



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:09 AM UTC

PDB ID : 5TAP / pdb_00005tap
EMDB ID : EMD-8381
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, all particles)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.40 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:

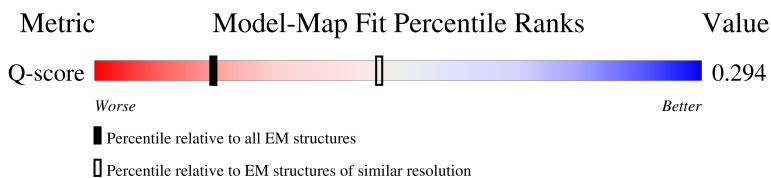
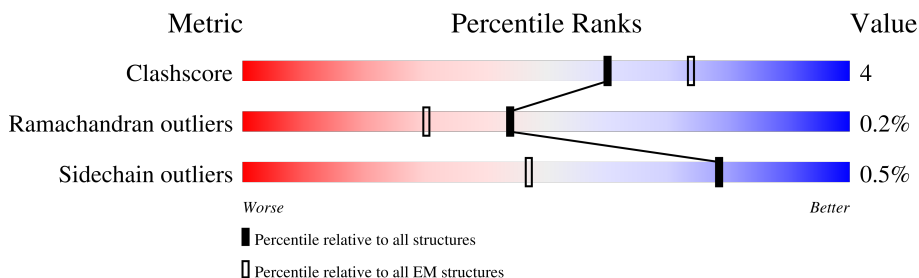
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.40 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	3132 (3.91 - 4.90)

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

Mol	Chain	Length	Quality of chain
1	A	108	
1	F	108	
1	H	108	
1	J	108	

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Mol	Chain	Length	Quality of chain
2	B	4416	35% 85% 9% 5%
2	E	4416	35% 85% 9% 5%
2	G	4416	35% 85% 9% 5%
2	I	4416	35% 85% 9% 5%

2 Entry composition

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

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

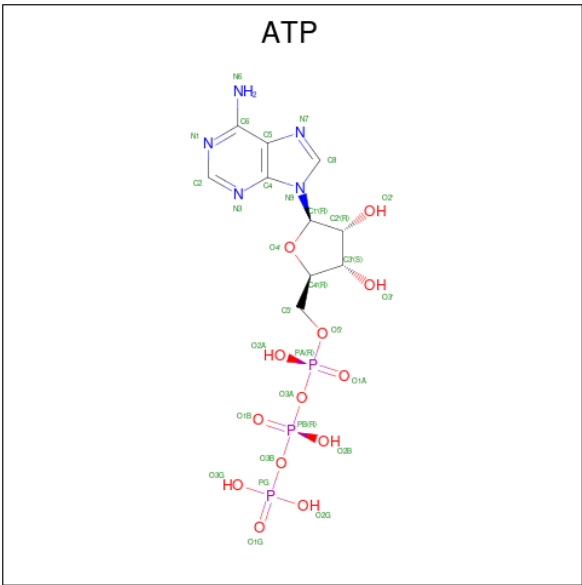
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

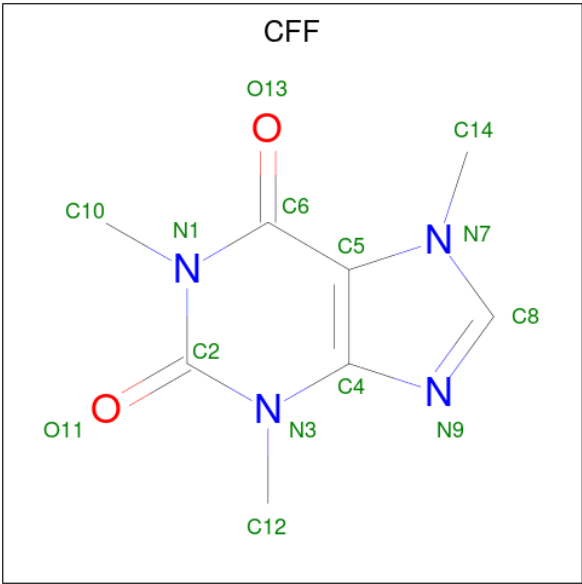
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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



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

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



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

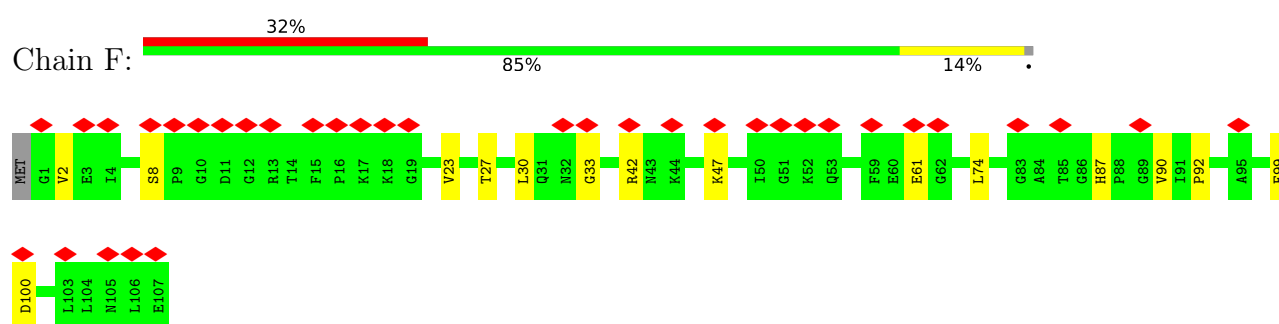
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

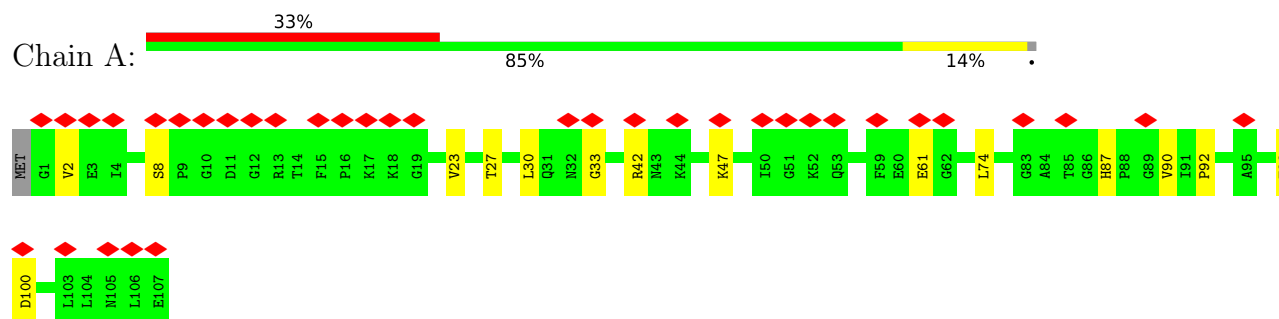
3 Residue-property plots [i](#)

