



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:57 PM UTC

PDB ID : 5TAL / pdb_00005tal
EMDB ID : EMD-8378
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 1&2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

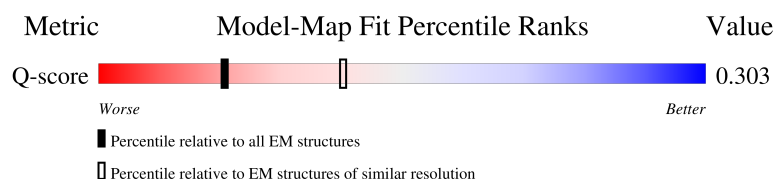
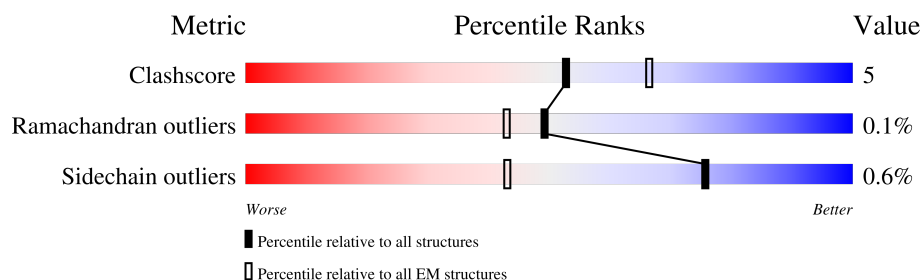
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



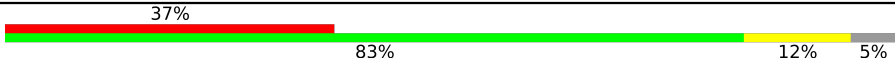
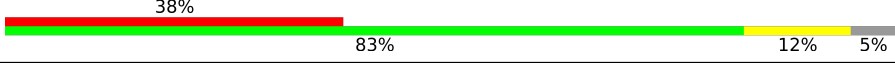
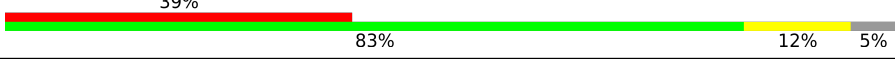
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	22% 83% 16%
1	F	108	23% 84% 15%
1	H	108	22% 85% 14%
1	J	108	23% 87% 12%

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Mol	Chain	Length	Quality of chain
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	B	5102	-	X	-	-
4	CFF	E	5102	-	X	-	-
4	CFF	G	5102	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

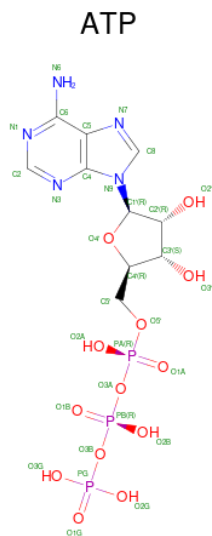
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

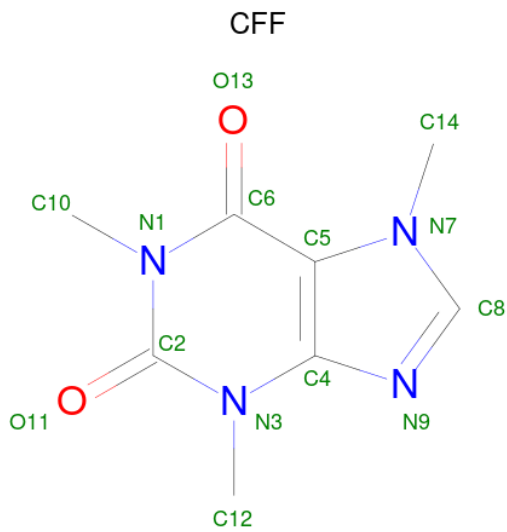
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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



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

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

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

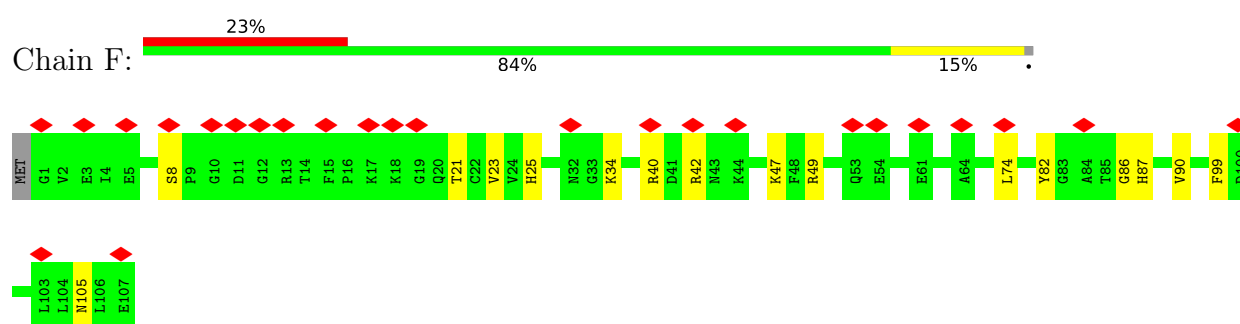
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

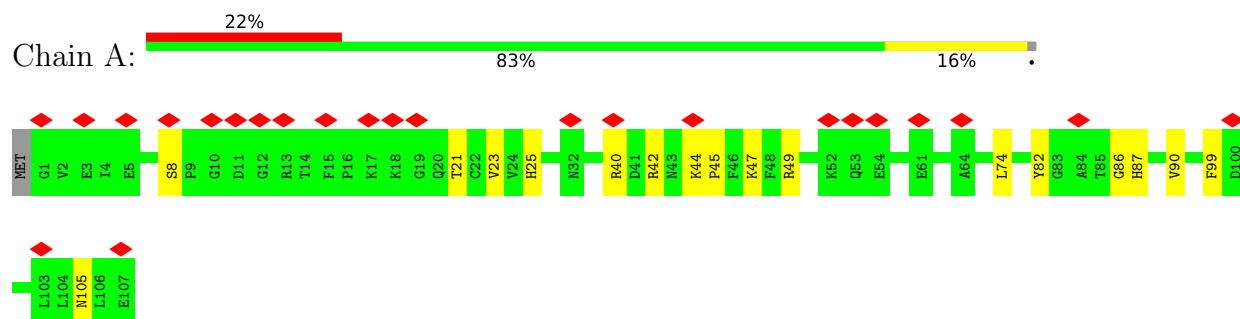
3 Residue-property plots [i](#)

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

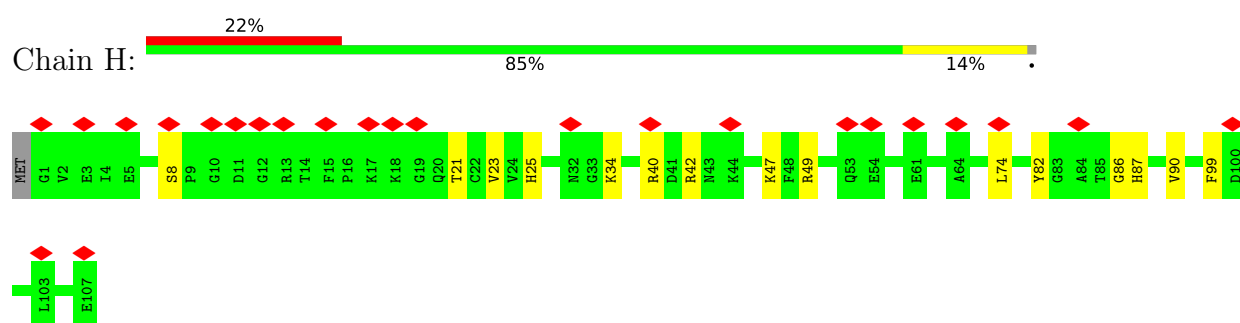
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



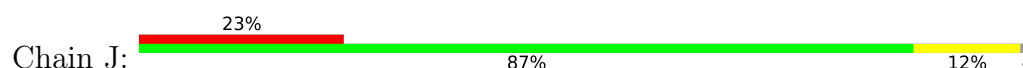
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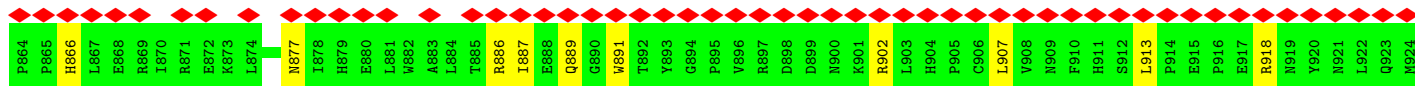


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

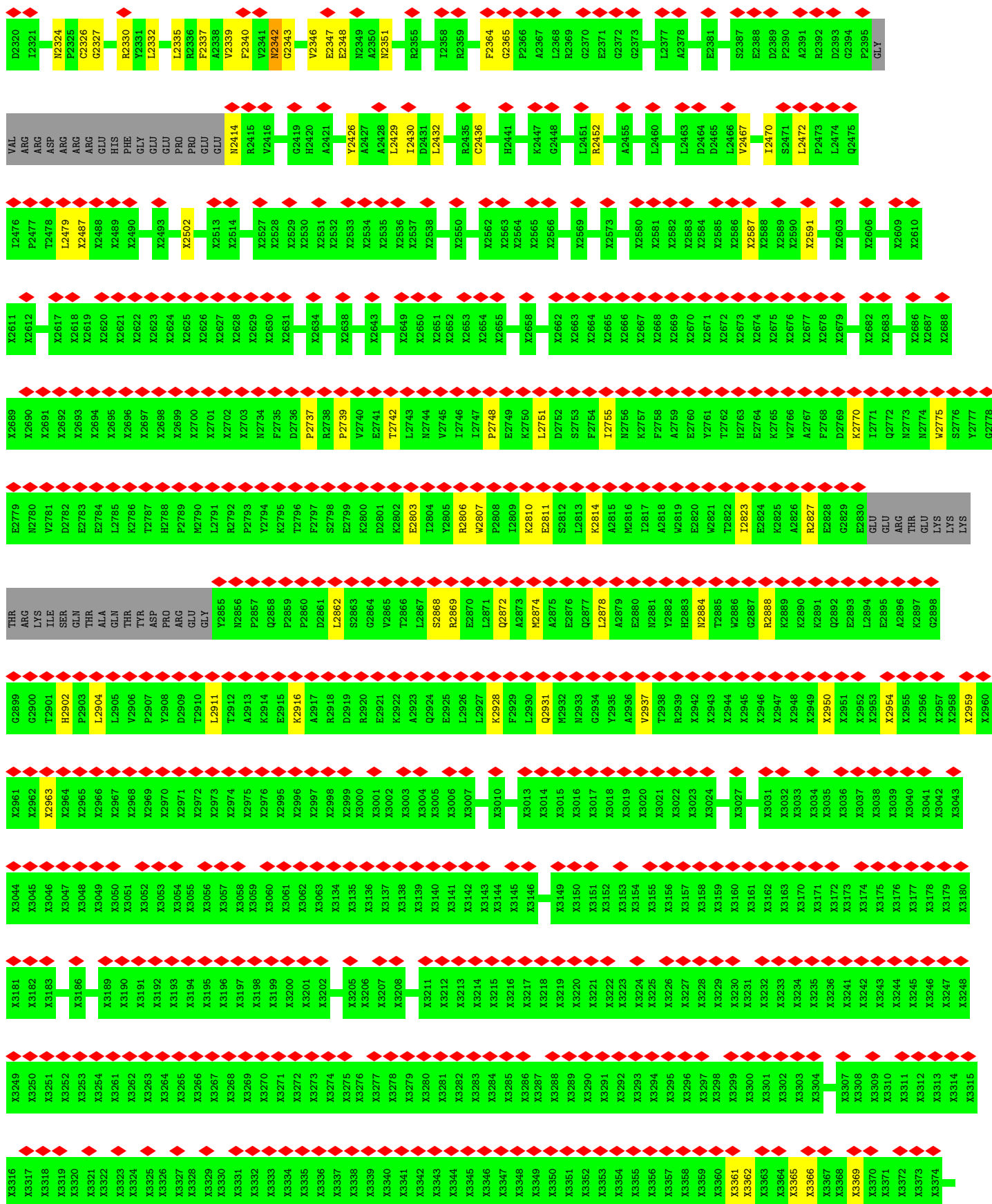


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





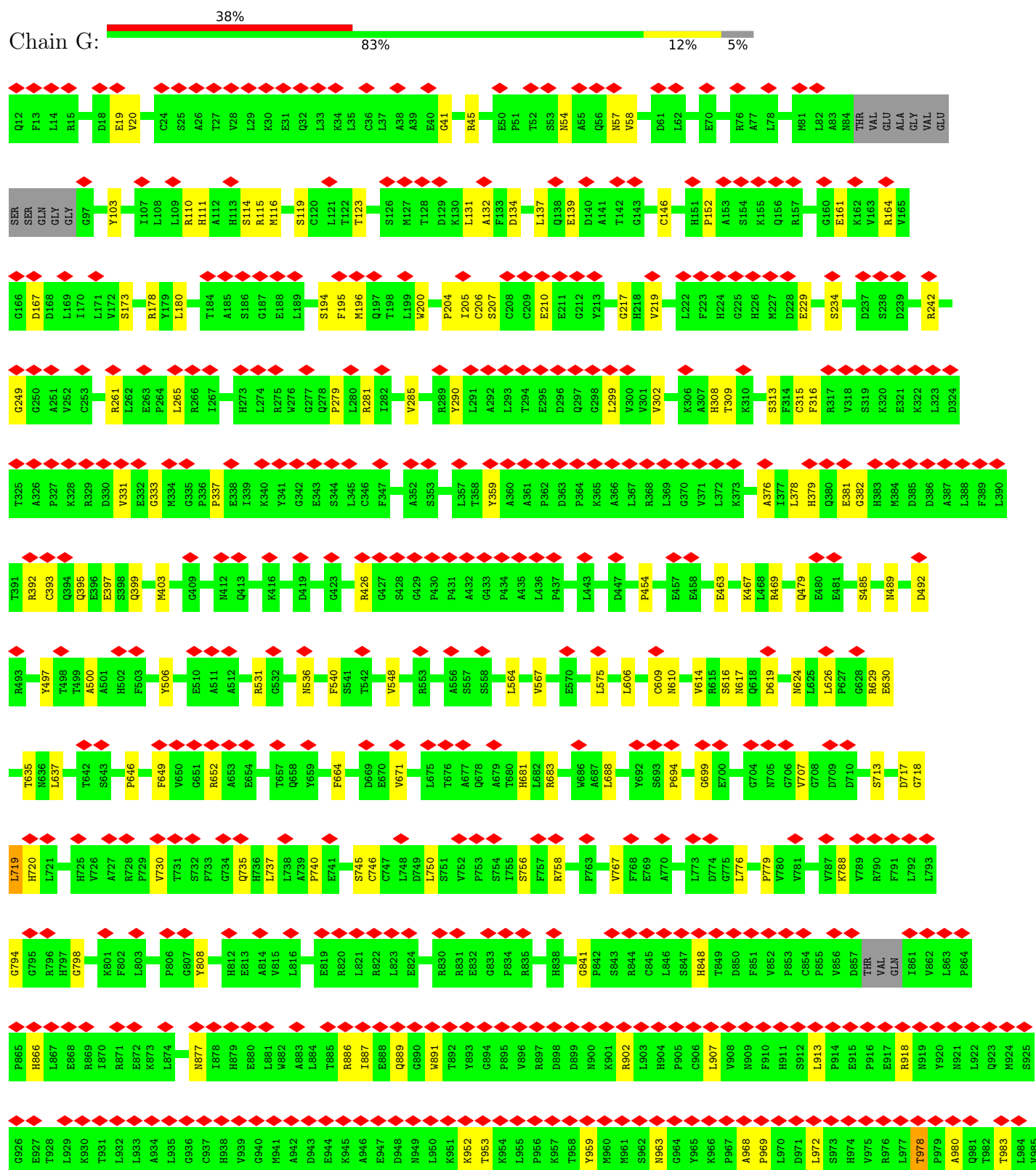






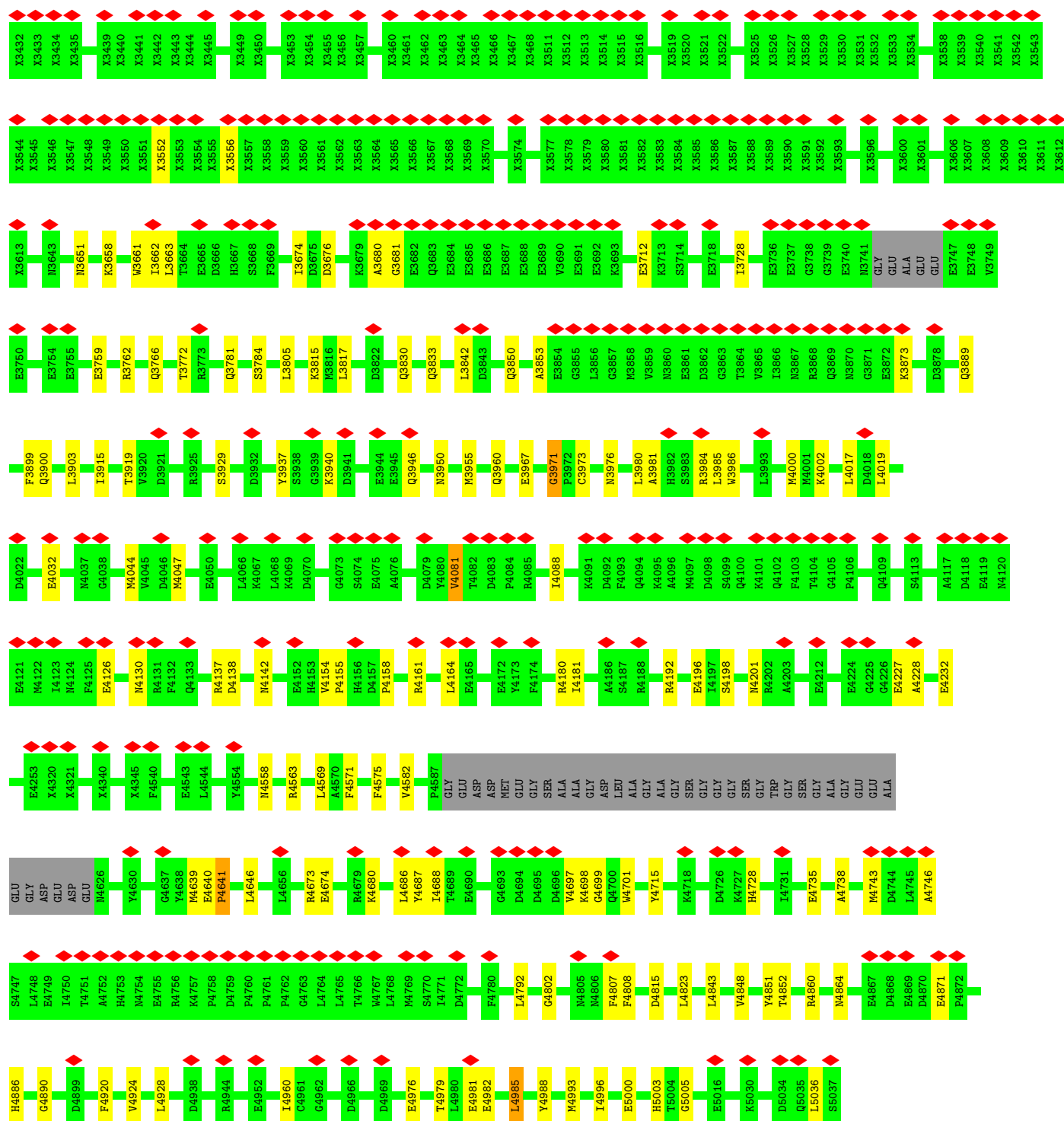
• Molecule 2: Ryanodine receptor 1

Chain G:

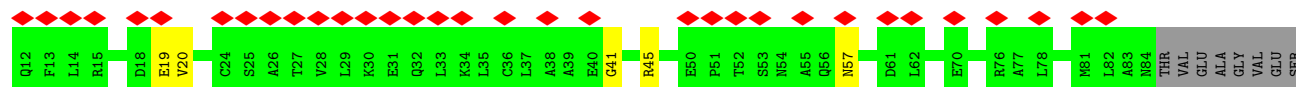
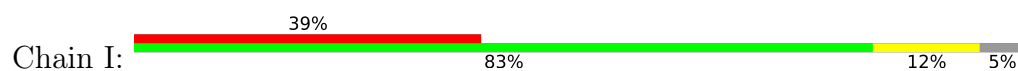




