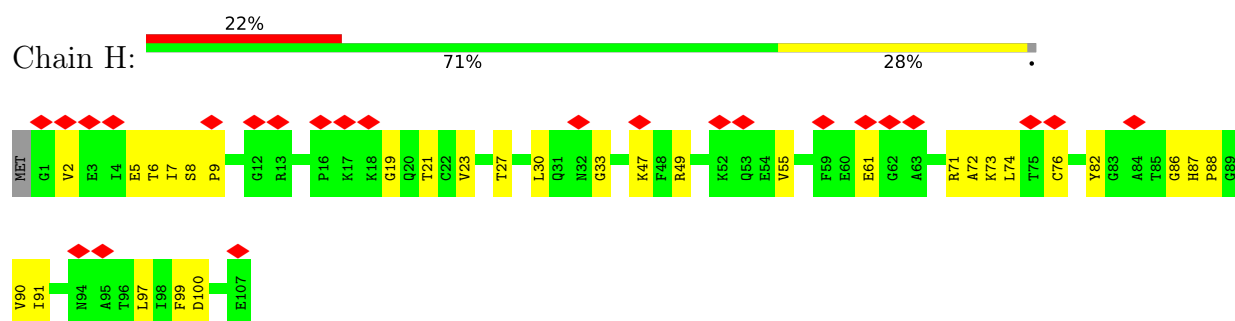
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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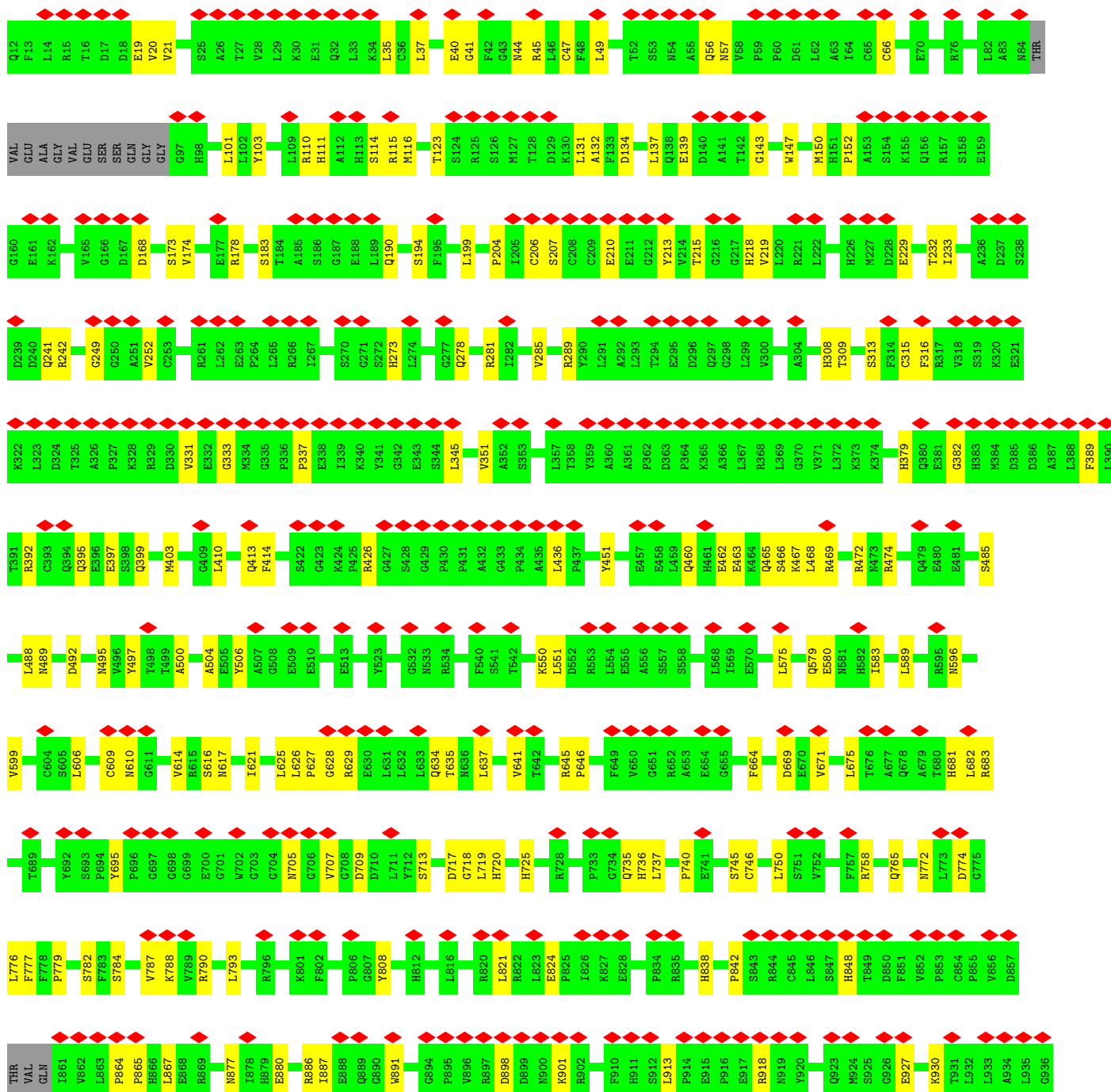
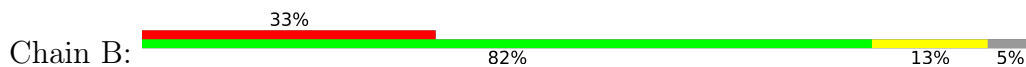
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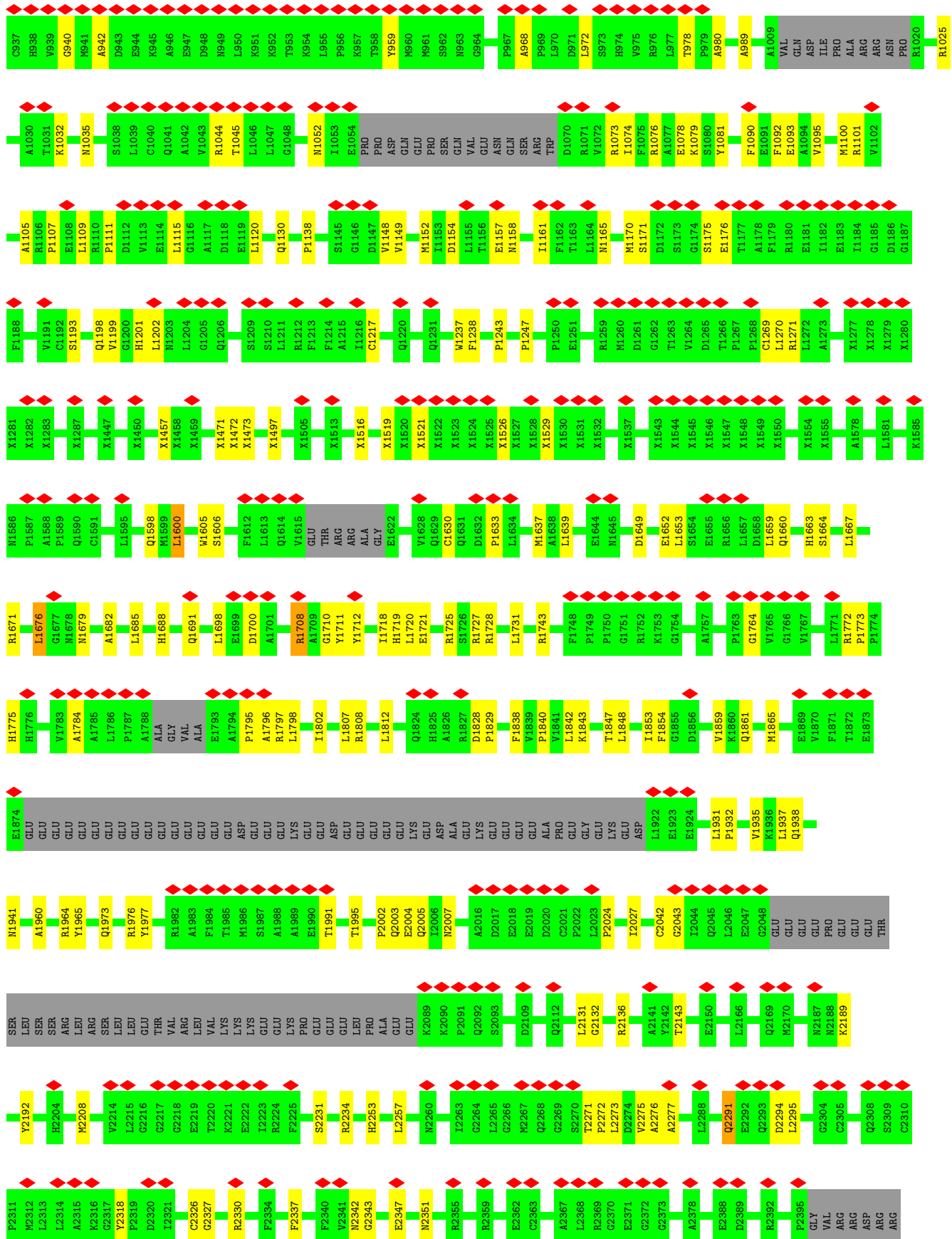


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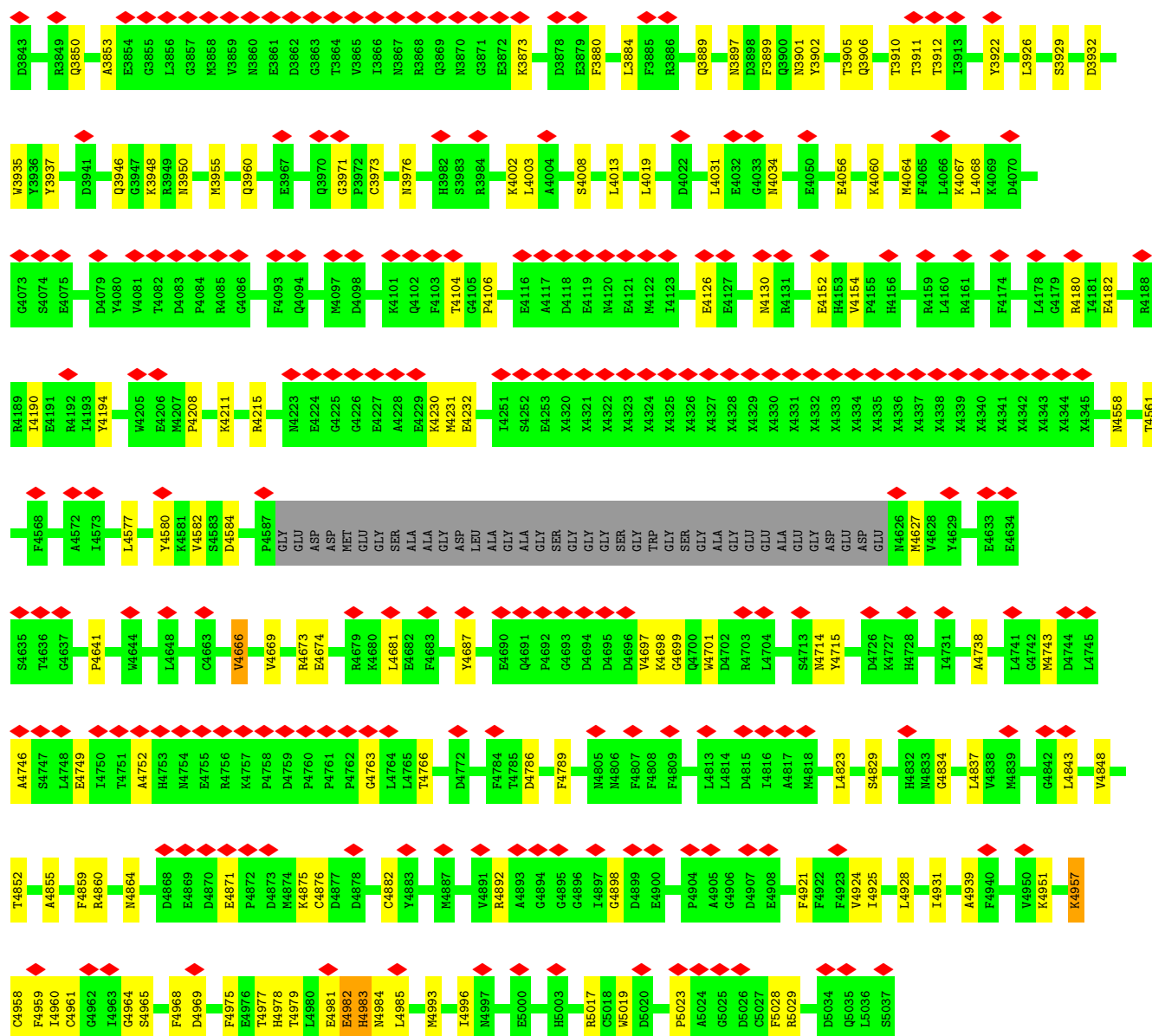


- Molecule 2: Ryanodine receptor 1

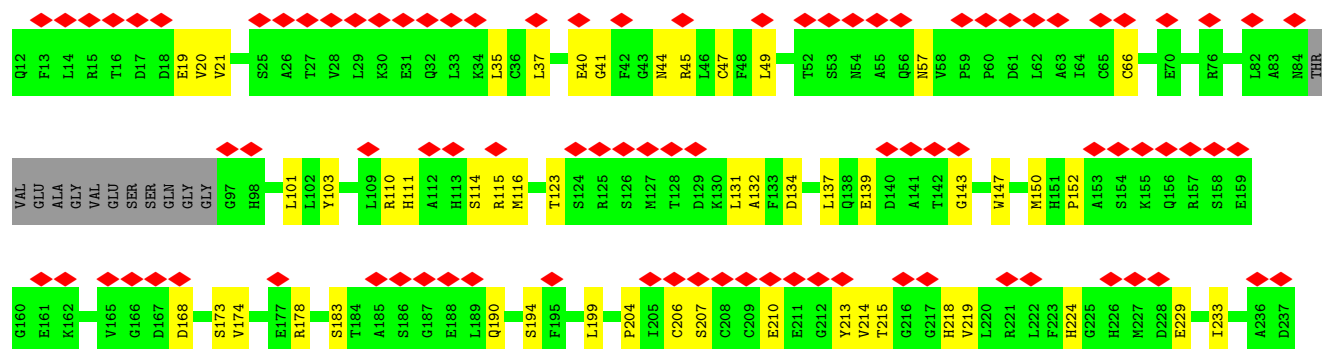
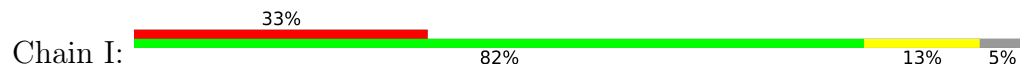








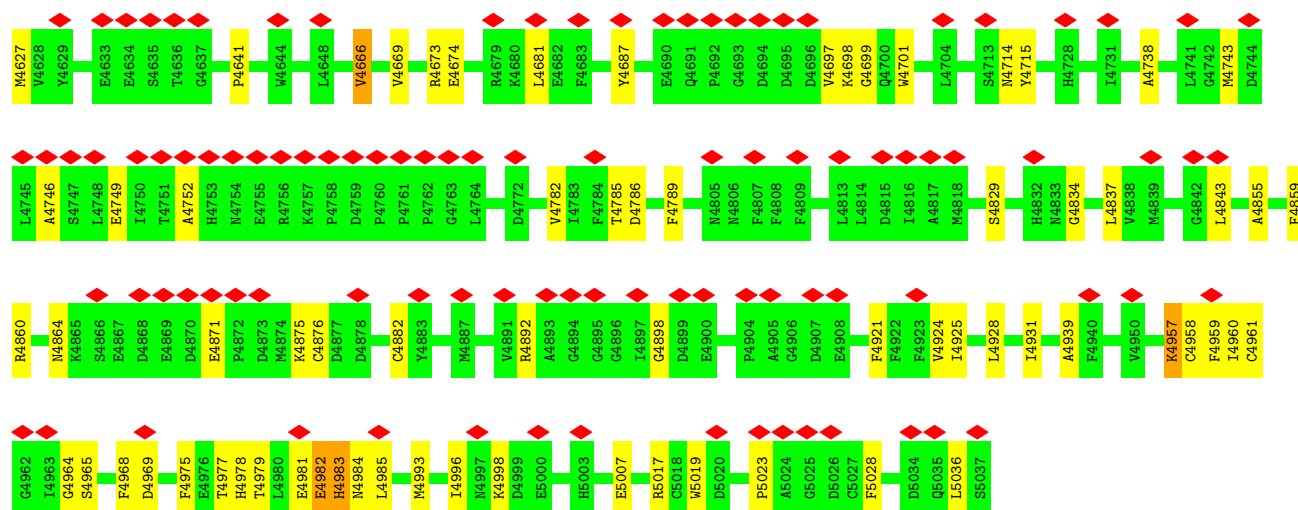
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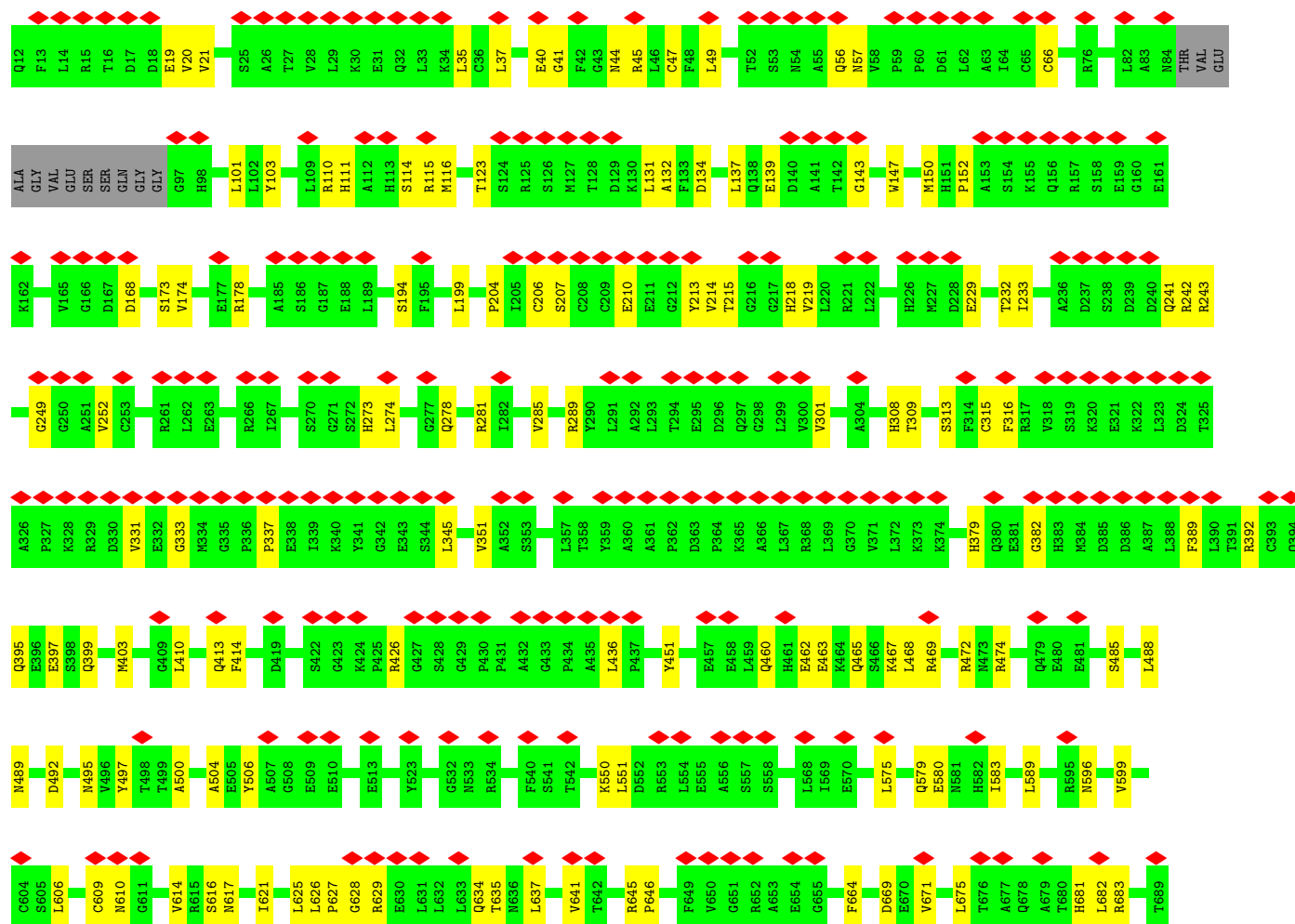
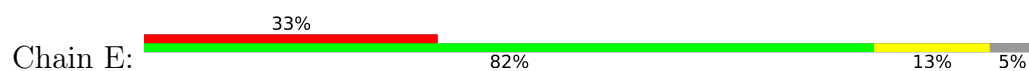
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A679	T680	H681	L682	R683	T689	Y692	S693	P694	Y695	P696	G697	G698	N617	Q618	I621	T622	L625	L626	P627	G628	R629	E630	F540	S541	L542	K550	L551	D552	R553	E555	A556	S557	S558	L568	I569	E570	L575	Q579	E580	N581	H582	I583	K584	S585	I586	L589	H593	G594	R595	N596	V599	C604	S605	L606	C609	N610	G611	V614	R615	S616	N617	Q618	I621	T622	L625	L626	P627	G628	R629	E630	F540	S541	L542	K550	L551	D552	R553	E555	A556	S557	S558	L568	I569	E570	L575	Q579	E580	N581	H582	I583	K584	S585	I586	L589	H593	G594																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
L488	N489	D492	N495	V496	Y497	T498	T499	A500	Y506	A507	G508	E509	E510	E513	Y523	R531	G532	N533	R534	F540	S541	L542	K550	L551	D552	R553	E555	A556	S557	S558	L568	I569	E570	L575	Q579	E580	N581	H582	I583	K584	S585	I586	L589	H593	G594	R595	N596	V599	C604	S605	L606	C609	N610	G611	V614	R615	S616	N617	Q618	I621	T622	L625	L626	P627	G628	R629	E630	F540	S541	L542	K550	L551	D552	R553	E555	A556	S557	S558	L568	I569	E570	L575	Q579	E580	N581	H582	I583	K584	S585	I586	L589	H593	G594																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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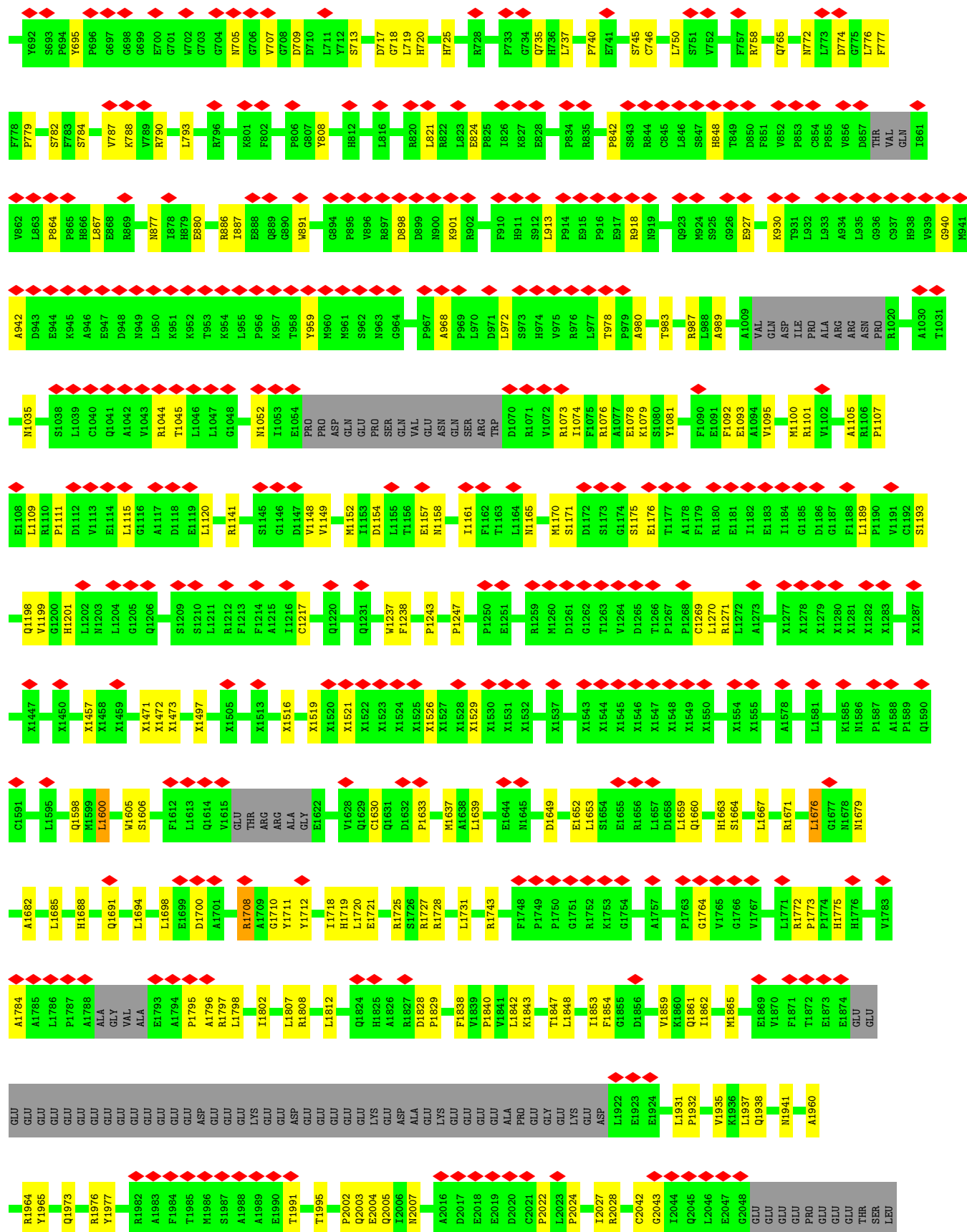