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

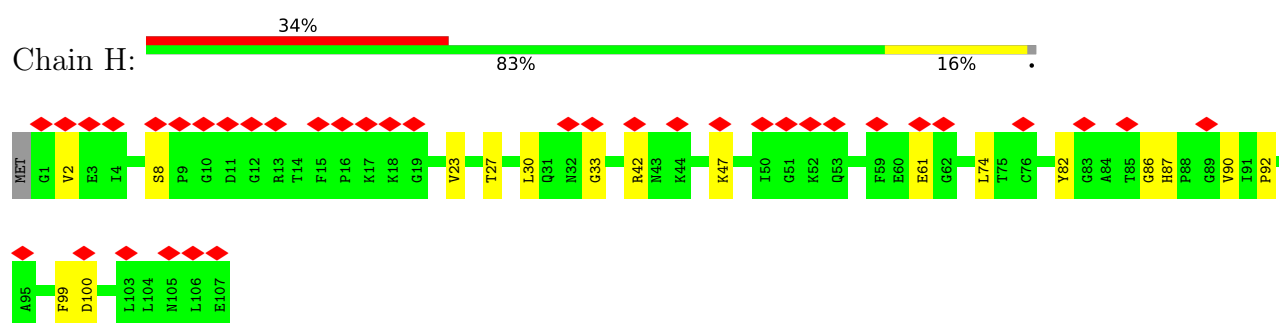
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



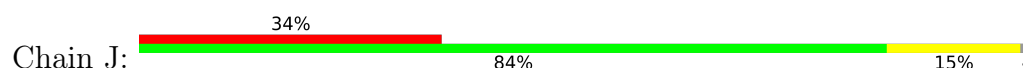
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

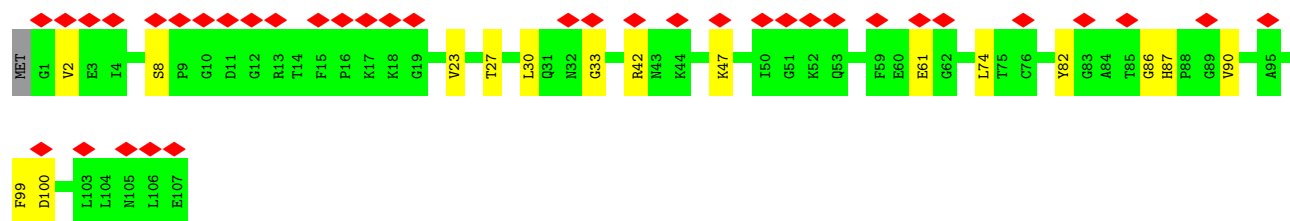


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

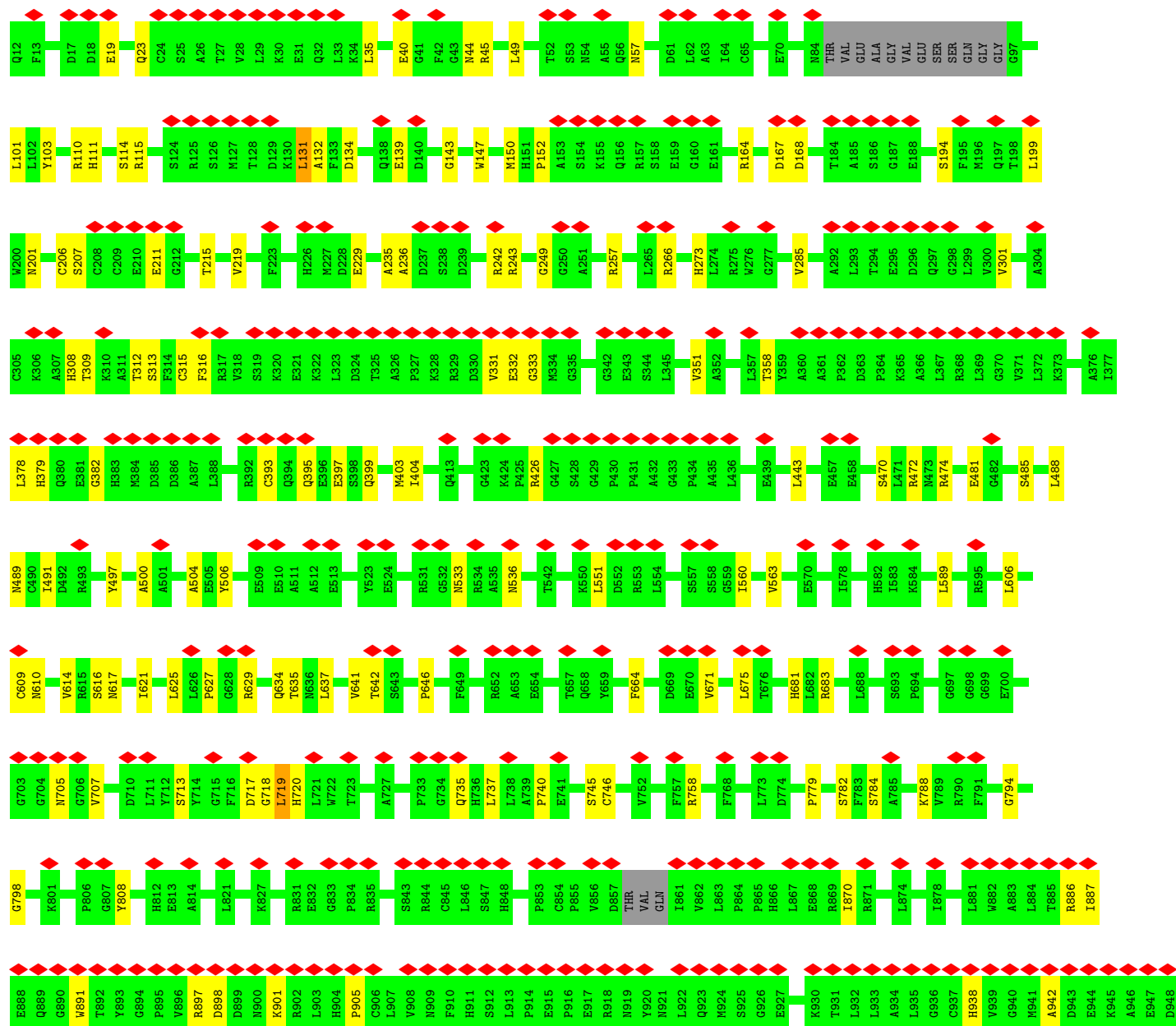
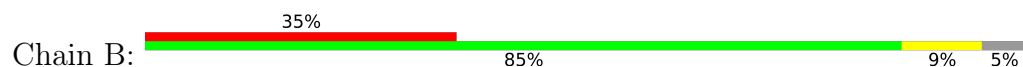