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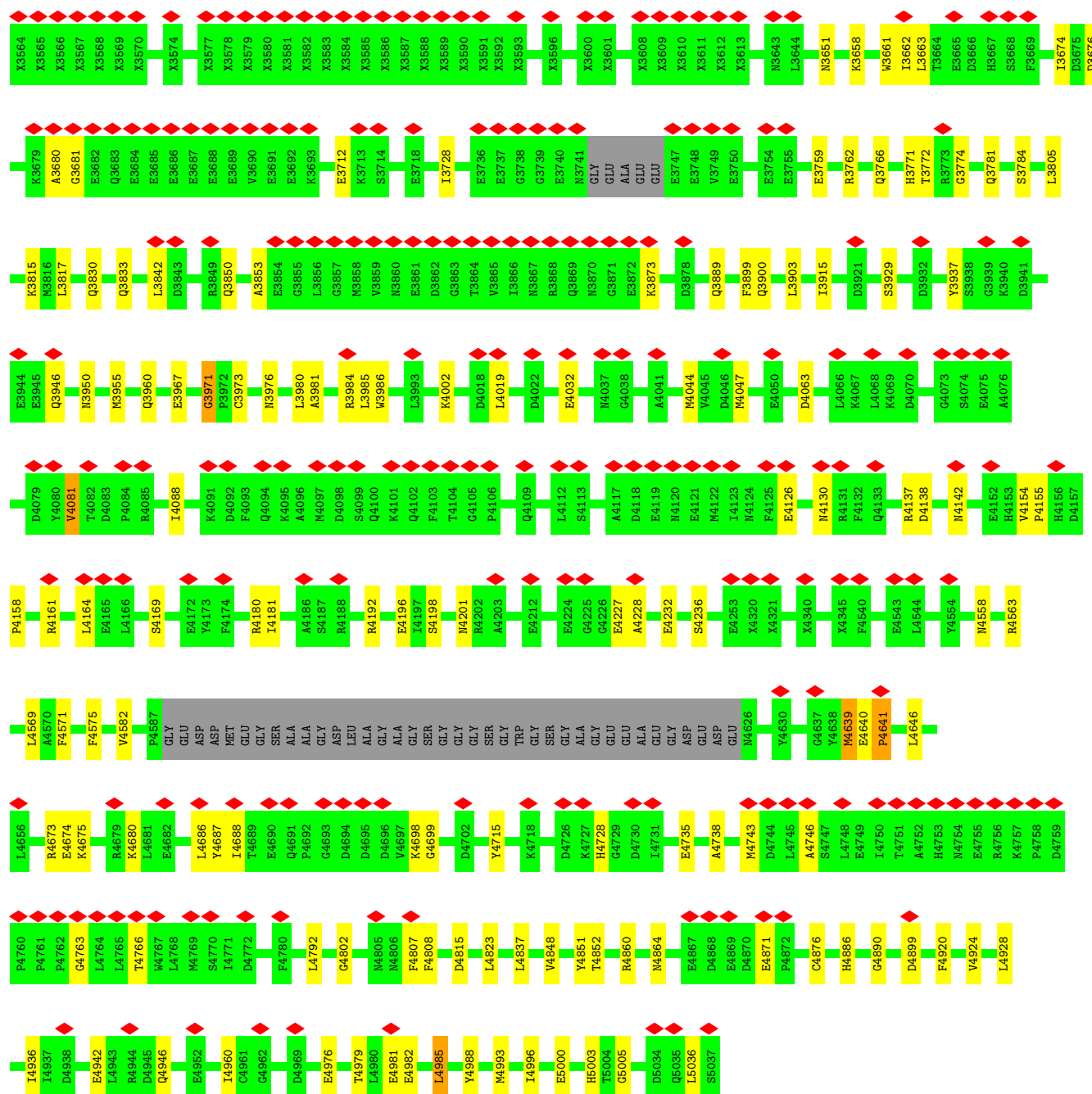
Chain I:



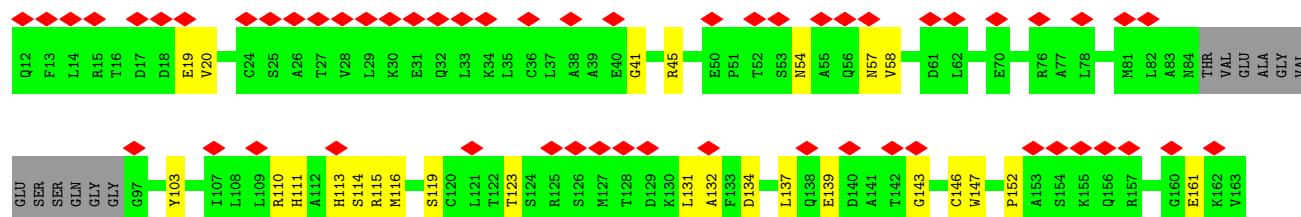
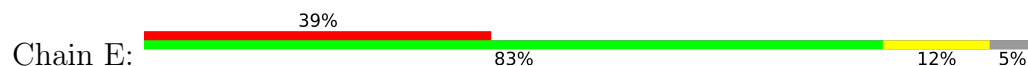




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X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445		X3449	X3450		X3453	X3454		X3557	X3558		X3559	X3560	X3561	X3562	X3458	
X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374			X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393							
X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304		X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3325		X3328	X3329	X3330	X3331	X3332								
X3198	X3199	X3200	X3201	X3202	X3203	X3204	X3207	X3208		X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255	X3256	X3257	X3258	X3259													
X3058	X3059	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3151		X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182		X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197								
X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3009	X3010		X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023		X3027	X3028	X3029	X3030	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3053	X3054	X3055	X3056	X3057								
E2915	K2916	A2917	R2918	D2919	K2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	N2932	Q2933	G2934	Y2935	A2936	W2937	T2938	R2939	K2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	K2951	K2952	K2953	Y2954	K2955	X2956	X2957	X2958	Y2959	K2960	X2961	K2962	Y2963	K2964	X2965	K2966	K2967	X2968	X2969	K2970	Y2971	K2972	K2973	X2974	K2975	X2976								
Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	Q2864	V2865	L2866	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	M2884	T2885	W2886	Q2887	R2888	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										
K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	E2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	K2829	E2830	GLU	GLU	ARG	THR	GLU	LVS	LVS	LVS	THR	ARG	LVS	ILE	SER	GLN	ALA	GLN	THR	TTR	ASP	PRO	ARG	GLU	GLY									
F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	P2754	L2755	N2756	P2757	P2758	E2759	E2760	V2761	T2762	H2763	E2764	K2765	W2766	A2767	P2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	P2777	Q2778	E2779	N2780	S2781	V2782	D2783	E2784	L2785	K2786	P2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794								
X2634		X2638	X2639	X2640		X2643		X2649	X2650	X2651		X2654	X2655		X2658		X2661	X2662	X2663	X2664	X2665	X2666	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685		X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734								
X2564	X2565	X2568	X2569		X2572	X2573		X2577		X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2587		X2591	X2592		X2595	X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2603	X2604	X2605	X2606		X2609	X2610	X2611	X2612	X2613	X2614		X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2632	X2633									



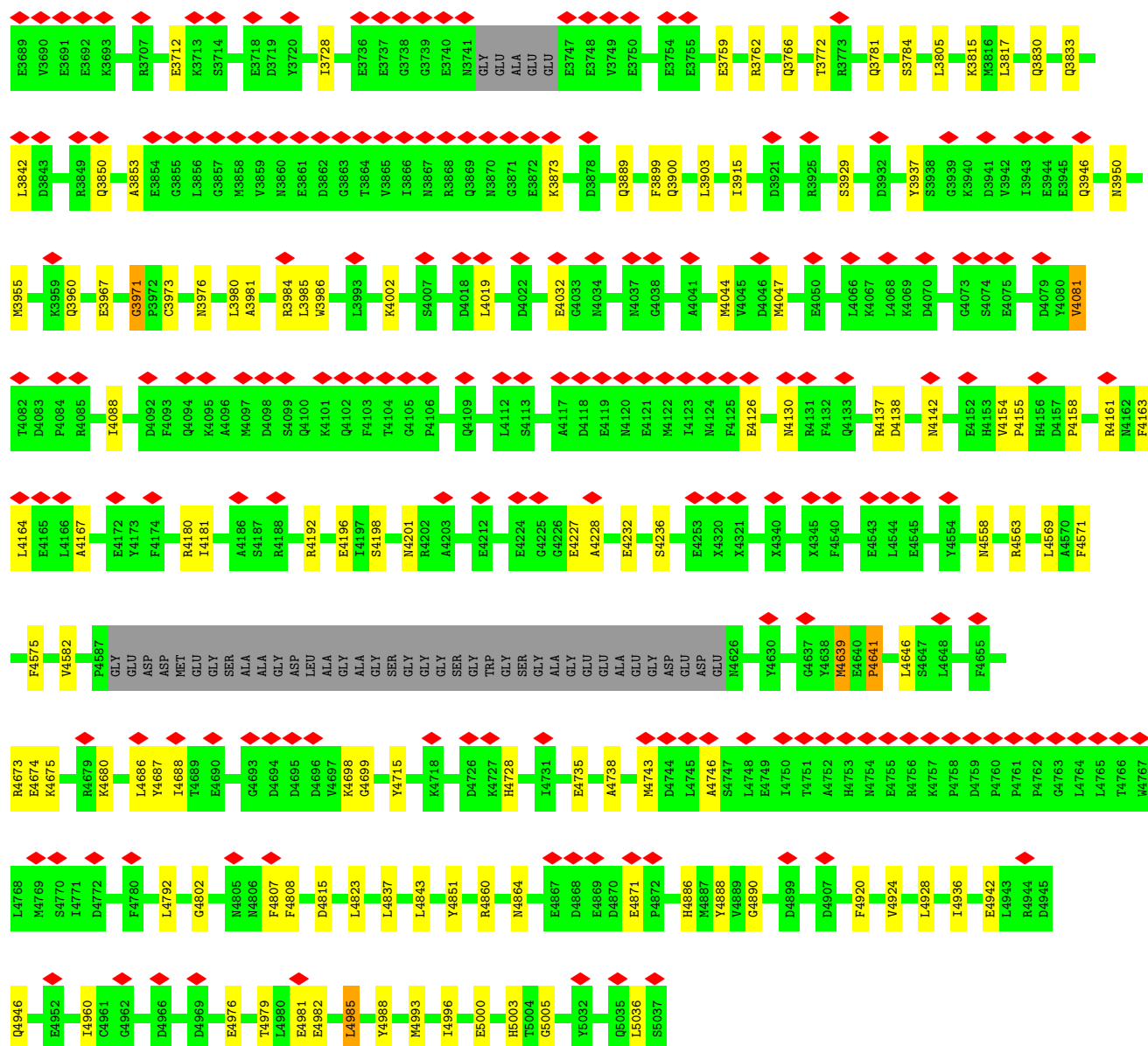
• Molecule 2: Ryanodine receptor 1



S1136	E1137	P1138	F1139	G1140	R1141	P1142	F1143	Q1144	D1147	V1148	V1149	G1150	C1151	M1152	L1155	T1156	E1157	I1161	F1162	T1163	L1164	N1165	G1166	L1169	M1170	S1171	D1172	S1173	F1174	E1176	T1177	A1178	F1179	R1180	E1181	I1182	E1183	T1184	G1185	G1195	Q1198	V1199	G1200	H1201	D1207	L1211	R1212	I1216	C1217									
PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	R1073	K1079	E1091	F1092	E1093	A1094	V1095	E1099	M1100	R1101	V1102	G1103	W1104	A1105	R1106	P1107	F1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	V1123	F1124	N1125	G1126	H1127	R1128	R1131	G1135					
T983	L984	S985	D986	R987	L988	A989	E990	D999	R1000	V1001	A1002	Q1003	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	PRO	R1020	L1021	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	R1033	L1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	N1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRO		
Q923	N924	S925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	N941	A942	D943	E944	K945	A946	E947	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	N960	H961	S962	N963	G964	Y965	K966	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	
V862	L863	P864	P865	H866	L867	E868	R869	L870	R871	E872	K873	L874	N877	I878	H879	E880	L881	W882	A883	L884	T885	R886	L887	E888	Q889	C890	W891	T892	Y893	C894	P895	W896	R897	D898	D899	N900	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922
R790	F791	L792	L793	G794	G795	G796	H797	G798	X801	F802	L803	P806	G807	Y808	H812	E813	A814	W815	L816	E819	R820	L821	R822	L823	E824	R831	E832	G833	P834	R835	H836	C841	P842	S843	R844	C845	L846	S847	H848	T849	D850	F851	W852	P853	C854	P855	V856	D857	I858	VAL	T861							
D717	G718	L719	H720	L721	H725	V726	A727	R728	P729	V730	T731	S732	P733	G734	Q735	H736	L737	L738	A739	P740	E741	S745	C746	C747	L748	D749	L750	S751	V752	P753	S754	G755	T756	F757	R758	I759	N760	P763	V767	F768	E769	A770	L773	D774	G775	L776	P779	V780	W781	V787	K788	V789						
E630	Q634	T635	N636	L637	T642	S643	P646	F649	V650	G651	R652	A653	E654	T657	Q658	Y659	F664	D669	E670	V671	L675	T676	A677	Q678	G679	H681	L682	R683	W686	A687	L688	Y692	S693	P694	G699	E700	G704	N705	G706	G708	D709	D710	S713															
D492	Y497	T498	T499	A500	A501	H502	F503	Y506	E510	A511	A512	R531	G532	N536	T542	V543	S549	K550	L551	D552	R553	A556	S557	S558	L564	E570	L575	L589	L606	C609	N610	V614	R615	S616	N617	Q618	D619	N624	L625	L626	R629																	
R242	G249	G250	A251	V252	C253	R261	L265	R266	I267	H273	L274	R275	W276	G277	Q278	P279	L280	R281	I282	V285	R289	Y290	L291	A292	L293	T294	E295	D296	Q297	G298	L299	V300	V301	V302	K306	A307	H308	T309	K310	S313	F314	C315	F316	R317	V318	S319	K320	E321	K322	L323								
R164	V165	G166	D167	D168	L169	L170	L171	S172	S173	E177	R178	Y179	L180	T184	A185	S186	G187	E188	L189	S194	F195	M196	Q197	T198	L199	W200	P204	I205	C206	S207	C208	C209	E210	E211	G212	Y213	G217	H218	V219	L222	F223	H224	G225	H226	M227	D228	E229	S234	D237	S238	D239							



X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3596	X3597	X3600	X3601	X3604	X3608	X3609	X3610	X3611	X3612	X3613	X3643	X3644	X3651	X3652	F3653	X3658	X3661	I3662	L3663	T3664	E3665	D3666	H3667	S3668	F3669	I3674	X3679	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688																			
X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3449	X3450	X3453	X3454	X3457	X3458	X3459	X3460	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514														
X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3574	X3577	X3578	X3579	X3580											
X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407										
X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346										
X3143	X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3151	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3198	X3199	X3200	X3201	X3202	X3203	X3204	X3207	X3208	X3211	X3212	X3213	X3214													
X3010	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3027	X3028	X3029	X3030	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3064	X3065	X3066	X3067	X3068	X3069	X3070	X3071	X3072	X3073	X3074	X3075	X3076	X3077	X3078	X3079	X3080	X3081	X3082	X3083
F2929	L2930	Q2931	M2932	N2933	Q2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2977	X2978	X2979	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3009												
R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	M2881	T2882	H2883	N2884	T2885	A2886	G2887	R2888	K2889	X2890	X2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	L2899	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928								
E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	T2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	K2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	T2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	I2804	Y2805	R2806	W2807	P2808									
I2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	T2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	Q2857	Q2858	P2859	P2860	D2861	L2862	S2863	Q2864	V2865	T2866	L2867	S2868										



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, CA, CFF, 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	0.21	0/834	0.48	0/1123
1	F	0.22	0/834	0.49	0/1123
1	H	0.21	0/834	0.49	0/1123
1	J	0.22	0/834	0.48	0/1123
2	B	0.23	0/25428	0.54	2/34534 (0.0%)
2	E	0.23	0/25428	0.54	2/34534 (0.0%)
2	G	0.23	0/25428	0.54	2/34534 (0.0%)
2	I	0.23	0/25428	0.54	2/34534 (0.0%)
All	All	0.23	0/105048	0.54	8/142628 (0.0%)

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

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4639	MET	CA-C-N	5.52	135.26	121.80
2	B	4639	MET	C-N-CA	5.52	135.26	121.80
2	I	4639	MET	CA-C-N	5.50	135.22	121.80
2	I	4639	MET	C-N-CA	5.50	135.22	121.80
2	G	4639	MET	CA-C-N	5.50	135.21	121.80
2	G	4639	MET	C-N-CA	5.50	135.21	121.80
2	E	4639	MET	CA-C-N	5.49	135.19	121.80
2	E	4639	MET	C-N-CA	5.49	135.19	121.80

There are no chirality outliers.