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P4208	T4082	T4082	G3857	GLU	X3601	X3534	X3400	X3336	X3251	X3154	L2930
K4211	P4083	P4083	M3858	ALA	X3606	X3535	X3401	X3337	X3252	Q2931	Q2931
R4215	R4085	R4085	V3859	GLU	X3607	X3537	X3402	X3338	X3253	R2932	R2932
M4223	G4086	G4086	V3860	GLU	X3608	X3538	X3403	X3339	X3254	R2933	R2933
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• Molecule 2: Ryanodine receptor 1



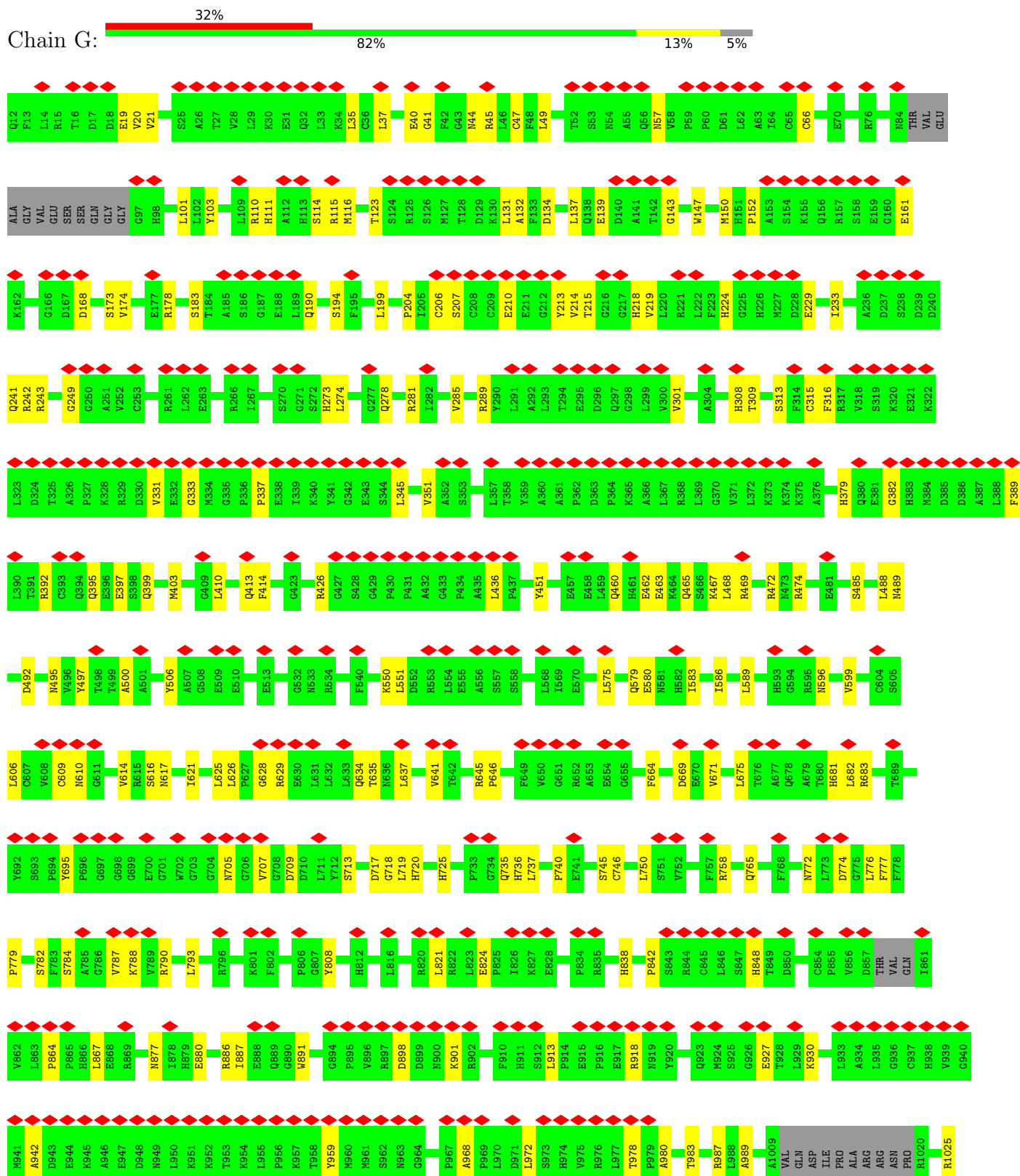


X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3420	X3424	X3431	X3432	X3433	X3434	X3435	X3436	X3439	X3440	X3441	X3442	X3443	X3453	X3454	X3458	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524									
X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394			
X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255	X3256	X3257	X3258	X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3301	X3302	X3303	X3313	X3314	X3318	X3325	X3326
X3046	X3047	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3176	X3177	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3230	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245								
K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	V2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2952	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X3006	X3009	X3016	X3019	X3020	X3021	X3022	X3023	X3027	X3034	X3035	X3036	X3037	X3038	X3043	X3044	X3045										
L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	G2886	G2887	A2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	E2915	K2916	A2917	D2918	D2919	E2920	E2921		
K2802	E2803	I2804	Y2805	R2806	V2807	P2808	I2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	I2817	A2818	V2819	E2820	V2821	T2822	I2823	E2824	K2825	A2826	E2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	THR	ARG	LYS	ILE	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861				
T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	X2623	X2624	X2625	X2649	X2650	X2651	X2669	X2670	X2671	X2672	X2673	X2682	X2683	X2688	X2689	X2690	X2691	X2692	X2693	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	F2735	P2736	E2738	P2739	V2740	E2741								
X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2585	X2605	X2606	X2614	X2618	X2622	X2623	X2624	X2625	X2649	X2650	X2651	X2669	X2670	X2671	X2672	X2673	X2682	X2683	X2688	X2689	X2690	X2691	X2692	X2693	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	F2735	P2736	E2738	P2739	V2740	E2741													
ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	GLU	GLU	N2414	R2415	H2420	G2434	H2441	G2446	R2452	L2463	D2464	D2465	L2466	I2469	I2470	S2471	L2472	P2473	L2474	Q2475	I2476	X2487	X2488	X2489	X2493	X2512	X2513	X2514	X2522	X2529	X2530	X2531	X2532	X2533	X2536	X2555																	
P2311	M2312	L2313	L2314	A2315	K2316	G2317	Y2318	D2319	D2320	I2321	C2326	G2327	R2330	F2334	F2337	F2340	N2341	G2342	G2343	E2347	N2351	R2355	R2359	E2362	C2363	F2364	A2367	L2368	R2369	G2370	E2371	G2372	G2373	A2378	E2388	D2389	R2392	P2395	GLY	VAL	ARG	ASP	ARG																	
Y2192	H2204	M2208	V2214	L2215	G2216	G2217	G2218	E2219	T2220	K2221	E2222	I2223	R2224	F2225	S2231	R2234	H2263	L2267	N2260	I2263	G2264	L2265	G2266	M2267	Q2268	G2269	S2270	P2271	P2272	L2273	D2274	V2275	A2276	A2277	L2288	Q2291	E2292	Q2293	D2294	L2295	G2304	C2305	Q2308	S2309	C2310															
SER	SER	ARG	LEU	ARG	SER	LEU	LEU	THR	VAL	LEU	VAL	LYS	LYS	GLU	GLU	PRO	GLU	LEU	PRO	ALA	GLU	K2089	K2090	P2091	Q2092	S2093	D2109	Q2112	F2121	L2131	G2132	R2136	A2141	T2142	T2143	E2150	L2166	Q2169	M2170	N2187	N2188	K2189																		

S5037	F4940	L4843	D1744	M4626	X4343	R4180	K4067	Q3833	E3718	X3525
V4950	V4950	V4848	L4745	M4627	X4344	I4181	L4068	S3840	D3719	X3526
K4951	K4951	T4852	A4746	V4628	X4345	E4182	D4070	S3841	X3527	X3527
K4957	K4957	T4852	S4747	Y4629	M4558	R4188	G4073	L3842	X3528	X3528
C4958	C4958	A4855	L4748	E4633	T4561	R4189	S4074	D3843	X3529	X3529
F4959	F4959	F4859	I4750	E4634	F4568	I4190	E4075	Q3849	X3530	X3530
I4960	I4960	R4860	T4751	S4635	F4568	E4191	E4075	Q3850	X3531	X3531
C4961	C4961	T4636	A4752	T4636	A4572	I4192	D4079	Q3853	X3532	X3532
G4962	G4962	G4637	H4753	G4637	I4573	I4193	Y4080	E3854	X3533	X3533
I4963	I4963	P4641	M4754	P4641	L4577	Y4194	Y4081	G3855	X3534	X3534
G4964	G4964	V4644	E4755	V4644	Y4580	E4205	D4082	E3856	X3535	X3535
S4965	S4965	L4648	R4756	L4648	K4581	E4206	P4084	G3857	X3536	X3536
F4968	F4968	C4663	K4757	C4663	V4582	D4207	R4085	M3858	X3537	X3537
D4969	D4969	V4666	P4758	V4666	D4584	P4208	G4086	V3859	X3538	X3538
F4975	F4975	V4669	D4759	V4669	F4587	K4211	G4086	E3747	X3539	X3539
E4976	E4976	D4772	P4760	D4772	GLY	R4215	F4093	GLU	X3540	X3540
T4977	T4977	V4782	L4761	V4782	GLU	E4224	D4094	ALA	X3541	X3541
H4978	H4978	I4783	L4765	I4783	ASP	E4225	M4097	GLU	X3542	X3542
T4979	T4979	T4785	T4766	T4785	ASP	G4226	D4098	GLU	X3543	X3543
L4980	L4980	T4791	L4766	T4791	ASP	E4227	K4101	N3867	X3544	X3544
E4981	E4981	M4805	L4766	M4805	ASP	A4228	Q4102	N3868	X3545	X3545
E4982	E4982	M4806	L4766	M4806	ASP	E4229	F4103	Q3869	X3546	X3546
H4983	H4983	G4894	L4766	G4894	ASP	E4230	T4104	N3870	X3547	X3547
N4984	N4984	G4895	L4766	G4895	ASP	E4231	G4105	L3866	X3548	X3548
L4985	L4985	I4897	L4766	I4897	ASP	E4232	P4106	N3867	X3549	X3549
M4993	M4993	D4898	L4766	D4898	ASP	E4233	E4116	Q3871	X3550	X3550
I4996	I4996	E4899	L4766	E4899	ASP	E4239	E4117	N3872	X3551	X3551
N4997	N4997	Q4691	L4766	Q4691	ASP	E4239	A4117	H3882	X3552	X3552
K4998	K4998	P4692	L4766	P4692	ASP	E4239	A4118	S3983	X3553	X3553
D4999	D4999	G4693	L4766	G4693	ASP	E4239	E4119	R3984	X3554	X3554
E5000	E5000	D4694	L4766	D4694	ASP	E4239	N4120	K4002	X3555	X3555
H5003	H5003	D4695	L4766	D4695	ASP	E4239	E4121	L4003	X3556	X3556
E5007	E5007	V4696	L4766	V4696	ASP	E4239	E4122	A4004	X3557	X3557
Y5014	Y5014	K4697	L4766	K4697	ASP	E4239	E4123	S4008	X3558	X3558
R5017	R5017	K4698	L4766	K4698	ASP	E4239	E4126	L4013	X3559	X3559
C5018	C5018	Q4700	L4766	Q4700	ASP	E4239	E4127	L4019	X3560	X3560
W5019	W5019	G4699	L4766	G4699	ASP	E4239	E4127	D4022	X3561	X3561
D5020	D5020	V4701	L4766	V4701	ASP	E4239	E4127	E4032	X3562	X3562
P5023	P5023	L4704	L4766	L4704	ASP	E4239	E4127	E4033	X3563	X3563
A5024	A5024	S4713	L4766	S4713	ASP	E4239	E4127	E4034	X3564	X3564
G5025	G5025	M4714	L4766	M4714	ASP	E4239	E4127	E4050	X3565	X3565
D5026	D5026	Y4715	L4766	Y4715	ASP	E4239	E4127	E4056	X3566	X3566
C5027	C5027	D4726	L4766	D4726	ASP	E4239	E4127	E4056	X3567	X3567
F5028	F5028	K4727	L4766	K4727	ASP	E4239	E4127	E4056	X3568	X3568
R5029	R5029	H4728	L4766	H4728	ASP	E4239	E4127	E4056	X3569	X3569
D5034	D5034	A4738	L4766	A4738	ASP	E4239	E4127	E4056	X3570	X3570
Q5035	Q5035	L4742	L4766	L4742	ASP	E4239	E4127	E4056	X3571	X3571
L5036	L5036	M4743	L4766	M4743	ASP	E4239	E4127	E4056	X3572	X3572
			L4743		ASP	E4239	E4127	E4056	X3573	X3573
					ASP	E4239	E4127	E4056	X3574	X3574
					ASP	E4239	E4127	E4056	X3575	X3575
					ASP	E4239	E4127	E4056	X3576	X3576
					ASP	E4239	E4127	E4056	X3577	X3577
					ASP	E4239	E4127	E4056	X3578	X3578
					ASP	E4239	E4127	E4056	X3579	X3579
					ASP	E4239	E4127	E4056	X3580	X3580
					ASP	E4239	E4127	E4056	X3581	X3581
					ASP	E4239	E4127	E4056	X3582	X3582
					ASP	E4239	E4127	E4056	X3583	X3583
					ASP	E4239	E4127	E4056	X3584	X3584
					ASP	E4239	E4127	E4056	X3585	X3585

• Molecule 2: Ryanodine receptor 1

Chain G:









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	0.077	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/834	0.48	0/1123
1	F	0.19	0/834	0.48	0/1123
1	H	0.19	0/834	0.48	0/1123
1	J	0.19	0/834	0.48	0/1123
2	B	0.19	0/25428	0.51	4/34534 (0.0%)
2	E	0.19	0/25428	0.51	4/34534 (0.0%)
2	G	0.19	0/25428	0.51	4/34534 (0.0%)
2	I	0.19	0/25428	0.51	4/34534 (0.0%)
All	All	0.19	0/105048	0.51	16/142628 (0.0%)

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

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

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4984	ASN	N-CA-C	-6.66	103.75	112.41
2	B	4984	ASN	N-CA-C	-6.65	103.76	112.41
2	I	4984	ASN	N-CA-C	-6.62	103.81	112.41
2	E	4984	ASN	N-CA-C	-6.59	103.84	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1829	PRO	N-CA-C	5.41	119.71	111.11
2	B	1829	PRO	N-CA-C	5.41	119.70	111.11
2	G	1829	PRO	N-CA-C	5.40	119.70	111.11
2	E	1829	PRO	N-CA-C	5.39	119.67	111.11
2	G	579	GLN	CA-C-N	5.02	131.13	121.54
2	G	579	GLN	C-N-CA	5.02	131.13	121.54
2	I	579	GLN	CA-C-N	5.02	131.13	121.54
2	I	579	GLN	C-N-CA	5.02	131.13	121.54
2	B	579	GLN	CA-C-N	5.01	131.12	121.54
2	B	579	GLN	C-N-CA	5.01	131.12	121.54
2	E	579	GLN	CA-C-N	5.01	131.11	121.54
2	E	579	GLN	C-N-CA	5.01	131.11	121.54

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	808	TYR	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	21	0
1	F	818	0	824	21	0
1	H	818	0	824	18	0
1	J	818	0	824	18	0
2	B	29499	0	24746	329	0
2	E	29499	0	24746	336	0
2	G	29499	0	24746	330	0
2	I	29499	0	24746	328	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102368	1374	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 6.