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



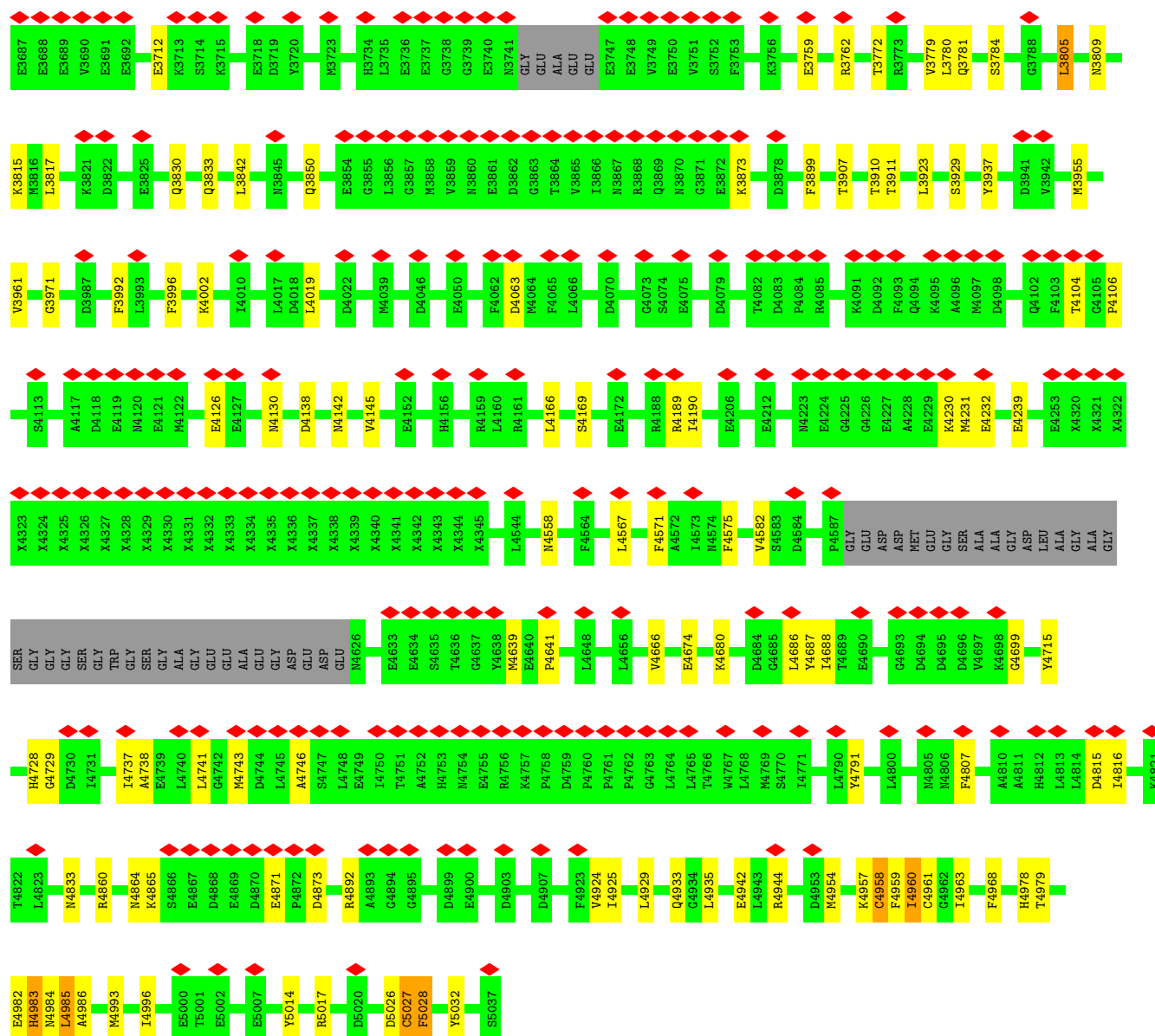


• Molecule 2: Ryanodine receptor 1

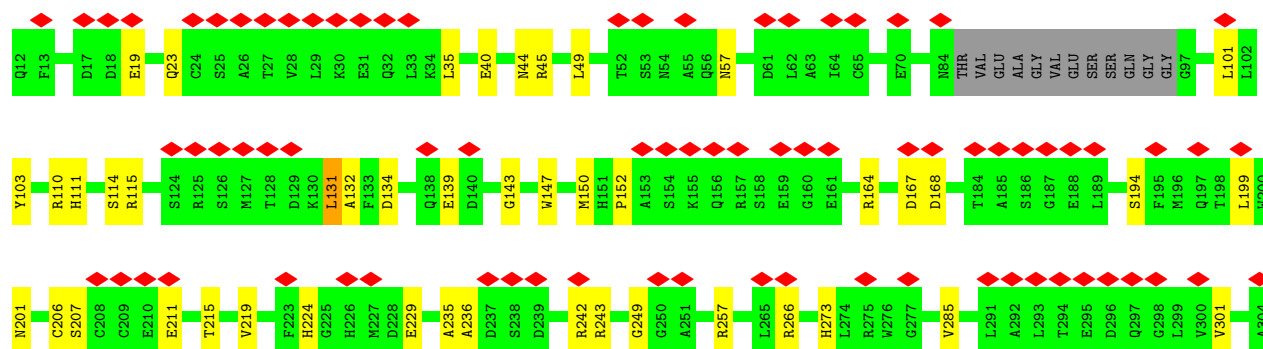
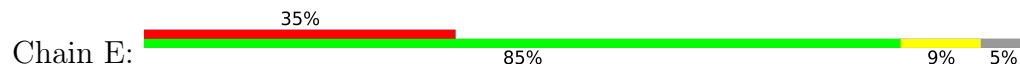