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1720	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	4807	PHE	Peptide
2	B	624	ASN	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1720	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	E	4641	PRO	Peptide
2	E	4807	PHE	Peptide
2	E	624	ASN	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1720	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	4807	PHE	Peptide
2	G	624	ASN	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1720	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4807	PHE	Peptide
2	I	624	ASN	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	10	0
1	F	818	0	824	11	0
1	H	818	0	824	8	0
1	J	818	0	824	7	0
2	B	29499	0	24746	298	0
2	E	29499	0	24747	290	0
2	G	29499	0	24747	289	0
2	I	29499	0	24747	298	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102371	1189	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1189) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.86	0.74
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.86	0.72
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.86	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.87	0.71
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.56	0.70
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.57	0.70
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.74	0.70
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.58	0.69
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.57	0.69
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.56	0.68
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.58	0.68
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.58	0.68
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.58	0.68
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.58	0.67
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.78	0.66
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.78	0.65
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.78	0.65
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.78	0.65
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.62	0.65
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.64
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.62	0.64
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.64
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.62	0.64
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.62	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.62	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.80	0.63
2:G:2266:GLY:O	2:G:2330:ARG:NH2	2.32	0.63
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.81	0.63
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.81	0.63
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.81	0.62
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.33	0.62
2:B:2266:GLY:O	2:B:2330:ARG:NH2	2.32	0.62
2:E:2266:GLY:O	2:E:2330:ARG:NH2	2.32	0.62
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.81	0.62
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.33	0.62
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.33	0.62
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.33	0.62
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.82	0.62
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.82	0.62
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.82	0.61
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.82	0.61
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.33	0.61
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.33	0.61
2:I:2266:GLY:O	2:I:2330:ARG:NH2	2.32	0.61
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.82	0.61
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.82	0.61
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.33	0.61
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.83	0.61
2:B:379:HIS:HD2	2:B:382:GLY:H	1.47	0.61
2:G:379:HIS:HD2	2:G:382:GLY:H	1.47	0.61
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.83	0.61
2:I:379:HIS:HD2	2:I:382:GLY:H	1.47	0.60
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.82	0.60
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.83	0.60
2:G:173:SER:HB3	2:G:178:ARG:H	1.66	0.60
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.66	0.60
2:I:173:SER:HB3	2:I:178:ARG:H	1.66	0.60
2:E:379:HIS:HD2	2:E:382:GLY:H	1.48	0.60
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.82	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.84	0.60
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.83	0.60
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.84	0.60
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.84	0.60
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.67	0.60
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.83	0.60
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.67	0.59
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.84	0.59
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.83	0.59
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.83	0.59
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.35	0.59
2:B:173:SER:HB3	2:B:178:ARG:H	1.66	0.59
2:G:132:ALA:HA	2:G:194:SER:HB2	1.85	0.59
2:I:132:ALA:HA	2:I:194:SER:HB2	1.85	0.59
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.84	0.59
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.83	0.59
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.59
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.59
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.35	0.59
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.59
2:E:173:SER:HB3	2:E:178:ARG:H	1.66	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.67	0.59
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.84	0.59
2:B:606:LEU:O	2:B:617:ASN:ND2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.76	0.59
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.85	0.59
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.36	0.59
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.36	0.59
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.67	0.59
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.85	0.59
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.36	0.58
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.67	0.58
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.84	0.58
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.67	0.58
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.85	0.58
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.67	0.58
2:E:132:ALA:HA	2:E:194:SER:HB2	1.85	0.58
2:B:132:ALA:HA	2:B:194:SER:HB2	1.85	0.58
2:I:606:LEU:O	2:I:617:ASN:ND2	2.36	0.58
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.76	0.58
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.84	0.58
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.85	0.58
2:G:606:LEU:O	2:G:617:ASN:ND2	2.36	0.58
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.84	0.58
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.37	0.58
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.36	0.58
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.84	0.58
2:I:978:THR:HB	2:I:980:ALA:H	1.69	0.58
2:E:606:LEU:O	2:E:617:ASN:ND2	2.36	0.58
2:E:978:THR:HB	2:E:980:ALA:H	1.69	0.58
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.76	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.37	0.58
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.37	0.58
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.86	0.58
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.37	0.58
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.35	0.58
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.37	0.58
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.37	0.58
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.37	0.58
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.37	0.58
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.76	0.58
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.37	0.58
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.35	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.58
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:978:THR:HB	2:B:980:ALA:H	1.69	0.57
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.35	0.57
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.86	0.57
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.86	0.57
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.85	0.57
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.86	0.57
2:G:978:THR:HB	2:G:980:ALA:H	1.69	0.57
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.85	0.57
2:G:2107:GLN:HG3	2:G:3681:GLY:HA2	1.87	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.86	0.57
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.87	0.57
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.37	0.57
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.86	0.57
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.86	0.57
2:I:359:TYR:HA	2:I:376:ALA:HA	1.86	0.57
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.86	0.57
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.86	0.56
2:I:2107:GLN:HG3	2:I:3681:GLY:HA2	1.87	0.56
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.56
2:B:4236:SER:OG	2:B:4675:LYS:NZ	2.38	0.56
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.87	0.56
2:B:359:TYR:HA	2:B:376:ALA:HA	1.86	0.56
2:E:2107:GLN:HG3	2:E:3681:GLY:HA2	1.87	0.56
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.70	0.56
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.56
2:B:2107:GLN:HG3	2:B:3681:GLY:HA2	1.87	0.56
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.88	0.56
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.88	0.56
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.88	0.56
2:G:217:GLY:O	2:G:261:ARG:NH1	2.39	0.56
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.88	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.56
2:E:4192:ARG:NH1	2:E:4982:GLU:OE2	2.39	0.56
2:B:217:GLY:O	2:B:261:ARG:NH1	2.39	0.56
2:I:217:GLY:O	2:I:261:ARG:NH1	2.39	0.56
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.88	0.56
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.88	0.56
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.86	0.56
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.87	0.56
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.70	0.56
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:265:LEU:HD12	2:I:279:PRO:HB2	1.88	0.56
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.86	0.56
2:B:265:LEU:HD12	2:B:279:PRO:HB2	1.88	0.56
2:G:359:TYR:HA	2:G:376:ALA:HA	1.86	0.56
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.88	0.56
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.86	0.56
2:E:359:TYR:HA	2:E:376:ALA:HA	1.86	0.55
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.88	0.55
2:B:4192:ARG:NH1	2:B:4982:GLU:OE2	2.39	0.55
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.39	0.55
2:G:4192:ARG:NH1	2:G:4982:GLU:OE2	2.39	0.55
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.37	0.55
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.86	0.55
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.88	0.55
2:G:614:VAL:HG22	2:G:616:SER:H	1.71	0.55
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.86	0.55
2:G:2347:GLU:O	2:G:2351:ASN:N	2.38	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.38	0.55
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.86	0.55
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.89	0.55
2:G:265:LEU:HD12	2:G:279:PRO:HB2	1.88	0.55
2:I:4192:ARG:NH1	2:I:4982:GLU:OE2	2.39	0.55
2:E:265:LEU:HD12	2:E:279:PRO:HB2	1.88	0.55
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.88	0.55
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.89	0.55
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.89	0.55
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.70	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.55
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.89	0.55
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.72	0.55
2:E:217:GLY:O	2:E:261:ARG:NH1	2.39	0.55
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.89	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.89	0.55
2:I:614:VAL:HG22	2:I:616:SER:H	1.71	0.55
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.88	0.55
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.89	0.55
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.70	0.55
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.89	0.55
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.89	0.55
2:I:180:LEU:O	2:I:200:TRP:NE1	2.36	0.55
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:315:CYS:SG	2:I:316:PHE:N	2.80	0.55
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.89	0.55
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.40	0.55
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.40	0.55
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.89	0.55
2:E:315:CYS:SG	2:E:316:PHE:N	2.80	0.55
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.40	0.55
2:E:2347:GLU:O	2:E:2351:ASN:N	2.38	0.55
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.89	0.55
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.89	0.55
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.39	0.55
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.40	0.55
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.89	0.54
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.88	0.54
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.89	0.54
2:B:614:VAL:HG22	2:B:616:SER:H	1.71	0.54
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.72	0.54
2:G:315:CYS:SG	2:G:316:PHE:N	2.80	0.54
2:B:315:CYS:SG	2:B:316:PHE:N	2.80	0.54
2:G:180:LEU:O	2:G:200:TRP:NE1	2.36	0.54
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.90	0.54
2:B:2347:GLU:O	2:B:2351:ASN:N	2.38	0.54
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.40	0.54
2:I:2347:GLU:O	2:I:2351:ASN:N	2.38	0.54
2:E:111:HIS:HD2	2:E:114:SER:H	1.54	0.54
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.90	0.54
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.40	0.54
2:B:4914:VAL:HG23	2:E:4888:TYR:HD1	1.72	0.54
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.89	0.54
2:E:683:ARG:NH1	2:E:707:VAL:O	2.38	0.54
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.40	0.54
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.89	0.54
2:E:614:VAL:HG22	2:E:616:SER:H	1.71	0.54
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.89	0.54
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.89	0.54
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.90	0.54
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.89	0.54
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.37	0.54
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.90	0.54
2:I:111:HIS:HD2	2:I:114:SER:H	1.54	0.54
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.89	0.54
2:E:1948:ASP:OD1	2:E:2126:ARG:NH2	2.39	0.54
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.90	0.53
2:B:111:HIS:HD2	2:B:114:SER:H	1.54	0.53
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.41	0.53
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.41	0.53
2:B:309:THR:O	2:B:313:SER:OG	2.27	0.53
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.90	0.53
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.90	0.53
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.40	0.53
2:B:4161:ARG:HD3	2:B:4164:LEU:HD12	1.90	0.53
2:G:111:HIS:HD2	2:G:114:SER:H	1.54	0.53
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.72	0.53
2:E:4161:ARG:HD3	2:E:4164:LEU:HD12	1.91	0.53
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.42	0.53
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.41	0.53
2:I:309:THR:O	2:I:313:SER:OG	2.27	0.53
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.53
2:G:309:THR:O	2:G:313:SER:OG	2.27	0.53
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.41	0.53
2:E:652:ARG:HB2	2:E:750:LEU:HD13	1.91	0.53
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.89	0.53
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.91	0.53
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.91	0.53
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.91	0.53
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.90	0.53
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.53
2:I:331:VAL:HG12	2:I:333:GLY:H	1.74	0.53
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.90	0.53
2:E:309:THR:O	2:E:313:SER:OG	2.27	0.53
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.39	0.52
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.91	0.52
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.90	0.52
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.89	0.52
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.42	0.52
2:I:652:ARG:HB2	2:I:750:LEU:HD13	1.91	0.52
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.41	0.52
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.43	0.52
2:G:2107:GLN:NE2	2:G:3680:ALA:O	2.43	0.52
2:I:4161:ARG:HD3	2:I:4164:LEU:HD12	1.90	0.52
2:G:2178:MET:HE1	2:G:2210:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:219:VAL:O	2:E:392:ARG:NH1	2.43	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.52
2:G:331:VAL:HG12	2:G:333:GLY:H	1.74	0.52
2:G:1636:MET:HE2	2:G:1638:ALA:HB2	1.91	0.52
2:I:2178:MET:HE1	2:I:2210:VAL:HG11	1.92	0.52
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.92	0.52
2:B:652:ARG:HB2	2:B:750:LEU:HD13	1.91	0.52
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.42	0.52
2:G:219:VAL:O	2:G:392:ARG:NH1	2.43	0.52
2:B:180:LEU:O	2:B:200:TRP:NE1	2.36	0.52
2:B:331:VAL:HG12	2:B:333:GLY:H	1.74	0.52
2:B:2178:MET:HE1	2:B:2210:VAL:HG11	1.92	0.52
2:I:1636:MET:HE2	2:I:1638:ALA:HB2	1.91	0.52
2:E:331:VAL:HG12	2:E:333:GLY:H	1.74	0.52
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.43	0.52
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.91	0.52
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.43	0.52
2:I:2107:GLN:NE2	2:I:3680:ALA:O	2.43	0.52
2:E:2178:MET:HE1	2:E:2210:VAL:HG11	1.92	0.52
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.90	0.52
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.92	0.52
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.52
2:G:652:ARG:HB2	2:G:750:LEU:HD13	1.91	0.52
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.91	0.52
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.43	0.52
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.43	0.52
2:G:4161:ARG:HD3	2:G:4164:LEU:HD12	1.90	0.51
2:B:683:ARG:NH1	2:B:707:VAL:O	2.38	0.51
2:I:219:VAL:O	2:I:392:ARG:NH1	2.43	0.51
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.43	0.51
2:E:889:GLN:O	2:E:902:ARG:NH1	2.44	0.51
1:A:82:TYR:O	1:A:86:GLY:N	2.43	0.51
2:B:219:VAL:O	2:B:392:ARG:NH1	2.43	0.51
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.43	0.51
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.93	0.51
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.93	0.51
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.51
2:B:1636:MET:HE2	2:B:1638:ALA:HB2	1.91	0.51
2:G:41:GLY:O	2:G:45:ARG:NH1	2.44	0.51
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.41	0.51
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1636:MET:HE2	2:E:1638:ALA:HB2	1.91	0.51
2:E:2107:GLN:NE2	2:E:3680:ALA:O	2.43	0.51
1:F:82:TYR:O	1:F:86:GLY:N	2.43	0.51
2:B:2107:GLN:NE2	2:B:3680:ALA:O	2.43	0.51
1:J:82:TYR:O	1:J:86:GLY:N	2.43	0.51
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.91	0.51
2:G:161:GLU:HA	2:I:3984:ARG:HH22	1.75	0.51
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.42	0.51
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.92	0.51
2:E:776:LEU:HG	2:E:848:HIS:HA	1.93	0.51
2:B:889:GLN:O	2:B:902:ARG:NH1	2.44	0.51
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.91	0.51
2:E:4198:SER:HB3	2:E:4201:ASN:HB2	1.93	0.51
2:E:4563:ARG:NH1	2:E:4815:ASP:OD1	2.44	0.51
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.93	0.51
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.43	0.51
2:G:889:GLN:O	2:G:902:ARG:NH1	2.44	0.51
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.51
2:E:3900:GLN:NE2	2:E:3967:GLU:O	2.44	0.51
2:B:776:LEU:HG	2:B:848:HIS:HA	1.93	0.50
2:G:683:ARG:NH1	2:G:707:VAL:O	2.38	0.50
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.92	0.50
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.93	0.50
2:B:1516:UNK:N	2:B:1529:UNK:O	2.44	0.50
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.44	0.50
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.44	0.50
2:I:889:GLN:O	2:I:902:ARG:NH1	2.44	0.50
2:I:4198:SER:HB3	2:I:4201:ASN:HB2	1.93	0.50
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.94	0.50
2:B:4563:ARG:NH1	2:B:4815:ASP:OD1	2.44	0.50
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.76	0.50
2:I:41:GLY:O	2:I:45:ARG:NH1	2.44	0.50
2:I:776:LEU:HG	2:I:848:HIS:HA	1.93	0.50
2:E:180:LEU:O	2:E:200:TRP:NE1	2.36	0.50
1:H:82:TYR:O	1:H:86:GLY:N	2.43	0.50
2:B:3900:GLN:NE2	2:B:3967:GLU:O	2.44	0.50
2:G:3900:GLN:NE2	2:G:3967:GLU:O	2.44	0.50
2:I:1516:UNK:N	2:I:1529:UNK:O	2.45	0.50
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.93	0.50
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.42	0.50
2:E:907:LEU:O	2:E:963:ASN:ND2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.44	0.50
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.44	0.50
2:G:776:LEU:HG	2:G:848:HIS:HA	1.93	0.50
2:G:1516:UNK:N	2:G:1529:UNK:O	2.45	0.50
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.93	0.50
2:B:41:GLY:O	2:B:45:ARG:NH1	2.44	0.50
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.44	0.50
2:G:4563:ARG:NH1	2:G:4815:ASP:OD1	2.44	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.45	0.50
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.38	0.50
2:B:4198:SER:HB3	2:B:4201:ASN:HB2	1.93	0.50
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.94	0.50
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.47	0.50
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.94	0.50
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.44	0.50
2:G:4198:SER:HB3	2:G:4201:ASN:HB2	1.93	0.50
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.93	0.50
2:I:4563:ARG:NH1	2:I:4815:ASP:OD1	2.44	0.50
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.44	0.50
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.47	0.49
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.45	0.49
2:E:4976:GLU:O	2:E:4979:THR:OG1	2.29	0.49
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.45	0.49
2:G:3759:GLU:HB3	2:G:3762:ARG:HH21	1.77	0.49
2:I:3900:GLN:NE2	2:I:3967:GLU:O	2.44	0.49
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.93	0.49
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.76	0.49
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.42	0.49
2:E:2332:LEU:HD13	2:E:2335:LEU:HD12	1.94	0.49
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.47	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.49
2:B:3759:GLU:HB3	2:B:3762:ARG:HH21	1.77	0.49
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.47	0.49
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.45	0.49
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.76	0.49
2:G:907:LEU:O	2:G:963:ASN:ND2	2.38	0.49
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.76	0.49
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.94	0.49
2:G:2318:TYR:OH	2:G:2414:ASN:N	2.45	0.49
2:B:1457:UNK:N	2:B:1497:UNK:O	2.46	0.49
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3759:GLU:HB3	2:I:3762:ARG:HH21	1.77	0.49
2:E:41:GLY:O	2:E:45:ARG:NH1	2.44	0.49
2:E:2318:TYR:OH	2:E:2414:ASN:N	2.46	0.49
2:B:2332:LEU:HD13	2:B:2335:LEU:HD12	1.94	0.49
2:G:164:ARG:N	2:G:167:ASP:OD2	2.43	0.49
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.95	0.49
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.44	0.49
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.48	0.49
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.95	0.49
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.94	0.49
2:I:1457:UNK:N	2:I:1497:UNK:O	2.46	0.49
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.41	0.49
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.48	0.49
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.41	0.49
2:B:907:LEU:O	2:B:963:ASN:ND2	2.38	0.49
2:B:2318:TYR:OH	2:B:2414:ASN:N	2.46	0.49
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.93	0.49
2:E:164:ARG:N	2:E:167:ASP:OD2	2.43	0.49
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.78	0.49
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.78	0.48
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.95	0.48
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.95	0.48
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.45	0.48
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.95	0.48
2:G:2305:CYS:HA	2:G:2324:ASN:HD22	1.79	0.48
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.95	0.48
2:E:3842:LEU:O	2:E:3929:SER:OG	2.32	0.48
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.78	0.48
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.37	0.48
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.96	0.48
2:I:1166:GLY:HA3	2:I:1216:ILE:HD13	1.96	0.48
2:I:4976:GLU:O	2:I:4979:THR:OG1	2.29	0.48
2:B:234:SER:O	2:B:242:ARG:NE	2.46	0.48
2:B:1166:GLY:HA3	2:B:1216:ILE:HD13	1.96	0.48
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.79	0.48
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.48	0.48
2:G:1166:GLY:HA3	2:G:1216:ILE:HD13	1.96	0.48
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.94	0.48
2:E:730:VAL:O	2:E:735:GLN:NE2	2.47	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.94	0.48
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.96	0.48
2:I:2332:LEU:HD13	2:I:2335:LEU:HD12	1.94	0.48
2:E:234:SER:O	2:E:242:ARG:NE	2.46	0.48
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.78	0.48
2:B:730:VAL:O	2:B:735:GLN:NE2	2.47	0.48
2:B:3842:LEU:O	2:B:3929:SER:OG	2.32	0.48
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.79	0.48
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.96	0.48
2:E:3759:GLU:HB3	2:E:3762:ARG:HH21	1.77	0.48
2:B:2950:UNK:O	2:B:2954:UNK:N	2.47	0.48
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.32	0.48
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.47	0.48
2:G:116:MET:HB2	2:G:137:LEU:HD12	1.96	0.48
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.42	0.48
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.79	0.48
2:E:1457:UNK:N	2:E:1497:UNK:O	2.46	0.48
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.79	0.48
2:B:116:MET:HB2	2:B:137:LEU:HD12	1.96	0.48
2:B:119:SER:HA	2:B:146:CYS:HA	1.96	0.48
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.79	0.48
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.48	0.48
2:I:2004:GLU:HA	2:I:2007:ASN:HB2	1.96	0.48
2:I:2318:TYR:OH	2:I:2414:ASN:N	2.45	0.48
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.37	0.48
2:E:2305:CYS:HA	2:E:2324:ASN:HD22	1.79	0.48
2:B:2004:GLU:HA	2:B:2007:ASN:HB2	1.96	0.48
2:B:4976:GLU:O	2:B:4979:THR:OG1	2.29	0.48
2:G:2332:LEU:HD13	2:G:2335:LEU:HD12	1.94	0.48
2:G:3842:LEU:O	2:G:3929:SER:OG	2.32	0.48
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.37	0.48
2:I:3903:LEU:HG	2:I:3915:ILE:HD12	1.96	0.48
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.96	0.48
2:E:1166:GLY:HA3	2:E:1216:ILE:HD13	1.96	0.48
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.95	0.48
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.79	0.48
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.32	0.48
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.96	0.48
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.96	0.48
2:G:3940:LYS:O	2:G:4002:LYS:NZ	2.42	0.48
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.96	0.48
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2305:CYS:HA	2:B:2324:ASN:HD22	1.79	0.47
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.96	0.47
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.79	0.47
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.97	0.47
2:G:1457:UNK:N	2:G:1497:UNK:O	2.46	0.47
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.96	0.47
2:G:2868:SER:O	2:G:2872:GLN:N	2.47	0.47
2:G:4843:LEU:HD12	2:I:4823:LEU:HD23	1.96	0.47
2:I:164:ARG:N	2:I:167:ASP:OD2	2.43	0.47
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.95	0.47
2:I:3842:LEU:O	2:I:3929:SER:OG	2.32	0.47
2:G:119:SER:HA	2:G:146:CYS:HA	1.96	0.47
2:G:730:VAL:O	2:G:735:GLN:NE2	2.47	0.47
2:I:730:VAL:O	2:I:735:GLN:NE2	2.47	0.47
2:I:4137:ARG:NH2	2:I:4196:GLU:OE2	2.48	0.47
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.96	0.47
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.79	0.47
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.78	0.47
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.48	0.47
2:E:2868:SER:O	2:E:2872:GLN:N	2.47	0.47
2:G:2950:UNK:O	2:G:2954:UNK:N	2.47	0.47
2:G:3903:LEU:HG	2:G:3915:ILE:HD12	1.96	0.47
2:E:4851:TYR:HD2	2:E:4920:PHE:HD1	1.62	0.47
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.97	0.47
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.78	0.47
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.97	0.47
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.78	0.47
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.95	0.47
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.96	0.47
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.96	0.47
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.97	0.47
2:B:123:THR:OG1	2:B:134:ASP:OD1	2.33	0.47
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.88	0.47
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.97	0.47
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.97	0.47
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.88	0.47
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.96	0.47
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.46	0.47
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.48	0.47
2:G:4137:ARG:NH2	2:G:4196:GLU:OE2	2.48	0.47
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.24	0.47
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.97	0.47
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.96	0.47
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.97	0.47
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.96	0.47
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.95	0.47
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.80	0.47
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.96	0.47
2:G:234:SER:O	2:G:242:ARG:NE	2.46	0.47
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.97	0.47
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.42	0.47
2:G:2004:GLU:HA	2:G:2007:ASN:HB2	1.96	0.47
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.79	0.47
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.97	0.47
2:I:119:SER:HA	2:I:146:CYS:HA	1.96	0.47
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.80	0.47
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.97	0.47
2:E:116:MET:HB2	2:E:137:LEU:HD12	1.96	0.47
2:E:123:THR:OG1	2:E:134:ASP:OD1	2.33	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.97	0.47
2:E:2950:UNK:O	2:E:2954:UNK:N	2.48	0.47
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.95	0.47
2:G:1817:GLU:O	2:G:1821:ASP:N	2.45	0.47
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.79	0.47
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.96	0.47
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.97	0.47
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.88	0.47
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.42	0.47
2:I:2305:CYS:HA	2:I:2324:ASN:HD22	1.79	0.47
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.48	0.47
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.79	0.47
2:E:3903:LEU:HG	2:E:3915:ILE:HD12	1.96	0.47
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.97	0.47
2:B:1747:LEU:HD21	2:B:2041:HIS:HB2	1.97	0.47
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.97	0.47
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.97	0.47
2:G:2452:ARG:HH12	2:E:177:GLU:HG3	1.79	0.47