All (1374) 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:4230:LYS:HD2	2:G:4959:PHE:CE2	1.25	1.69
2:E:4230:LYS:HD2	2:E:4959:PHE:CE2	1.25	1.64
2:I:4230:LYS:HD2	2:I:4959:PHE:CE2	1.25	1.60
2:B:4230:LYS:HD2	2:B:4959:PHE:CE2	1.25	1.58
2:B:4230:LYS:HD2	2:B:4959:PHE:CZ	1.55	1.42
2:E:4230:LYS:HD2	2:E:4959:PHE:CZ	1.55	1.42
2:E:4230:LYS:CD	2:E:4959:PHE:CZ	2.04	1.41
2:B:4230:LYS:CD	2:B:4959:PHE:CZ	2.04	1.41
2:I:4230:LYS:HD2	2:I:4959:PHE:CZ	1.55	1.40
2:G:4230:LYS:HD2	2:G:4959:PHE:CZ	1.55	1.40
2:I:4230:LYS:CD	2:I:4959:PHE:CZ	2.04	1.40
2:G:4230:LYS:CD	2:G:4959:PHE:CZ	2.04	1.39
2:I:4230:LYS:CD	2:I:4959:PHE:CE2	2.15	1.29
2:B:4230:LYS:CD	2:B:4959:PHE:CE2	2.15	1.27
2:E:4230:LYS:CD	2:E:4959:PHE:CE2	2.15	1.25
2:G:4230:LYS:CD	2:G:4959:PHE:CE2	2.15	1.20
2:I:4230:LYS:HD3	2:I:4959:PHE:CZ	1.76	1.19
2:G:4230:LYS:HD3	2:G:4959:PHE:CZ	1.76	1.13
2:B:4230:LYS:HD3	2:B:4959:PHE:HZ	1.07	1.12
2:E:4230:LYS:HD3	2:E:4959:PHE:CZ	1.76	1.12
2:B:4230:LYS:HD3	2:B:4959:PHE:CZ	1.76	1.09
2:E:4230:LYS:HD3	2:E:4959:PHE:HZ	1.07	1.09
2:I:4230:LYS:HD3	2:I:4959:PHE:HZ	1.07	1.07
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.37	1.06
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.37	1.06
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.37	1.06
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4230:LYS:HD3	2:G:4959:PHE:HZ	1.07	1.04
2:I:4230:LYS:HD2	2:I:4959:PHE:HE2	1.25	0.96
2:B:4230:LYS:HD2	2:B:4959:PHE:HE2	1.26	0.96
2:E:4230:LYS:HD2	2:E:4959:PHE:HE2	1.26	0.92
2:G:4230:LYS:HD2	2:G:4959:PHE:HE2	1.26	0.90
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.51	0.75
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.51	0.75
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.51	0.74
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.51	0.73
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.89	0.70
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.57	0.69
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.57	0.69
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.57	0.69
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.57	0.68
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.89	0.68
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.91	0.68
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.91	0.67
2:G:379:HIS:HD2	2:G:382:GLY:H	1.42	0.67
2:I:379:HIS:HD2	2:I:382:GLY:H	1.42	0.66
2:E:379:HIS:HD2	2:E:382:GLY:H	1.42	0.66
2:E:4957:LYS:CG	2:E:4964:GLY:HA2	2.23	0.66
2:B:379:HIS:HD2	2:B:382:GLY:H	1.42	0.65
2:I:4957:LYS:CG	2:I:4964:GLY:HA2	2.22	0.64
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.79	0.64
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.64
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.79	0.64
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.16	0.64
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.64
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.79	0.63
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.64	0.63
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.16	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.81	0.63
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.79	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.80	0.63
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.16	0.63
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.81	0.62
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.64	0.62
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.81	0.62
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.81	0.62
2:B:4957:LYS:CG	2:B:4964:GLY:HA2	2.22	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.64	0.62
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.64	0.62
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.81	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.62
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.33	0.62
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.33	0.62
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.33	0.62
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.33	0.62
2:E:313:SER:HB3	2:E:351:VAL:HB	1.82	0.61
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.16	0.61
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.82	0.61
2:B:313:SER:HB3	2:B:351:VAL:HB	1.82	0.61
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.61
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.81	0.61
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.81	0.61
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.34	0.61
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.34	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.33	0.61
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.33	0.61
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.82	0.61
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.81	0.61
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.33	0.61
2:B:111:HIS:HD2	2:B:114:SER:H	1.49	0.61
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.34	0.61
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.33	0.61
2:G:313:SER:HB3	2:G:351:VAL:HB	1.82	0.61
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.34	0.61
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.83	0.60
2:E:111:HIS:HD2	2:E:114:SER:H	1.49	0.60
2:G:111:HIS:HD2	2:G:114:SER:H	1.49	0.60
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.82	0.60
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.83	0.60
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.60
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.60
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.34	0.60
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.84	0.60
2:I:313:SER:HB3	2:I:351:VAL:HB	1.83	0.60
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.83	0.60
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.33	0.60
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.83	0.60
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.34	0.60
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.84	0.60
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.84	0.60
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.84	0.60
2:I:111:HIS:HD2	2:I:114:SER:H	1.49	0.60
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.83	0.60
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.82	0.60
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.85	0.59
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.84	0.59
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.82	0.59
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.84	0.59
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.83	0.59
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.84	0.59
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.84	0.59
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.85	0.59
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.84	0.59
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.84	0.59
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.84	0.59
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.59
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.84	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.84	0.59
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.84	0.58
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.36	0.58
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.33	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.58
1:H:6:THR:HA	1:H:72:ALA:HA	1.85	0.58
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.33	0.58
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.36	0.58
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.37	0.58
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.58
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.37	0.58
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.86	0.58
2:E:331:VAL:HG12	2:E:333:GLY:H	1.68	0.58
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.85	0.58
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.36	0.58
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.36	0.58
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.85	0.58
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.36	0.58
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.37	0.58
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.36	0.58
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.85	0.58
2:I:4230:LYS:HE3	2:I:4231:MET:HE2	1.86	0.58
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.85	0.58
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.85	0.58
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.36	0.58
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.36	0.58
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.37	0.58
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.85	0.58
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.58
2:G:331:VAL:HG12	2:G:333:GLY:H	1.68	0.58
1:A:6:THR:HA	1:A:72:ALA:HA	1.85	0.57
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.85	0.57
2:I:331:VAL:HG12	2:I:333:GLY:H	1.68	0.57
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.69	0.57
2:G:4230:LYS:HE3	2:G:4231:MET:HE2	1.86	0.57
2:G:4957:LYS:CG	2:G:4964:GLY:HA2	2.22	0.57
1:J:6:THR:HA	1:J:72:ALA:HA	1.85	0.57
2:B:331:VAL:HG12	2:B:333:GLY:H	1.68	0.57
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.87	0.57
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.85	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.57
2:E:4898:GLY:O	2:G:4892:ARG:NH2	2.37	0.57
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.86	0.57
1:F:6:THR:HA	1:F:72:ALA:HA	1.85	0.57
1:H:87:HIS:H	1:H:91:ILE:HB	1.69	0.57
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.87	0.57
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.38	0.57
1:F:87:HIS:H	1:F:91:ILE:HB	1.69	0.57
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.69	0.57
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.85	0.57
2:I:4829:SER:HB2	2:I:4939:ALA:HB1	1.86	0.57
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.86	0.57
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.37	0.57
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.70	0.57
2:B:4230:LYS:HE3	2:B:4231:MET:HE2	1.85	0.57
2:B:4960:ILE:HG22	2:B:4960:ILE:O	2.05	0.57
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.70	0.57
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.73	0.57
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.85	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.69	0.57
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.38	0.57
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.70	0.57
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.85	0.57
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.57
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.57
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.70	0.57
2:E:1271:ARG:HA	2:E:1471:UNK:HA	1.86	0.57
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.70	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.57
2:B:1271:ARG:HA	2:B:1471:UNK:HA	1.86	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.57
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.70	0.57
2:E:4829:SER:HB2	2:E:4939:ALA:HB1	1.86	0.57
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.38	0.57
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.73	0.56
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.38	0.56
2:E:4230:LYS:HE3	2:E:4231:MET:HE2	1.85	0.56
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.69	0.56
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.86	0.56
2:G:1271:ARG:HA	2:G:1471:UNK:HA	1.86	0.56
2:G:4829:SER:HB2	2:G:4939:ALA:HB1	1.86	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.69	0.56
2:I:4957:LYS:HG2	2:I:4964:GLY:CA	2.25	0.56
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.73	0.56
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.86	0.56
2:E:4960:ILE:HG22	2:E:4960:ILE:O	2.05	0.56
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.88	0.56
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.69	0.56
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.87	0.56
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.87	0.56
2:I:1271:ARG:HA	2:I:1471:UNK:HA	1.86	0.56
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.69	0.56
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.87	0.56
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.86	0.56
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.86	0.56
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.38	0.56
1:A:87:HIS:H	1:A:91:ILE:HB	1.69	0.56
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.85	0.56
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.38	0.56
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.69	0.56
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.70	0.56
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.73	0.56
2:I:669:ASP:OD2	2:I:790:ARG:NH2	2.39	0.56
2:I:4960:ILE:O	2:I:4960:ILE:HG22	2.05	0.56
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.34	0.56
2:B:4829:SER:HB2	2:B:4939:ALA:HB1	1.86	0.56
2:G:683:ARG:NH1	2:G:707:VAL:O	2.37	0.56
2:G:4957:LYS:HG2	2:G:4964:GLY:CA	2.25	0.56
1:J:87:HIS:H	1:J:91:ILE:HB	1.69	0.55
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.70	0.55
2:E:4230:LYS:CD	2:E:4959:PHE:HE2	1.94	0.55
2:G:4230:LYS:CD	2:G:4959:PHE:HE2	1.94	0.55
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.39	0.55
2:G:4960:ILE:HG22	2:G:4960:ILE:O	2.05	0.55
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.86	0.55
2:B:669:ASP:OD2	2:B:790:ARG:NH2	2.39	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.38	0.55
2:G:4230:LYS:CG	2:G:4959:PHE:CE2	2.88	0.55
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.34	0.55
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.89	0.55
2:B:4957:LYS:HG2	2:B:4964:GLY:CA	2.25	0.55
2:E:683:ARG:NH1	2:E:707:VAL:O	2.37	0.55
2:G:41:GLY:O	2:G:45:ARG:NH1	2.40	0.55
2:G:609:CYS:SG	2:G:610:ASN:N	2.80	0.55
2:G:4230:LYS:CG	2:G:4959:PHE:HE2	2.19	0.55
2:B:4230:LYS:CG	2:B:4959:PHE:HE2	2.19	0.55
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.40	0.55
2:I:4230:LYS:CG	2:I:4959:PHE:HE2	2.19	0.55
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.89	0.55
2:B:41:GLY:O	2:B:45:ARG:NH1	2.40	0.55
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.40	0.55
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.89	0.55
2:G:669:ASP:OD2	2:G:790:ARG:NH2	2.39	0.55
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.40	0.54
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.89	0.54
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.89	0.54
2:I:41:GLY:O	2:I:45:ARG:NH1	2.40	0.54
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.89	0.54
2:I:609:CYS:SG	2:I:610:ASN:N	2.80	0.54
2:E:609:CYS:SG	2:E:610:ASN:N	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4190:ILE:HD13	2:E:5028:PHE:H	1.73	0.54
2:B:4232:GLU:OE1	2:B:5019:TRP:NE1	2.40	0.54
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.89	0.54
2:E:4230:LYS:CG	2:E:4959:PHE:HE2	2.19	0.54
2:E:4232:GLU:OE1	2:E:5019:TRP:NE1	2.40	0.54
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.89	0.54
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.89	0.54
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.90	0.54
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.90	0.54
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.89	0.54
2:E:41:GLY:O	2:E:45:ARG:NH1	2.40	0.54
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.89	0.54
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.89	0.54
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.89	0.54
2:B:1727:ARG:HH12	2:B:1772:ARG:HB3	1.73	0.54
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	1.90	0.54
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.40	0.54
2:B:4190:ILE:HD13	2:B:5028:PHE:H	1.73	0.54
2:I:4232:GLU:OE1	2:I:5019:TRP:NE1	2.40	0.54
1:F:5:GLU:HB2	1:F:73:LYS:HB3	1.90	0.54
1:A:5:GLU:HB2	1:A:73:LYS:HB3	1.90	0.54
2:B:609:CYS:SG	2:B:610:ASN:N	2.80	0.54
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.76	0.54
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.90	0.54
2:E:451:TYR:O	2:E:474:ARG:NH1	2.41	0.53
2:E:669:ASP:OD2	2:E:790:ARG:NH2	2.39	0.53
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.90	0.53
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.76	0.53
2:G:4190:ILE:HD13	2:G:5028:PHE:H	1.73	0.53
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.76	0.53
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.89	0.53
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.90	0.53
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.91	0.53
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.90	0.53
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.91	0.53
2:E:1727:ARG:HH12	2:E:1772:ARG:HB3	1.73	0.53
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.34	0.53
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.89	0.53
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.90	0.53
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.91	0.53
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.89	0.53
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.40	0.53
2:I:4190:ILE:HD13	2:I:5028:PHE:H	1.73	0.53
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.74	0.53
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.89	0.53
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.89	0.53
2:B:168:ASP:HB3	2:B:199:LEU:HD22	1.91	0.53
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.90	0.53
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.90	0.53
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.89	0.53
2:G:315:CYS:SG	2:G:316:PHE:N	2.82	0.53
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.74	0.53
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.89	0.53
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.89	0.53
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.90	0.53
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.74	0.53
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.91	0.53
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.91	0.53
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.34	0.53
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.74	0.53
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.74	0.53
2:I:315:CYS:SG	2:I:316:PHE:N	2.82	0.53
2:I:1727:ARG:HH12	2:I:1772:ARG:HB3	1.73	0.53
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.91	0.53
2:E:241:GLN:O	2:E:289:ARG:NH1	2.42	0.53
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.90	0.53
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.74	0.53
2:G:451:TYR:O	2:G:474:ARG:NH1	2.41	0.53
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	1.90	0.53
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.90	0.53
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.42	0.53
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.76	0.53
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.91	0.53
2:I:451:TYR:O	2:I:474:ARG:NH1	2.41	0.53
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.91	0.53
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.90	0.53
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.89	0.52
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.91	0.52
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.91	0.52
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.90	0.52
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:168:ASP:HB3	2:I:199:LEU:HD22	1.91	0.52
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.91	0.52
2:G:1727:ARG:HH12	2:G:1772:ARG:HB3	1.73	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.42	0.52
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.89	0.52
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.91	0.52
1:H:5:GLU:HB2	1:H:73:LYS:HB3	1.90	0.52
1:J:5:GLU:HB2	1:J:73:LYS:HB3	1.90	0.52
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.90	0.52
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.91	0.52
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.91	0.52
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.74	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.42	0.52
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.91	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.90	0.52
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.92	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.42	0.52
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.90	0.52
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.91	0.52
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.91	0.52
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.92	0.52
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.89	0.52
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.91	0.52
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	1.90	0.52
2:E:315:CYS:SG	2:E:316:PHE:N	2.82	0.52
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.92	0.52
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.91	0.52
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.92	0.52
2:B:315:CYS:SG	2:B:316:PHE:N	2.82	0.52
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.91	0.52
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.91	0.52
2:G:168:ASP:HB3	2:G:199:LEU:HD22	1.91	0.52
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.92	0.52
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.91	0.52
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.91	0.52
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.92	0.52
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.92	0.52
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.92	0.52
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.74	0.52
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.92	0.52
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.92	0.52
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.92	0.52
2:E:168:ASP:HB3	2:E:199:LEU:HD22	1.91	0.51
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.92	0.51
2:E:4230:LYS:CG	2:E:4959:PHE:CE2	2.88	0.51
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.51
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.93	0.51
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.43	0.51
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.91	0.51
2:I:132:ALA:HA	2:I:194:SER:HB2	1.93	0.51
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.44	0.51
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.91	0.51
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.92	0.51
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.93	0.51
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.91	0.51
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.93	0.51
2:G:132:ALA:HA	2:G:194:SER:HB2	1.93	0.51
2:B:451:TYR:O	2:B:474:ARG:NH1	2.41	0.51
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.44	0.51
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.91	0.51
2:B:4230:LYS:CG	2:B:4959:PHE:CE2	2.88	0.51
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.76	0.51
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.91	0.51
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.91	0.51
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.92	0.51
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.91	0.51
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.92	0.51
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.93	0.51
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.44	0.51
2:I:4230:LYS:CG	2:I:4959:PHE:CE2	2.88	0.51
2:I:4958:CYS:SG	2:I:4961:CYS:N	2.84	0.51
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.44	0.51
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.93	0.51
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.91	0.51
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.51
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.93	0.51
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.91	0.51
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.44	0.51
2:G:682:LEU:HD13	2:G:787:VAL:HG11	1.92	0.51
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.84	0.51
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4064:MET:HA	2:B:4067:LYS:HZ2	1.75	0.51
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.92	0.51
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.84	0.51
2:B:4958:CYS:SG	2:B:4961:CYS:N	2.84	0.51
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.44	0.51
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.84	0.51
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.76	0.51
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.27	0.51
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.91	0.51
2:B:4182:GLU:OE1	2:B:4983:HIS:NE2	2.44	0.51
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.92	0.51
2:I:682:LEU:HD13	2:I:787:VAL:HG11	1.92	0.51
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.93	0.51
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.27	0.51
2:E:682:LEU:HD13	2:E:787:VAL:HG11	1.92	0.51
1:J:27:THR:HB	1:J:100:ASP:HB3	1.93	0.51
2:B:682:LEU:HD13	2:B:787:VAL:HG11	1.92	0.51
2:I:241:GLN:O	2:I:289:ARG:NH1	2.42	0.51
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.92	0.51
2:E:132:ALA:HA	2:E:194:SER:HB2	1.93	0.51
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.84	0.51
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.76	0.51
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.93	0.51
1:H:27:THR:HB	1:H:100:ASP:HB3	1.93	0.50
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.92	0.50
2:B:683:ARG:NH1	2:B:707:VAL:O	2.37	0.50
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.44	0.50
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.93	0.50
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.93	0.50
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.76	0.50
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.93	0.50
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.93	0.50
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.44	0.50
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.50
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.93	0.50
2:I:2347:GLU:O	2:I:2351:ASN:N	2.40	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.92	0.50
1:F:27:THR:HB	1:F:100:ASP:HB3	1.93	0.50
2:B:1269:CYS:HA	2:B:1473:UNK:HA	1.93	0.50
2:I:485:SER:O	2:I:489:ASN:N	2.40	0.50
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.94	0.50
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.93	0.50
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.94	0.50
2:B:132:ALA:HA	2:B:194:SER:HB2	1.93	0.50
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.93	0.50
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.94	0.50
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.29	0.50
2:G:485:SER:O	2:G:489:ASN:N	2.40	0.50
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.93	0.50
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.29	0.50
2:G:4958:CYS:SG	2:G:4961:CYS:N	2.84	0.50
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.92	0.50
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.94	0.50
2:I:4064:MET:HA	2:I:4067:LYS:HZ1	1.76	0.50
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.29	0.50
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.94	0.50
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.93	0.50
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.76	0.50
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.94	0.50
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.93	0.50
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.94	0.50
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.94	0.50
2:G:4064:MET:HA	2:G:4067:LYS:HZ1	1.77	0.50
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.93	0.50
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.27	0.50
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.76	0.50
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.93	0.50
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.94	0.50
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.41	0.50
1:F:11:ASP:OD1	1:F:67:SER:OG	2.27	0.50
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.94	0.50
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.41	0.50
2:E:218:HIS:HB3	2:E:392:ARG:HD3	1.94	0.50
2:E:1269:CYS:HA	2:E:1473:UNK:HA	1.93	0.50
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.94	0.50
2:G:173:SER:HB3	2:G:178:ARG:H	1.77	0.50
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.93	0.50
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.94	0.50
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.94	0.50
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.45	0.50
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.29	0.50
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.93	0.50
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.50
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.93	0.50
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.93	0.50
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.93	0.50
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.45	0.49
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.94	0.49
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.94	0.49
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.94	0.49
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.45	0.49
2:E:4958:CYS:SG	2:E:4961:CYS:N	2.84	0.49
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.76	0.49
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.39	0.49
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.93	0.49
2:I:3922:TYR:O	2:I:3926:LEU:N	2.44	0.49
2:E:1516:UNK:N	2:E:1529:UNK:O	2.45	0.49
2:E:4064:MET:HA	2:E:4067:LYS:HZ1	1.77	0.49
2:G:241:GLN:O	2:G:289:ARG:NH1	2.42	0.49
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.46	0.49
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.94	0.49
2:B:173:SER:HB3	2:B:178:ARG:H	1.77	0.49
2:B:218:HIS:HB3	2:B:392:ARG:HD3	1.94	0.49
2:B:1848:LEU:HB3	2:B:1853:ILE:HB	1.95	0.49
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.94	0.49
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.49
2:I:1516:UNK:N	2:I:1529:UNK:O	2.45	0.49
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.45	0.49
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.94	0.49
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.94	0.49
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.39	0.49
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.78	0.49
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.94	0.49
2:G:1660:GLN:O	2:G:1664:SER:N	2.45	0.49
1:A:27:THR:HB	1:A:100:ASP:HB3	1.93	0.49
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.94	0.49
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.94	0.49
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.42	0.49
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.94	0.49
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.94	0.49
2:E:1848:LEU:HB3	2:E:1853:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.95	0.49
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.49
2:G:1269:CYS:HA	2:G:1473:UNK:HA	1.93	0.49
2:G:1516:UNK:N	2:G:1529:UNK:O	2.45	0.49
2:B:241:GLN:O	2:B:289:ARG:NH1	2.42	0.49
2:B:2758:PHE:O	2:B:2762:THR:N	2.45	0.49
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.95	0.49
2:I:1148:VAL:HB	2:I:1165:ASN:HA	1.94	0.49
2:I:1269:CYS:HA	2:I:1473:UNK:HA	1.93	0.49
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.93	0.49
2:E:2758:PHE:O	2:E:2762:THR:N	2.45	0.49
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.49
2:G:4975:PHE:O	2:G:4979:THR:HG23	2.12	0.49
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.46	0.49
2:B:1516:UNK:N	2:B:1529:UNK:O	2.45	0.49
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.94	0.49
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.95	0.49
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.46	0.49
2:E:3840:SER:O	2:E:3922:TYR:OH	2.31	0.49
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.94	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.44	0.49
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.93	0.49
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.94	0.49
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.95	0.49
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.44	0.49
2:B:4928:LEU:HD23	2:B:4931:ILE:HD12	1.95	0.49
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.95	0.49
2:I:880:GLU:OE1	2:I:968:ALA:N	2.44	0.49
2:I:978:THR:HB	2:I:980:ALA:H	1.78	0.49
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.46	0.49
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.39	0.49
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.94	0.49
2:I:4892:ARG:NH2	2:G:4898:GLY:O	2.46	0.49
2:I:4998:LYS:NZ	2:I:5007:GLU:OE1	2.43	0.49
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.93	0.49
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.46	0.49
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.95	0.49
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.46	0.49
2:I:4928:LEU:HD23	2:I:4931:ILE:HD12	1.95	0.49
2:E:485:SER:O	2:E:489:ASN:N	2.40	0.49
2:E:1991:THR:O	2:E:1995:THR:OG1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2347:GLU:O	2:E:2351:ASN:N	2.40	0.49
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.95	0.49
2:G:1848:LEU:HB3	2:G:1853:ILE:HB	1.95	0.49
2:G:1991:THR:O	2:G:1995:THR:OG1	2.31	0.49
2:G:4056:GLU:O	2:G:4060:LYS:N	2.43	0.49
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.94	0.49
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.94	0.49
2:B:978:THR:HB	2:B:980:ALA:H	1.78	0.49
2:I:709:ASP:HA	2:I:725:HIS:H	1.78	0.49
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.94	0.49
2:E:3922:TYR:O	2:E:3926:LEU:N	2.44	0.49
2:E:4182:GLU:OE1	2:E:4983:HIS:NE2	2.44	0.49
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.42	0.49
2:E:4928:LEU:HD23	2:E:4931:ILE:HD12	1.95	0.49
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.95	0.49
2:G:4928:LEU:HD23	2:G:4931:ILE:HD12	1.95	0.49
2:B:4975:PHE:O	2:B:4979:THR:HG23	2.12	0.48
2:I:173:SER:HB3	2:I:178:ARG:H	1.77	0.48
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.46	0.48
2:I:4056:GLU:O	2:I:4060:LYS:N	2.43	0.48
2:E:1660:GLN:O	2:E:1664:SER:N	2.45	0.48
2:G:978:THR:HB	2:G:980:ALA:H	1.78	0.48
2:G:1148:VAL:HB	2:G:1165:ASN:HA	1.95	0.48
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.94	0.48
2:B:709:ASP:HA	2:B:725:HIS:H	1.78	0.48
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.95	0.48
2:B:1148:VAL:HB	2:B:1165:ASN:HA	1.94	0.48
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.46	0.48
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.78	0.48
2:I:1848:LEU:HB3	2:I:1853:ILE:HB	1.95	0.48
2:I:3840:SER:O	2:I:3922:TYR:OH	2.31	0.48
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.46	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.44	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.48
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.47	0.48
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.94	0.48
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.27	0.48
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.45	0.48
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.94	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.95	0.48
2:B:645:ARG:N	2:B:824:GLU:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.94	0.48
2:E:1148:VAL:HB	2:E:1165:ASN:HA	1.95	0.48
2:E:4056:GLU:O	2:E:4060:LYS:N	2.43	0.48
2:G:3840:SER:O	2:G:3922:TYR:OH	2.31	0.48
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.95	0.48
2:I:4975:PHE:O	2:I:4979:THR:HG23	2.12	0.48
2:E:173:SER:HB3	2:E:178:ARG:H	1.77	0.48
2:E:278:GLN:N	2:E:315:CYS:SG	2.87	0.48
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.95	0.48
2:E:4921:PHE:HA	2:E:4925:ILE:HD13	1.95	0.48
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.95	0.48
2:G:4182:GLU:OE1	2:G:4983:HIS:NE2	2.44	0.48
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.95	0.48
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.46	0.48
2:G:218:HIS:HB3	2:G:392:ARG:HD3	1.94	0.48
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.48
2:G:3767:GLN:HA	2:G:3770:LEU:HB2	1.95	0.48
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.78	0.48
2:I:626:LEU:HG	2:I:628:GLY:H	1.79	0.48
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.93	0.48
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.95	0.48
2:G:626:LEU:HG	2:G:628:GLY:H	1.79	0.48
2:G:2347:GLU:O	2:G:2351:ASN:N	2.40	0.48