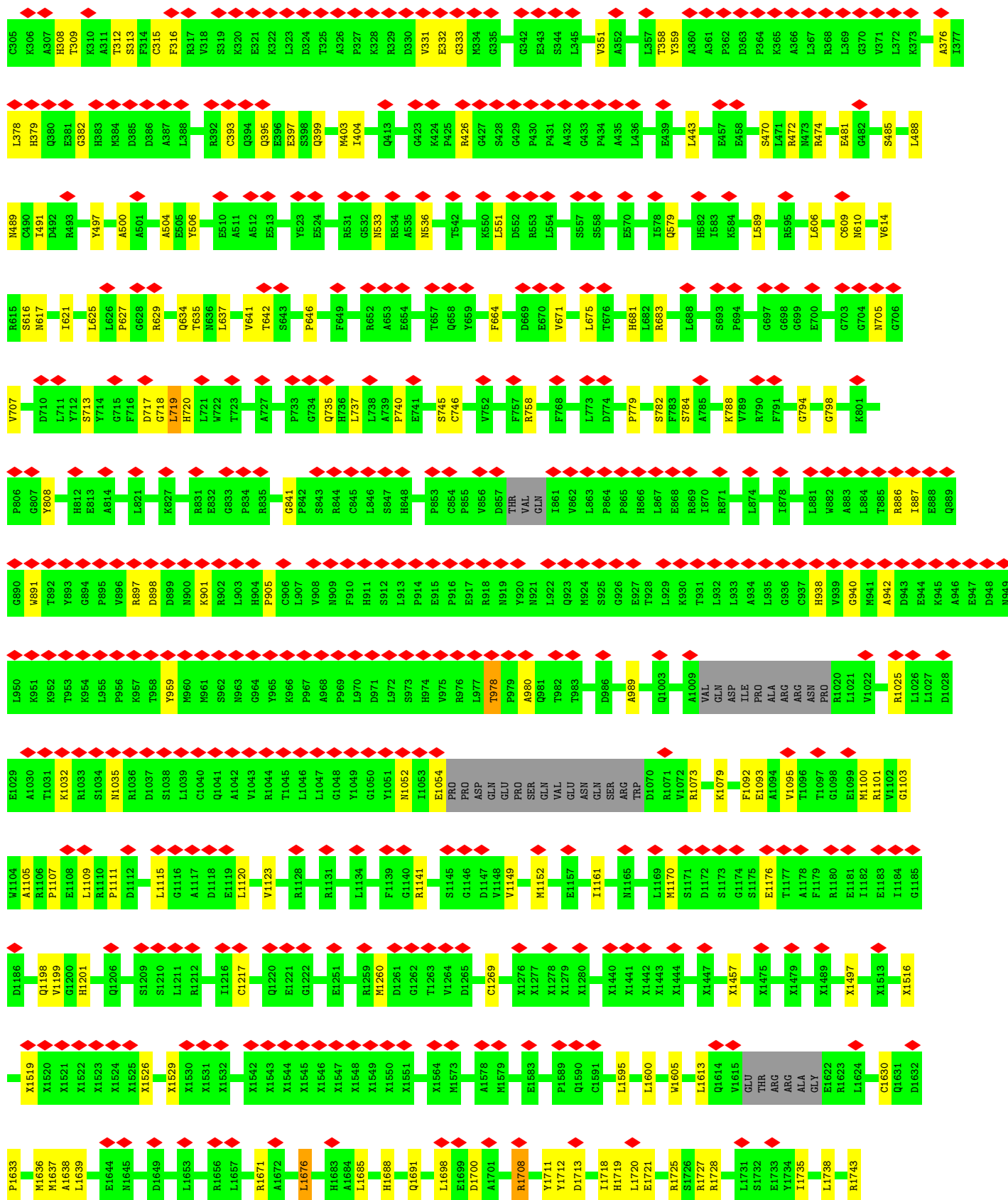


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X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3574	X3575	X3576	X3577	X3578	
X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3422	X3423	X3427	X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3442	X3443	X3450	X3451	X3452	X3453	X3454	X3455	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516							
X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3361	X3362	X3363	X3364	X3365	X3366	X3369	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395				
X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3308	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3323	X3324	X3325	X3330	X3331	X3332	X3333	X3334						
X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3053	X3057	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3151	X3152	X3153	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3181	X3182	X3183	X3190					
X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2961	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3009	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3032	X3033	X3034	X3038	X3039	X3040	X3041	X3042						
N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	G2897	G2898	G2899	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	T2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	P2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	Y2942	
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Y2761	T2762	H2763	E2764	T2765	W2766	A2767	P2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	T2777	Q2778	L2779	N2780	D2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	T2792	P2793	Y2794	K2795	T2796	S2797	T2798	V2799	E2740	E2741	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760
W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	D2860	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880			