2:G:4851:TYR:HD2	2:G:4920:PHE:HD1	1.62	0.47
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.88	0.47
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.97	0.47
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.46	0.46
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.48	0.46
2:I:234:SER:O	2:I:242:ARG:NE	2.46	0.46
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.97	0.46
2:I:4236:SER:OG	2:I:4675:LYS:NZ	2.38	0.46
2:I:907:LEU:O	2:I:963:ASN:ND2	2.38	0.46
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.97	0.46
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.97	0.46
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.97	0.46
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.96	0.46
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.78	0.46
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.97	0.46
2:B:4137:ARG:NH2	2:B:4196:GLU:OE2	2.48	0.46
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.48	0.46
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.32	0.46
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.38	0.46
2:E:1747:LEU:HD21	2:E:2041:HIS:HB2	1.97	0.46
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.98	0.46
2:G:206:CYS:SG	2:G:207:SER:N	2.88	0.46
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.97	0.46
2:G:4976:GLU:O	2:G:4979:THR:OG1	2.29	0.46
2:I:116:MET:HB2	2:I:137:LEU:HD12	1.96	0.46
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.48	0.46
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.46	0.46
2:B:3903:LEU:HG	2:B:3915:ILE:HD12	1.96	0.46
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.81	0.46
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.98	0.46
2:G:3361:UNK:O	2:G:3365:UNK:N	2.49	0.46
2:I:1695:LEU:HB3	2:I:1810:LYS:HZ2	1.80	0.46
2:I:2868:SER:O	2:I:2872:GLN:N	2.47	0.46
2:E:4886:HIS:O	2:E:4890:GLY:N	2.44	0.46
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.98	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.98	0.46
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.97	0.46
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.97	0.46
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.97	0.46
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.97	0.46
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.97	0.46
2:I:123:THR:OG1	2:I:134:ASP:OD1	2.33	0.46
2:I:2950:UNK:O	2:I:2954:UNK:N	2.48	0.46
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1954:ARG:HE	2:B:2041:HIS:HD2	1.63	0.46
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.51	0.46
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.98	0.46
2:I:4851:TYR:HD2	2:I:4920:PHE:HD1	1.62	0.46
2:E:206:CYS:SG	2:E:207:SER:N	2.88	0.46
2:E:2004:GLU:HA	2:E:2007:ASN:HB2	1.96	0.46
2:E:4137:ARG:NH2	2:E:4196:GLU:OE2	2.48	0.46
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.38	0.46
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.51	0.46
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.80	0.46
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.88	0.46
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.80	0.46
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.51	0.46
2:I:3361:UNK:O	2:I:3365:UNK:N	2.48	0.46
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.97	0.46
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.97	0.46
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.46	0.46
2:E:3361:UNK:O	2:E:3365:UNK:N	2.48	0.46
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.97	0.46
2:B:866:HIS:O	2:B:1051:TYR:OH	2.34	0.46
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.48	0.46
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.98	0.46
2:G:123:THR:OG1	2:G:134:ASP:OD1	2.33	0.46
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.98	0.46
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.98	0.46
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.48	0.46
2:B:1695:LEU:HB3	2:B:1810:LYS:HZ2	1.79	0.46
2:B:2024:PRO:O	2:B:2028:ARG:NE	2.45	0.46
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.97	0.46
2:I:2479:LEU:O	2:I:2487:UNK:N	2.49	0.46
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.32	0.46
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.99	0.45
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.81	0.45
2:G:626:LEU:HD23	2:G:630:GLU:H	1.82	0.45
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.81	0.45
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.97	0.45
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.81	0.45
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.97	0.45
2:E:290:TYR:O	2:E:302:VAL:N	2.49	0.45
2:B:2868:SER:O	2:B:2872:GLN:N	2.47	0.45
2:G:290:TYR:O	2:G:302:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.81	0.45
2:E:119:SER:HA	2:E:146:CYS:HA	1.96	0.45
2:E:866:HIS:O	2:E:1051:TYR:OH	2.34	0.45
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.97	0.45
2:E:3552:UNK:O	2:E:3556:UNK:N	2.49	0.45
2:B:206:CYS:SG	2:B:207:SER:N	2.88	0.45
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.50	0.45
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.98	0.45
2:G:1707:LEU:O	2:G:1710:GLY:N	2.33	0.45
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.99	0.45
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.98	0.45
2:E:626:LEU:HD23	2:E:630:GLU:H	1.82	0.45
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.88	0.45
1:J:21:THR:HA	1:J:49:ARG:HA	1.99	0.45
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.99	0.45
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.98	0.45
2:E:1954:ARG:HE	2:E:2041:HIS:HD2	1.63	0.45
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.50	0.45
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.99	0.45
2:B:2874:MET:O	2:B:2878:LEU:N	2.44	0.45
2:B:4851:TYR:HD2	2:B:4920:PHE:HD1	1.62	0.45
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.82	0.45
2:I:1747:LEU:HD21	2:I:2041:HIS:HB2	1.97	0.45
2:I:3552:UNK:O	2:I:3556:UNK:N	2.50	0.45
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.81	0.45
2:B:626:LEU:HD23	2:B:630:GLU:H	1.82	0.45
2:B:2012:PHE:CG	2:B:2022:PRO:HD3	2.52	0.45
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.99	0.45
2:G:1747:LEU:HD21	2:G:2041:HIS:HB2	1.97	0.45
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.97	0.45
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.98	0.45
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.50	0.45
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.97	0.45
2:G:3552:UNK:O	2:G:3556:UNK:N	2.50	0.45
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.98	0.45
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.99	0.45
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.50	0.45
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.98	0.45
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.99	0.45
2:G:1695:LEU:HB3	2:G:1810:LYS:HZ2	1.82	0.45
2:I:206:CYS:SG	2:I:207:SER:N	2.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2029:GLN:O	2:I:2033:ASP:N	2.48	0.45
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.99	0.45
1:F:21:THR:HA	1:F:49:ARG:HA	1.99	0.45
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.46	0.45
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.82	0.45
2:B:3552:UNK:O	2:B:3556:UNK:N	2.50	0.45
2:B:4848:VAL:O	2:B:4852:THR:OG1	2.24	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
2:G:2012:PHE:CG	2:G:2022:PRO:HD3	2.52	0.45
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.45
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.97	0.45
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.50	0.45
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.50	0.45
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.99	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.45
2:B:290:TYR:O	2:B:302:VAL:N	2.49	0.44
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.50	0.44
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.98	0.44
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.82	0.44
2:I:1954:ARG:HE	2:I:2041:HIS:HD2	1.63	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.50	0.44
2:E:2012:PHE:CG	2:E:2022:PRO:HD3	2.52	0.44
2:B:161:GLU:HG2	2:E:3984:ARG:HH12	1.82	0.44
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.44
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.50	0.44
2:G:1675:ALA:HB1	2:G:1676:LEU:HD13	1.99	0.44
2:G:1954:ARG:HE	2:G:2041:HIS:HD2	1.63	0.44
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.98	0.44
2:I:290:TYR:O	2:I:302:VAL:N	2.49	0.44
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.46	0.44
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.50	0.44
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.50	0.44
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	2.00	0.44
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.81	0.44
2:E:4942:GLU:O	2:E:4946:GLN:N	2.47	0.44
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.00	0.44
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	2.00	0.44
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.81	0.44
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	2.00	0.44
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.83	0.44
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2012:PHE:CG	2:I:2022:PRO:HD3	2.52	0.44
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.30	0.44
1:H:21:THR:HA	1:H:49:ARG:HA	1.99	0.44
2:B:1101:ARG:HH21	2:B:1115:LEU:H	1.65	0.44
2:B:1720:LEU:HD23	2:B:1721:GLU:HA	2.00	0.44
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.83	0.44
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.32	0.44
2:G:4823:LEU:HD23	2:E:4843:LEU:HD12	1.98	0.44
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.83	0.44
2:I:626:LEU:HD23	2:I:630:GLU:H	1.82	0.44
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.50	0.44
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.44
2:G:1720:LEU:HD23	2:G:1721:GLU:HA	2.00	0.44
2:I:1675:ALA:HB1	2:I:1676:LEU:HD13	1.99	0.44
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.99	0.44
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.33	0.44
2:B:3361:UNK:O	2:B:3365:UNK:N	2.50	0.44
2:B:4044:MET:HA	2:B:4047:MET:HG2	2.00	0.44
2:I:548:VAL:HG12	2:I:564:LEU:HD22	2.00	0.44
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.50	0.44
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.82	0.44
2:E:1720:LEU:HD23	2:E:1721:GLU:HA	2.00	0.44
2:E:2479:LEU:O	2:E:2487:UNK:N	2.50	0.44
2:E:4639:MET:HE2	2:E:4639:MET:HB3	1.87	0.44
2:B:983:THR:O	2:B:987:ARG:N	2.49	0.44
2:B:3781:GLN:HA	2:B:3784:SER:HB3	2.00	0.44
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.83	0.44
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.00	0.44
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.88	0.44
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	2.00	0.44
2:E:1675:ALA:HB1	2:E:1676:LEU:HD13	1.99	0.44
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.38	0.44
2:B:164:ARG:N	2:B:167:ASP:OD2	2.43	0.44
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.50	0.44
2:B:719:LEU:HD22	2:B:735:GLN:HG2	2.00	0.44
2:B:794:GLY:H	2:B:798:GLY:HA3	1.83	0.44
2:B:2034:PHE:O	2:B:2038:LEU:N	2.51	0.44
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.98	0.44
2:B:4886:HIS:O	2:B:4890:GLY:N	2.44	0.44
2:G:1101:ARG:HH21	2:G:1115:LEU:H	1.65	0.44
2:G:4044:MET:HA	2:G:4047:MET:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.50	0.44
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.99	0.44
2:B:1865:MET:SD	2:B:1865:MET:N	2.91	0.44
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	1.99	0.44
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	2.00	0.44
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	2.00	0.44
2:G:2034:PHE:O	2:G:2038:LEU:N	2.51	0.44
2:I:1720:LEU:HD23	2:I:1721:GLU:HA	2.00	0.44
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.00	0.44
2:I:1737:PRO:HD3	2:I:1771:LEU:HD21	2.00	0.44
2:I:2034:PHE:O	2:I:2038:LEU:N	2.51	0.44
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.00	0.44
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.83	0.44
2:E:1865:MET:SD	2:E:1865:MET:N	2.91	0.44
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	2.00	0.43
2:G:2874:MET:O	2:G:2878:LEU:N	2.44	0.43
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	2.00	0.43
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.50	0.43
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.98	0.43
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.99	0.43
2:E:548:VAL:HG12	2:E:564:LEU:HD22	2.00	0.43
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.50	0.43
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	1.99	0.43
2:E:4802:GLY:HA2	2:E:4808:PHE:HB2	2.00	0.43
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.82	0.43
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.83	0.43
2:B:1737:PRO:HD3	2:B:1771:LEU:HD21	2.00	0.43
2:B:2432:LEU:O	2:B:2436:CYS:N	2.50	0.43
2:G:1737:PRO:HD3	2:G:1771:LEU:HD21	2.00	0.43
2:G:3365:UNK:O	2:G:3369:UNK:N	2.51	0.43
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.99	0.43
2:E:195:PHE:HB3	2:E:196:MET:HG2	2.00	0.43
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.00	0.43
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.00	0.43
1:A:21:THR:HA	1:A:49:ARG:HA	1.99	0.43
2:B:195:PHE:HB3	2:B:196:MET:HG2	2.00	0.43
2:B:886:ARG:HB3	2:B:891:TRP:HB2	2.01	0.43
2:B:2029:GLN:O	2:B:2033:ASP:N	2.48	0.43
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.00	0.43
2:I:485:SER:O	2:I:489:ASN:N	2.38	0.43
2:I:4044:MET:HA	2:I:4047:MET:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:794:GLY:H	2:E:798:GLY:HA3	1.83	0.43
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.99	0.43
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.92	0.43
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.00	0.43
2:I:699:GLY:O	2:I:1647:CYS:N	2.50	0.43
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	2.00	0.43
2:I:4848:VAL:O	2:I:4852:THR:OG1	2.24	0.43
2:E:54:ASN:O	2:E:58:VAL:N	2.46	0.43
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.01	0.43
2:B:2364:PHE:HD1	2:B:2429:LEU:HD21	1.83	0.43
2:B:4843:LEU:HD12	2:E:4823:LEU:HD23	2.01	0.43
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.00	0.43
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.00	0.43
2:I:195:PHE:HB3	2:I:196:MET:HG2	2.01	0.43
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.00	0.43
2:E:4044:MET:HA	2:E:4047:MET:HG2	2.00	0.43
2:E:4163:PHE:O	2:E:4167:ALA:N	2.45	0.43
2:B:548:VAL:HG12	2:B:564:LEU:HD22	2.00	0.43
2:B:1675:ALA:HB1	2:B:1676:LEU:HD13	1.99	0.43
2:G:719:LEU:HD22	2:G:735:GLN:HG2	2.00	0.43
2:G:794:GLY:H	2:G:798:GLY:HA3	1.83	0.43
2:I:794:GLY:H	2:I:798:GLY:HA3	1.83	0.43
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	2.01	0.43
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.01	0.43
2:I:2364:PHE:HD1	2:I:2429:LEU:HD21	1.84	0.43
2:I:2432:LEU:O	2:I:2436:CYS:N	2.50	0.43
2:B:489:ASN:HA	2:B:492:ASP:HB2	2.00	0.43
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	2.00	0.43
2:I:489:ASN:HA	2:I:492:ASP:HB2	2.00	0.43
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	2.01	0.43
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	1.99	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	2.00	0.43
2:E:719:LEU:HD22	2:E:735:GLN:HG2	2.00	0.43
2:E:1101:ARG:HH21	2:E:1115:LEU:H	1.65	0.43
2:E:1695:LEU:HB3	2:E:1810:LYS:HZ2	1.84	0.43
2:E:1817:GLU:O	2:E:1821:ASP:N	2.45	0.43
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.92	0.43
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.52	0.43
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.00	0.43
2:B:2587:UNK:O	2:B:2591:UNK:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:548:VAL:HG12	2:G:564:LEU:HD22	2.00	0.43
2:G:886:ARG:HB3	2:G:891:TRP:HB2	2.01	0.43
2:G:2029:GLN:O	2:G:2033:ASP:N	2.48	0.43
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.01	0.43
2:G:2364:PHE:HD1	2:G:2429:LEU:HD21	1.84	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.84	0.43
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.00	0.43
2:I:2587:UNK:O	2:I:2591:UNK:N	2.52	0.43
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.99	0.43
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.00	0.43
2:E:2587:UNK:O	2:E:2591:UNK:N	2.52	0.43
2:E:4558:ASN:OD1	2:E:4558:ASN:N	2.52	0.43
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.00	0.43
2:B:2479:LEU:O	2:B:2487:UNK:N	2.52	0.43
2:G:134:ASP:OD1	2:G:134:ASP:N	2.52	0.43
2:G:681:HIS:HE2	2:G:683:ARG:NE	2.17	0.43
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.49	0.43
2:I:1101:ARG:HH21	2:I:1115:LEU:H	1.65	0.43
2:I:1866:ILE:HG13	2:I:1926:LEU:HB3	2.01	0.43
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.00	0.43
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.82	0.43
2:E:681:HIS:HE2	2:E:683:ARG:NE	2.17	0.43
2:E:3781:GLN:HA	2:E:3784:SER:HB3	2.00	0.43
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.01	0.43
2:B:4138:ASP:O	2:B:4142:ASN:ND2	2.52	0.43
2:G:2215:LEU:HD23	2:G:2260:ASN:HB3	2.01	0.43
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	1.99	0.43
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.52	0.43
2:I:1865:MET:SD	2:I:1865:MET:N	2.91	0.43
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.84	0.43
2:E:699:GLY:O	2:E:1647:CYS:N	2.50	0.43
2:E:1737:PRO:HD3	2:E:1771:LEU:HD21	2.00	0.43
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.00	0.43
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.92	0.43
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.84	0.43
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.84	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.42
2:G:299:LEU:HD13	2:G:378:LEU:HG	2.01	0.42
2:G:866:HIS:O	2:G:1051:TYR:OH	2.34	0.42
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	2.01	0.42
2:I:719:LEU:HD22	2:I:735:GLN:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.92	0.42
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	2.01	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.42
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.01	0.42
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.30	0.42
2:G:195:PHE:HB3	2:G:196:MET:HG2	2.00	0.42
2:G:699:GLY:O	2:G:1647:CYS:N	2.50	0.42
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	2.01	0.42
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.84	0.42
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.52	0.42
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.52	0.42
2:E:2364:PHE:HD1	2:E:2429:LEU:HD21	1.84	0.42
2:B:681:HIS:HE2	2:B:683:ARG:NE	2.17	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.33	0.42
2:B:4639:MET:HE2	2:B:4639:MET:HB3	1.87	0.42
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.52	0.42
2:G:1865:MET:SD	2:G:1865:MET:N	2.91	0.42
2:G:2479:LEU:O	2:G:2487:UNK:N	2.52	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.42
2:G:3984:ARG:HH22	2:E:161:GLU:HA	1.83	0.42
2:I:866:HIS:O	2:I:1051:TYR:OH	2.34	0.42
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.99	0.42
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.84	0.42
2:I:2215:LEU:HD23	2:I:2260:ASN:HB3	2.01	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.52	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:E:4138:ASP:O	2:E:4142:ASN:ND2	2.52	0.42
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.42
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	2.01	0.42
2:B:1641:ILE:HA	2:B:1642:PRO:HD3	1.89	0.42
2:B:3365:UNK:O	2:B:3369:UNK:N	2.52	0.42
2:B:4942:GLU:O	2:B:4946:GLN:N	2.47	0.42
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.84	0.42
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.52	0.42
2:G:4138:ASP:O	2:G:4142:ASN:ND2	2.52	0.42
2:G:4571:PHE:O	2:G:4575:PHE:N	2.53	0.42
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.00	0.42
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.52	0.42
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.92	0.42
2:I:4571:PHE:O	2:I:4575:PHE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:489:ASN:HA	2:E:492:ASP:HB2	2.00	0.42
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.84	0.42
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.01	0.42
2:B:54:ASN:O	2:B:58:VAL:N	2.46	0.42
2:B:299:LEU:HD13	2:B:378:LEU:HG	2.01	0.42
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.37	0.42
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.00	0.42
2:G:1240:LYS:HB3	2:G:1604:SER:H	1.84	0.42
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.92	0.42
2:I:1817:GLU:O	2:I:1821:ASP:N	2.45	0.42
2:I:2024:PRO:O	2:I:2028:ARG:NE	2.45	0.42
2:I:4942:GLU:O	2:I:4946:GLN:N	2.47	0.42
1:F:34:LYS:HE3	2:E:634:GLN:HB3	2.02	0.42
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.52	0.42
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.00	0.42
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.92	0.42
2:G:4697:VAL:O	2:G:4701:TRP:N	2.52	0.42
2:I:886:ARG:HB3	2:I:891:TRP:HB2	2.01	0.42
2:I:2902:HIS:HE1	2:I:2904:LEU:HD12	1.85	0.42
2:E:913:LEU:O	2:E:918:ARG:NH2	2.53	0.42
2:E:983:THR:O	2:E:987:ARG:N	2.49	0.42
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	2.00	0.42
2:B:1866:ILE:HG13	2:B:1926:LEU:HB3	2.01	0.42
2:B:2902:HIS:HE1	2:B:2904:LEU:HD12	1.85	0.42
2:G:913:LEU:O	2:G:918:ARG:NH2	2.53	0.42
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.46	0.42
2:G:1866:ILE:HG13	2:G:1926:LEU:HB3	2.01	0.42
2:I:1641:ILE:HA	2:I:1642:PRO:HD3	1.90	0.42
2:I:4138:ASP:O	2:I:4142:ASN:ND2	2.52	0.42
2:I:4158:PRO:HA	2:I:4161:ARG:HB2	2.01	0.42
2:E:134:ASP:OD1	2:E:134:ASP:N	2.52	0.42
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	2.02	0.42
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.52	0.42
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.84	0.42
2:G:489:ASN:HA	2:G:492:ASP:HB2	2.00	0.42
2:I:756:SER:HB3	2:I:767:VAL:HG22	2.01	0.42
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.00	0.42
2:E:395:GLN:HG3	2:E:397:GLU:H	1.85	0.42
2:B:4558:ASN:OD1	2:B:4558:ASN:N	2.52	0.42
2:G:2587:UNK:O	2:G:2591:UNK:N	2.52	0.42
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:681:HIS:HE2	2:I:683:ARG:NE	2.17	0.42
2:I:913:LEU:O	2:I:918:ARG:NH2	2.53	0.42
2:I:2874:MET:O	2:I:2878:LEU:N	2.44	0.42
2:I:3771:HIS:O	2:I:3774:GLY:N	2.43	0.42
2:E:299:LEU:HD13	2:E:378:LEU:HG	2.01	0.42
2:B:913:LEU:O	2:B:918:ARG:NH2	2.53	0.42
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.92	0.42
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.85	0.42
2:I:299:LEU:HD13	2:I:378:LEU:HG	2.01	0.42
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.85	0.42
2:I:4181:ILE:HD11	2:I:4988:TYR:CD1	2.55	0.42
2:E:756:SER:HB3	2:E:767:VAL:HG22	2.01	0.42
2:E:953:THR:HB	2:E:969:PRO:HD2	2.02	0.42
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	2.01	0.42
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.85	0.42
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.45	0.42
2:E:4158:PRO:HA	2:E:4161:ARG:HB2	2.01	0.42
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	2.01	0.41
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.85	0.41
2:G:395:GLN:HG3	2:G:397:GLU:H	1.85	0.41
2:G:983:THR:O	2:G:987:ARG:N	2.50	0.41
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	2.02	0.41
2:G:4569:LEU:HD11	2:G:4646:LEU:HD22	2.02	0.41
2:I:1240:LYS:HB3	2:I:1604:SER:H	1.84	0.41
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	2.02	0.41
2:I:4138:ASP:N	2:I:4138:ASP:OD1	2.53	0.41
2:I:4886:HIS:O	2:I:4890:GLY:N	2.44	0.41
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.18	0.41
2:E:1866:ILE:HG13	2:E:1926:LEU:HB3	2.01	0.41
2:E:2215:LEU:HD23	2:E:2260:ASN:HB3	2.01	0.41
2:E:4181:ILE:HD11	2:E:4988:TYR:CD1	2.55	0.41
1:F:25:HIS:HB3	1:F:40:ARG:HD3	2.03	0.41
2:B:756:SER:HB3	2:B:767:VAL:HG22	2.01	0.41
2:B:1240:LYS:HB3	2:B:1604:SER:H	1.85	0.41
2:B:2215:LEU:HD23	2:B:2260:ASN:HB3	2.01	0.41
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.84	0.41
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	2.02	0.41
2:G:4735:GLU:HA	2:G:4738:ALA:HB3	2.02	0.41
2:I:4228:ALA:O	2:I:4232:GLU:N	2.52	0.41
2:I:5000:GLU:HA	2:I:5003:HIS:CD2	2.55	0.41
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:GLN:HG3	2:B:397:GLU:H	1.85	0.41
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.18	0.41
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.18	0.41
2:G:2024:PRO:O	2:G:2028:ARG:NE	2.45	0.41
2:G:4158:PRO:HA	2:G:4161:ARG:HB2	2.01	0.41
2:G:4558:ASN:OD1	2:G:4558:ASN:N	2.52	0.41
2:I:395:GLN:HG3	2:I:397:GLU:H	1.85	0.41
2:I:710:ASP:OD1	2:I:710:ASP:N	2.54	0.41
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	2.02	0.41
2:E:4228:ALA:O	2:E:4232:GLU:N	2.52	0.41
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.84	0.41
2:B:1707:LEU:O	2:B:1710:GLY:N	2.33	0.41
2:G:54:ASN:O	2:G:58:VAL:N	2.46	0.41
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.41
2:I:953:THR:HB	2:I:969:PRO:HD2	2.02	0.41
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	2.01	0.41
2:E:2297:LYS:O	2:E:2300:SER:OG	2.35	0.41
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.49	0.41
2:E:4735:GLU:HA	2:E:4738:ALA:HB3	2.02	0.41
2:B:710:ASP:OD1	2:B:710:ASP:N	2.54	0.41
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.00	0.41
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	2.02	0.41
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.02	0.41
2:B:5000:GLU:HA	2:B:5003:HIS:CD2	2.56	0.41
2:G:205:ILE:HD12	2:G:205:ILE:HA	1.95	0.41
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.02	0.41
2:G:2959:UNK:O	2:G:2963:UNK:N	2.54	0.41
2:I:134:ASP:OD1	2:I:134:ASP:N	2.52	0.41
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	2.01	0.41
2:I:4558:ASN:OD1	2:I:4558:ASN:N	2.52	0.41
1:F:23:VAL:H	1:F:105:ASN:HB3	1.86	0.41
2:B:485:SER:HA	2:B:488:LEU:HB2	2.03	0.41
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.03	0.41
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	2.02	0.41
2:B:2467:VAL:HA	2:B:2470:ILE:HD12	2.03	0.41
2:B:2959:UNK:O	2:B:2963:UNK:N	2.53	0.41
2:B:4928:LEU:HD13	2:B:4928:LEU:HA	1.92	0.41
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	2.02	0.41
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.35	0.41
2:I:983:THR:O	2:I:987:ARG:N	2.50	0.41
2:E:710:ASP:OD1	2:E:710:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	2.01	0.41
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.02	0.41
2:E:4569:LEU:HD11	2:E:4646:LEU:HD22	2.02	0.41
1:A:25:HIS:HB3	1:A:40:ARG:HD3	2.02	0.41
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.86	0.41
2:B:4181:ILE:HD11	2:B:4988:TYR:CD1	2.55	0.41
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.38	0.41
2:G:4138:ASP:N	2:G:4138:ASP:OD1	2.53	0.41
2:G:4228:ALA:O	2:G:4232:GLU:N	2.52	0.41
2:I:582:HIS:O	2:I:585:SER:OG	2.32	0.41
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.03	0.41
2:I:2517:UNK:O	2:I:2521:UNK:N	2.53	0.41
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	2.03	0.41
2:E:2467:VAL:HA	2:E:2470:ILE:HD12	2.03	0.41
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.03	0.41
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.52	0.41
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.53	0.41
2:B:4158:PRO:HA	2:B:4161:ARG:HB2	2.01	0.41
2:B:4228:ALA:O	2:B:4232:GLU:N	2.52	0.41
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	2.01	0.41
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.03	0.41
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.84	0.41
2:G:2902:HIS:HE1	2:G:2904:LEU:HD12	1.85	0.41
2:G:4181:ILE:HD11	2:G:4988:TYR:CD1	2.55	0.41
1:F:23:VAL:HB	1:F:105:ASN:HA	2.03	0.41
1:A:23:VAL:H	1:A:105:ASN:HB3	1.86	0.41
1:H:25:HIS:HB3	1:H:40:ARG:HD3	2.03	0.41
1:J:23:VAL:H	1:J:105:ASN:HB3	1.86	0.41
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	2.02	0.41
2:B:4569:LEU:HD11	2:B:4646:LEU:HD22	2.02	0.41
2:G:756:SER:HB3	2:G:767:VAL:HG22	2.01	0.41
2:G:953:THR:HB	2:G:969:PRO:HD2	2.02	0.41
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.03	0.41
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.41
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	2.02	0.41
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.03	0.41
2:G:5000:GLU:HA	2:G:5003:HIS:CD2	2.56	0.41
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.18	0.41
2:I:485:SER:HA	2:I:488:LEU:HB2	2.03	0.41
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.42	0.41
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.46	0.41
2:I:4639:MET:HE2	2:I:4639:MET:HB3	1.87	0.41
2:E:1240:LYS:HB3	2:E:1604:SER:H	1.84	0.41
2:E:2432:LEU:O	2:E:2436:CYS:N	2.50	0.41
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.03	0.41
2:E:5000:GLU:HA	2:E:5003:HIS:CD2	2.56	0.41
1:A:23:VAL:HB	1:A:105:ASN:HA	2.03	0.41
2:B:953:THR:HB	2:B:969:PRO:HD2	2.02	0.41
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.32	0.41
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.86	0.41
2:B:4000:MET:HE3	2:B:4017:LEU:HD21	2.03	0.41
2:B:4837:LEU:HD22	2:B:4936:ILE:HD11	2.02	0.41
2:G:4000:MET:HE3	2:G:4017:LEU:HD21	2.03	0.41
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.86	0.41
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	2.02	0.41
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.03	0.41
2:I:4837:LEU:HD22	2:I:4936:ILE:HD11	2.02	0.41
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.86	0.41
2:E:2365:GLY:HA3	2:E:2426:TYR:HE1	1.86	0.41
2:B:699:GLY:O	2:B:1647:CYS:N	2.50	0.40
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.03	0.40
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	2.02	0.40
2:B:4735:GLU:HA	2:B:4738:ALA:HB3	2.02	0.40
2:G:485:SER:O	2:G:489:ASN:N	2.38	0.40
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.02	0.40
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.86	0.40
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.86	0.40
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	2.02	0.40
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.86	0.40
2:I:1592:PRO:HA	2:I:1593:PRO:HD3	1.96	0.40
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.03	0.40
2:I:2467:VAL:HA	2:I:2470:ILE:HD12	2.03	0.40
2:I:2959:UNK:O	2:I:2963:UNK:N	2.54	0.40
2:I:4569:LEU:HD11	2:I:4646:LEU:HD22	2.02	0.40
2:I:4735:GLU:HA	2:I:4738:ALA:HB3	2.02	0.40
2:E:485:SER:HA	2:E:488:LEU:HB2	2.03	0.40
2:E:2034:PHE:O	2:E:2038:LEU:N	2.51	0.40
2:G:2467:VAL:HA	2:G:2470:ILE:HD12	2.03	0.40
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.03	0.40
2:E:1739:THR:H	2:E:1742:THR:HB	1.86	0.40
2:E:2517:UNK:O	2:E:2521:UNK:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2902:HIS:HE1	2:E:2904:LEU:HD12	1.85	0.40
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.86	0.40
1:A:44:LYS:HA	1:A:45:PRO:HD3	1.89	0.40
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.42	0.40
2:B:1817:GLU:O	2:B:1821:ASP:N	2.45	0.40
2:B:2365:GLY:HA3	2:B:2426:TYR:HE1	1.87	0.40
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.86	0.40
2:B:3915:ILE:O	2:B:3919:THR:N	2.52	0.40
2:G:1641:ILE:HA	2:G:1642:PRO:HD3	1.89	0.40
2:G:3915:ILE:O	2:G:3919:THR:N	2.52	0.40
2:G:4886:HIS:O	2:G:4890:GLY:N	2.44	0.40
2:I:540:PHE:HD2	2:I:567:VAL:HG11	1.87	0.40
2:I:1739:THR:H	2:I:1742:THR:HB	1.87	0.40
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.02	0.40
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.86	0.40
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	2.03	0.40
2:E:4837:LEU:HD22	2:E:4936:ILE:HD11	2.02	0.40
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.86	0.40
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.86	0.40
2:B:2297:LYS:O	2:B:2300:SER:OG	2.35	0.40
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.03	0.40
2:B:3840:SER:OG	2:B:3875:MET:O	2.32	0.40
2:B:3940:LYS:O	2:B:4002:LYS:NZ	2.42	0.40
2:B:4822:THR:O	2:B:4825:THR:OG1	2.33	0.40
2:G:540:PHE:HD2	2:G:567:VAL:HG11	1.87	0.40
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.86	0.40
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	2.02	0.40
2:E:551:LEU:HD21	2:E:589:LEU:HD13	2.03	0.40
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.04	0.40
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.86	0.40
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.53	0.40
2:B:4571:PHE:O	2:B:4575:PHE:N	2.53	0.40
2:I:1092:PHE:N	2:I:1149:VAL:O	2.43	0.40
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.39	0.40
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.86	0.40
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.49	0.40
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.57	0.40
2:E:4571:PHE:O	2:E:4575:PHE:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