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.95	0.48
2:I:4182:GLU:OE1	2:I:4983:HIS:NE2	2.44	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.48
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.95	0.48
2:E:4975:PHE:O	2:E:4979:THR:HG23	2.12	0.48
2:G:4215:ARG:NH2	3:G:5101:ATP:O1A	2.47	0.48
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.46	0.48
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.48
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.41	0.48
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.47	0.48
2:I:218:HIS:HB3	2:I:392:ARG:HD3	1.94	0.48
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.48
2:I:4230:LYS:CD	2:I:4959:PHE:HE2	1.94	0.48
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.94	0.48
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.46	0.48
2:G:709:ASP:HA	2:G:725:HIS:H	1.79	0.48
2:B:1991:THR:O	2:B:1995:THR:OG1	2.31	0.48
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:645:ARG:N	2:G:824:GLU:O	2.45	0.48
2:B:1660:GLN:O	2:B:1664:SER:N	2.45	0.48
2:B:3767:GLN:HA	2:B:3770:LEU:HB2	1.95	0.48
2:I:1991:THR:O	2:I:1995:THR:OG1	2.31	0.48
2:E:709:ASP:HA	2:E:725:HIS:H	1.79	0.48
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.48
2:E:1694:LEU:O	2:E:1712:TYR:OH	2.27	0.48
2:G:278:GLN:N	2:G:315:CYS:SG	2.87	0.48
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.46	0.48
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.78	0.48
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.32	0.48
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.95	0.48
2:B:278:GLN:N	2:B:315:CYS:SG	2.87	0.47
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.32	0.47
2:B:4921:PHE:HA	2:B:4925:ILE:HD13	1.95	0.47
2:I:1171:SER:OG	2:I:1175:SER:N	2.45	0.47
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.95	0.47
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.79	0.47
2:I:4921:PHE:HA	2:I:4925:ILE:HD13	1.95	0.47
2:E:1171:SER:OG	2:E:1175:SER:N	2.45	0.47
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.47
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.46	0.47
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.96	0.47
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.96	0.47
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.97	0.47
2:I:2758:PHE:O	2:I:2762:THR:N	2.45	0.47
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.96	0.47
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.48	0.47
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.96	0.47
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.94	0.47
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.94	0.47
2:B:3840:SER:O	2:B:3922:TYR:OH	2.31	0.47
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.97	0.47
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.32	0.47
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.46	0.47
2:B:4056:GLU:O	2:B:4060:LYS:N	2.43	0.47
2:I:2880:GLU:O	2:I:2884:ASN:N	2.47	0.47
1:A:82:TYR:O	1:A:86:GLY:N	2.48	0.47
1:H:82:TYR:O	1:H:86:GLY:N	2.48	0.47
2:B:4898:GLY:O	2:E:4892:ARG:NH2	2.47	0.47
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	1.96	0.47
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.97	0.47
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	1.96	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.95	0.47
2:E:309:THR:O	2:E:313:SER:OG	2.33	0.47
2:E:978:THR:HB	2:E:980:ALA:H	1.78	0.47
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.32	0.47
2:E:4957:LYS:HG2	2:E:4964:GLY:CA	2.25	0.47
2:G:1663:HIS:O	2:G:1667:LEU:N	2.47	0.47
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.38	0.47
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.96	0.47
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.48	0.47
2:B:4215:ARG:NH2	3:B:5101:ATP:O1A	2.47	0.47
2:I:645:ARG:N	2:I:824:GLU:O	2.45	0.47
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.48	0.47
2:I:3767:GLN:HA	2:I:3770:LEU:HB2	1.95	0.47
2:E:626:LEU:HG	2:E:628:GLY:H	1.79	0.47
2:E:3767:GLN:HA	2:E:3770:LEU:HB2	1.96	0.47
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.46	0.47
2:G:101:LEU:HB3	2:G:150:MET:HE1	1.97	0.47
2:B:626:LEU:HG	2:B:628:GLY:H	1.79	0.47
2:B:2880:GLU:O	2:B:2884:ASN:N	2.47	0.47
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.47	0.47
2:G:309:THR:O	2:G:313:SER:OG	2.33	0.47
2:G:880:GLU:OE1	2:G:968:ALA:N	2.44	0.47
2:G:4921:PHE:HA	2:G:4925:ILE:HD13	1.95	0.47
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.43	0.47
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.96	0.47
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.96	0.47
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.96	0.47
1:J:82:TYR:O	1:J:86:GLY:N	2.48	0.47
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.97	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.50	0.47
2:I:1663:HIS:O	2:I:1667:LEU:N	2.47	0.47
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.44	0.47
2:G:842:PRO:HD3	2:G:1073:ARG:HG3	1.97	0.47
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	1.96	0.47
1:F:82:TYR:O	1:F:86:GLY:N	2.48	0.46
1:A:11:ASP:OD1	1:A:67:SER:OG	2.27	0.46
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.96	0.46
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	1.96	0.46
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.46	0.46
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.97	0.46
2:B:309:THR:O	2:B:313:SER:OG	2.33	0.46
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.97	0.46
2:B:1965:TYR:OH	2:B:2027:ILE:O	2.33	0.46
2:E:645:ARG:N	2:E:824:GLU:O	2.45	0.46
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.97	0.46
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.98	0.46
2:E:2868:SER:O	2:E:2872:GLN:N	2.45	0.46
2:E:4998:LYS:NZ	2:E:5007:GLU:OE1	2.43	0.46
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.96	0.46
2:E:880:GLU:OE1	2:E:968:ALA:N	2.44	0.46
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.96	0.46
2:G:913:LEU:O	2:G:918:ARG:NH2	2.49	0.46
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.96	0.46
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.98	0.46
2:B:4892:ARG:NH2	2:I:4898:GLY:O	2.49	0.46
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.96	0.46
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.80	0.46
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.80	0.46
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.97	0.46
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.96	0.46
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.49	0.46
2:I:101:LEU:HB3	2:I:150:MET:HE1	1.97	0.46
2:E:842:PRO:HD3	2:E:1073:ARG:HG3	1.97	0.46
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.50	0.46
2:E:4215:ARG:NH2	3:E:5101:ATP:O1A	2.47	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.41	0.46
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.81	0.46
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.98	0.46
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.97	0.46
2:B:488:LEU:O	2:B:492:ASP:N	2.47	0.46
2:B:1101:ARG:HE	2:B:1115:LEU:HB3	1.81	0.46
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.46
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.98	0.46
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.96	0.46
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.98	0.46
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.46
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.81	0.46
2:I:278:GLN:N	2:I:315:CYS:SG	2.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.96	0.46
2:G:2880:GLU:O	2:G:2884:ASN:N	2.47	0.46
2:B:913:LEU:O	2:B:918:ARG:NH2	2.49	0.46
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.98	0.46
2:E:101:LEU:HB3	2:E:150:MET:HE1	1.97	0.46
2:E:913:LEU:O	2:E:918:ARG:NH2	2.49	0.46
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.50	0.46
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.46
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.50	0.45
2:E:488:LEU:O	2:E:492:ASP:N	2.47	0.45
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.97	0.45
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.98	0.45
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.98	0.45
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.49	0.45
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.98	0.45
2:E:1663:HIS:O	2:E:1667:LEU:N	2.47	0.45
2:E:1965:TYR:OH	2:E:2027:ILE:O	2.33	0.45
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.81	0.45
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.99	0.45
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.99	0.45
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.99	0.45
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.99	0.45
2:B:842:PRO:HD3	2:B:1073:ARG:HG3	1.97	0.45
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.81	0.45
2:B:3922:TYR:O	2:B:3926:LEU:N	2.44	0.45
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	1.97	0.45
2:I:309:THR:O	2:I:313:SER:OG	2.33	0.45
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.50	0.45
2:I:842:PRO:HD3	2:I:1073:ARG:HG3	1.97	0.45
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.98	0.45
2:I:913:LEU:O	2:I:918:ARG:NH2	2.49	0.45
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.81	0.45
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.98	0.45
2:B:2347:GLU:O	2:B:2351:ASN:N	2.40	0.45
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.82	0.45
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.99	0.45
2:E:621:ILE:O	2:E:625:LEU:N	2.47	0.45
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.81	0.45
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.99	0.45
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.81	0.45
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:488:LEU:O	2:G:492:ASP:N	2.47	0.45
2:G:776:LEU:HG	2:G:848:HIS:HA	1.98	0.45
2:G:1101:ARG:HE	2:G:1115:LEU:HB3	1.81	0.45
2:G:2868:SER:O	2:G:2872:GLN:N	2.45	0.45
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.49	0.45
1:H:21:THR:HA	1:H:49:ARG:HA	1.99	0.45
2:I:776:LEU:HG	2:I:848:HIS:HA	1.98	0.45
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.49	0.45
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.99	0.45
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.98	0.45
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.98	0.45
2:G:4558:ASN:HB2	2:G:4561:THR:HB	1.99	0.45
1:A:19:GLY:HA2	1:A:49:ARG:HH21	1.81	0.45
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.82	0.45
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.98	0.45
2:I:793:LEU:HD22	2:I:821:LEU:HD13	1.99	0.45
2:I:1660:GLN:O	2:I:1664:SER:N	2.45	0.45
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.99	0.45
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.99	0.45
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.81	0.45
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.50	0.45
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.98	0.45
1:A:21:THR:HA	1:A:49:ARG:HA	1.99	0.45
2:I:1154:ASP:O	2:I:1158:ASN:N	2.50	0.45
2:I:1843:LYS:HB2	2:I:1938:GLN:HE22	1.82	0.45
2:G:621:ILE:O	2:G:625:LEU:N	2.47	0.45
1:H:19:GLY:HA2	1:H:49:ARG:HH21	1.81	0.45
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.82	0.45
2:I:4558:ASN:HB2	2:I:4561:THR:HB	1.99	0.45
2:E:1101:ARG:HE	2:E:1115:LEU:HB3	1.81	0.45
2:E:1843:LYS:HB2	2:E:1938:GLN:HE22	1.82	0.45
2:E:2880:GLU:O	2:E:2884:ASN:N	2.47	0.45
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.81	0.45
2:G:1154:ASP:O	2:G:1158:ASN:N	2.50	0.45
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	1.99	0.45
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.50	0.44
2:B:776:LEU:HG	2:B:848:HIS:HA	1.98	0.44
2:I:614:VAL:HG22	2:I:616:SER:H	1.82	0.44
2:I:1101:ARG:HE	2:I:1115:LEU:HB3	1.81	0.44
2:E:776:LEU:HG	2:E:848:HIS:HA	1.98	0.44
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.98	0.44
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.46	0.44
2:G:3932:ASP:HA	2:G:3935:TRP:HD1	1.81	0.44
2:G:4855:ALA:HA	2:G:4859:PHE:HB2	1.99	0.44
1:H:30:LEU:HD23	1:H:33:GLY:HA3	1.99	0.44
1:J:21:THR:HA	1:J:49:ARG:HA	1.99	0.44
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.98	0.44
2:I:1965:TYR:OH	2:I:2027:ILE:O	2.33	0.44
2:I:3932:ASP:HA	2:I:3935:TRP:HD1	1.81	0.44
2:E:468:LEU:HB3	2:E:472:ARG:HH12	1.82	0.44
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.98	0.44
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.99	0.44
2:G:614:VAL:HG22	2:G:616:SER:H	1.82	0.44
2:G:1171:SER:OG	2:G:1175:SER:N	2.45	0.44
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.91	0.44
2:G:3922:TYR:O	2:G:3926:LEU:N	2.44	0.44
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.99	0.44
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.99	0.44
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.91	0.44
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.83	0.44
2:E:614:VAL:HG22	2:E:616:SER:H	1.82	0.44
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.50	0.44
2:E:4924:VAL:HG23	2:E:4925:ILE:HD12	2.00	0.44
2:G:395:GLN:HG3	2:G:397:GLU:H	1.82	0.44
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	1.99	0.44
2:B:614:VAL:HG22	2:B:616:SER:H	1.82	0.44
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.99	0.44
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.98	0.44
2:B:1171:SER:OG	2:B:1175:SER:N	2.45	0.44
2:B:4697:VAL:O	2:B:4701:TRP:N	2.51	0.44
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.98	0.44
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.81	0.44
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.51	0.44
2:E:460:GLN:HG2	2:E:462:GLU:H	1.83	0.44
2:E:793:LEU:HD22	2:E:821:LEU:HD13	1.99	0.44
2:G:1843:LYS:HB2	2:G:1938:GLN:HE22	1.82	0.44
2:G:2758:PHE:O	2:G:2762:THR:N	2.44	0.44
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.82	0.44
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.99	0.44
1:J:19:GLY:HA2	1:J:49:ARG:HH21	1.81	0.44
2:B:793:LEU:HD22	2:B:821:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:880:GLU:OE1	2:B:968:ALA:N	2.44	0.44
2:B:1973:GLN:O	2:B:1977:TYR:N	2.45	0.44
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.00	0.44
2:I:460:GLN:HG2	2:I:462:GLU:H	1.83	0.44
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.98	0.44
2:I:3362:UNK:O	2:I:3366:UNK:N	2.51	0.44
2:E:2810:LYS:O	2:E:2814:LYS:N	2.45	0.44
2:E:3362:UNK:O	2:E:3366:UNK:N	2.51	0.44
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.51	0.44
2:G:460:GLN:HG2	2:G:462:GLU:H	1.83	0.44
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.31	0.44
2:G:3362:UNK:O	2:G:3366:UNK:N	2.51	0.44
2:G:4924:VAL:HG23	2:G:4925:ILE:HD12	2.00	0.44
1:F:30:LEU:HD23	1:F:33:GLY:HA3	1.99	0.44
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.83	0.44
2:B:1154:ASP:O	2:B:1158:ASN:N	2.50	0.44
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.83	0.44
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.82	0.44
2:E:395:GLN:HG3	2:E:397:GLU:H	1.82	0.44
2:E:1457:UNK:N	2:E:1497:UNK:O	2.51	0.44
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.82	0.44
2:E:4843:LEU:HD12	2:G:4823:LEU:HD23	1.99	0.44
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.82	0.44
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.99	0.44
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.98	0.44
1:F:19:GLY:HA2	1:F:49:ARG:HH21	1.81	0.44
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.83	0.44
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.99	0.44
2:B:460:GLN:HG2	2:B:462:GLU:H	1.83	0.44
2:I:621:ILE:O	2:I:625:LEU:N	2.47	0.44
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.42	0.44
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.00	0.44
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	1.99	0.44
2:G:468:LEU:HB3	2:G:472:ARG:HH12	1.82	0.44
1:F:21:THR:HA	1:F:49:ARG:HA	1.99	0.44
2:B:206:CYS:SG	2:B:207:SER:N	2.91	0.44
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.00	0.44
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.91	0.44
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.46	0.44
2:B:3842:LEU:O	2:B:3929:SER:OG	2.36	0.44
2:I:1457:UNK:N	2:I:1497:UNK:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	2.00	0.44
2:I:4924:VAL:HG23	2:I:4925:ILE:HD12	2.00	0.44
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.83	0.44
2:G:793:LEU:HD22	2:G:821:LEU:HD13	1.99	0.44
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	2.00	0.44
2:B:56:GLN:O	2:B:309:THR:OG1	2.33	0.44
2:B:395:GLN:HG3	2:B:397:GLU:H	1.82	0.44
2:B:468:LEU:HB3	2:B:472:ARG:HH12	1.82	0.44
2:B:1843:LYS:HB2	2:B:1938:GLN:HE22	1.82	0.44
2:I:395:GLN:HG3	2:I:397:GLU:H	1.82	0.44
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.00	0.44
2:E:206:CYS:SG	2:E:207:SER:N	2.91	0.44
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.83	0.43
2:B:116:MET:HB2	2:B:137:LEU:HD12	2.00	0.43
2:B:3932:ASP:HA	2:B:3935:TRP:HD1	1.81	0.43
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.51	0.43
2:I:463:GLU:O	2:I:466:SER:OG	2.35	0.43
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.99	0.43
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	1.99	0.43
2:I:4855:ALA:HA	2:I:4859:PHE:HB2	1.99	0.43
2:E:3905:THR:HA	2:E:3912:THR:HG23	2.00	0.43
2:E:3932:ASP:HA	2:E:3935:TRP:HD1	1.81	0.43
2:G:3905:THR:HA	2:G:3912:THR:HG23	2.00	0.43
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.99	0.43
2:B:2868:SER:O	2:B:2872:GLN:N	2.45	0.43
2:B:4924:VAL:HG23	2:B:4925:ILE:HD12	2.00	0.43
2:I:468:LEU:HB3	2:I:472:ARG:HH12	1.82	0.43
2:I:4215:ARG:NH2	3:I:5101:ATP:O1A	2.47	0.43
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.99	0.43
2:E:765:GLN:NE2	2:E:1521:UNK:O	2.52	0.43
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.41	0.43
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.84	0.43
2:G:3842:LEU:O	2:G:3929:SER:OG	2.36	0.43
2:G:4031:LEU:HB3	2:G:4034:ASN:HB2	2.00	0.43
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	2.01	0.43
1:A:30:LEU:HD23	1:A:33:GLY:HA3	1.99	0.43
2:B:210:GLU:HG3	2:B:337:PRO:HG3	2.00	0.43
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.51	0.43
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.99	0.43
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.00	0.43
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:MET:HB2	2:E:137:LEU:HD12	2.00	0.43
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.99	0.43
1:J:30:LEU:HD23	1:J:33:GLY:HA3	1.99	0.43
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.84	0.43
2:B:3362:UNK:O	2:B:3366:UNK:N	2.51	0.43
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.83	0.43
2:B:4855:ALA:HA	2:B:4859:PHE:HB2	1.99	0.43
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.51	0.43
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	2.00	0.43
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	2.00	0.43
2:E:3842:LEU:O	2:E:3929:SER:OG	2.36	0.43
2:G:1973:GLN:O	2:G:1977:TYR:N	2.45	0.43
2:G:4003:LEU:HB2	2:G:4013:LEU:HD13	2.00	0.43
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.83	0.43
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.00	0.43
2:B:4003:LEU:HB2	2:B:4013:LEU:HD13	2.00	0.43
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	2.00	0.43
2:B:4558:ASN:HB2	2:B:4561:THR:HB	1.99	0.43
2:I:210:GLU:HG3	2:I:337:PRO:HG3	2.00	0.43
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.99	0.43
2:I:1865:MET:SD	2:I:1865:MET:N	2.92	0.43
2:I:3842:LEU:O	2:I:3929:SER:OG	2.36	0.43
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.83	0.43
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.00	0.43
2:G:765:GLN:NE2	2:G:1521:UNK:O	2.52	0.43
2:G:1937:LEU:O	2:G:1941:ASN:ND2	2.52	0.43
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.82	0.43
2:G:4834:GLY:HA2	2:G:4837:LEU:HD12	2.00	0.43
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.00	0.43
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.84	0.43
2:I:183:SER:N	2:I:190:GLN:O	2.51	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.83	0.43
2:I:4031:LEU:HB3	2:I:4034:ASN:HB2	2.00	0.43
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.84	0.43
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.83	0.43
2:E:4697:VAL:O	2:E:4701:TRP:N	2.51	0.43
2:G:206:CYS:SG	2:G:207:SER:N	2.91	0.43
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.00	0.43
1:F:7:ILE:N	1:F:71:ARG:O	2.46	0.43
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	1.99	0.43
2:B:1937:LEU:O	2:B:1941:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4977:THR:HG22	2:B:4981:GLU:HB2	2.01	0.43
2:I:2103:VAL:O	2:I:2107:GLN:N	2.47	0.43
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.84	0.43
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.52	0.43
2:E:4558:ASN:HB2	2:E:4561:THR:HB	1.99	0.43
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.83	0.43
2:B:1457:UNK:N	2:B:1497:UNK:O	2.51	0.43
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.52	0.43
2:E:1154:ASP:O	2:E:1158:ASN:N	2.50	0.43
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.83	0.43
2:E:4003:LEU:HB2	2:E:4013:LEU:HD13	2.00	0.43
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	2.01	0.43
2:E:4834:GLY:HA2	2:E:4837:LEU:HD12	2.00	0.43
2:E:4977:THR:HG22	2:E:4981:GLU:HB2	2.01	0.43
2:G:1238:PHE:O	2:G:1606:SER:N	2.50	0.43
2:G:1457:UNK:N	2:G:1497:UNK:O	2.51	0.43
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.00	0.43
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.51	0.43
2:G:4239:GLU:OE2	2:G:5014:TYR:OH	2.34	0.43
2:G:4875:LYS:HB3	2:G:4882:CYS:HA	2.01	0.43
2:B:485:SER:O	2:B:489:ASN:N	2.40	0.43
2:B:1865:MET:SD	2:B:1865:MET:N	2.92	0.43
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.83	0.43
2:B:3552:UNK:O	2:B:3556:UNK:N	2.52	0.43
2:I:1937:LEU:O	2:I:1941:ASN:ND2	2.52	0.43
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	2.00	0.43
2:I:4782:VAL:O	2:I:4785:THR:OG1	2.37	0.43
2:I:4977:THR:HG22	2:I:4981:GLU:HB2	2.01	0.43
2:E:1154:ASP:HB3	2:E:1157:GLU:HB3	2.01	0.43
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.00	0.43
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	2.01	0.43
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.00	0.43
2:G:1865:MET:SD	2:G:1865:MET:N	2.92	0.43
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.84	0.43
2:B:21:VAL:HG12	2:B:66:CYS:HA	2.01	0.43
2:B:1154:ASP:HB3	2:B:1157:GLU:HB3	2.01	0.43
2:B:1663:HIS:O	2:B:1667:LEU:N	2.47	0.43
2:I:206:CYS:SG	2:I:207:SER:N	2.91	0.43
2:I:4834:GLY:HA2	2:I:4837:LEU:HD12	2.00	0.43
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.84	0.43
2:E:3365:UNK:O	2:E:3369:UNK:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3902:TYR:O	2:E:3906:GLN:NE2	2.52	0.43
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.00	0.43
2:G:3880:PHE:O	2:G:3884:LEU:N	2.52	0.43
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	2.00	0.42
2:B:3365:UNK:O	2:B:3369:UNK:N	2.52	0.42
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.84	0.42
2:I:116:MET:HB2	2:I:137:LEU:HD12	2.00	0.42
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.84	0.42
2:I:2868:SER:O	2:I:2872:GLN:N	2.45	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.52	0.42
2:E:1238:PHE:O	2:E:1606:SER:N	2.50	0.42
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	2.00	0.42
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.83	0.42
2:E:4031:LEU:HB3	2:E:4034:ASN:HB2	2.00	0.42
2:G:2863:SER:OG	2:G:2928:LYS:NZ	2.48	0.42
2:G:4064:MET:O	2:G:4068:LEU:N	2.52	0.42
2:B:183:SER:N	2:B:190:GLN:O	2.51	0.42
2:B:1659:LEU:O	2:B:1663:HIS:N	2.49	0.42
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.84	0.42
2:B:3880:PHE:O	2:B:3884:LEU:N	2.52	0.42
2:B:3902:TYR:O	2:B:3906:GLN:NE2	2.52	0.42
2:B:3905:THR:HA	2:B:3912:THR:HG23	2.00	0.42
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.52	0.42
2:I:4003:LEU:HB2	2:I:4013:LEU:HD13	2.00	0.42
2:E:21:VAL:HG12	2:E:66:CYS:HA	2.01	0.42
2:E:210:GLU:HG3	2:E:337:PRO:HG3	2.00	0.42
2:E:606:LEU:O	2:E:617:ASN:ND2	2.52	0.42
2:E:1937:LEU:O	2:E:1941:ASN:ND2	2.52	0.42
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.54	0.42
2:E:4875:LYS:HB3	2:E:4882:CYS:HA	2.01	0.42
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.02	0.42
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.83	0.42
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.41	0.42
2:G:4977:THR:HG22	2:G:4981:GLU:HB2	2.01	0.42
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.89	0.42
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.53	0.42
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	2.01	0.42
2:B:4834:GLY:HA2	2:B:4837:LEU:HD12	2.00	0.42
2:I:606:LEU:O	2:I:617:ASN:ND2	2.52	0.42
2:I:765:GLN:NE2	2:I:1521:UNK:O	2.52	0.42
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3880:PHE:O	2:I:3884:LEU:N	2.52	0.42
2:I:3905:THR:HA	2:I:3912:THR:HG23	2.00	0.42
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.53	0.42
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.84	0.42
2:G:21:VAL:HG12	2:G:66:CYS:HA	2.01	0.42
2:G:3902:TYR:O	2:G:3906:GLN:NE2	2.52	0.42
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.84	0.42
1:F:7:ILE:HG22	1:F:9:PRO:HD2	2.01	0.42
2:B:606:LEU:O	2:B:617:ASN:ND2	2.52	0.42
2:B:4031:LEU:HB3	2:B:4034:ASN:HB2	2.00	0.42
2:I:21:VAL:HG12	2:I:66:CYS:HA	2.01	0.42
2:I:4697:VAL:O	2:I:4701:TRP:N	2.51	0.42
2:E:123:THR:OG1	2:E:134:ASP:OD1	2.38	0.42
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.02	0.42
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.36	0.42
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	2.01	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.52	0.42
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.85	0.42
2:B:233:ILE:HD12	2:B:242:ARG:HB3	2.01	0.42
2:B:765:GLN:NE2	2:B:1521:UNK:O	2.52	0.42
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.53	0.42
2:E:1973:GLN:O	2:E:1977:TYR:N	2.45	0.42
2:E:2132:GLY:O	2:E:2136:ARG:N	2.53	0.42
2:G:116:MET:HB2	2:G:137:LEU:HD12	2.00	0.42
2:G:183:SER:N	2:G:190:GLN:O	2.51	0.42
2:G:210:GLU:HG3	2:G:337:PRO:HG3	2.00	0.42
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.84	0.42
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.52	0.42
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.54	0.42
1:H:55:VAL:HA	2:G:1784:ALA:HA	2.02	0.42
2:B:37:LEU:HD11	2:B:47:CYS:HB3	2.01	0.42
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.85	0.42
2:I:488:LEU:O	2:I:492:ASP:N	2.48	0.42
2:I:3902:TYR:O	2:I:3906:GLN:NE2	2.52	0.42
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.84	0.42
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.00	0.42
2:E:1865:MET:SD	2:E:1865:MET:N	2.92	0.42
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.85	0.42
2:E:4855:ALA:HA	2:E:4859:PHE:HB2	1.99	0.42
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.52	0.42
2:G:3552:UNK:O	2:G:3556:UNK:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HG22	1:A:9:PRO:HD2	2.01	0.42
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.84	0.42
2:I:1154:ASP:HB3	2:I:1157:GLU:HB3	2.01	0.42
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.02	0.42
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.02	0.42
2:I:4064:MET:O	2:I:4068:LEU:N	2.52	0.42
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.46	0.42
2:E:3880:PHE:O	2:E:3884:LEU:N	2.52	0.42
2:E:4064:MET:O	2:E:4068:LEU:N	2.52	0.42
2:G:37:LEU:HD11	2:G:47:CYS:HB3	2.01	0.42
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.83	0.42
2:E:37:LEU:HD11	2:E:47:CYS:HB3	2.01	0.42
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.34	0.42
2:G:215:THR:H	2:G:218:HIS:CE1	2.38	0.42
2:G:224:HIS:N	2:G:229:GLU:O	2.44	0.42
2:G:606:LEU:O	2:G:617:ASN:ND2	2.52	0.42
2:G:1154:ASP:HB3	2:G:1157:GLU:HB3	2.01	0.42
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.85	0.42
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.02	0.42
1:H:7:ILE:HG22	1:H:9:PRO:HD2	2.01	0.42
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.54	0.42
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.51	0.42
2:I:123:THR:OG1	2:I:134:ASP:OD1	2.38	0.42
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	2.02	0.42
2:E:1105:ALA:N	2:E:1189:LEU:O	2.53	0.42
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.52	0.42
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.52	0.42
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.51	0.42
2:G:233:ILE:HD12	2:G:242:ARG:HB3	2.01	0.42
2:G:1074:ILE:HA	2:G:1193:SER:HA	2.02	0.42
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	2.01	0.42
2:I:37:LEU:HD11	2:I:47:CYS:HB3	2.01	0.42
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.52	0.42
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.85	0.42
2:E:940:GLY:O	2:E:1052:ASN:N	2.52	0.42
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.02	0.42
2:E:4848:VAL:O	2:E:4852:THR:OG1	2.34	0.42
2:E:4965:SER:O	2:E:4969:ASP:N	2.53	0.42
2:E:4993:MET:HA	2:E:4996:ILE:HD12	2.02	0.42
2:G:2103:VAL:O	2:G:2107:GLN:N	2.47	0.42
2:B:927:GLU:HA	2:B:930:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.02	0.41
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.52	0.41
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.02	0.41
2:I:224:HIS:N	2:I:229:GLU:O	2.44	0.41
2:E:56:GLN:O	2:E:309:THR:OG1	2.33	0.41
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.35	0.41
2:E:1074:ILE:HA	2:E:1193:SER:HA	2.02	0.41
2:E:2143:THR:H	2:E:3651:ASN:HD21	1.68	0.41
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.02	0.41
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.53	0.41
2:I:582:HIS:O	2:I:585:SER:OG	2.30	0.41
2:I:838:HIS:HA	2:I:1201:HIS:HB3	2.02	0.41
2:I:4965:SER:O	2:I:4969:ASP:N	2.53	0.41
2:E:1659:LEU:O	2:E:1663:HIS:N	2.49	0.41
2:E:4782:VAL:O	2:E:4785:THR:OG1	2.37	0.41
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.42	0.41
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.02	0.41
2:B:4993:MET:HA	2:B:4996:ILE:HD12	2.02	0.41
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.52	0.41
2:E:3552:UNK:O	2:E:3556:UNK:N	2.52	0.41
2:G:983:THR:O	2:G:987:ARG:N	2.51	0.41
2:G:1105:ALA:N	2:G:1189:LEU:O	2.53	0.41
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.35	0.41
2:B:1074:ILE:HA	2:B:1193:SER:HA	2.02	0.41
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.31	0.41
2:B:4848:VAL:O	2:B:4852:THR:OG1	2.34	0.41
2:B:4965:SER:O	2:B:4969:ASP:N	2.53	0.41
2:I:215:THR:H	2:I:218:HIS:CE1	2.38	0.41
2:I:233:ILE:HD12	2:I:242:ARG:HB3	2.01	0.41
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.86	0.41
2:I:983:THR:O	2:I:987:ARG:N	2.51	0.41
2:I:3552:UNK:O	2:I:3556:UNK:N	2.52	0.41
2:E:215:THR:H	2:E:218:HIS:CE1	2.38	0.41
2:E:233:ILE:HD12	2:E:242:ARG:HB3	2.01	0.41
2:E:927:GLU:HA	2:E:930:LYS:HB2	2.02	0.41
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.85	0.41
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.35	0.41
2:G:4697:VAL:O	2:G:4701:TRP:N	2.51	0.41
1:A:7:ILE:N	1:A:71:ARG:O	2.46	0.41
1:A:8:SER:H	2:B:736:HIS:HB3	1.85	0.41
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.30	0.41
2:B:4951:LYS:HE2	2:B:4951:LYS:HB3	1.94	0.41
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.02	0.41
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.86	0.41
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	2.02	0.41
2:G:485:SER:HA	2:G:488:LEU:HB2	2.03	0.41
2:G:4983:HIS:CE1	2:G:5023:PRO:HG2	2.56	0.41
2:B:940:GLY:O	2:B:1052:ASN:N	2.52	0.41
2:B:4064:MET:O	2:B:4068:LEU:N	2.52	0.41
2:B:4843:LEU:HD12	2:E:4823:LEU:HD23	2.02	0.41
2:I:4993:MET:HA	2:I:4996:ILE:HD12	2.02	0.41
2:E:414:PHE:HE1	2:E:436:LEU:HB3	1.86	0.41
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.03	0.41
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.02	0.41
2:E:4983:HIS:CE1	2:E:5023:PRO:HG2	2.56	0.41
2:G:4993:MET:HA	2:G:4996:ILE:HD12	2.01	0.41
1:H:8:SER:H	2:G:736:HIS:HB3	1.84	0.41
2:B:213:TYR:CG	2:B:337:PRO:HB2	2.56	0.41
2:B:1238:PHE:O	2:B:1606:SER:N	2.50	0.41
2:I:215:THR:HG22	2:I:273:HIS:HA	2.03	0.41
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.85	0.41
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.56	0.41
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.03	0.41
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	2.01	0.41
2:E:485:SER:HA	2:E:488:LEU:HB2	2.03	0.41
2:G:134:ASP:OD1	2:G:134:ASP:N	2.54	0.41
2:G:215:THR:HG22	2:G:273:HIS:HA	2.03	0.41
2:G:1720:LEU:HD12	2:G:1847:THR:HG23	2.02	0.41
2:G:4965:SER:O	2:G:4969:ASP:N	2.53	0.41
1:J:7:ILE:HG22	1:J:9:PRO:HD2	2.01	0.41
2:B:123:THR:OG1	2:B:134:ASP:OD1	2.38	0.41
2:B:621:ILE:O	2:B:625:LEU:N	2.47	0.41
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	2.02	0.41
2:I:618:GLN:O	2:I:622:THR:OG1	2.37	0.41
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.41	0.41
2:I:4983:HIS:CE1	2:I:5023:PRO:HG2	2.56	0.41
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.38	0.41
1:J:7:ILE:N	1:J:71:ARG:O	2.46	0.41
2:B:215:THR:H	2:B:218:HIS:CE1	2.38	0.41
2:B:232:THR:HB	2:B:252:VAL:HG11	2.03	0.41
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.56	0.41
2:B:2132:GLY:O	2:B:2136:ARG:N	2.53	0.41
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.03	0.41
2:B:4875:LYS:HB3	2:B:4882:CYS:HA	2.01	0.41
2:I:134:ASP:OD1	2:I:134:ASP:N	2.54	0.41
2:I:485:SER:HA	2:I:488:LEU:HB2	2.03	0.41
2:I:629:ARG:HB3	2:I:634:GLN:NE2	2.36	0.41
2:I:1141:ARG:HD2	2:I:1141:ARG:H	1.86	0.41
2:I:1720:LEU:HD12	2:I:1847:THR:HG23	2.02	0.41
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.02	0.41
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.36	0.41
2:I:2810:LYS:O	2:I:2814:LYS:N	2.45	0.41
2:I:4875:LYS:HB3	2:I:4882:CYS:HA	2.01	0.41
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.02	0.41
2:E:215:THR:HG22	2:E:273:HIS:HA	2.03	0.41
2:E:243:ARG:NH1	2:E:301:VAL:O	2.42	0.41
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.56	0.41
2:E:4951:LYS:HE2	2:E:4951:LYS:HB3	1.94	0.41
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.02	0.41
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.03	0.41
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.56	0.41
2:G:2143:THR:H	2:G:3651:ASN:HD21	1.68	0.41
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.89	0.41
2:B:1270:LEU:N	2:B:1472:UNK:O	2.54	0.41
2:B:4983:HIS:CE1	2:B:5023:PRO:HG2	2.56	0.41
2:I:213:TYR:CG	2:I:337:PRO:HB2	2.56	0.41
2:I:583:ILE:HA	2:I:586:ILE:HD12	2.03	0.41
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	2.03	0.41
2:E:1720:LEU:HD12	2:E:1847:THR:HG23	2.02	0.41
2:G:1965:TYR:OH	2:G:2027:ILE:O	2.33	0.41
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.46	0.40
2:I:1238:PHE:O	2:I:1606:SER:N	2.50	0.40
2:E:232:THR:HB	2:E:252:VAL:HG11	2.03	0.40
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.03	0.40
2:E:983:THR:O	2:E:987:ARG:N	2.51	0.40
2:E:1270:LEU:N	2:E:1472:UNK:O	2.54	0.40
2:G:123:THR:OG1	2:G:134:ASP:OD1	2.38	0.40
2:G:1092:PHE:N	2:G:1149:VAL:O	2.39	0.40
2:G:1659:LEU:O	2:G:1663:HIS:N	2.49	0.40
2:G:4821:LYS:HE2	2:G:4821:LYS:HB3	1.97	0.40
2:B:215:THR:HG22	2:B:273:HIS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:ASN:HD21	2:B:550:LYS:HE3	1.87	0.40
2:B:838:HIS:HA	2:B:1201:HIS:HB3	2.02	0.40
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	2.02	0.40
2:E:134:ASP:OD1	2:E:134:ASP:N	2.54	0.40
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.87	0.40
2:E:4787:ASN:O	2:E:4791:TYR:N	2.49	0.40
2:G:750:LEU:HD21	2:G:777:PHE:HE2	1.86	0.40
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.97	0.40
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.85	0.40
2:I:927:GLU:HA	2:I:930:LYS:HB2	2.02	0.40
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.87	0.40
2:E:4968:PHE:HE1	2:E:5029:ARG:HD3	1.86	0.40
2:G:213:TYR:CG	2:G:337:PRO:HB2	2.56	0.40
2:G:414:PHE:HE1	2:G:436:LEU:HB3	1.86	0.40
2:G:495:ASN:HD21	2:G:550:LYS:HE3	1.87	0.40
2:G:838:HIS:HA	2:G:1201:HIS:HB3	2.02	0.40
2:G:927:GLU:HA	2:G:930:LYS:HB2	2.02	0.40
2:B:414:PHE:HE1	2:B:436:LEU:HB3	1.86	0.40
2:B:1130:GLN:HG2	2:B:1138:PRO:HA	2.04	0.40
2:I:1074:ILE:HA	2:I:1193:SER:HA	2.02	0.40
2:E:213:TYR:CG	2:E:337:PRO:HB2	2.56	0.40
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.03	0.40
2:G:243:ARG:NH1	2:G:301:VAL:O	2.42	0.40
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.03	0.40
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.03	0.40
2:B:463:GLU:O	2:B:466:SER:OG	2.35	0.40
2:B:1090:PHE:HD2	2:B:1202:LEU:HD11	1.87	0.40
2:B:2143:THR:H	2:B:3651:ASN:HD21	1.68	0.40
2:B:4968:PHE:HE1	2:B:5029:ARG:HD3	1.86	0.40
2:I:495:ASN:HD21	2:I:550:LYS:HE3	1.87	0.40
2:I:1694:LEU:O	2:I:1712:TYR:OH	2.27	0.40
2:I:1804:LEU:O	2:I:1808:ARG:N	2.53	0.40
2:E:495:ASN:HD21	2:E:550:LYS:HE3	1.87	0.40
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.36	0.40
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.52	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%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4416 (73%)	2929 (90%)	302 (9%)	4 (0%)	48	83
2	E	3235/4416 (73%)	2930 (91%)	301 (9%)	4 (0%)	48	83
2	G	3235/4416 (73%)	2930 (91%)	301 (9%)	4 (0%)	48	83
2	I	3235/4416 (73%)	2928 (90%)	303 (9%)	4 (0%)	48	83
All	All	13360/18096 (74%)	12101 (91%)	1243 (9%)	16 (0%)	49	83