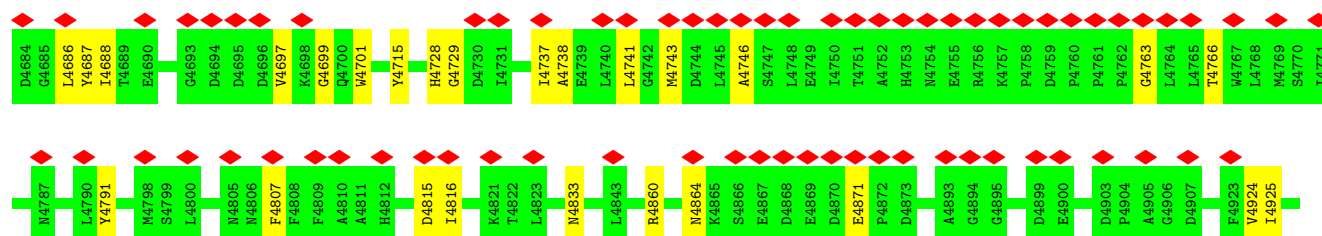
• Molecule 2: Ryanodine receptor 1



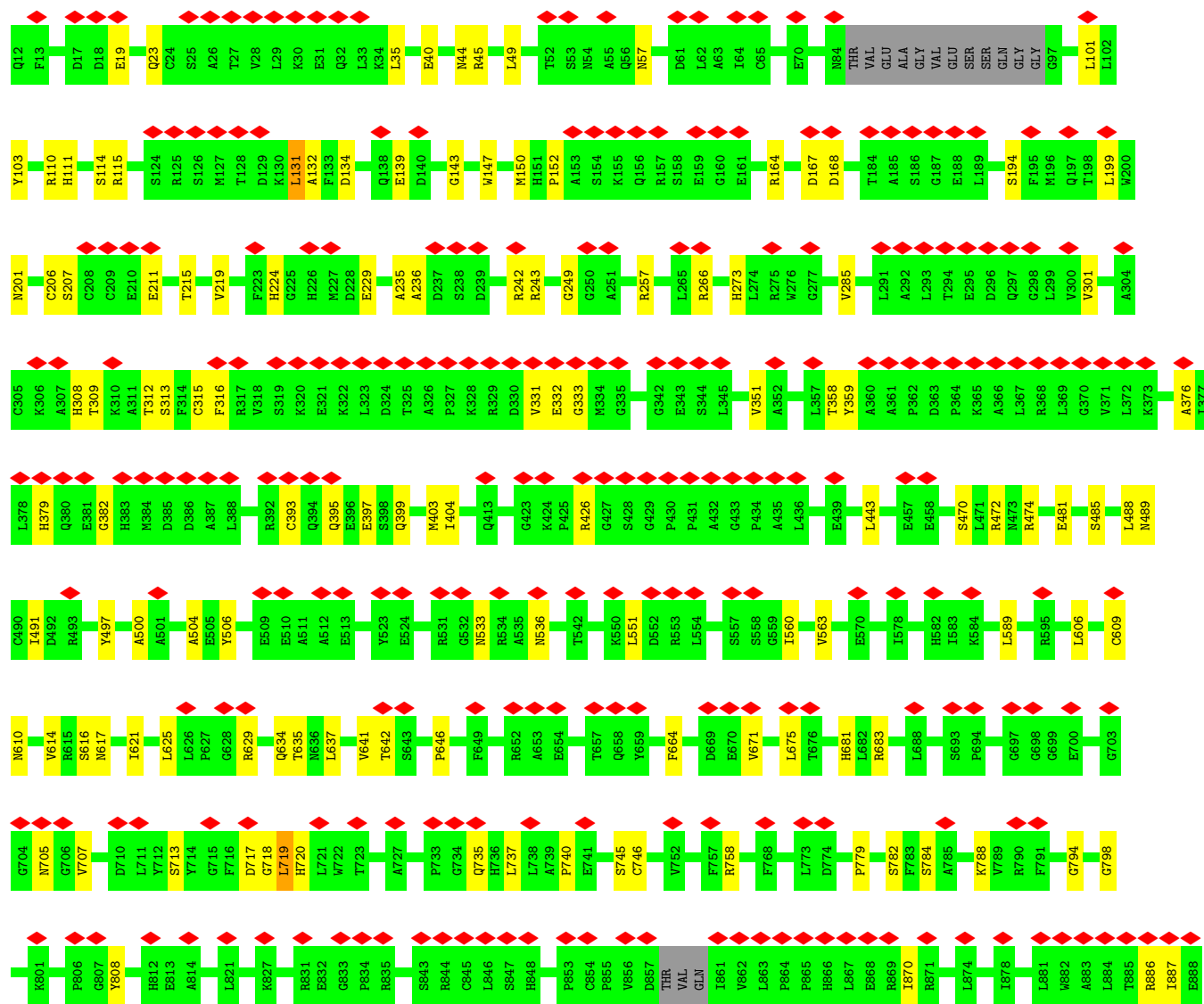
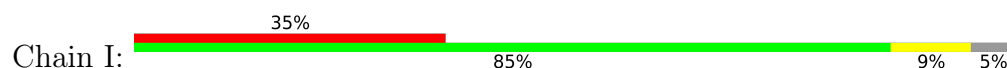




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ALA	X3039	X3178	X3252	X3323	X3389	X3469	X3570	X3671	D3941	M4097	M4231	ALA
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GLY	X3046	X3193	X3259	X3330	X3396	X3476	X3577	E3685	L3817	S4113	X4323	GLY
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GLY	X3049	X3196	X3262	X3333	X3399	X3479	X3580	E3688	L3993	E4127	X4326	GLY
GLY	X3050	X3197	X3263	X3334	X3400	X3480	X3581	E3689	F3996	E4128	X4327	GLY
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GLY	X3134	X3211	X3271	X3342	X3408	X3488	X3589	Y3720	D4022	N4130	X4335	GLY
GLY	X3135	X3212	X3272	X3343	X3409	X3489	X3590	H3723	M4039	D4138	X4336	GLY
GLY	X3136	X3213	X3273	X3344	X3410	X3490	X3591	L3735	D4046	N4142	X4337	GLY
GLY	X3137	X3214	X3274	X3345	X3411	X3491	X3592	H3734	E4050	V4145	X4338	GLY
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GLY	X3144	X3221	X3281	X3352	X3424	X3498	X3599	GLY	D4072	L4166	L4544	GLY
GLY	X3145	X3222	X3282	X3353	X3425	X3499	X3600	ALA	V4073	E4172	F4564	GLY
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GLY	X3148	X3225	X3285	X3356	X3428	X3502	X3603	GLU	E4076	R4188	A4572	GLY
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GLY	X3150	X3227	X3287	X3358	X3430	X3504	X3605	E3748	D4083	E4190	N4574	GLY
GLY	X3151	X3230	X3288	X3359	X3431	X3505	X3606	T3699	P4084	E4206	I4575	GLY
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GLY	X3243	X3243	X3301	X3372	X3444	X3518	X3619					GLY
GLY	X3244	X3244	X3302	X3373	X3445	X3519	X3620					GLY
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GLY			X3307	X3378	X3450	X3524	X3625					GLY
GLY			X3308	X3379	X3451	X3525	X3626					GLY
GLY			X3309	X3380	X3452	X3526	X3627					GLY
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GLY			X3311	X3382	X3454	X3528	X3629					GLY
GLY			X3312	X3383	X3455	X3529	X3630					GLY
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GLY			X3317	X3388	X3460	X3534	X3635					GLY
GLY			X3318	X3389	X3461	X3535	X3636					GLY
GLY			X3319	X3390	X3462	X3536	X3637					GLY
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GLY			X3321	X3392	X3464	X3538	X3639					GLY
GLY			X3322	X3393	X3465	X3539	X3640					GLY
GLY			X3323	X3394	X3466	X3540	X3641					GLY
GLY			X3324	X3395	X3467	X3541	X3642					GLY
GLY			X3325	X3396	X3468	X3542	X3643					GLY
GLY			X3326	X3397	X3469	X3543	X3644					GLY
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GLY			X3362	X3433	X3505	X3579	X3680					GLY
GLY			X3363	X3434	X3506	X3580	X3681					GLY
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GLY			X3365	X3436	X3508	X3582	X3683					GLY
GLY			X3366	X3437	X3509	X3583	X3684					GLY
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GLY												