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%)	2886 (89%)	345 (11%)	4 (0%)	48	83
2	E	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	48	83
2	G	3235/4416 (73%)	2889 (89%)	341 (10%)	5 (0%)	43	77
2	I	3235/4416 (73%)	2888 (89%)	342 (11%)	5 (0%)	43	77
All	All	13360/18096 (74%)	11935 (89%)	1407 (10%)	18 (0%)	49	83

All (18) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
2	I	4640	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
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%)	2477 (99%)	16 (1%)	78	80
2	E	2493/3022 (82%)	2477 (99%)	16 (1%)	78	80
2	G	2493/3022 (82%)	2477 (99%)	16 (1%)	78	80
2	I	2493/3022 (82%)	2477 (99%)	16 (1%)	78	80
All	All	10324/12444 (83%)	10260 (99%)	64 (1%)	76	80

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	688	LEU
2	B	719	LEU
2	B	978	THR
2	B	1600	LEU
2	B	1676	LEU
2	B	2010	LEU
2	B	2144	ILE
2	B	2339	VAL
2	B	2342	ASN
2	B	3663	LEU
2	B	3805	LEU
2	B	4081	VAL
2	B	4154	VAL

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Mol	Chain	Res	Type
2	B	4792	LEU
2	B	4985	LEU
2	G	131	LEU
2	G	688	LEU
2	G	719	LEU
2	G	978	THR
2	G	1600	LEU
2	G	1676	LEU
2	G	2010	LEU
2	G	2144	ILE
2	G	2339	VAL
2	G	2342	ASN
2	G	3663	LEU
2	G	3805	LEU
2	G	4081	VAL
2	G	4154	VAL
2	G	4792	LEU
2	G	4985	LEU
2	I	131	LEU
2	I	688	LEU
2	I	719	LEU
2	I	978	THR
2	I	1600	LEU
2	I	1676	LEU
2	I	2010	LEU
2	I	2144	ILE
2	I	2339	VAL
2	I	2342	ASN
2	I	3663	LEU
2	I	3805	LEU
2	I	4081	VAL
2	I	4154	VAL
2	I	4792	LEU
2	I	4985	LEU
2	E	131	LEU
2	E	688	LEU
2	E	719	LEU
2	E	978	THR
2	E	1600	LEU
2	E	1676	LEU
2	E	2010	LEU
2	E	2144	ILE

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Mol	Chain	Res	Type
2	E	2339	VAL
2	E	2342	ASN
2	E	3663	LEU
2	E	3805	LEU
2	E	4081	VAL
2	E	4154	VAL
2	E	4792	LEU
2	E	4985	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (218) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	31	GLN
1	F	87	HIS
1	A	31	GLN
1	A	87	HIS
1	H	31	GLN
1	H	87	HIS
1	J	31	GLN
1	J	87	HIS
2	B	32	GLN
2	B	57	ASN
2	B	113	HIS
2	B	201	ASN
2	B	273	HIS
2	B	379	HIS
2	B	395	GLN
2	B	479	GLN
2	B	489	ASN
2	B	520	ASN
2	B	582	HIS
2	B	593	HIS
2	B	725	HIS
2	B	797	HIS
2	B	1206	GLN
2	B	1598	GLN
2	B	1679	ASN
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	1952	GLN

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Mol	Chain	Res	Type
2	B	2041	HIS
2	B	2127	GLN
2	B	2260	ASN
2	B	2291	GLN
2	B	2349	ASN
2	B	2773	ASN
2	B	3781	GLN
2	B	3809	ASN
2	B	3814	GLN
2	B	3896	ASN
2	B	3900	GLN
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	4043	GLN
2	B	4054	ASN
2	B	4078	GLN
2	B	4109	GLN
2	B	4142	ASN
2	B	4201	ASN
2	B	4209	GLN
2	B	4776	GLN
2	B	4806	ASN
2	B	4832	HIS
2	B	4946	GLN
2	B	4973	HIS
2	B	5003	HIS
2	B	5031	GLN
2	G	32	GLN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	151	HIS
2	G	201	ASN
2	G	273	HIS
2	G	379	HIS
2	G	395	GLN
2	G	479	GLN
2	G	489	ASN

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Mol	Chain	Res	Type
2	G	495	ASN
2	G	520	ASN
2	G	593	HIS
2	G	725	HIS
2	G	797	HIS
2	G	838	HIS
2	G	1598	GLN
2	G	1679	ASN
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	2041	HIS
2	G	2127	GLN
2	G	2260	ASN
2	G	2349	ASN
2	G	2773	ASN
2	G	2931	GLN
2	G	3781	GLN
2	G	3809	ASN
2	G	3814	GLN
2	G	3896	ASN
2	G	3900	GLN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	4020	GLN
2	G	4034	ASN
2	G	4078	GLN
2	G	4109	GLN
2	G	4142	ASN
2	G	4201	ASN
2	G	4209	GLN
2	G	4246	GLN
2	G	4776	GLN
2	G	4806	ASN
2	G	4946	GLN
2	G	4973	HIS
2	G	5003	HIS
2	G	5031	GLN
2	I	32	GLN

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Mol	Chain	Res	Type
2	I	57	ASN
2	I	113	HIS
2	I	201	ASN
2	I	273	HIS
2	I	379	HIS
2	I	395	GLN
2	I	479	GLN
2	I	489	ASN
2	I	495	ASN
2	I	520	ASN
2	I	582	HIS
2	I	593	HIS
2	I	725	HIS
2	I	797	HIS
2	I	1220	GLN
2	I	1598	GLN
2	I	1679	ASN
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	1952	GLN
2	I	2041	HIS
2	I	2107	GLN
2	I	2127	GLN
2	I	2260	ASN
2	I	2349	ASN
2	I	2763	HIS
2	I	2773	ASN
2	I	2788	HIS
2	I	3781	GLN
2	I	3809	ASN
2	I	3814	GLN
2	I	3896	ASN
2	I	3900	GLN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	4034	ASN
2	I	4043	GLN
2	I	4078	GLN

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Mol	Chain	Res	Type
2	I	4109	GLN
2	I	4142	ASN
2	I	4201	ASN
2	I	4209	GLN
2	I	4776	GLN
2	I	4806	ASN
2	I	4832	HIS
2	I	4946	GLN
2	I	5003	HIS
2	I	5031	GLN
2	E	32	GLN
2	E	57	ASN
2	E	113	HIS
2	E	201	ASN
2	E	273	HIS
2	E	379	HIS
2	E	395	GLN
2	E	479	GLN
2	E	489	ASN
2	E	495	ASN
2	E	520	ASN
2	E	582	HIS
2	E	593	HIS
2	E	725	HIS
2	E	797	HIS
2	E	1220	GLN
2	E	1598	GLN
2	E	1679	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	1952	GLN
2	E	2041	HIS
2	E	2127	GLN
2	E	2260	ASN
2	E	2291	GLN
2	E	2349	ASN
2	E	2763	HIS
2	E	2773	ASN
2	E	3781	GLN
2	E	3809	ASN

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Mol	Chain	Res	Type
2	E	3814	GLN
2	E	3896	ASN
2	E	3900	GLN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	4034	ASN
2	E	4043	GLN
2	E	4078	GLN
2	E	4109	GLN
2	E	4142	ASN
2	E	4201	ASN
2	E	4209	GLN
2	E	4246	GLN
2	E	4776	GLN
2	E	4806	ASN
2	E	4946	GLN
2	E	5003	HIS
2	E	5031	GLN

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	5101	-	32,33,33	1.36	5 (15%)	48,52,52	1.74	10 (20%)
4	CFF	E	5102	-	15,15,15	2.01	7 (46%)	23,23,23	2.71	9 (39%)
4	CFF	G	5102	-	15,15,15	2.01	7 (46%)	23,23,23	2.71	9 (39%)
4	CFF	I	5102	-	15,15,15	2.02	7 (46%)	23,23,23	2.71	8 (34%)
3	ATP	I	5101	-	32,33,33	1.36	5 (15%)	48,52,52	1.74	10 (20%)
3	ATP	G	5101	-	32,33,33	1.35	5 (15%)	48,52,52	1.73	10 (20%)
3	ATP	E	5101	-	32,33,33	1.35	5 (15%)	48,52,52	1.73	9 (18%)
4	CFF	B	5102	-	15,15,15	2.01	7 (46%)	23,23,23	2.71	9 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	4/22/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	G	5101	-	-	4/22/38/38	0/3/3/3
3	ATP	E	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	5101	ATP	C5-C4	4.50	1.47	1.39
3	B	5101	ATP	C5-C4	4.47	1.47	1.39
3	E	5101	ATP	C5-C4	4.45	1.47	1.39
3	G	5101	ATP	C5-C4	4.44	1.47	1.39
4	G	5102	CFF	C6-N1	-3.98	1.32	1.40
4	I	5102	CFF	C6-N1	-3.98	1.32	1.40
4	E	5102	CFF	C6-N1	-3.96	1.32	1.40
4	B	5102	CFF	C6-N1	-3.94	1.32	1.40
4	G	5102	CFF	C4-N3	-2.89	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	C4-N3	-2.86	1.33	1.38
4	B	5102	CFF	C4-N3	-2.85	1.33	1.38
4	E	5102	CFF	C4-N3	-2.80	1.33	1.38
3	B	5101	ATP	C5-N7	-2.59	1.34	1.39
3	G	5101	ATP	C5-N7	-2.58	1.34	1.39
3	E	5101	ATP	C5-N7	-2.57	1.34	1.39
3	I	5101	ATP	C5-N7	-2.57	1.34	1.39
3	E	5101	ATP	C5-C6	2.47	1.47	1.41
3	B	5101	ATP	C5-C6	2.47	1.47	1.41
3	I	5101	ATP	C5-C6	2.46	1.47	1.41
3	G	5101	ATP	C5-C6	2.46	1.47	1.41
4	E	5102	CFF	C5-N7	-2.43	1.34	1.38
4	B	5102	CFF	C5-N7	-2.41	1.34	1.38
4	G	5102	CFF	C5-N7	-2.40	1.34	1.38
4	I	5102	CFF	C5-N7	-2.40	1.34	1.38
4	I	5102	CFF	C2-N3	-2.39	1.34	1.39
4	B	5102	CFF	C2-N3	-2.37	1.34	1.39
4	G	5102	CFF	C2-N3	-2.36	1.34	1.39
4	E	5102	CFF	C2-N3	-2.36	1.34	1.39
3	I	5101	ATP	C4-N9	-2.32	1.32	1.37
3	G	5101	ATP	C4-N9	-2.31	1.32	1.37
3	B	5101	ATP	C4-N9	-2.31	1.32	1.37
3	I	5101	ATP	C8-N7	2.27	1.36	1.31
3	E	5101	ATP	C4-N9	-2.25	1.33	1.37
3	E	5101	ATP	C8-N7	2.25	1.36	1.31
3	G	5101	ATP	C8-N7	2.25	1.36	1.31
3	B	5101	ATP	C8-N7	2.24	1.36	1.31
4	B	5102	CFF	C2-N1	-2.19	1.34	1.39
4	I	5102	CFF	C2-N1	-2.19	1.34	1.39
4	G	5102	CFF	C2-N1	-2.17	1.34	1.39
4	E	5102	CFF	C2-N1	-2.17	1.34	1.39
4	G	5102	CFF	O13-C6	-2.15	1.18	1.23
4	B	5102	CFF	O11-C2	-2.14	1.18	1.22
4	E	5102	CFF	O13-C6	-2.14	1.18	1.23
4	E	5102	CFF	O11-C2	-2.14	1.18	1.22
4	I	5102	CFF	O11-C2	-2.14	1.18	1.22
4	G	5102	CFF	O11-C2	-2.12	1.18	1.22
4	B	5102	CFF	O13-C6	-2.11	1.18	1.23
4	I	5102	CFF	O13-C6	-2.10	1.18	1.23