All (16) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2484 (100%)	9 (0%)	84	84
2	E	2493/3022 (82%)	2484 (100%)	9 (0%)	84	84
2	G	2493/3022 (82%)	2484 (100%)	9 (0%)	84	84
2	I	2493/3022 (82%)	2484 (100%)	9 (0%)	84	84
All	All	10324/12444 (83%)	10288 (100%)	36 (0%)	84	85

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	1600	LEU
2	B	1676	LEU
2	B	3663	LEU
2	B	3805	LEU
2	B	4154	VAL
2	B	4957	LYS
2	B	4982	GLU
2	B	4983	HIS
2	I	131	LEU
2	I	1600	LEU
2	I	1676	LEU
2	I	3663	LEU
2	I	3805	LEU
2	I	4154	VAL
2	I	4957	LYS
2	I	4982	GLU
2	I	4983	HIS
2	E	131	LEU

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Mol	Chain	Res	Type
2	E	1600	LEU
2	E	1676	LEU
2	E	3663	LEU
2	E	3805	LEU
2	E	4154	VAL
2	E	4957	LYS
2	E	4982	GLU
2	E	4983	HIS
2	G	131	LEU
2	G	1600	LEU
2	G	1676	LEU
2	G	3663	LEU
2	G	3805	LEU
2	G	4154	VAL
2	G	4957	LYS
2	G	4982	GLU
2	G	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (237) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	43	ASN
1	F	87	HIS
1	A	43	ASN
1	A	87	HIS
1	H	43	ASN
1	H	87	HIS
1	J	43	ASN
1	J	87	HIS
2	B	44	ASN
2	B	57	ASN
2	B	98	HIS
2	B	105	HIS
2	B	113	HIS
2	B	379	HIS
2	B	383	HIS
2	B	412	ASN
2	B	413	GLN
2	B	461	HIS
2	B	465	GLN
2	B	520	ASN
2	B	582	HIS

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Mol	Chain	Res	Type
2	B	597	HIS
2	B	765	GLN
2	B	838	HIS
2	B	877	ASN
2	B	1244	GLN
2	B	1598	GLN
2	B	1660	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	1941	ASN
2	B	1949	GLN
2	B	2005	GLN
2	B	2007	ASN
2	B	2127	GLN
2	B	2260	ASN
2	B	2763	HIS
2	B	2773	ASN
2	B	2856	ASN
2	B	3647	HIS
2	B	3761	GLN
2	B	3809	ASN
2	B	3814	GLN
2	B	3830	GLN
2	B	3889	GLN
2	B	3895	HIS
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	3994	HIS
2	B	4034	ASN
2	B	4037	ASN
2	B	4054	ASN
2	B	4109	GLN
2	B	4120	ASN
2	B	4142	ASN
2	B	4691	GLN

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Mol	Chain	Res	Type
2	B	4803	HIS
2	B	4947	GLN
2	B	4987	ASN
2	B	5003	HIS
2	I	57	ASN
2	I	98	HIS
2	I	105	HIS
2	I	113	HIS
2	I	379	HIS
2	I	383	HIS
2	I	412	ASN
2	I	413	GLN
2	I	461	HIS
2	I	465	GLN
2	I	520	ASN
2	I	582	HIS
2	I	597	HIS
2	I	765	GLN
2	I	838	HIS
2	I	877	ASN
2	I	1244	GLN
2	I	1598	GLN
2	I	1660	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	1941	ASN
2	I	1949	GLN
2	I	2005	GLN
2	I	2007	ASN
2	I	2127	GLN
2	I	2184	ASN
2	I	2260	ASN
2	I	2324	ASN
2	I	2763	HIS
2	I	2773	ASN
2	I	2856	ASN
2	I	3647	HIS
2	I	3761	GLN

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Mol	Chain	Res	Type
2	I	3809	ASN
2	I	3814	GLN
2	I	3830	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	3994	HIS
2	I	4034	ASN
2	I	4054	ASN
2	I	4109	GLN
2	I	4120	ASN
2	I	4142	ASN
2	I	4691	GLN
2	I	4803	HIS
2	I	4947	GLN
2	I	4987	ASN
2	I	5003	HIS
2	E	44	ASN
2	E	57	ASN
2	E	105	HIS
2	E	113	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	412	ASN
2	E	413	GLN
2	E	520	ASN
2	E	597	HIS
2	E	765	GLN
2	E	838	HIS
2	E	877	ASN
2	E	1220	GLN
2	E	1244	GLN
2	E	1598	GLN
2	E	1660	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS

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Mol	Chain	Res	Type
2	E	1775	HIS
2	E	1861	GLN
2	E	1941	ASN
2	E	1949	GLN
2	E	2005	GLN
2	E	2007	ASN
2	E	2127	GLN
2	E	2184	ASN
2	E	2260	ASN
2	E	2324	ASN
2	E	2763	HIS
2	E	2773	ASN
2	E	2856	ASN
2	E	3647	HIS
2	E	3761	GLN
2	E	3809	ASN
2	E	3814	GLN
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	3994	HIS
2	E	4034	ASN
2	E	4054	ASN
2	E	4109	GLN
2	E	4120	ASN
2	E	4142	ASN
2	E	4691	GLN
2	E	4803	HIS
2	E	4947	GLN
2	E	4987	ASN
2	E	5003	HIS
2	G	57	ASN
2	G	98	HIS
2	G	105	HIS
2	G	113	HIS
2	G	379	HIS
2	G	383	HIS
2	G	412	ASN

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Mol	Chain	Res	Type
2	G	413	GLN
2	G	520	ASN
2	G	582	HIS
2	G	597	HIS
2	G	765	GLN
2	G	838	HIS
2	G	877	ASN
2	G	1244	GLN
2	G	1598	GLN
2	G	1660	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	1941	ASN
2	G	1949	GLN
2	G	2005	GLN
2	G	2007	ASN
2	G	2127	GLN
2	G	2260	ASN
2	G	2324	ASN
2	G	2763	HIS
2	G	2773	ASN
2	G	2856	ASN
2	G	3647	HIS
2	G	3761	GLN
2	G	3809	ASN
2	G	3814	GLN
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	3994	HIS
2	G	4034	ASN
2	G	4054	ASN
2	G	4109	GLN
2	G	4120	ASN

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Mol	Chain	Res	Type
2	G	4142	ASN
2	G	4691	GLN
2	G	4803	HIS
2	G	4947	GLN
2	G	4987	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	E	5101	-	32,33,33	1.38	5 (15%)	48,52,52	1.72	9 (18%)
3	ATP	I	5101	-	32,33,33	1.39	5 (15%)	48,52,52	1.73	9 (18%)
4	CFF	E	5102	-	15,15,15	1.76	5 (33%)	23,23,23	2.80	10 (43%)
4	CFF	I	5102	-	15,15,15	1.76	5 (33%)	23,23,23	2.80	10 (43%)
3	ATP	G	5101	-	32,33,33	1.40	5 (15%)	48,52,52	1.73	9 (18%)
3	ATP	B	5101	-	32,33,33	1.39	5 (15%)	48,52,52	1.73	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CFF	B	5102	-	15,15,15	1.76	5 (33%)	23,23,23	2.80	10 (43%)
4	CFF	G	5102	-	15,15,15	1.76	5 (33%)	23,23,23	2.79	10 (43%)