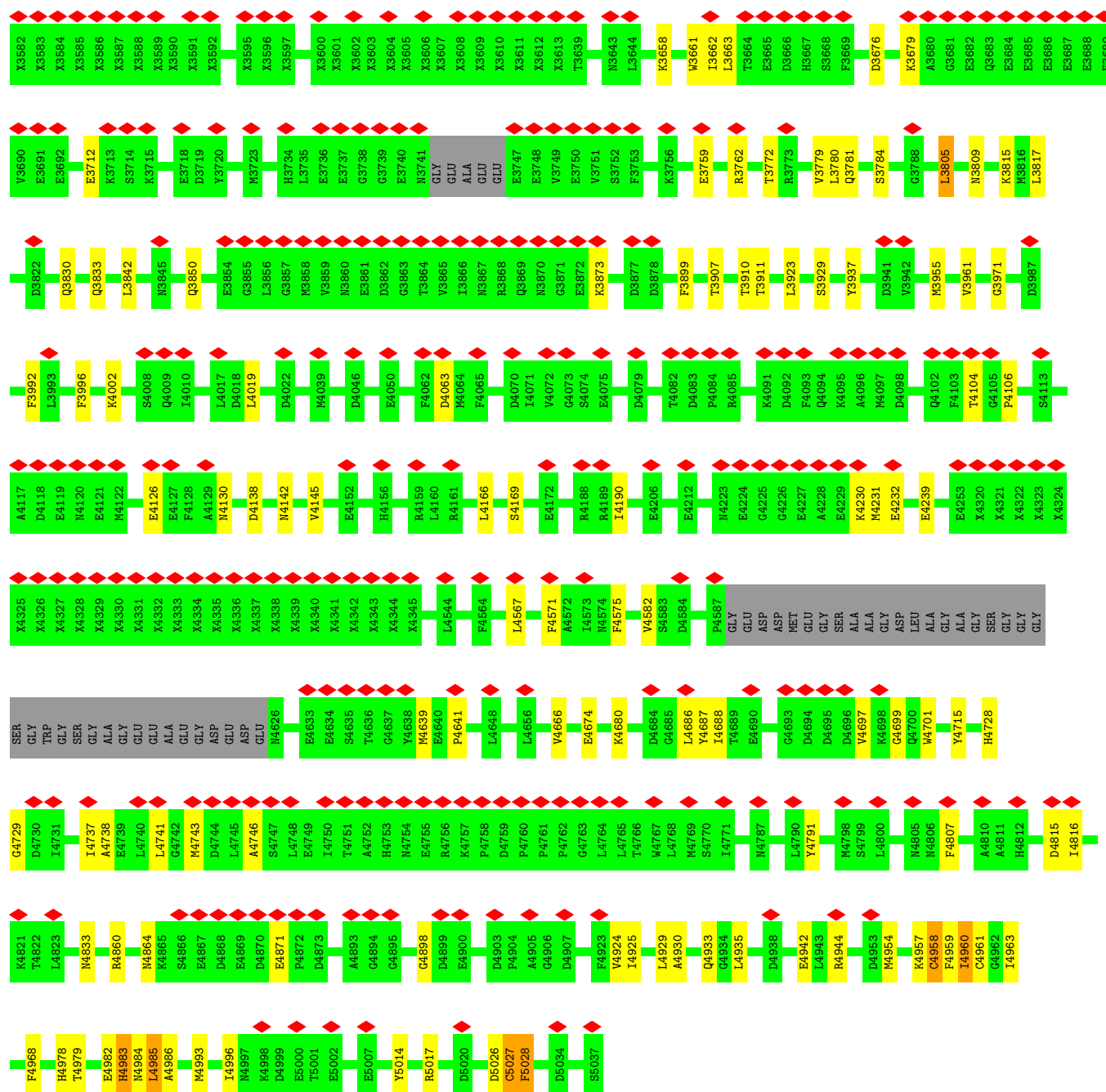


• Molecule 2: Ryanodine receptor 1

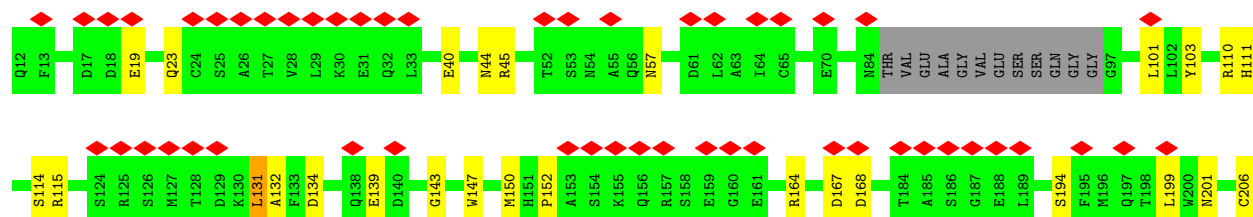
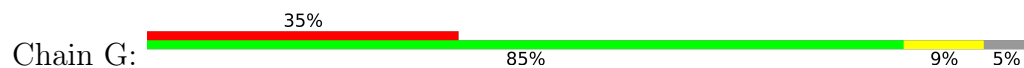