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5102	CFF	C14-N7-C8	-7.73	111.82	126.28
4	G	5102	CFF	C14-N7-C8	-7.69	111.90	126.28
4	I	5102	CFF	C14-N7-C8	-7.68	111.91	126.28
4	E	5102	CFF	C14-N7-C8	-7.67	111.93	126.28
3	E	5101	ATP	C5-C4-N3	-5.53	119.11	126.72
3	B	5101	ATP	C5-C4-N3	-5.49	119.16	126.72
3	I	5101	ATP	C5-C4-N3	-5.47	119.19	126.72
3	G	5101	ATP	C5-C4-N3	-5.43	119.24	126.72
4	B	5102	CFF	C14-N7-C5	5.20	140.14	127.77
4	E	5102	CFF	C14-N7-C5	5.16	140.05	127.77
4	G	5102	CFF	C14-N7-C5	5.16	140.05	127.77
4	I	5102	CFF	C14-N7-C5	5.14	140.00	127.77
3	E	5101	ATP	N3-C4-N9	4.22	134.35	127.17
3	B	5101	ATP	N3-C4-N9	4.20	134.32	127.17
3	I	5101	ATP	N3-C4-N9	4.20	134.31	127.17
3	G	5101	ATP	N3-C4-N9	4.17	134.26	127.17
4	I	5102	CFF	C5-C6-N1	4.12	119.61	112.06
4	E	5102	CFF	C5-C6-N1	4.10	119.57	112.06
4	G	5102	CFF	C5-C6-N1	4.09	119.55	112.06
4	B	5102	CFF	C5-C6-N1	4.08	119.54	112.06
3	I	5101	ATP	C2-N3-C4	3.57	120.55	111.83
3	B	5101	ATP	C2-N3-C4	3.57	120.55	111.83
3	G	5101	ATP	C2-N3-C4	3.56	120.53	111.83
3	E	5101	ATP	C2-N3-C4	3.56	120.52	111.83
3	I	5101	ATP	C4-C5-N7	-3.49	106.60	110.58
3	B	5101	ATP	C4-C5-N7	-3.48	106.60	110.58
3	E	5101	ATP	C4-C5-N7	-3.45	106.64	110.58
3	G	5101	ATP	C4-C5-N7	-3.43	106.67	110.58
3	G	5101	ATP	N3-C2-N1	-3.32	123.56	128.58
3	B	5101	ATP	N3-C2-N1	-3.29	123.60	128.58
3	I	5101	ATP	N3-C2-N1	-3.29	123.61	128.58
3	E	5101	ATP	N3-C2-N1	-3.22	123.70	128.58
4	E	5102	CFF	C6-N1-C2	-3.13	120.57	125.66
4	G	5102	CFF	C6-N1-C2	-3.11	120.60	125.66
4	I	5102	CFF	C6-N1-C2	-3.11	120.60	125.66
4	B	5102	CFF	C6-N1-C2	-3.09	120.64	125.66
4	B	5102	CFF	C6-C5-C4	-2.86	119.31	122.92
4	I	5102	CFF	C6-C5-C4	-2.86	119.32	122.92
4	G	5102	CFF	C6-C5-C4	-2.84	119.34	122.92
4	I	5102	CFF	N7-C8-N9	-2.82	108.38	113.48
4	B	5102	CFF	N7-C8-N9	-2.82	108.38	113.48
4	E	5102	CFF	N7-C8-N9	-2.81	108.38	113.48
4	E	5102	CFF	N3-C4-N9	2.81	130.69	126.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	N7-C8-N9	-2.79	108.42	113.48
4	E	5102	CFF	C6-C5-C4	-2.79	119.40	122.92
4	B	5102	CFF	N3-C4-N9	2.78	130.64	126.27
4	G	5102	CFF	N3-C4-N9	2.77	130.63	126.27
4	I	5102	CFF	N3-C4-N9	2.76	130.60	126.27
4	G	5102	CFF	O13-C6-C5	-2.61	121.04	126.38
3	I	5101	ATP	C4-N9-C8	2.60	108.47	105.74
4	E	5102	CFF	O13-C6-C5	-2.59	121.07	126.38
4	I	5102	CFF	O13-C6-C5	-2.57	121.11	126.38
3	G	5101	ATP	C4-N9-C8	2.57	108.44	105.74
4	B	5102	CFF	O13-C6-C5	-2.57	121.12	126.38
3	B	5101	ATP	C4-N9-C8	2.56	108.43	105.74
3	E	5101	ATP	C3'-C2'-C1'	2.52	106.23	101.46
3	G	5101	ATP	C3'-C2'-C1'	2.50	106.19	101.46
3	I	5101	ATP	C3'-C2'-C1'	2.50	106.19	101.46
3	E	5101	ATP	C4-N9-C8	2.49	108.35	105.74
3	B	5101	ATP	C3'-C2'-C1'	2.48	106.16	101.46
3	I	5101	ATP	C5-N7-C8	2.42	107.25	103.45
3	B	5101	ATP	C5-N7-C8	2.41	107.24	103.45
3	E	5101	ATP	C5-N7-C8	2.40	107.22	103.45
3	G	5101	ATP	C5-N7-C8	2.39	107.21	103.45
3	B	5101	ATP	C6-C5-N7	2.33	136.59	132.09
3	I	5101	ATP	C6-C5-N7	2.33	136.58	132.09
3	G	5101	ATP	C6-C5-N7	2.29	136.51	132.09
3	E	5101	ATP	C6-C5-N7	2.26	136.44	132.09
3	G	5101	ATP	C2-N1-C6	2.09	122.16	118.73
3	I	5101	ATP	C2-N1-C6	2.06	122.12	118.73
3	B	5101	ATP	C2-N1-C6	2.04	122.09	118.73
4	E	5102	CFF	N3-C2-N1	2.04	119.69	117.14
4	G	5102	CFF	N3-C2-N1	2.02	119.66	117.14
4	B	5102	CFF	N3-C2-N1	2.00	119.64	117.14

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

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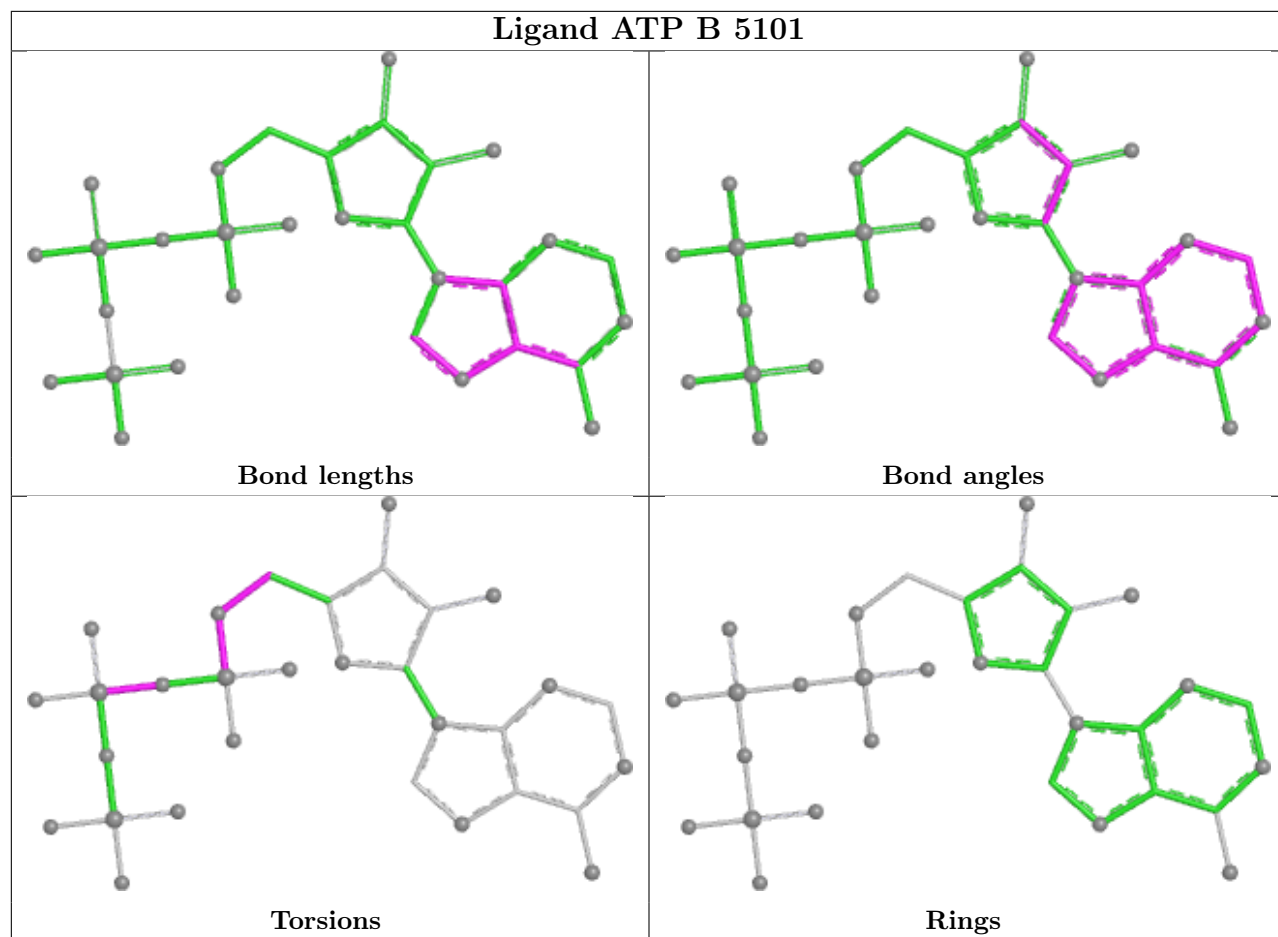
Mol	Chain	Res	Type	Atoms
3	E	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C4'-C5'-O5'-PA
3	I	5101	ATP	C4'-C5'-O5'-PA
3	E	5101	ATP	C4'-C5'-O5'-PA
3	B	5101	ATP	C4'-C5'-O5'-PA
3	B	5101	ATP	PA-O3A-PB-O2B
3	G	5101	ATP	PA-O3A-PB-O2B
3	I	5101	ATP	PA-O3A-PB-O2B
3	E	5101	ATP	PA-O3A-PB-O2B

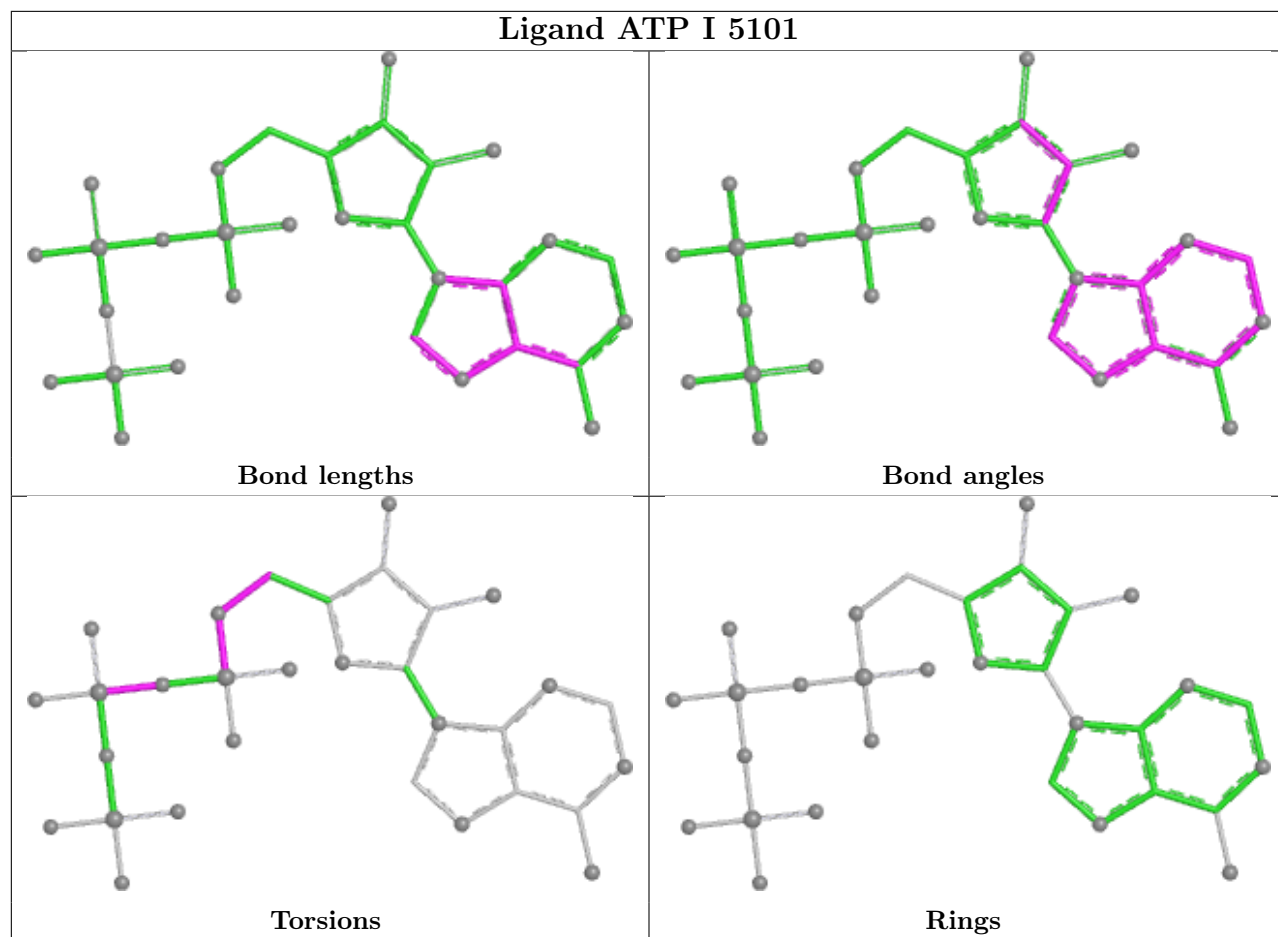
There are no ring outliers.

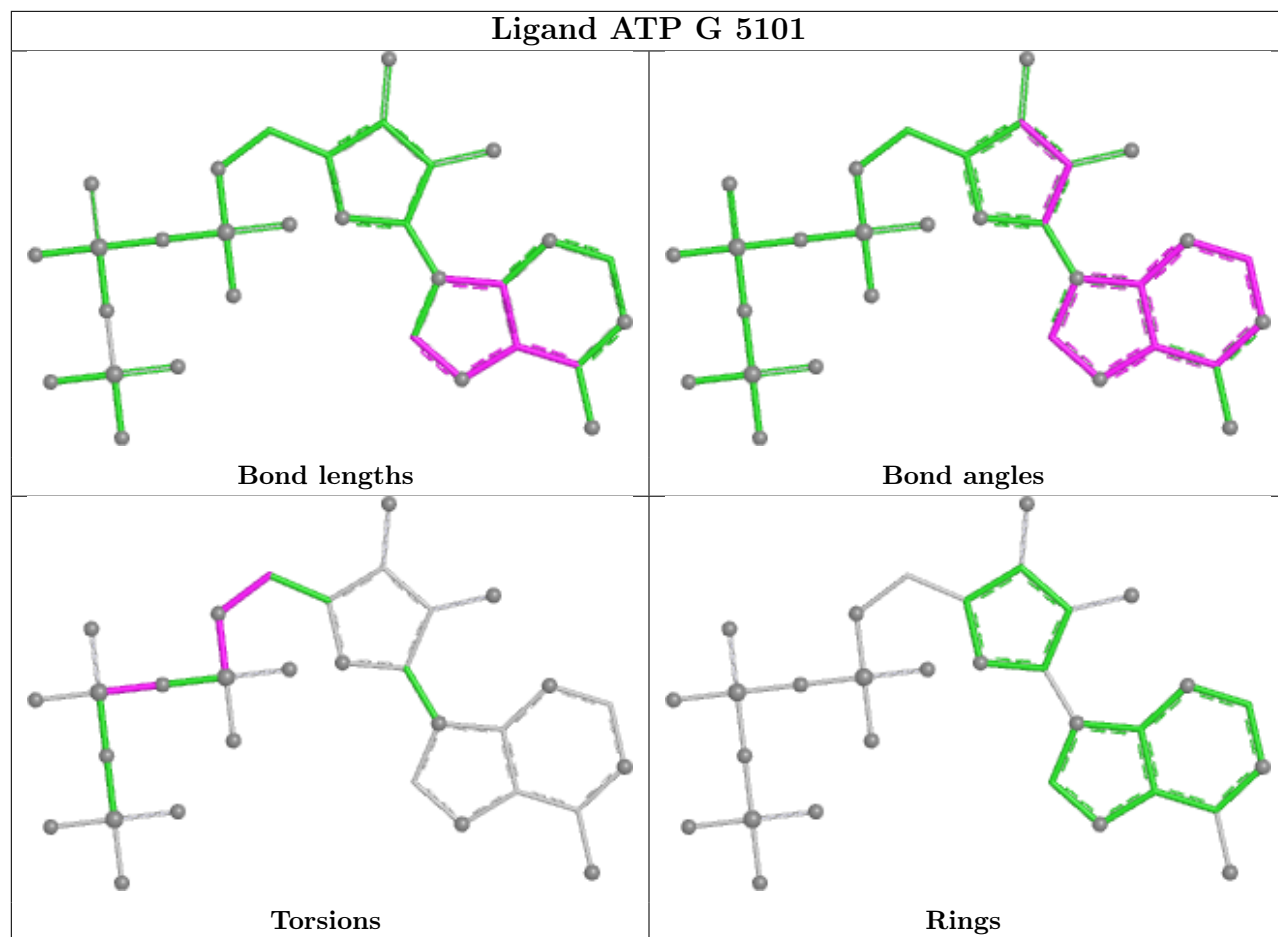
4 monomers are involved in 4 short contacts:

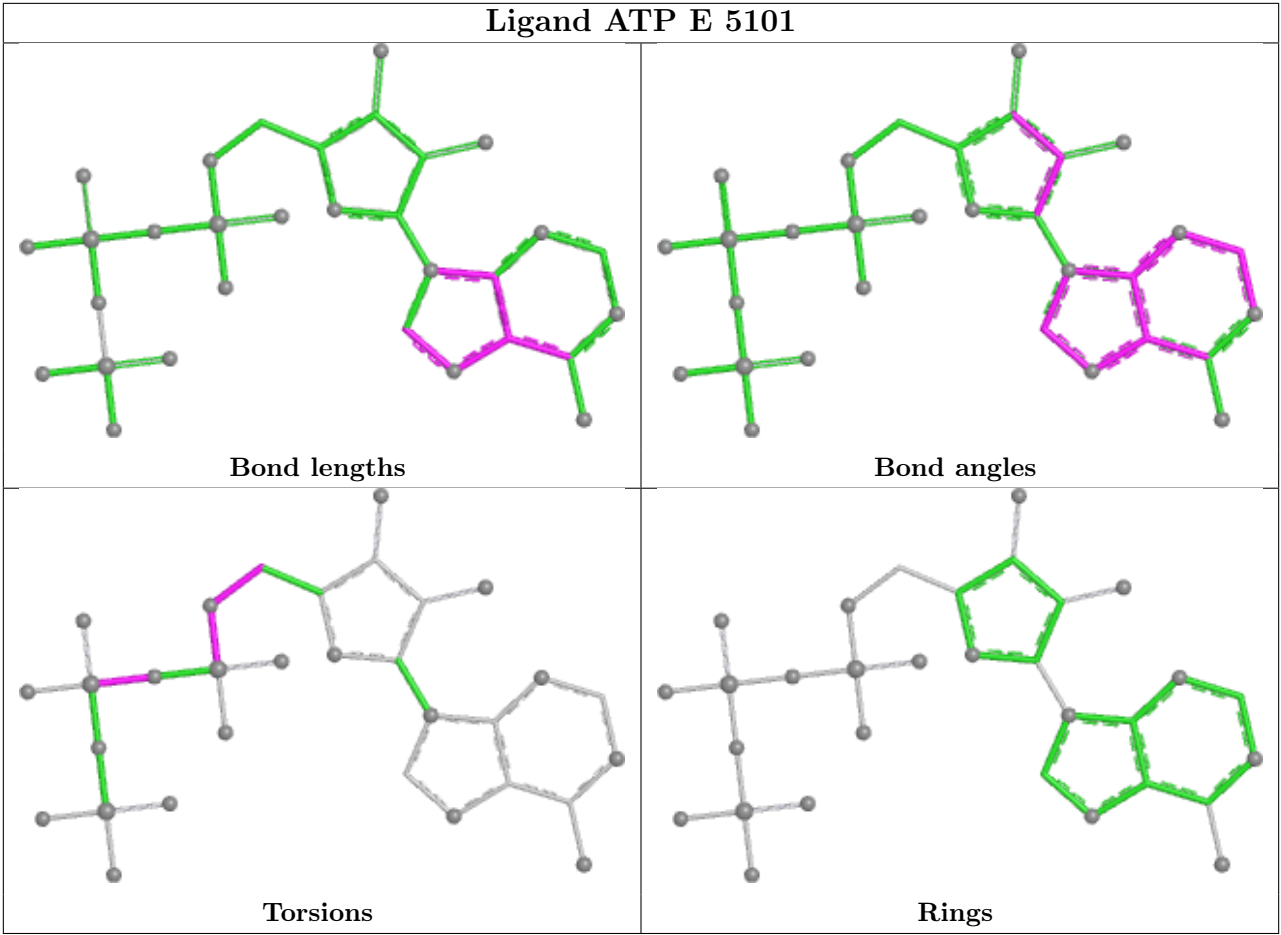
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
3	I	5101	ATP	1	0
3	G	5101	ATP	1	0
3	E	5101	ATP	1	0

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

All chain breaks are listed below:

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

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

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

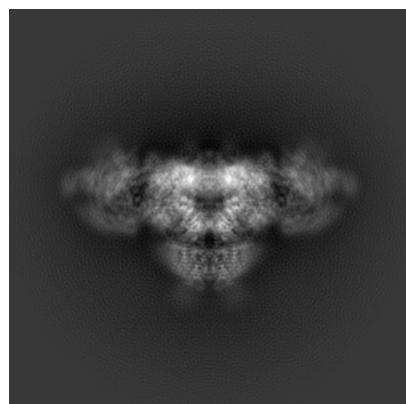
6 Map visualisation [i](#)

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

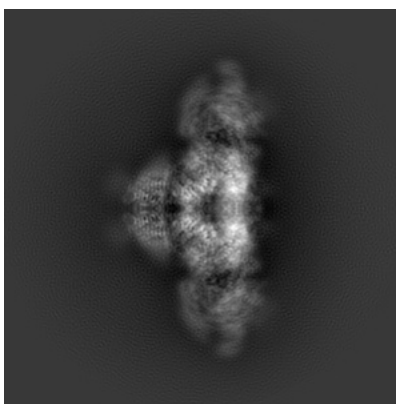
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

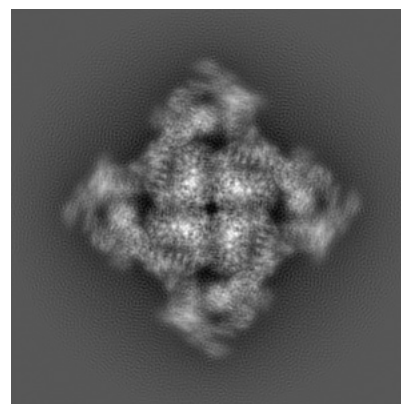
6.1.1 Primary map



X

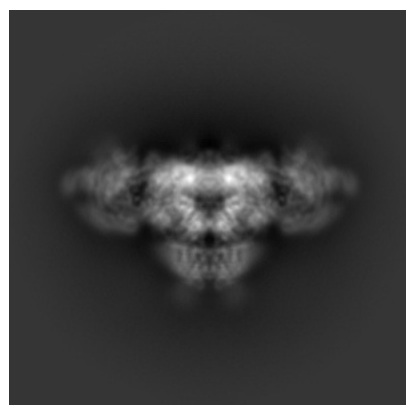


Y

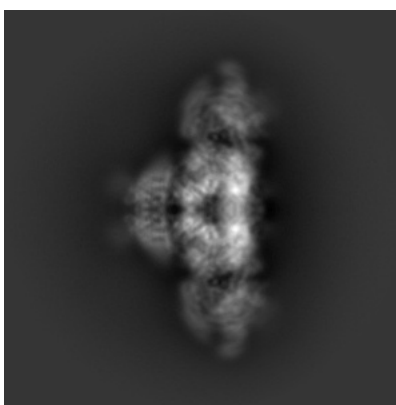


Z

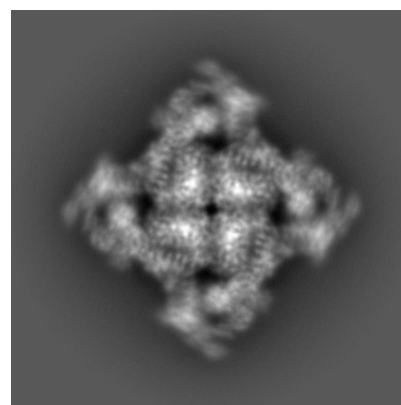
6.1.2 Raw map



X



Y

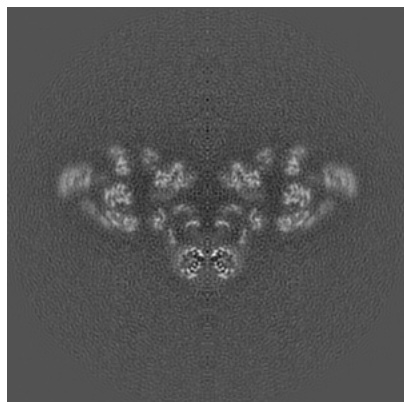


Z

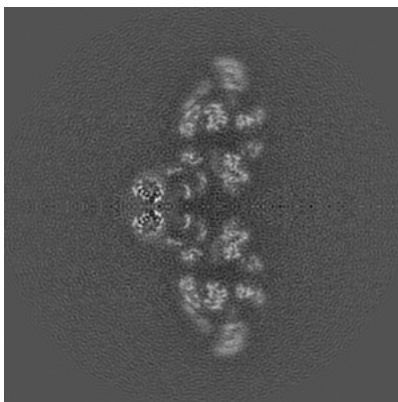
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

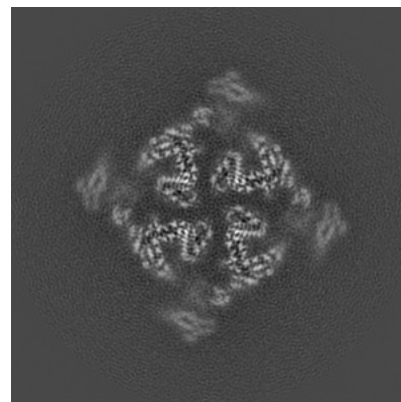
6.2.1 Primary map



X Index: 200

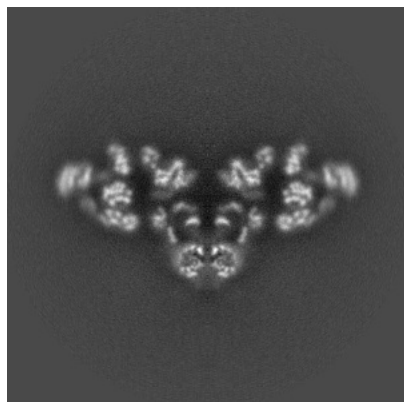


Y Index: 200

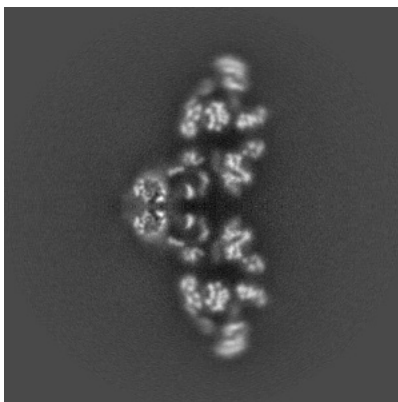


Z Index: 200

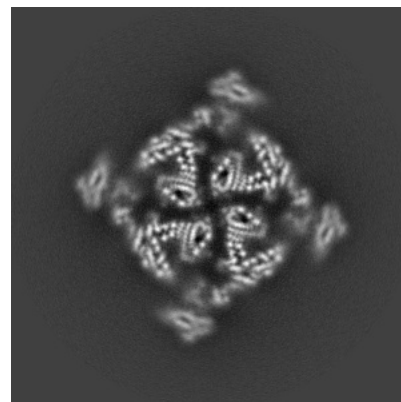
6.2.2 Raw map



X Index: 200



Y Index: 200

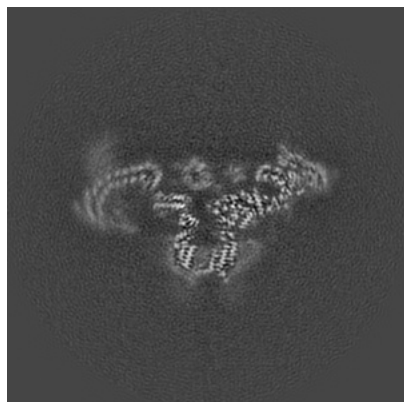


Z Index: 200

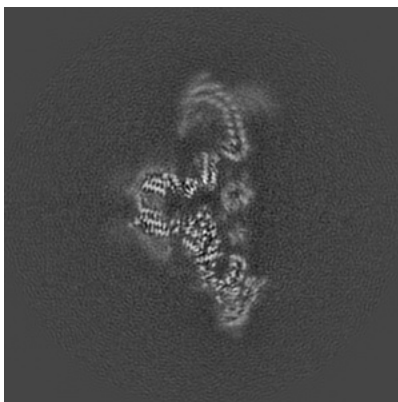
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

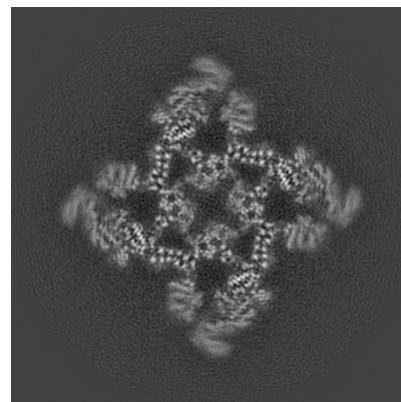
6.3.1 Primary map



X Index: 175

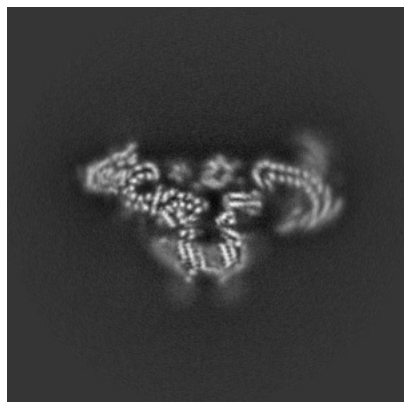


Y Index: 175

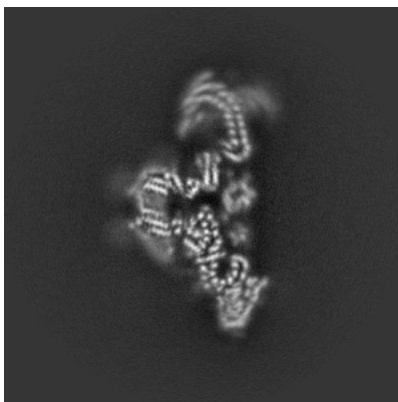


Z Index: 225

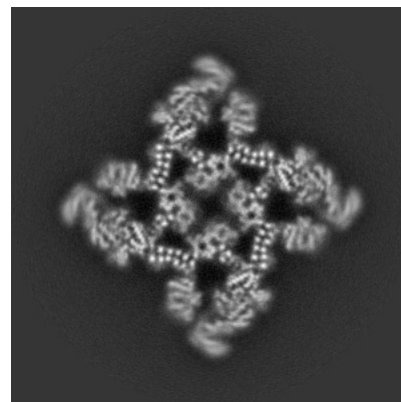
6.3.2 Raw map



X Index: 225



Y Index: 175

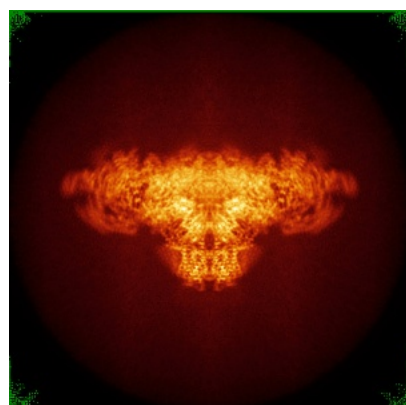


Z Index: 227

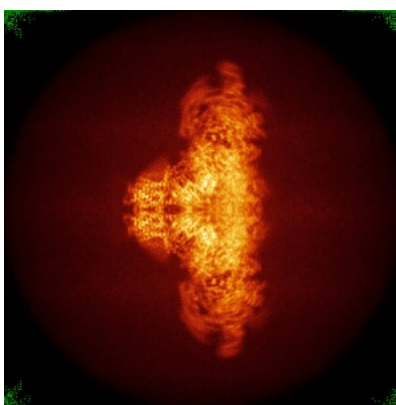
The images above show the largest variance slices of the map in three orthogonal directions.

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

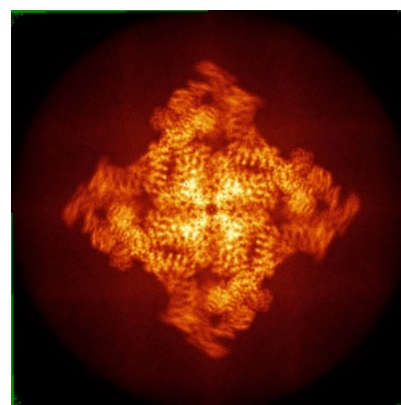
6.4.1 Primary map



X

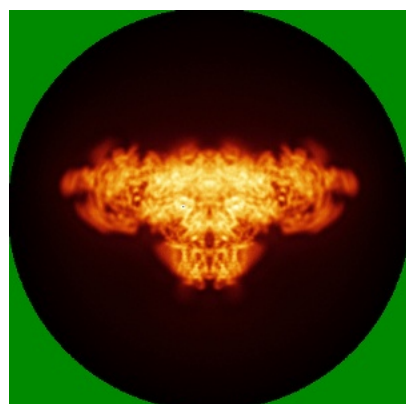


Y

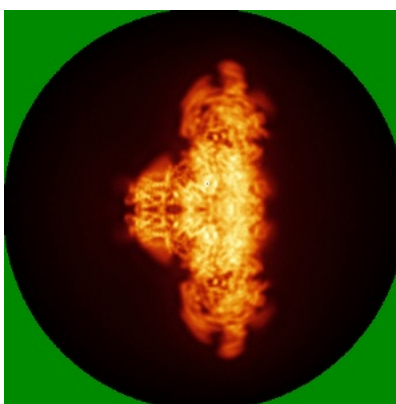


Z

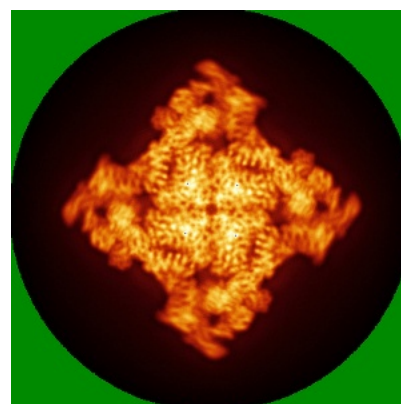
6.4.2 Raw map



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](#)

This section was not generated.

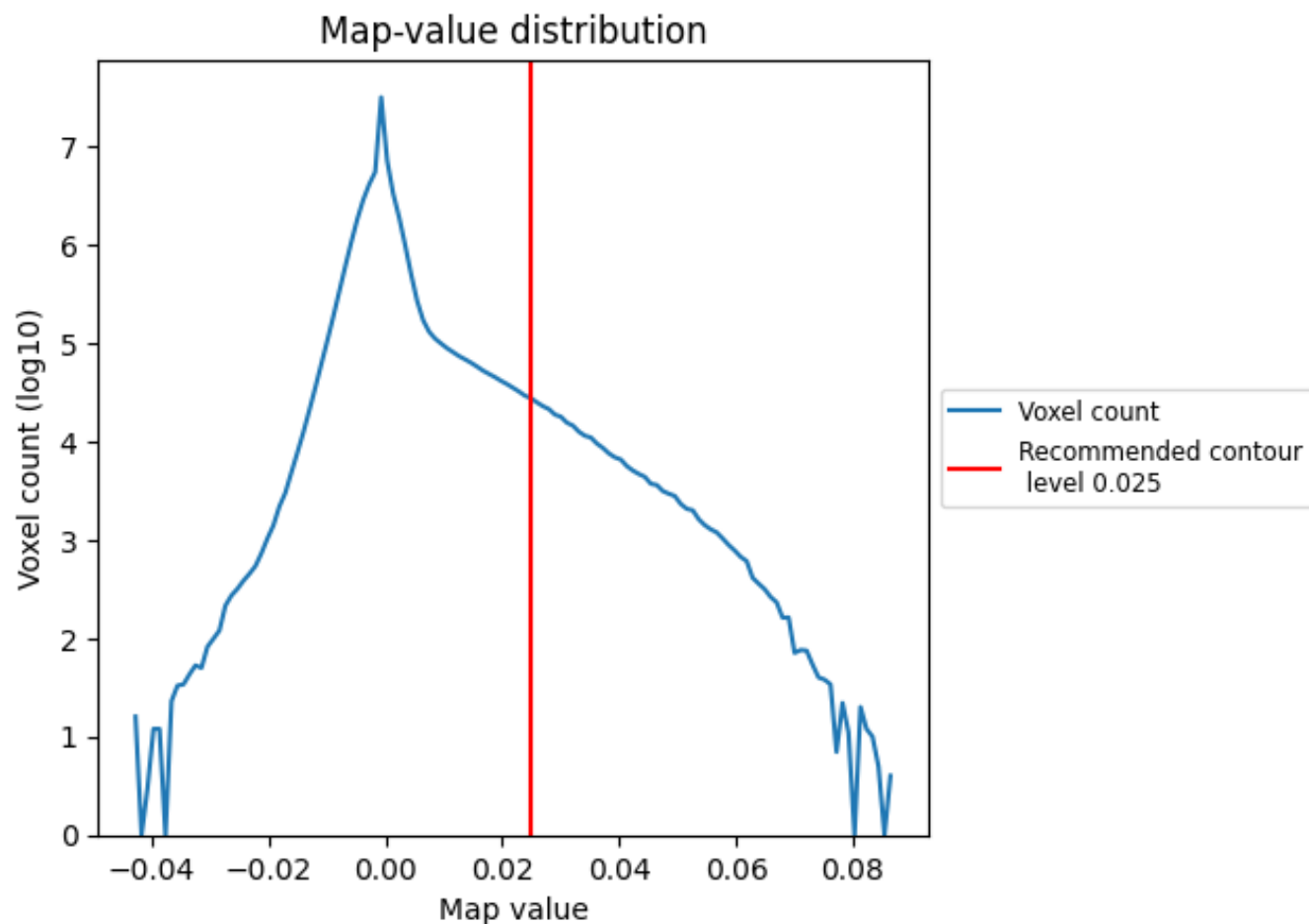
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