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	-	-	6/22/38/38	0/3/3/3
3	ATP	I	5101	-	-	6/22/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	6/22/38/38	0/3/3/3
3	ATP	B	5101	-	-	6/22/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	5101	ATP	C5-C4	4.63	1.47	1.39
3	I	5101	ATP	C5-C4	4.61	1.47	1.39
3	E	5101	ATP	C5-C4	4.61	1.47	1.39
3	B	5101	ATP	C5-C4	4.61	1.47	1.39
4	B	5102	CFF	C6-N1	-3.74	1.32	1.40
4	E	5102	CFF	C6-N1	-3.74	1.32	1.40
4	G	5102	CFF	C6-N1	-3.74	1.32	1.40
4	I	5102	CFF	C6-N1	-3.71	1.32	1.40
3	G	5101	ATP	C5-C6	2.63	1.48	1.41
3	I	5101	ATP	C5-C6	2.63	1.48	1.41
3	B	5101	ATP	C5-C6	2.62	1.48	1.41
3	E	5101	ATP	C5-C6	2.61	1.48	1.41
3	G	5101	ATP	C5-N7	-2.39	1.34	1.39
3	B	5101	ATP	C5-N7	-2.37	1.34	1.39
3	E	5101	ATP	C5-N7	-2.35	1.34	1.39
3	I	5101	ATP	C5-N7	-2.35	1.34	1.39
3	G	5101	ATP	C8-N7	2.33	1.36	1.31
3	I	5101	ATP	C8-N7	2.32	1.36	1.31
3	B	5101	ATP	C8-N7	2.29	1.36	1.31
3	E	5101	ATP	C8-N7	2.28	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	C4-N3	-2.23	1.34	1.38
4	G	5102	CFF	C4-N3	-2.23	1.34	1.38
4	B	5102	CFF	C4-N3	-2.21	1.34	1.38
4	E	5102	CFF	C4-N3	-2.21	1.34	1.38
4	G	5102	CFF	C5-N7	-2.17	1.34	1.38
4	B	5102	CFF	C5-N7	-2.14	1.34	1.38
4	I	5102	CFF	C5-N7	-2.11	1.34	1.38
4	G	5102	CFF	O13-C6	-2.11	1.18	1.23
3	G	5101	ATP	C4-N9	-2.10	1.33	1.37
4	E	5102	CFF	C5-N7	-2.09	1.34	1.38
4	B	5102	CFF	O13-C6	-2.07	1.18	1.23
4	B	5102	CFF	O11-C2	-2.07	1.18	1.22
4	E	5102	CFF	O11-C2	-2.07	1.18	1.22
4	G	5102	CFF	O11-C2	-2.07	1.18	1.22
3	B	5101	ATP	C4-N9	-2.06	1.33	1.37
3	I	5101	ATP	C4-N9	-2.06	1.33	1.37
4	I	5102	CFF	O11-C2	-2.04	1.18	1.22
4	I	5102	CFF	O13-C6	-2.03	1.18	1.23
4	E	5102	CFF	O13-C6	-2.03	1.18	1.23
3	E	5101	ATP	C4-N9	-2.02	1.33	1.37

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5102	CFF	C14-N7-C8	-7.71	111.86	126.28
4	G	5102	CFF	C14-N7-C8	-7.70	111.87	126.28
4	I	5102	CFF	C14-N7-C8	-7.70	111.87	126.28
4	E	5102	CFF	C14-N7-C8	-7.69	111.89	126.28
3	G	5101	ATP	C5-C4-N3	-5.60	119.01	126.72
3	I	5101	ATP	C5-C4-N3	-5.57	119.05	126.72
3	B	5101	ATP	C5-C4-N3	-5.56	119.06	126.72
3	E	5101	ATP	C5-C4-N3	-5.52	119.11	126.72
4	I	5102	CFF	C14-N7-C5	5.19	140.11	127.77
4	G	5102	CFF	C14-N7-C5	5.18	140.09	127.77
4	B	5102	CFF	C14-N7-C5	5.17	140.08	127.77
4	E	5102	CFF	C14-N7-C5	5.16	140.05	127.77
3	G	5101	ATP	N3-C4-N9	4.45	134.73	127.17
3	I	5101	ATP	N3-C4-N9	4.42	134.68	127.17
3	E	5101	ATP	N3-C4-N9	4.41	134.66	127.17
3	B	5101	ATP	N3-C4-N9	4.40	134.65	127.17
4	I	5102	CFF	C5-C6-N1	4.34	120.01	112.06
4	B	5102	CFF	C5-C6-N1	4.34	120.01	112.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5102	CFF	C5-C6-N1	4.34	120.01	112.06
4	G	5102	CFF	C5-C6-N1	4.31	119.96	112.06
3	G	5101	ATP	C2-N3-C4	3.65	120.74	111.83
3	I	5101	ATP	C2-N3-C4	3.64	120.73	111.83
3	B	5101	ATP	C2-N3-C4	3.63	120.70	111.83
3	E	5101	ATP	C2-N3-C4	3.62	120.67	111.83
4	I	5102	CFF	C6-N1-C2	-3.55	119.89	125.66
3	I	5101	ATP	C4-C5-N7	-3.54	106.53	110.58
3	B	5101	ATP	C4-C5-N7	-3.54	106.53	110.58
3	G	5101	ATP	C4-C5-N7	-3.53	106.55	110.58
4	B	5102	CFF	C6-N1-C2	-3.52	119.93	125.66
4	E	5102	CFF	C6-N1-C2	-3.52	119.94	125.66
3	E	5101	ATP	C4-C5-N7	-3.50	106.58	110.58
4	G	5102	CFF	C6-N1-C2	-3.48	120.00	125.66
3	I	5101	ATP	N3-C2-N1	-3.33	123.54	128.58
3	G	5101	ATP	N3-C2-N1	-3.30	123.58	128.58
3	B	5101	ATP	N3-C2-N1	-3.30	123.58	128.58
3	E	5101	ATP	N3-C2-N1	-3.28	123.61	128.58
4	G	5102	CFF	N3-C4-N9	3.20	131.30	126.27
4	E	5102	CFF	N3-C4-N9	3.19	131.29	126.27
4	B	5102	CFF	N3-C4-N9	3.19	131.29	126.27
4	I	5102	CFF	N3-C4-N9	3.19	131.28	126.27
4	E	5102	CFF	N7-C8-N9	-2.93	108.17	113.48
4	B	5102	CFF	N7-C8-N9	-2.93	108.17	113.48
4	I	5102	CFF	N7-C8-N9	-2.92	108.19	113.48
3	G	5101	ATP	C4-N9-C8	2.91	108.80	105.74
4	G	5102	CFF	N7-C8-N9	-2.91	108.20	113.48
3	I	5101	ATP	C4-N9-C8	2.90	108.78	105.74
4	E	5102	CFF	O13-C6-C5	-2.89	120.46	126.38
4	B	5102	CFF	O13-C6-C5	-2.89	120.47	126.38
4	G	5102	CFF	O13-C6-C5	-2.88	120.48	126.38
3	E	5101	ATP	C4-N9-C8	2.87	108.75	105.74
3	B	5101	ATP	C4-N9-C8	2.86	108.74	105.74
4	I	5102	CFF	O13-C6-C5	-2.86	120.53	126.38
4	G	5102	CFF	C6-C5-C4	-2.69	119.53	122.92
4	B	5102	CFF	C6-C5-C4	-2.68	119.55	122.92
4	E	5102	CFF	C6-C5-C4	-2.65	119.58	122.92
4	I	5102	CFF	C6-C5-C4	-2.64	119.59	122.92
3	B	5101	ATP	C5-N7-C8	2.60	107.54	103.45
3	I	5101	ATP	C5-N7-C8	2.60	107.53	103.45
3	E	5101	ATP	C5-N7-C8	2.59	107.51	103.45
3	G	5101	ATP	C5-N7-C8	2.58	107.51	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	5102	CFF	N3-C2-N1	2.49	120.25	117.14
4	B	5102	CFF	N3-C2-N1	2.48	120.23	117.14
4	G	5102	CFF	N3-C2-N1	2.46	120.22	117.14
4	E	5102	CFF	N3-C2-N1	2.45	120.20	117.14
3	B	5101	ATP	C6-C5-N7	2.21	136.35	132.09
3	E	5101	ATP	C6-C5-N7	2.21	136.34	132.09
3	I	5101	ATP	C6-C5-N7	2.19	136.32	132.09
3	G	5101	ATP	C6-C5-N7	2.19	136.31	132.09
3	I	5101	ATP	N9-C8-N7	-2.15	110.88	113.94
3	G	5101	ATP	N9-C8-N7	-2.15	110.88	113.94
3	B	5101	ATP	N9-C8-N7	-2.14	110.90	113.94
3	E	5101	ATP	N9-C8-N7	-2.13	110.92	113.94
4	E	5102	CFF	C8-N9-C4	2.04	107.88	102.98
4	B	5102	CFF	C8-N9-C4	2.04	107.88	102.98
4	I	5102	CFF	C8-N9-C4	2.04	107.86	102.98
4	G	5102	CFF	C8-N9-C4	2.03	107.86	102.98

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O2A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O2A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	B	5101	ATP	C3'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	C3'-C4'-C5'-O5'
3	E	5101	ATP	O4'-C4'-C5'-O5'
3	E	5101	ATP	C3'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	C3'-C4'-C5'-O5'
3	B	5101	ATP	C4'-C5'-O5'-PA

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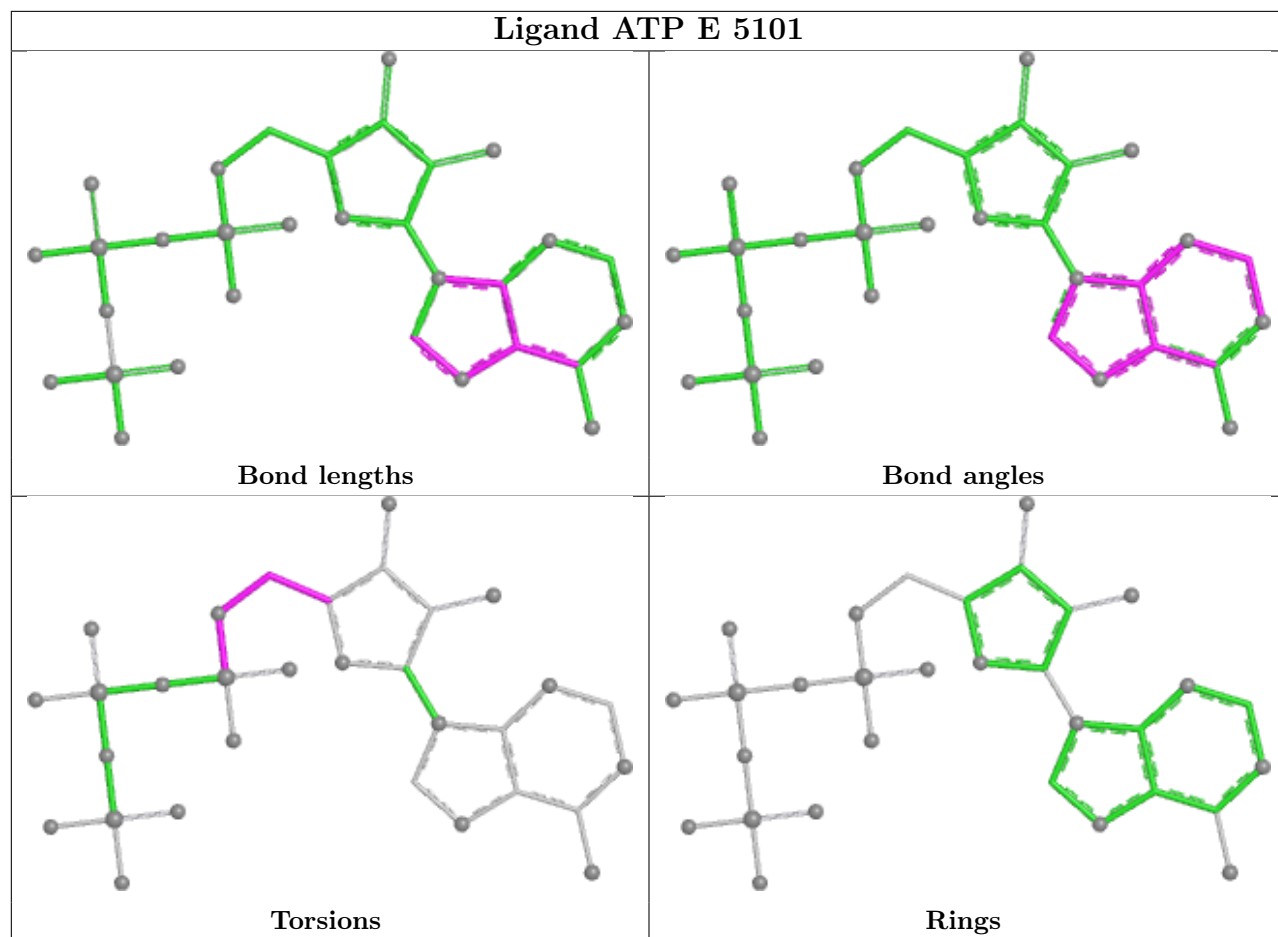
Mol	Chain	Res	Type	Atoms
3	I	5101	ATP	C4'-C5'-O5'-PA
3	E	5101	ATP	C4'-C5'-O5'-PA
3	G	5101	ATP	C4'-C5'-O5'-PA

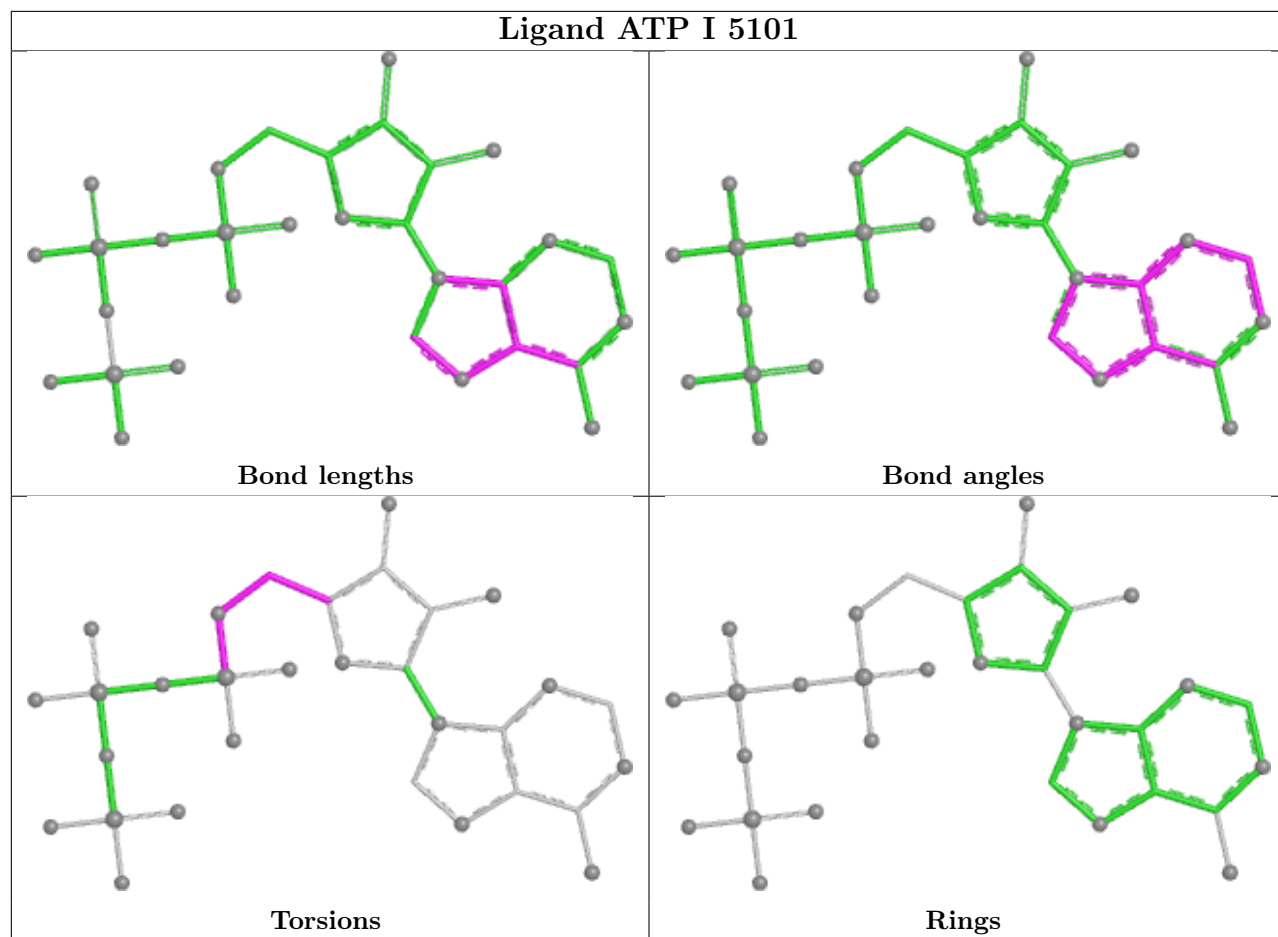
There are no ring outliers.

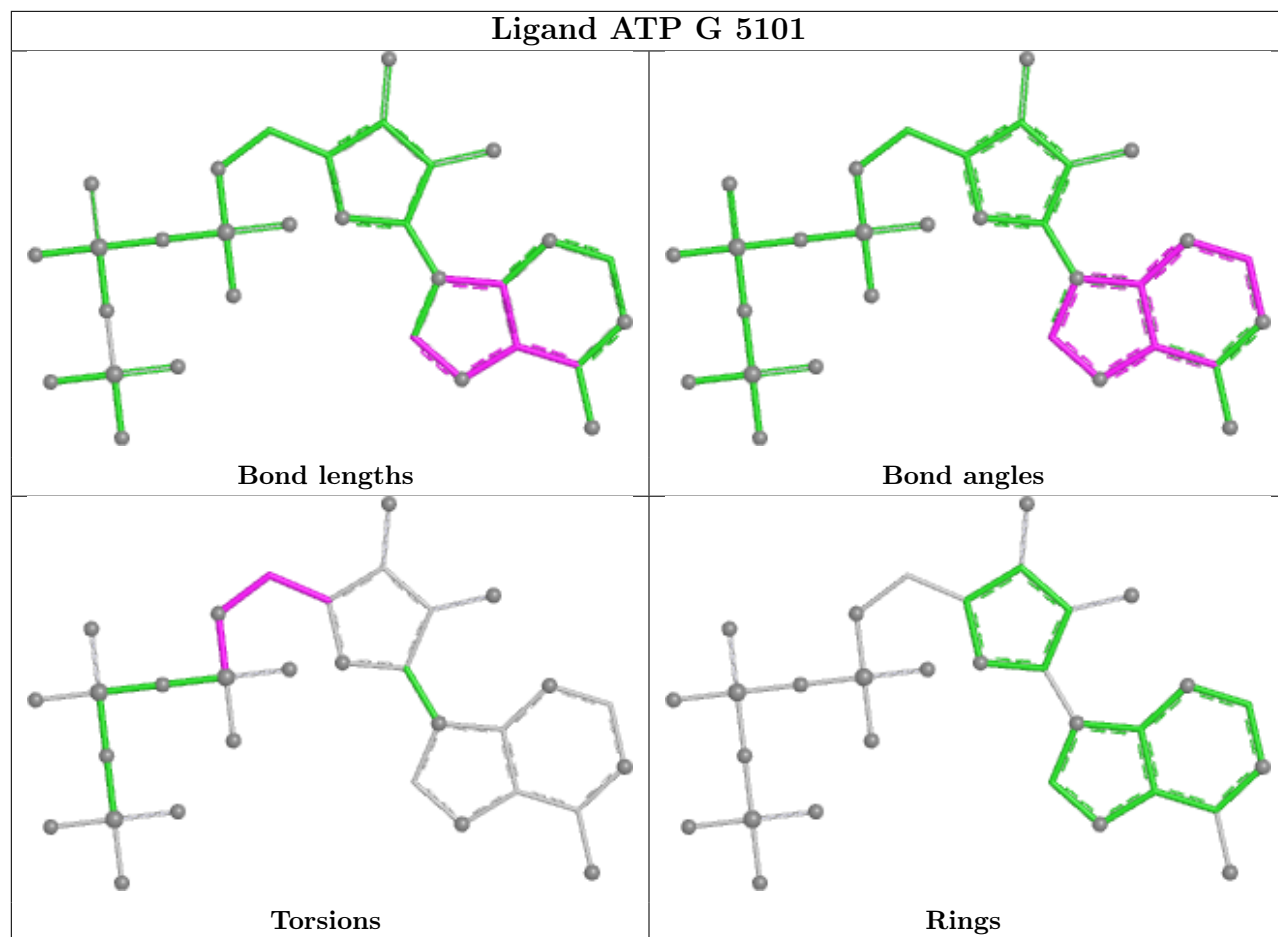
4 monomers are involved in 8 short contacts:

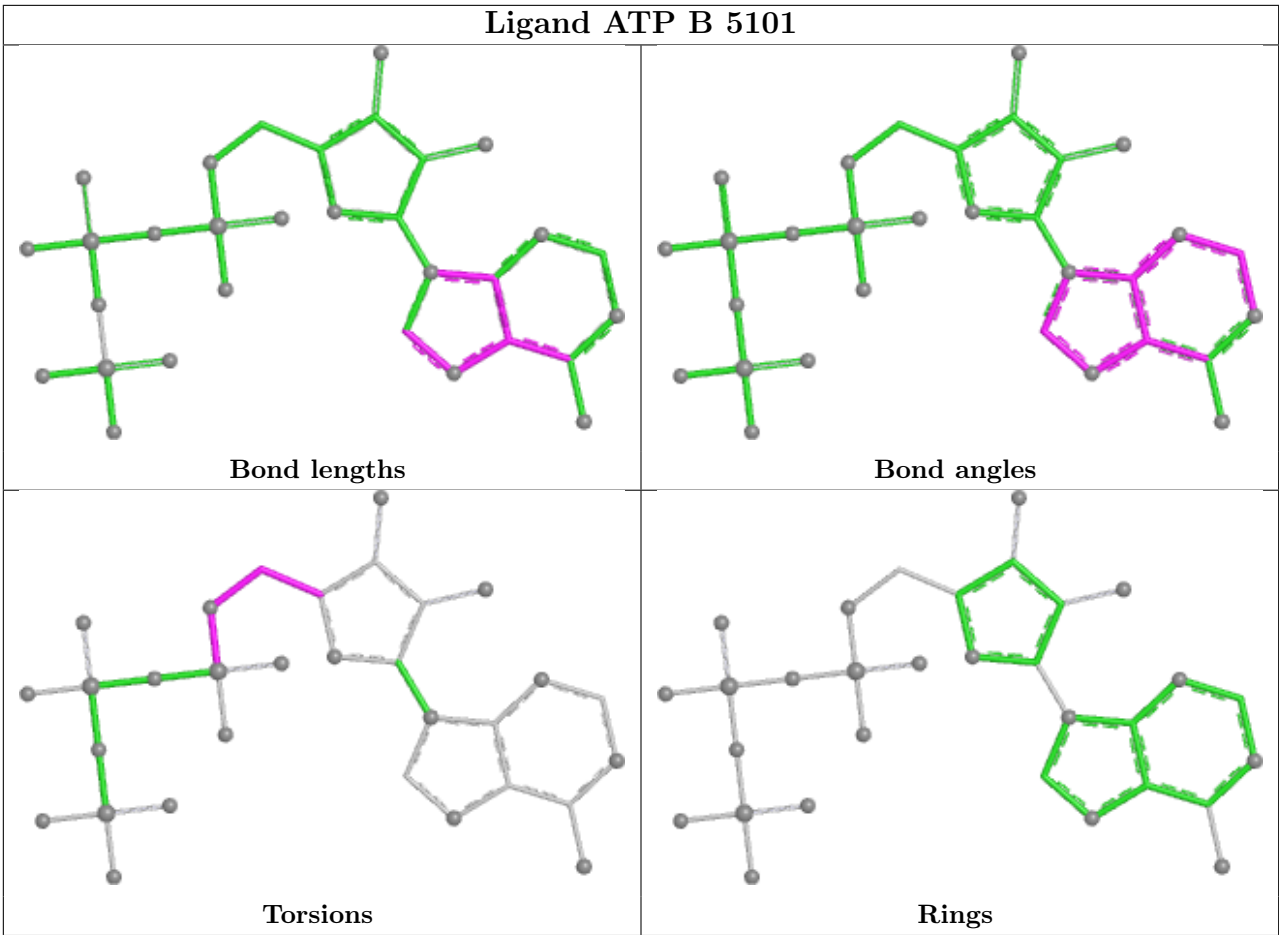
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	2	0
3	I	5101	ATP	2	0
3	G	5101	ATP	2	0
3	B	5101	ATP	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.19
1	I	4345:UNK	C	4540:PHE	N	73.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4345:UNK	C	4540:PHE	N	73.19
1	G	4345:UNK	C	4540:PHE	N	73.19
1	B	3613:UNK	C	3639:THR	N	44.63
1	I	3613:UNK	C	3639:THR	N	44.63
1	E	3613:UNK	C	3639:THR	N	44.63
1	G	3613:UNK	C	3639:THR	N	44.63
1	B	4253:GLU	C	4320:UNK	N	27.52
1	I	4253:GLU	C	4320:UNK	N	27.52
1	G	4253:GLU	C	4320:UNK	N	27.52
1	E	4253:GLU	C	4320:UNK	N	27.51
1	B	3163:UNK	C	3170:UNK	N	16.25
1	I	3163:UNK	C	3170:UNK	N	16.25
1	E	3163:UNK	C	3170:UNK	N	16.25
1	G	3163:UNK	C	3170:UNK	N	16.25
1	B	3063:UNK	C	3134:UNK	N	14.93
1	I	3063:UNK	C	3134:UNK	N	14.93
1	E	3063:UNK	C	3134:UNK	N	14.93
1	G	3063:UNK	C	3134:UNK	N	14.93
1	B	3468:UNK	C	3511:UNK	N	14.63
1	I	3468:UNK	C	3511:UNK	N	14.63
1	E	3468:UNK	C	3511:UNK	N	14.63
1	G	3468:UNK	C	3511:UNK	N	14.63
1	B	2703:UNK	C	2734:ASN	N	14.10
1	I	2703:UNK	C	2734:ASN	N	14.10
1	E	2703:UNK	C	2734:ASN	N	14.10
1	G	2703:UNK	C	2734:ASN	N	14.10
1	B	3236:UNK	C	3241:UNK	N	13.44
1	I	3236:UNK	C	3241:UNK	N	13.44
1	E	3236:UNK	C	3241:UNK	N	13.44
1	G	3236:UNK	C	3241:UNK	N	13.44
1	B	2976:UNK	C	2995:UNK	N	12.48
1	I	2976:UNK	C	2995:UNK	N	12.48
1	E	2976:UNK	C	2995:UNK	N	12.48
1	G	2976:UNK	C	2995:UNK	N	12.48
1	B	1564:UNK	C	1573:MET	N	12.21
1	I	1564:UNK	C	1573:MET	N	12.21
1	E	1564:UNK	C	1573:MET	N	12.21
1	G	1564:UNK	C	1573:MET	N	12.21
1	B	3254:UNK	C	3261:UNK	N	8.37
1	I	3254:UNK	C	3261:UNK	N	8.37
1	E	3254:UNK	C	3261:UNK	N	8.37
1	G	3254:UNK	C	3261:UNK	N	8.37

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	5.79
1	I	1297:UNK	C	1430:UNK	N	5.79
1	E	1297:UNK	C	1430:UNK	N	5.79
1	G	1297:UNK	C	1430:UNK	N	5.79
1	B	2479:LEU	C	2487:UNK	N	3.60
1	I	2479:LEU	C	2487:UNK	N	3.60
1	E	2479:LEU	C	2487:UNK	N	3.60
1	G	2479:LEU	C	2487:UNK	N	3.60
1	B	2939:ARG	C	2942:UNK	N	3.57
1	I	2939:ARG	C	2942:UNK	N	3.57
1	E	2939:ARG	C	2942:UNK	N	3.57
1	G	2939:ARG	C	2942:UNK	N	3.57

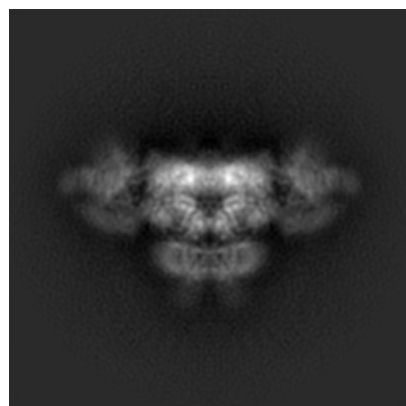
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8383. These allow visual inspection of the internal detail of the map and identification of artifacts.

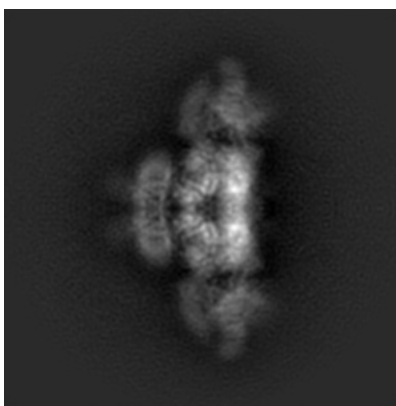
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

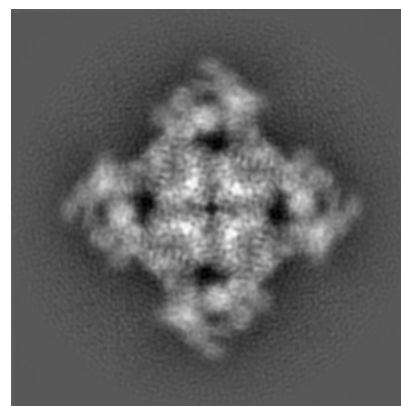
6.1.1 Primary map



X

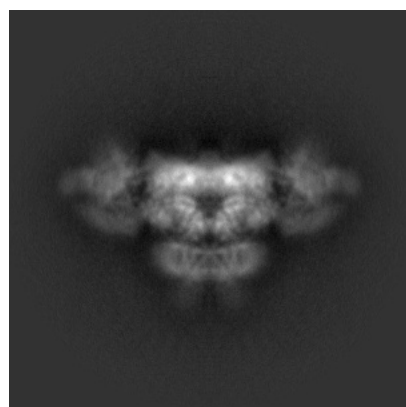


Y

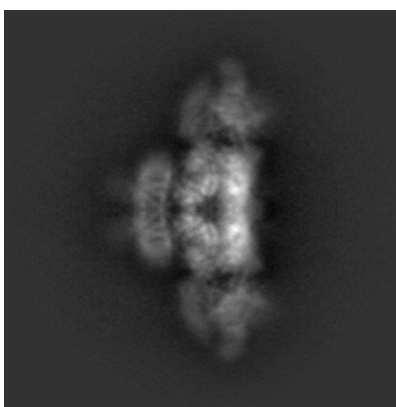


Z

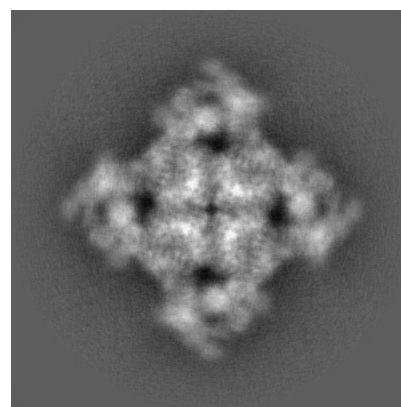
6.1.2 Raw map



X



Y

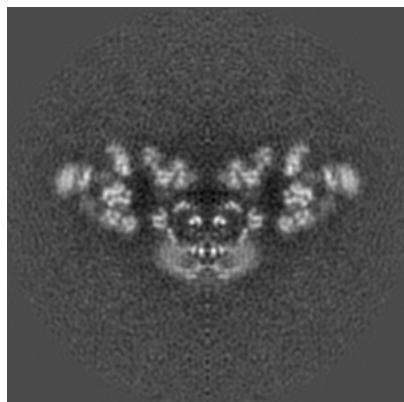


Z

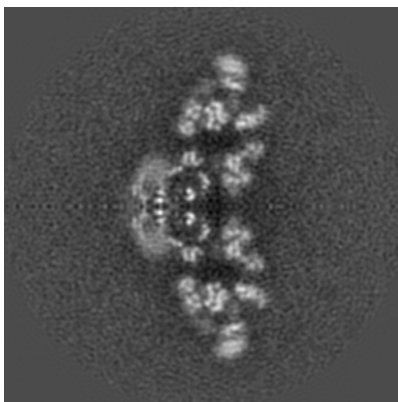
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

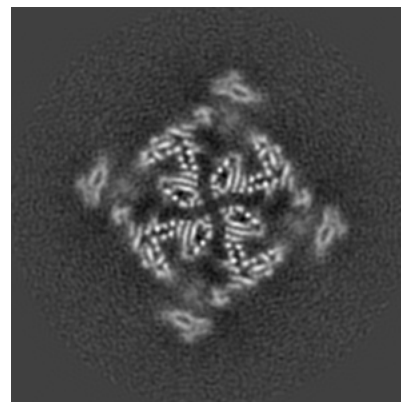
6.2.1 Primary map



X Index: 200

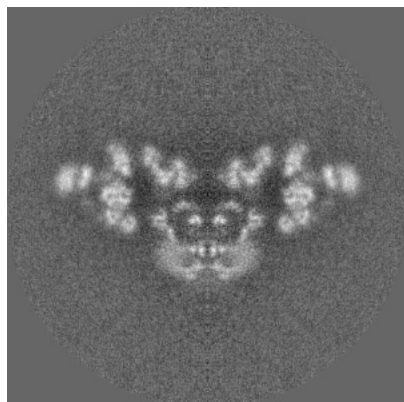


Y Index: 200

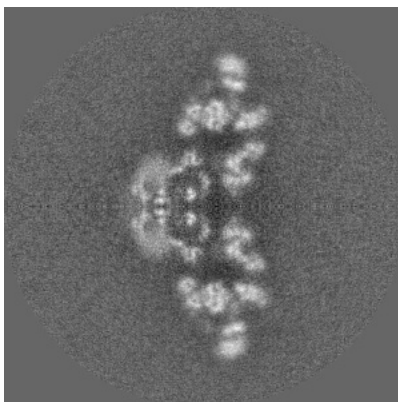


Z Index: 200

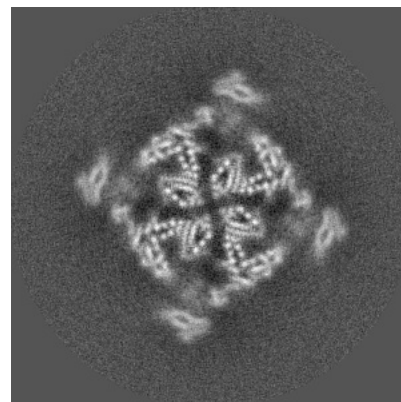
6.2.2 Raw map



X Index: 200



Y Index: 200

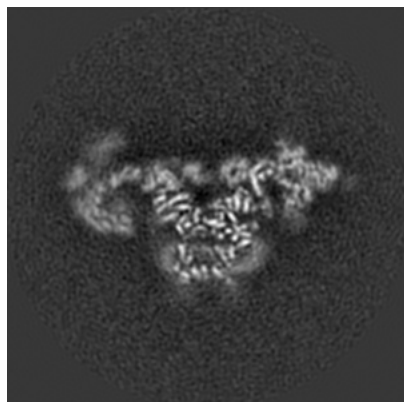


Z Index: 200

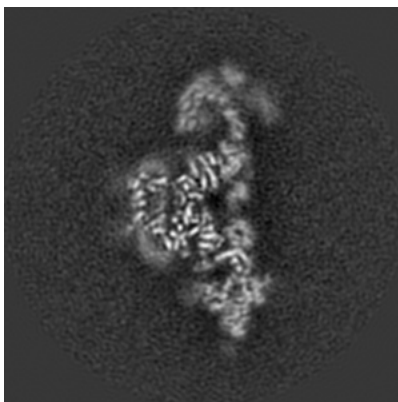
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

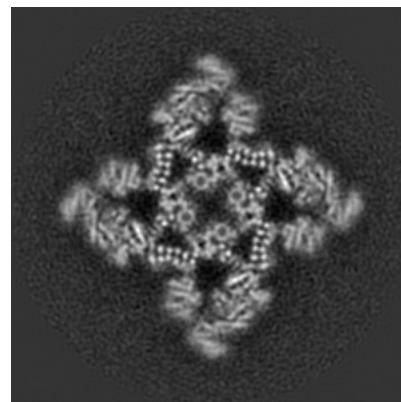
6.3.1 Primary map



X Index: 183

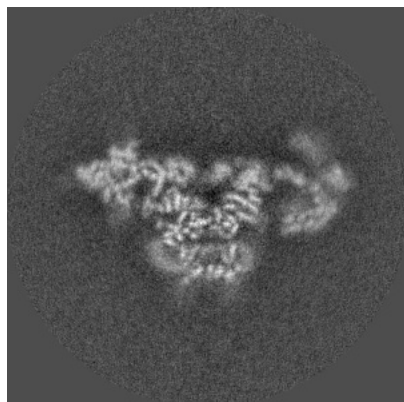


Y Index: 183

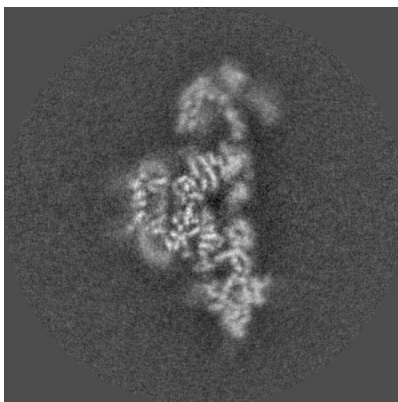


Z Index: 226

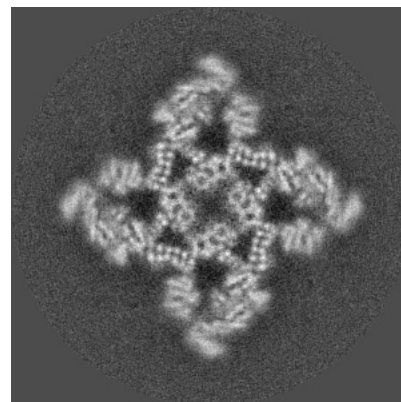
6.3.2 Raw map



X Index: 217



Y Index: 183

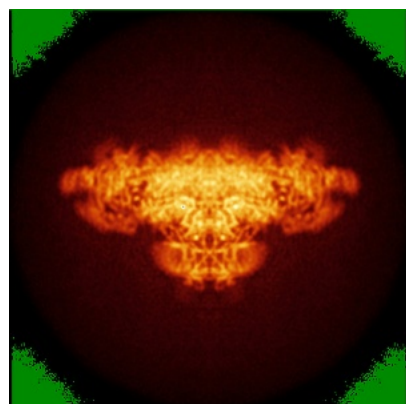


Z Index: 227

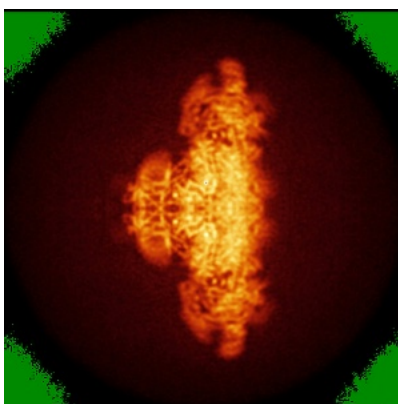
The images above show the largest variance slices of the map in three orthogonal directions.

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

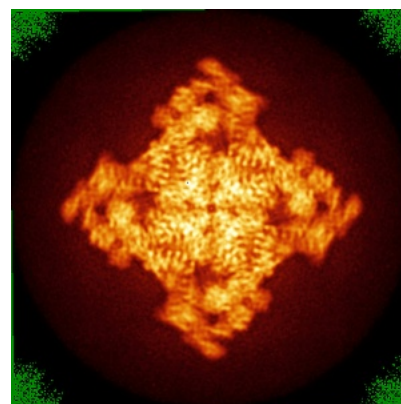
6.4.1 Primary map



X

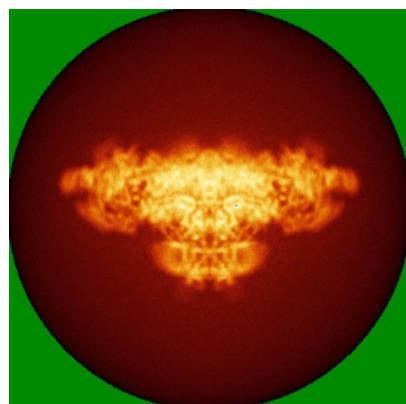


Y

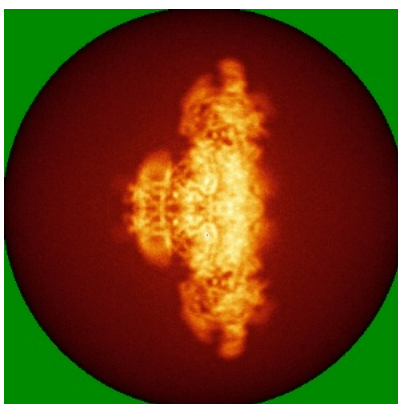


Z

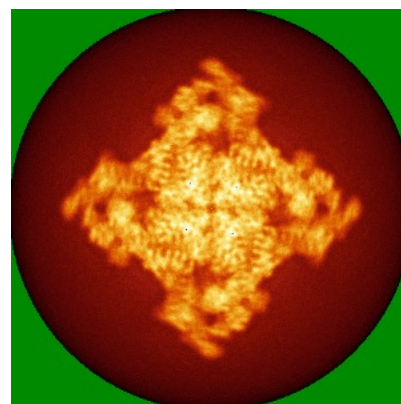
6.4.2 Raw map



X



Y

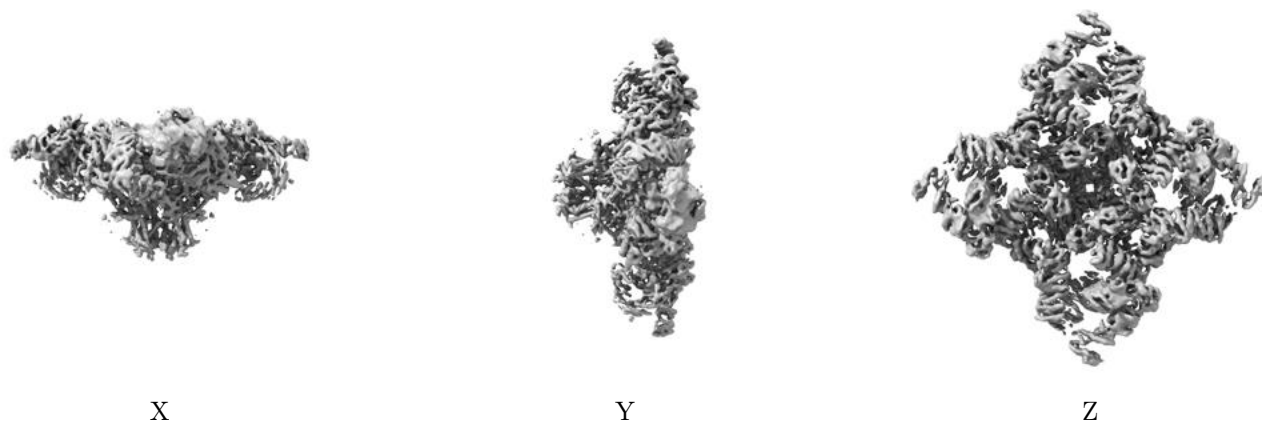


Z

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

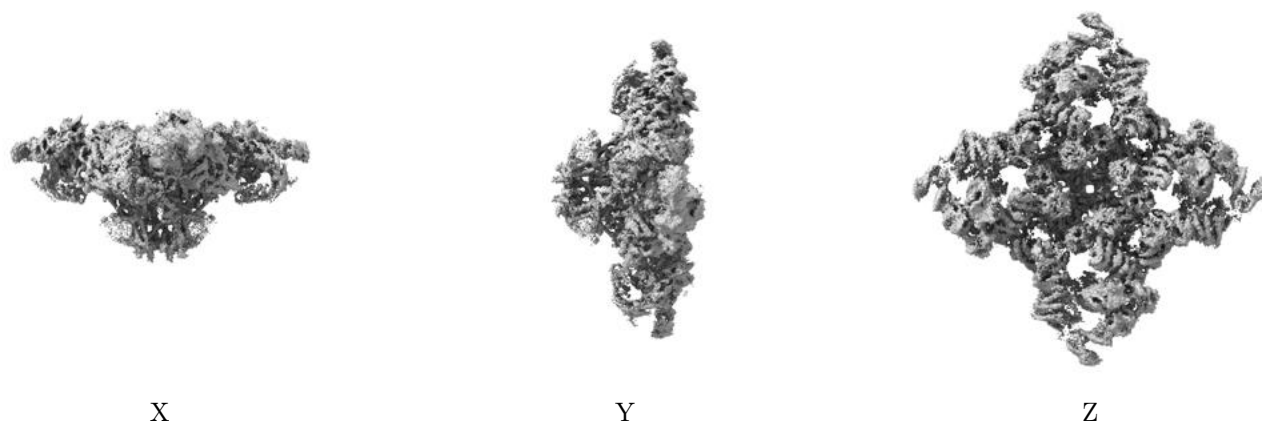
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