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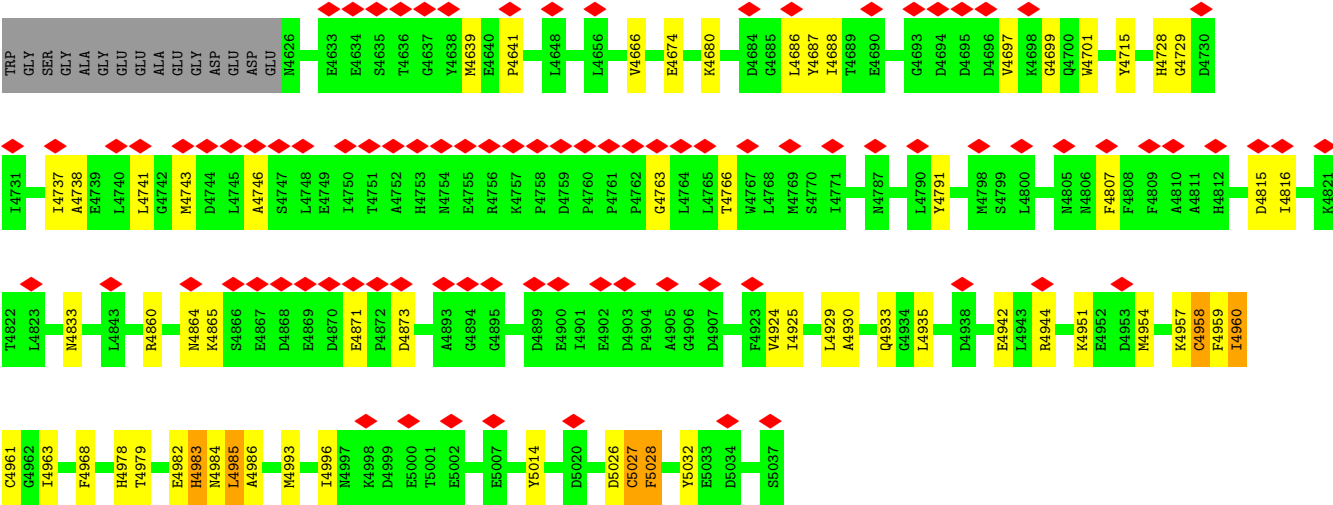
• Molecule 2: Ryanodine receptor 1







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X4337	L4018	L4019	E3718	X3590	X3528	X3407	X3347	X3276	X3202	X3052	X2953
X4338	L4019	Q3850	D3719	X3591	X3529	X3408	X3348	X3277	X3203	X3053	X2954
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X4368	D3941	S3668	V3779	X3626	X3559	X3438	X3378	X3307	X3233	X3127	X2984
X4369	F4103	F3669	L3780	X3627	X3560	X3439	X3379	X3308	X3234	X3128	X2985
X4370	T4104	D3676	Q3781	X3628	X3561	X3440	X3380	X3309	X3235	X3129	X2986
X4371	M3955	K3679	S3784	X3629	X3562	X3441	X3381	X3310	X3236	X3130	X2987
X4372	P4106	A3680	G3788	X3630	X3563	X3442	X3382	X3311	X3237	X3131	X2988
X4373	S4113	G3681	L3805	X3631	X3564	X3443	X3383	X3312	X3238	X3132	X2989
X4374	A4117	E3682	N3809	X3632	X3565	X3444	X3384	X3313	X3239	X3133	X2990
X4375	D4118	E3683	K3815	X3633	X3566	X3445	X3385	X3314	X3240	X3134	X2991
X4376		E3684		X3634	X3567	X3446	X3386	X3315	X3241	X3135	X2992
X4377		E3685		X3635	X3568	X3447	X3387	X3316	X3242	X3136	X2993
X4378		E3686		X3636	X3569	X3448	X3388	X3317	X3243	X3137	X2994
X4379		E3687		X3637	X3570	X3449	X3389	X3318	X3244	X3138	X2995
X4380				X3638	X3571	X3450	X3390	X3319	X3245	X3139	X2996
X4381				X3639	X3572	X3451	X3391	X3320	X3246	X3140	X2997
X4382				X3640	X3573	X3452	X3392	X3321	X3247	X3141	X2998
X4383				X3641	X3574	X3453	X3393	X3322	X3248	X3142	X2999
X4384				X3642	X3575	X3454	X3394	X3323	X3249	X3143	X3000
X4385				X3643	X3576	X3455	X3395	X3324	X3250	X3144	X3001
X4386				X3644	X3577	X3456	X3396	X3325	X3251	X3145	X3002
X4387				X3645	X3578	X3457	X3397	X3326	X3252	X3146	X3003
X4388				X3646	X3579	X3458	X3398	X3327	X3253	X3147	X3004
X4389				X3647	X3580	X3459	X3399	X3328	X3254	X3148	X3005
X4390				X3648	X3581	X3460	X3400	X3329	X3255	X3149	X3006
X4391				X3649	X3582	X3461	X3401	X3330	X3256	X3150	X3007
X4392				X3650	X3583	X3462	X3402	X3331	X3257	X3151	X3008
X4393				X3651	X3584	X3463	X3403	X3332	X3258	X3152	X3009
X4394				X3652	X3585	X3464	X3404	X3333	X3259	X3153	X3010
X4395				X3653	X3586	X3465	X3405	X3334	X3260	X3154	X3011
X4396				X3654	X3587	X3466	X3406	X3335	X3261	X3155	X3012
X4397				X3655	X3588	X3467	X3407	X3336	X3262	X3156	X3013
X4398				X3656	X3589	X3468	X3408	X3337	X3263	X3157	X3014
X4399				X3657	X3590	X3469	X3409	X3338	X3264	X3158	X3015
X4400				X3658	X3591	X3470	X3410	X3339	X3265	X3159	X3016
X4401				X3659	X3592	X3471	X3411	X3340	X3266	X3160	X3017
X4402				X3660	X3593	X3472	X3412	X3341	X3267	X3161	X3018
X4403				X3661	X3594	X3473	X3413	X3342	X3268	X3162	X3019
X4404				X3662	X3595	X3474	X3414	X3343	X3269	X3163	X3020
X4405				X3663	X3596	X3475	X3415	X3344	X3270	X3164	X3021
X4406				X3664	X3597	X3476	X3416	X3345	X3271	X3165	X3022
X4407				X3665	X3598	X3477	X3417	X3346	X3272	X3166	X3023
X4408				X3666	X3599	X3478	X3418	X3347	X3273	X3167	X3024
X4409				X3667	X3600	X3479	X3419	X3348	X3274	X3168	X3025
X4410				X3668	X3601	X3480	X3420	X3349	X3275	X3169	X3026
X4411				X3669	X3602	X3481	X3421	X3350	X3276	X3170	X3027
X4412				X3670	X3603	X3482	X3422	X3351	X3277	X3171	X3028
X4413				X3671	X3604	X3483	X3423	X3352	X3278	X3172	X3029
X4414				X3672	X3605	X3484	X3424	X3353	X3279	X3173	X3030
X4415				X3673	X3606	X3485	X3425	X3354	X3280	X3174	X3031
X4416				X3674	X3607	X3486	X3426	X3355	X3281	X3175	X3032
X4417				X3675	X3608	X3487	X3427	X3356	X3282	X3176	X3033
X4418				X3676	X3609	X3488	X3428	X3357	X3283	X3177	X3034
X4419				X3677	X3610	X3489	X3429	X3358	X3284	X3178	X3035
X4420				X3678	X3611	X3490	X3430	X3359	X3285	X3179	X3036
X4421				X3679	X3612	X3491	X3431	X3360	X3286	X3180	X3037
X4422				X3680	X3613	X3492	X3432	X3361	X3287	X3181	X3038
X4423				X3681	X3614	X3493	X3433	X3362	X3288	X3182	X3039
X4424				X3682	X3615	X3494	X3434	X3363	X3289	X3183	X3040
X4425				X3683	X3616	X3495	X3435	X3364	X3290	X3184	X3041
X4426				X3684	X3617	X3496	X3436	X3365	X3291	X3185	X3042
X4427				X3685	X3618	X3497	X3437	X3366	X3292	X3186	X3043
X4428				X3686	X3619	X3498	X3438	X3367	X3293	X3187	X3044
X4429				X3687	X3620	X3499	X3439	X3368	X3294	X3188	X3045
X4430				X3688	X3621	X3500	X3440	X3369	X3295	X3189	X3046
X4431				X3689	X3622	X3501	X3441	X3370	X3296	X3190	X3047
X4432				X3690	X3623	X3502	X3442	X3371	X3297	X3191	X3048
X4433				X3691	X3624	X3503	X3443	X3372	X3298	X3192	X3049
X4434				X3692	X3625	X3504	X3444	X3373	X3299	X3193	X3050
X4435				X3693	X3626	X3505	X3445	X3374	X3300	X3194	X3051
X4436				X3694	X3627	X3506	X3446	X3375	X3301	X3195	X3052
X4437				X3695	X3628	X3507	X3447	X3376	X3302	X3196	X3053
X4438				X3696	X3629	X3508	X3448	X3377	X3303	X3197	X3054
X4439				X3697	X3630	X3509	X3449	X3378	X3304	X3198	X3055
X4440				X3698	X3631	X3510	X3450	X3379	X3305	X3199	X3056
X4441				X3699	X3632	X3511	X3451	X3380	X3306	X3200	X3057
X4442				X3700	X3633	X3512	X3452	X3381	X3307	X3201	X3058
X4443				X3701	X3634	X3513	X3453	X3382	X3308	X3202	X3059
X4444				X3702	X3635	X3514	X3454	X3383	X3309	X3203	X3060
X4445				X3703	X3636	X3515					