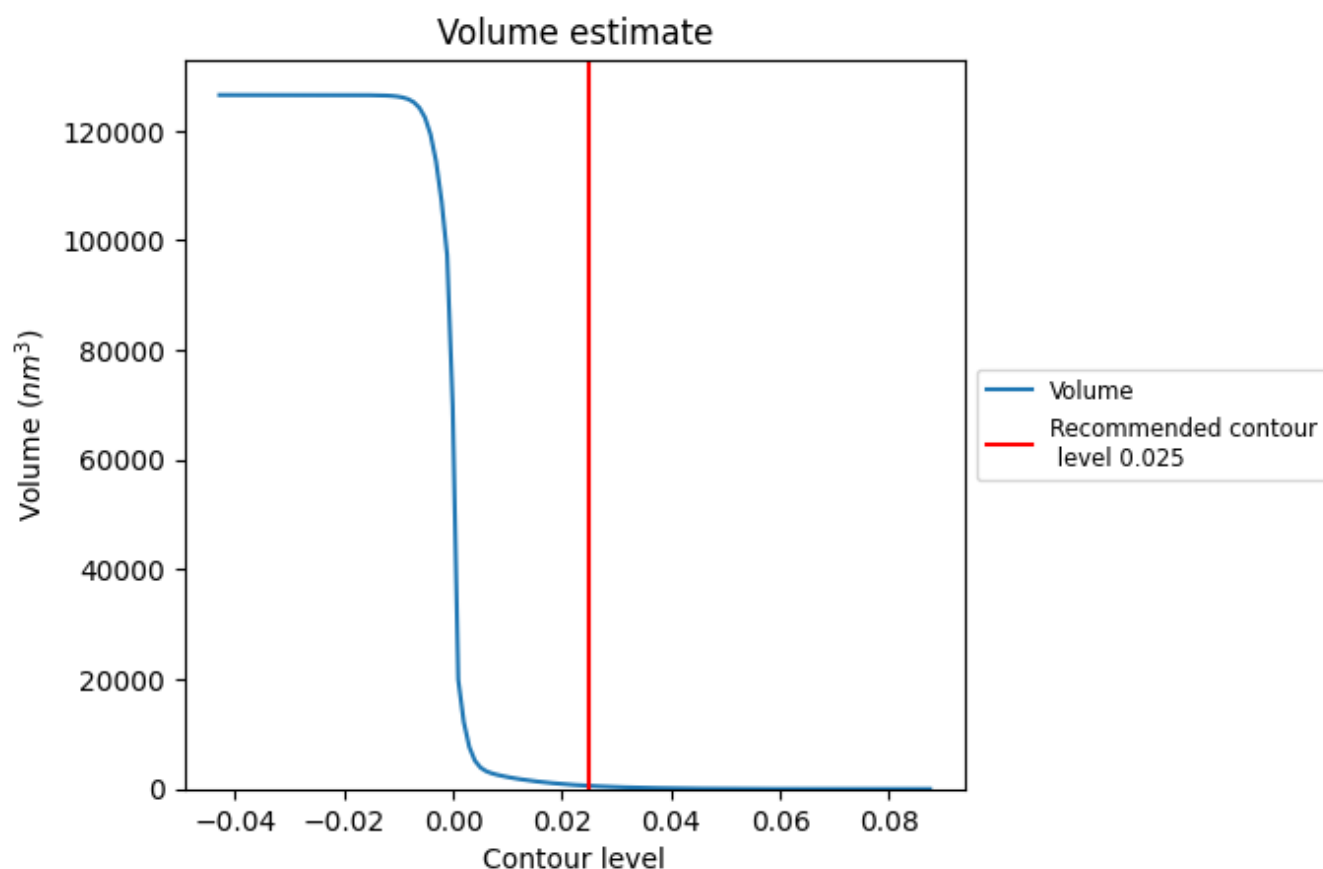
This section contains the results of statistical analysis of the map.

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.

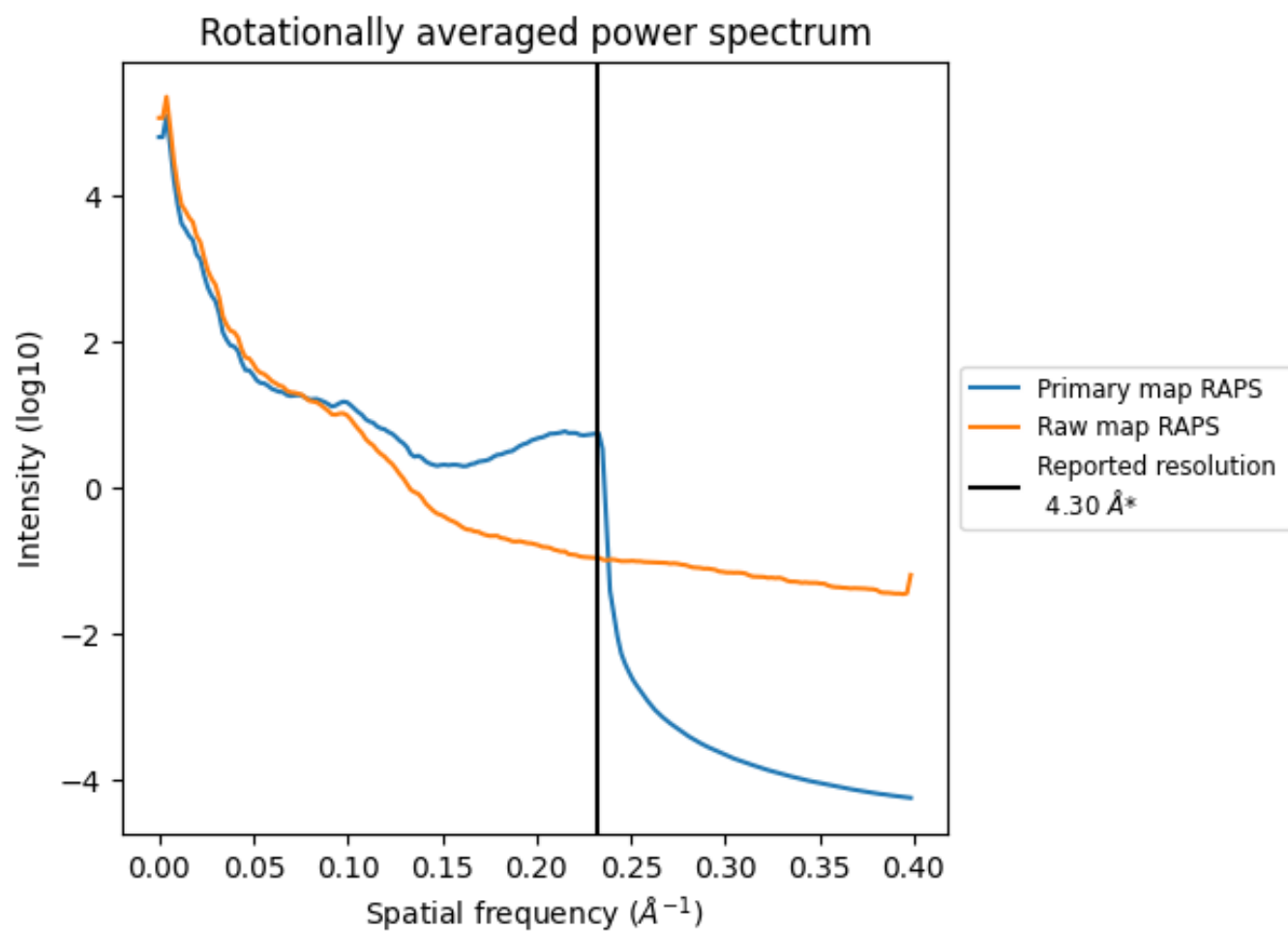
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

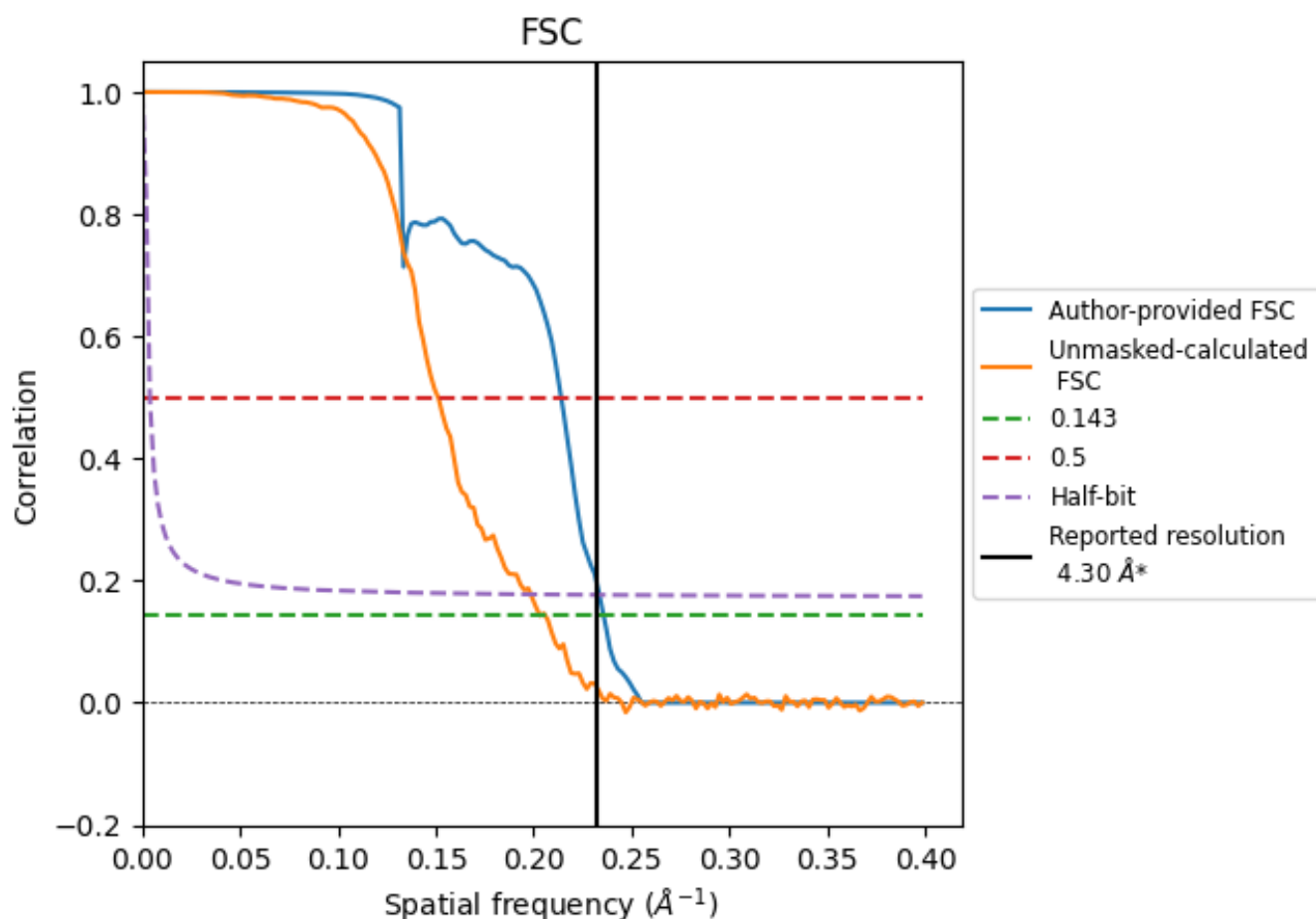


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.233 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

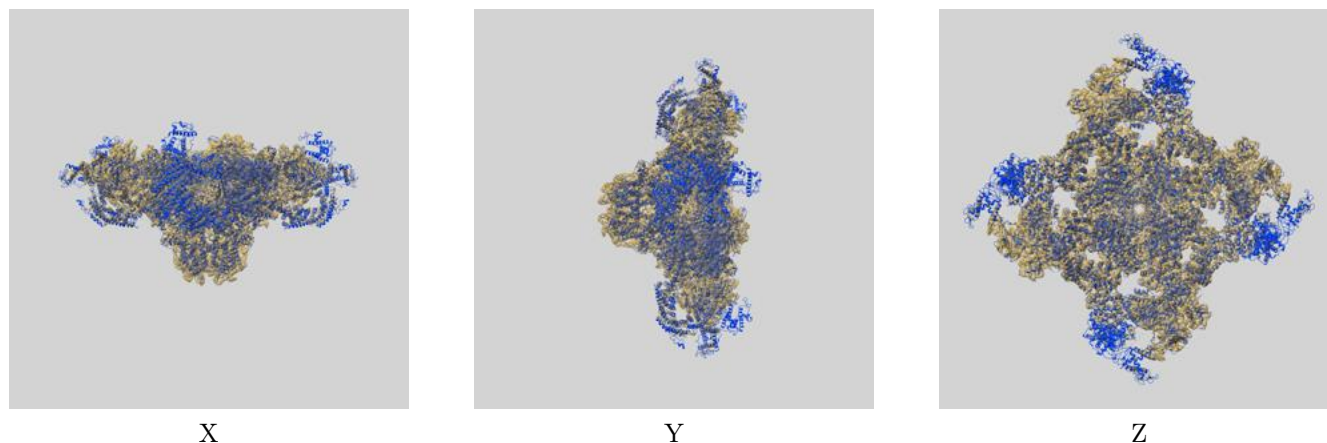
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.24	4.67	4.28
Unmasked-calculated*	4.92	6.61	5.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.92 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

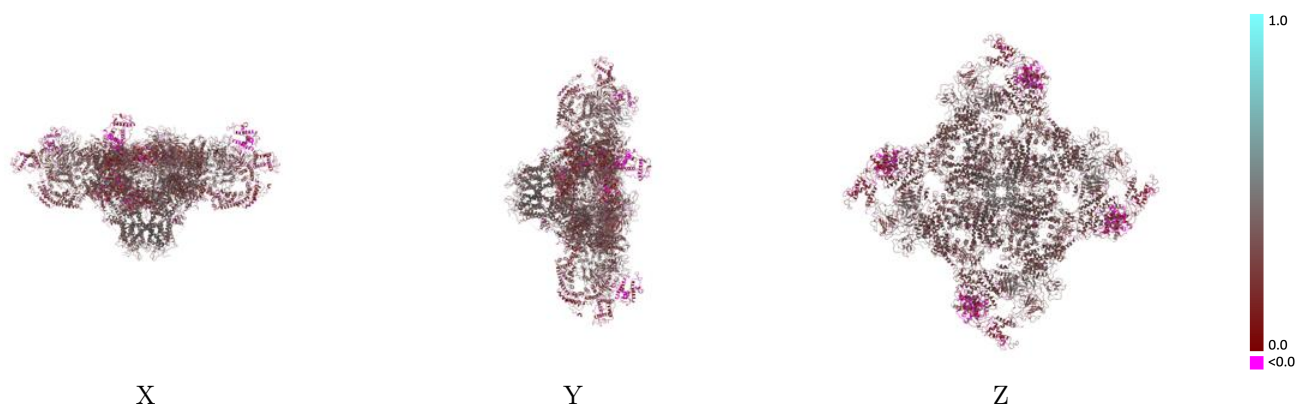
This section contains information regarding the fit between EMDB map EMD-8378 and PDB model 5TAL. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



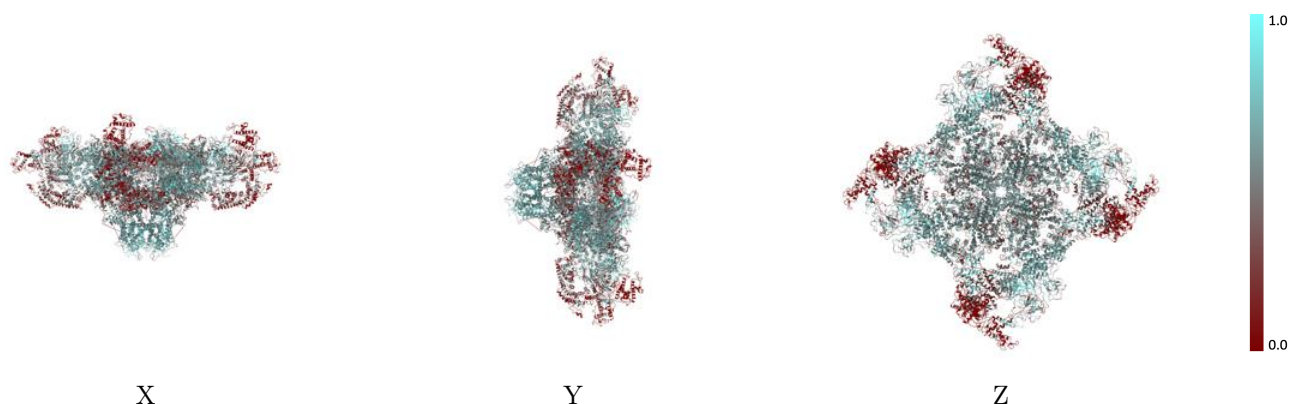
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



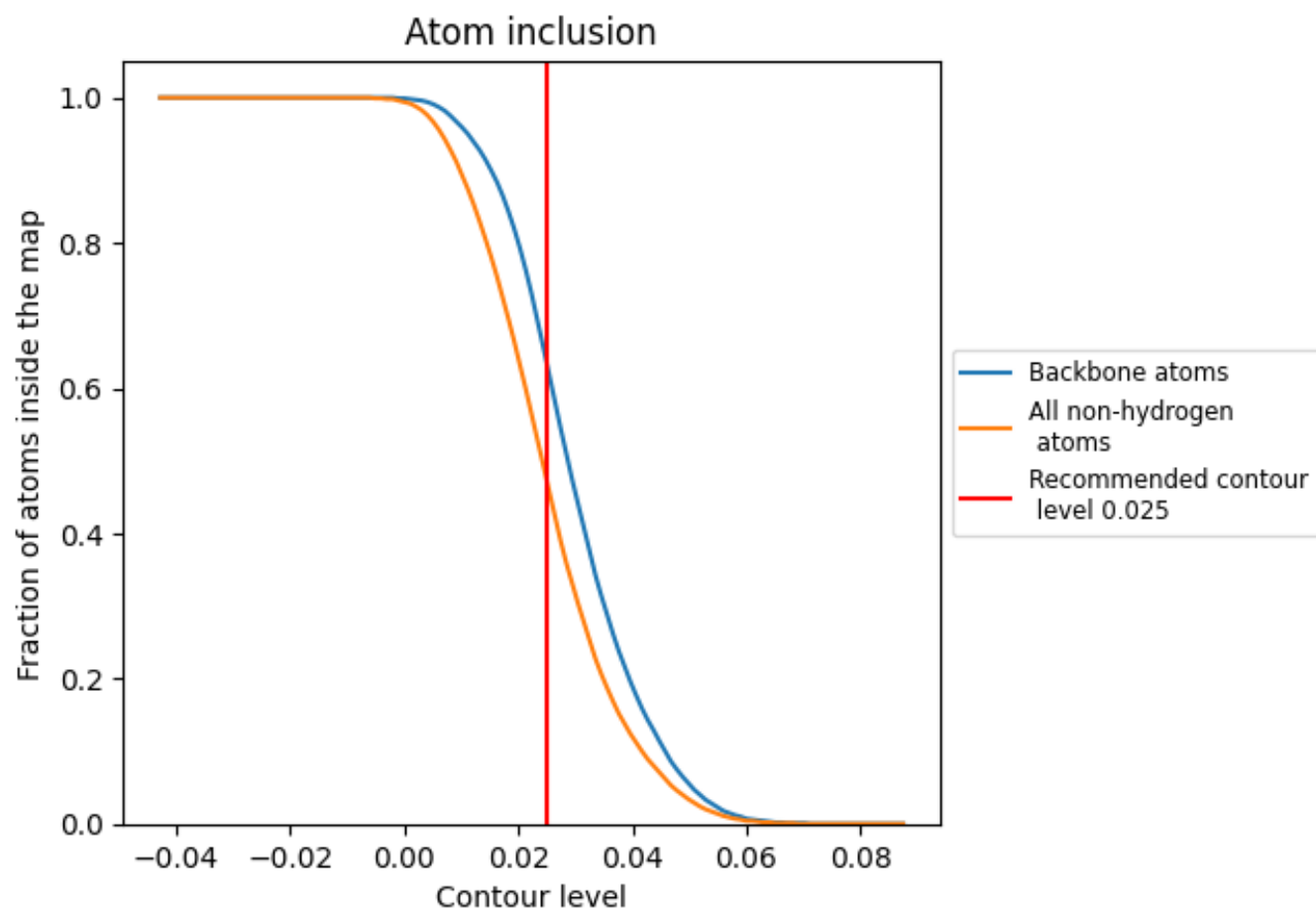
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4710	0.3030
A	0.5380	0.3550
B	0.4720	0.3050
E	0.4660	0.2980
F	0.5430	0.3580
G	0.4700	0.3030
H	0.5360	0.3570
I	0.4660	0.2990
J	0.5360	0.3550

1.0

0.0

<0.0