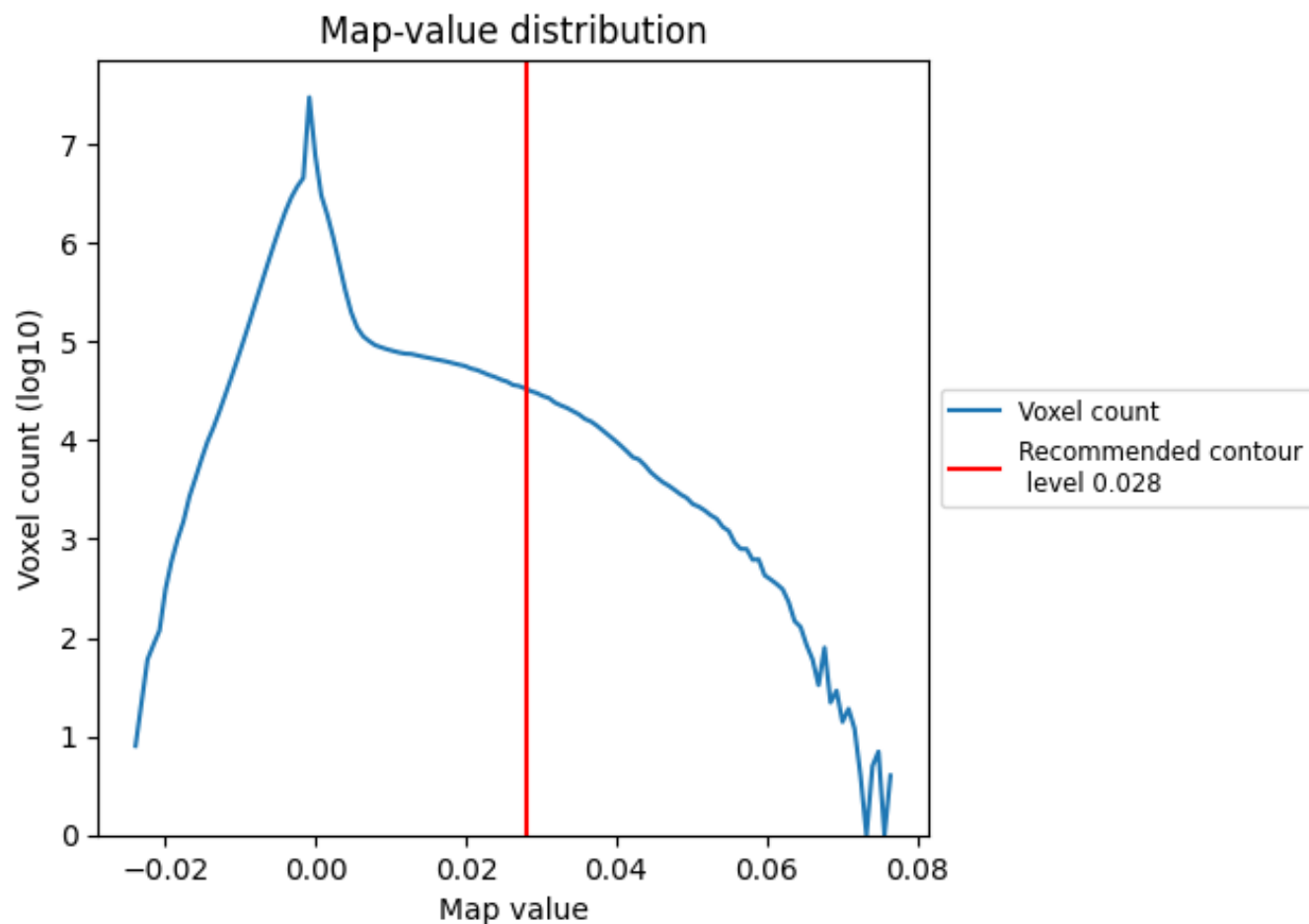
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

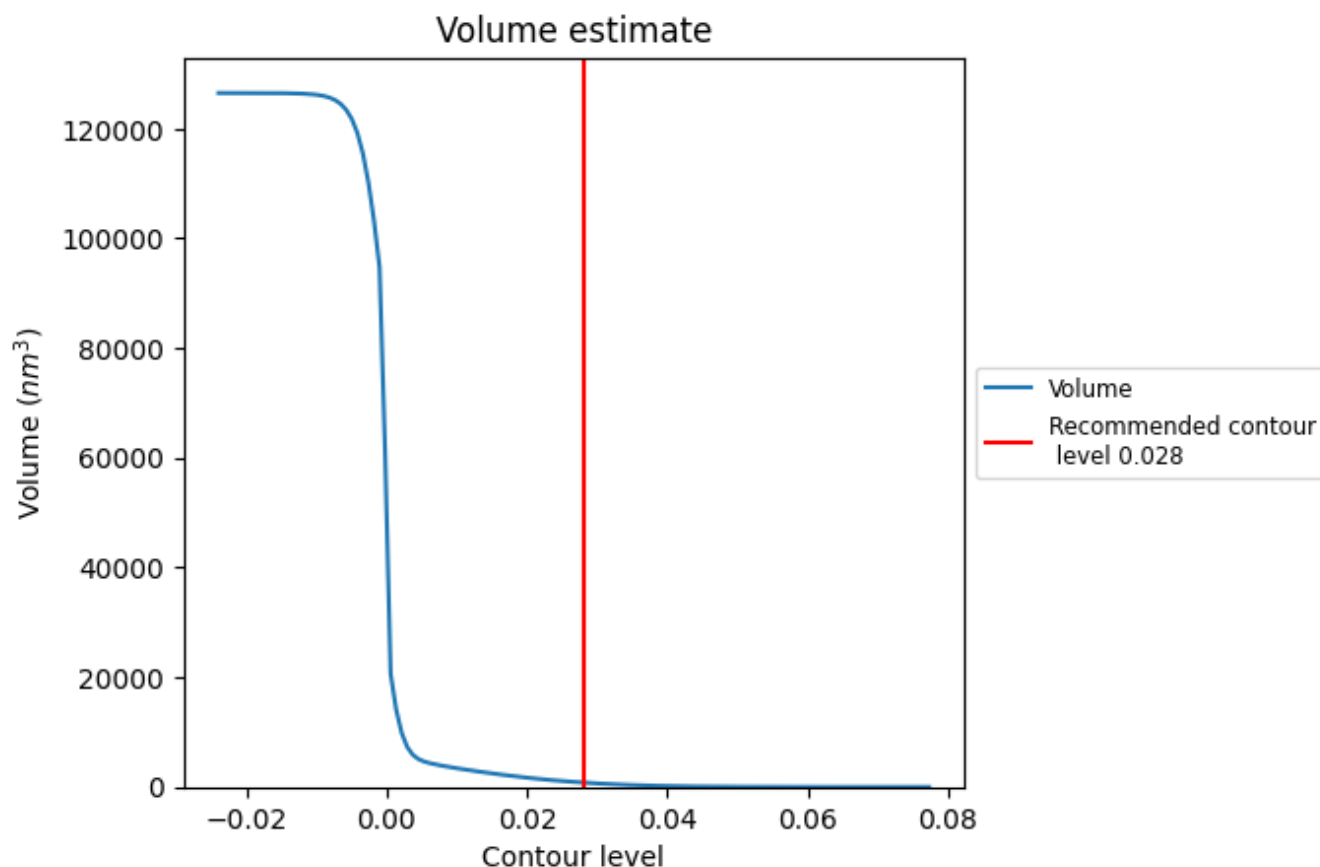
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

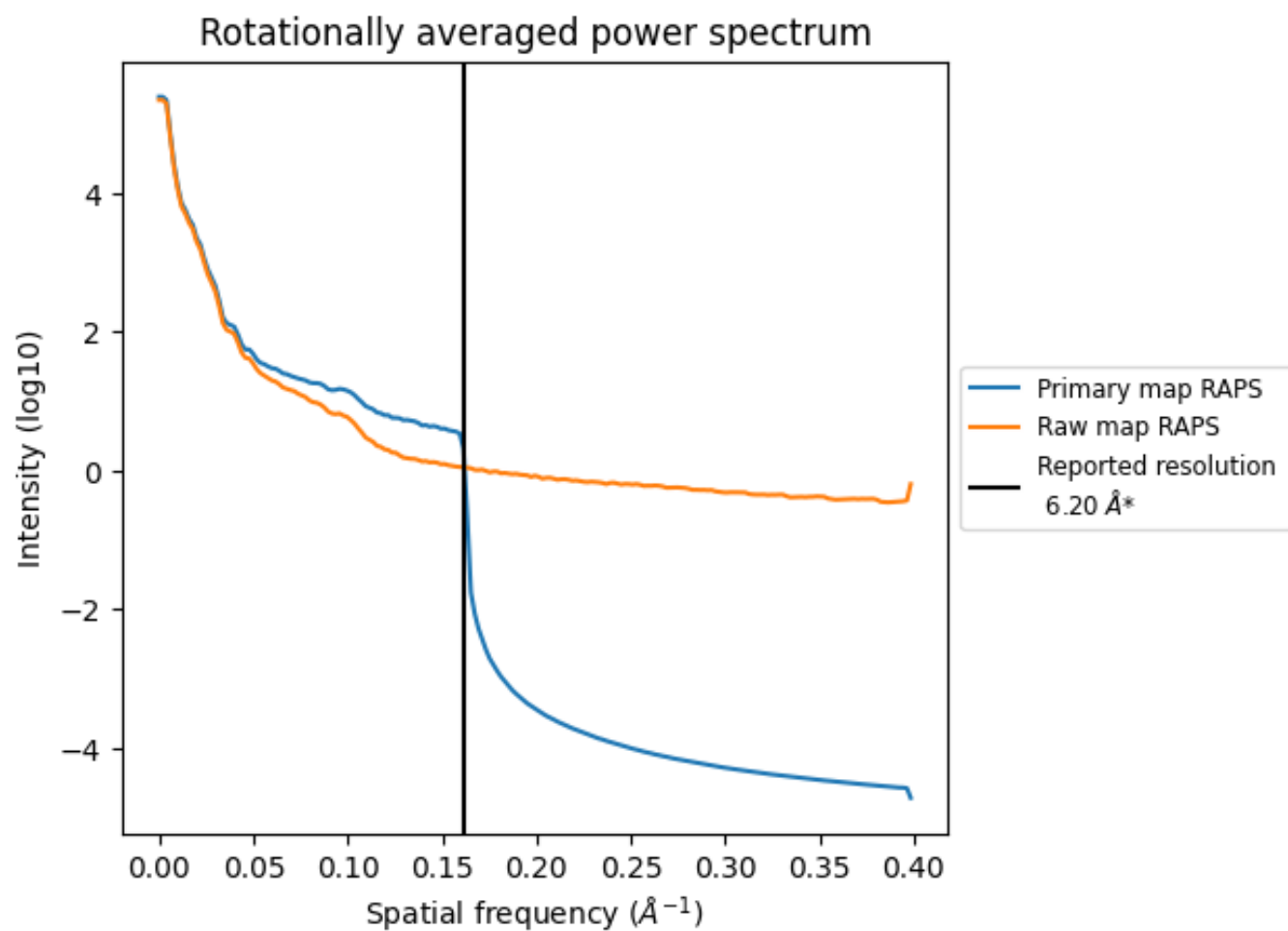
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 804 nm^3 ; this corresponds to an approximate mass of 726 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 ⓘ

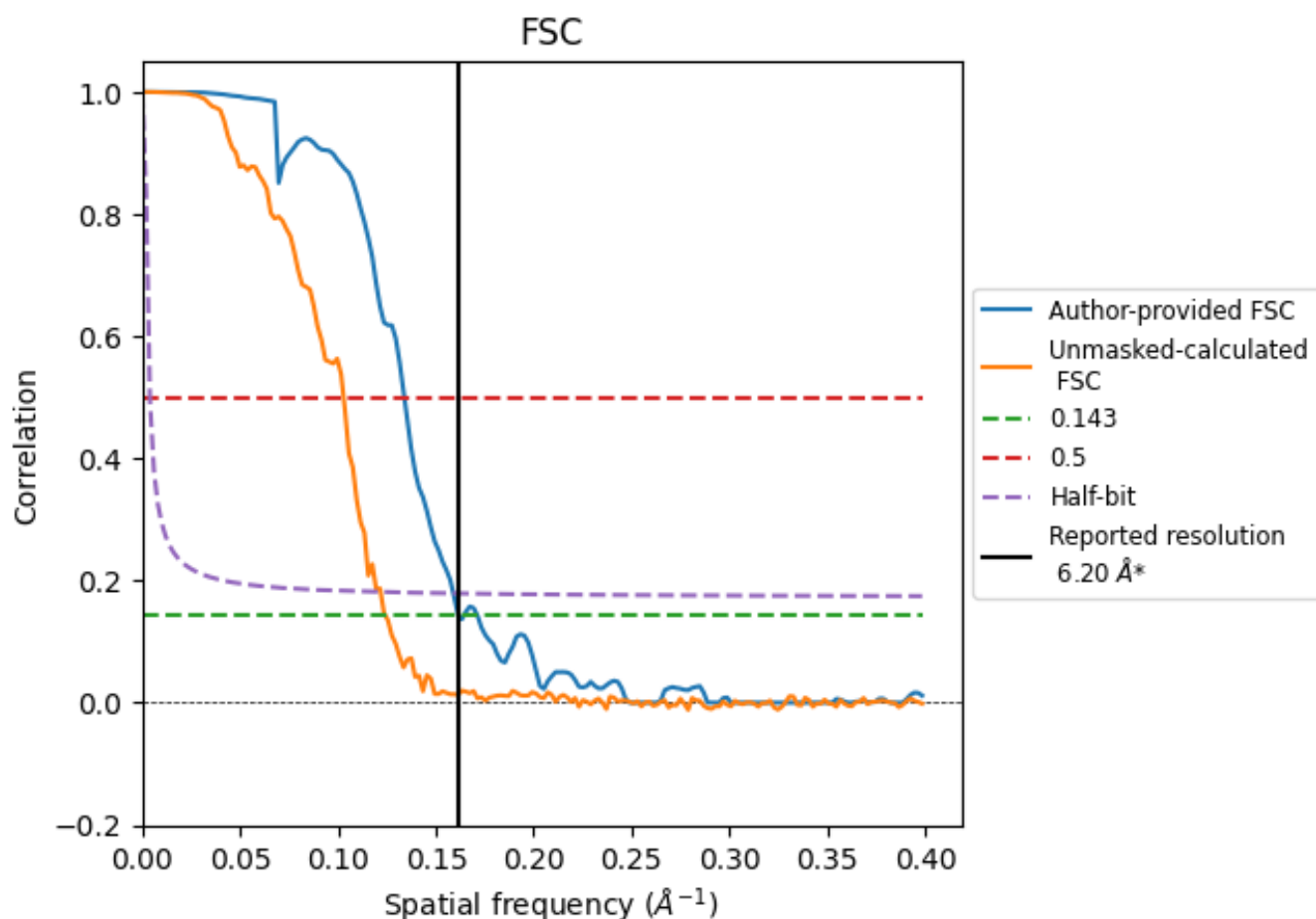


*Reported resolution corresponds to spatial frequency of 0.161 Å⁻¹

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 0.161 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

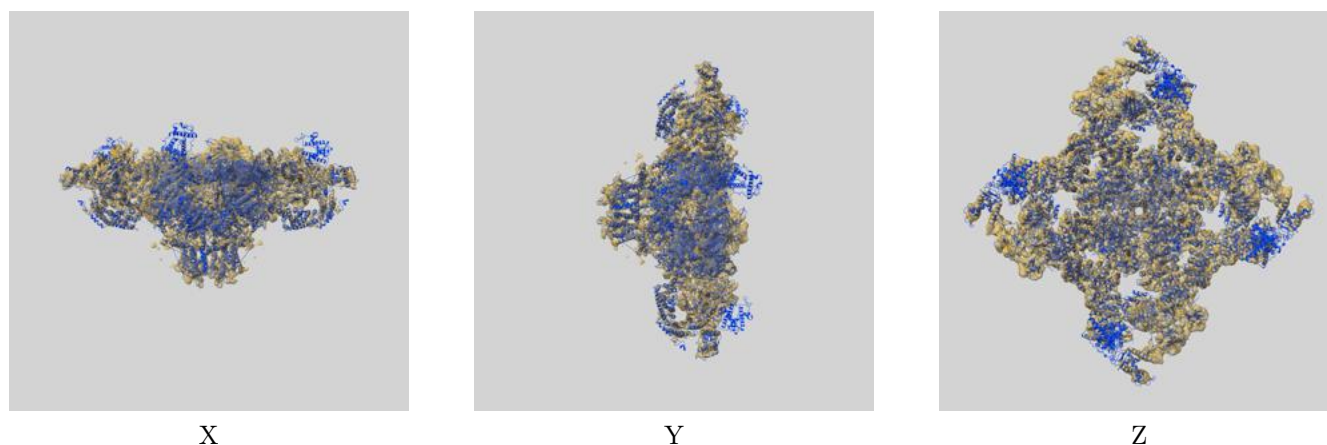
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.19	7.47	6.29
Unmasked-calculated*	8.06	9.72	8.21

*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 8.06 differs from the reported value 6.2 by more than 10 %

9 Map-model fit [i](#)

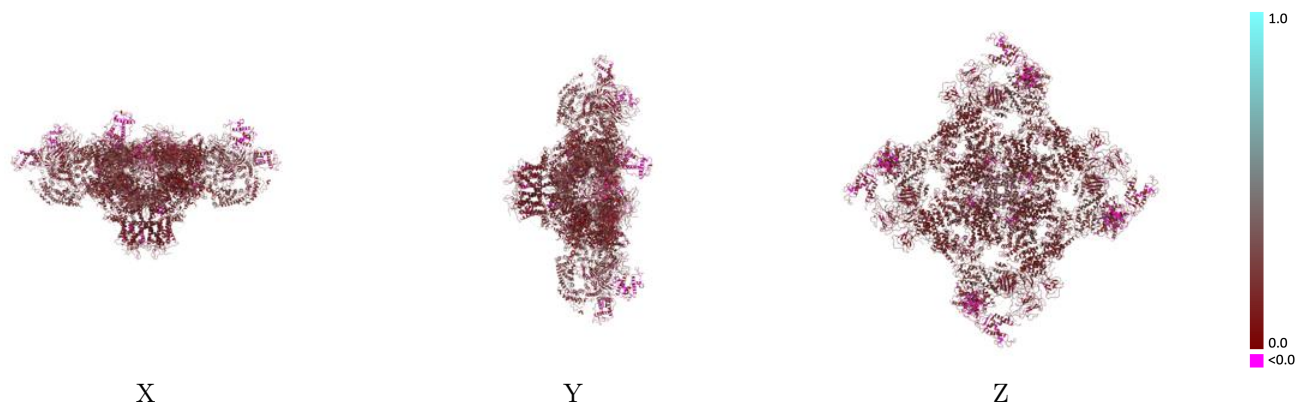
This section contains information regarding the fit between EMDB map EMD-8383 and PDB model 5TAS. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.028 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](#)

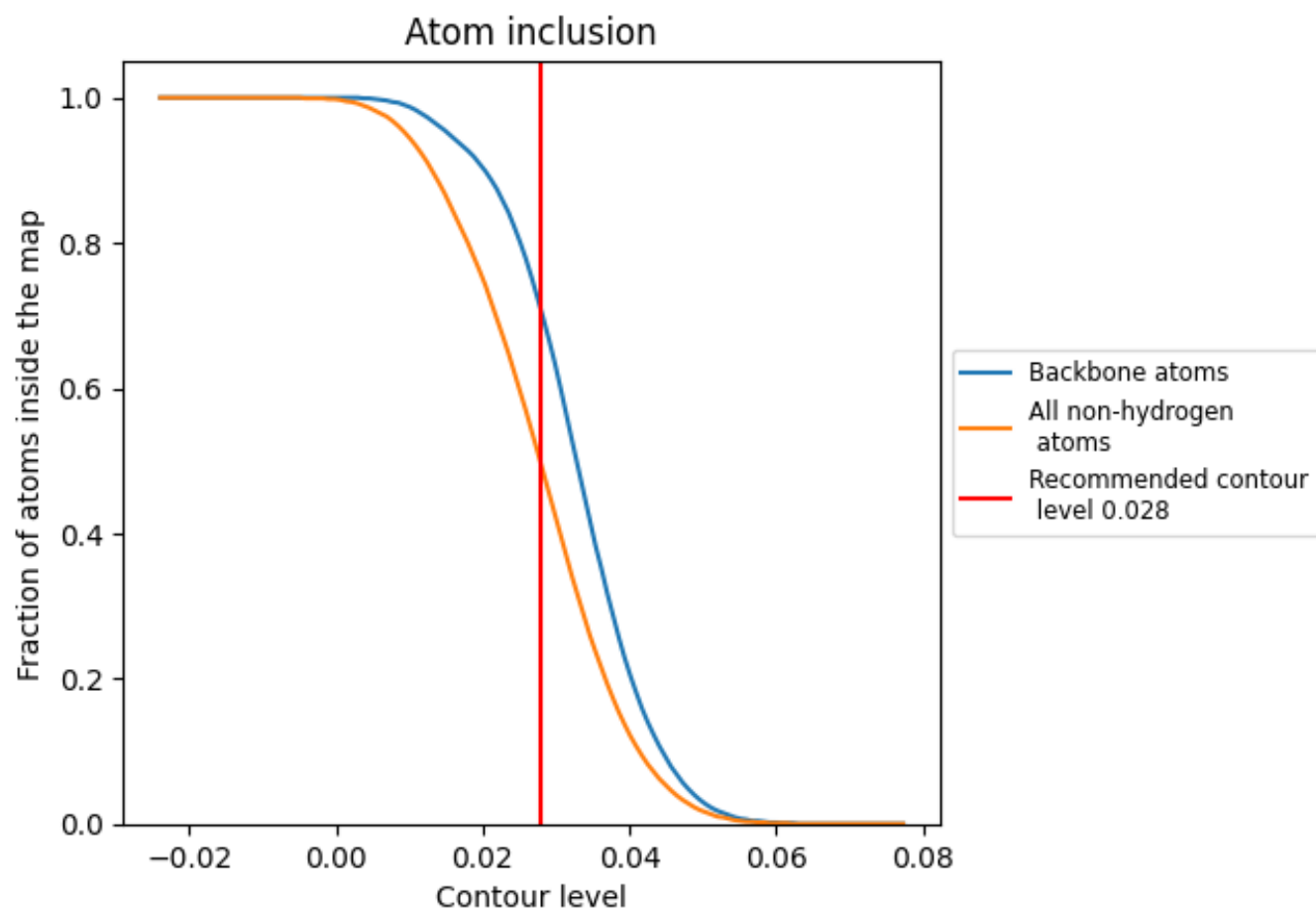


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 49% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4930	0.1830
A	0.5400	0.1700
B	0.4910	0.1840
E	0.4910	0.1830
F	0.5470	0.1750
G	0.4930	0.1840
H	0.5450	0.1730
I	0.4920	0.1830
J	0.5450	0.1720

1.0

0.0

<0.0