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	0.116	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.21	0/834	0.45	0/1123
1	F	0.21	0/834	0.45	0/1123
1	H	0.21	0/834	0.45	0/1123
1	J	0.21	0/834	0.45	0/1123
2	B	0.22	0/25428	0.52	3/34534 (0.0%)
2	E	0.22	0/25428	0.52	5/34534 (0.0%)
2	G	0.22	0/25428	0.52	3/34534 (0.0%)
2	I	0.22	0/25428	0.52	3/34534 (0.0%)
All	All	0.22	0/105048	0.51	14/142628 (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	15
2	E	0	15
2	G	0	15
2	I	0	15
All	All	0	64

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	5.16	134.37	116.30
2	G	131	LEU	CA-CB-CG	5.16	134.35	116.30
2	B	131	LEU	CA-CB-CG	5.15	134.32	116.30
2	E	131	LEU	CA-CB-CG	5.15	134.32	116.30
2	I	4639	MET	CA-C-N	5.13	134.32	121.80
2	I	4639	MET	C-N-CA	5.13	134.32	121.80
2	E	4639	MET	CA-C-N	5.11	134.27	121.80
2	E	4639	MET	C-N-CA	5.11	134.27	121.80
2	G	4639	MET	CA-C-N	5.11	134.27	121.80
2	G	4639	MET	C-N-CA	5.11	134.27	121.80
2	B	4639	MET	CA-C-N	5.11	134.26	121.80
2	B	4639	MET	C-N-CA	5.11	134.26	121.80
2	E	579	GLN	CA-C-N	5.02	131.12	121.54
2	E	579	GLN	C-N-CA	5.02	131.12	121.54

There are no chirality outliers.

All (64) 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	1720	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1720	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1720	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	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	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	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	8	0
1	F	818	0	824	8	0
1	H	818	0	824	9	0
1	J	818	0	824	8	0
2	B	29499	0	24749	249	0
2	E	29499	0	24749	249	0
2	G	29499	0	24749	245	0
2	I	29499	0	24749	247	0
3	B	31	0	12	3	0
3	E	31	0	12	3	0
3	G	31	0	12	3	0
3	I	31	0	12	3	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
All	All	121452	0	102380	1004	0

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

All (1004) 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:I:4230:LYS:HD2	2:I:4959:PHE:HE1	1.38	0.88
2:E:4230:LYS:HD2	2:E:4959:PHE:HE1	1.38	0.88
2:B:4230:LYS:HD2	2:B:4959:PHE:HE1	1.38	0.87
2:G:4230:LYS:HD2	2:G:4959:PHE:HE1	1.38	0.87
2:B:4983:HIS:CD2	2:B:4983:HIS:H	1.94	0.86
2:G:4983:HIS:CD2	2:G:4983:HIS:H	1.94	0.86
2:I:4983:HIS:H	2:I:4983:HIS:CD2	1.94	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4230:LYS:CD	2:B:4959:PHE:HE1	1.92	0.83
2:I:4230:LYS:CD	2:I:4959:PHE:HE1	1.92	0.82
2:E:4983:HIS:CD2	2:E:4983:HIS:H	1.94	0.82
2:E:4230:LYS:CD	2:E:4959:PHE:HE1	1.92	0.82
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.15	0.81
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.15	0.81
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.15	0.81
2:G:4230:LYS:CD	2:G:4959:PHE:HE1	1.92	0.81
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.15	0.80
2:G:4983:HIS:H	2:G:4983:HIS:HD2	1.29	0.79
2:B:4983:HIS:H	2:B:4983:HIS:HD2	1.29	0.77
2:I:4983:HIS:H	2:I:4983:HIS:HD2	1.29	0.77
2:E:4983:HIS:H	2:E:4983:HIS:HD2	1.29	0.77
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.77	0.73
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.77	0.73
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.77	0.72
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.77	0.72
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.04	0.72
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.04	0.71
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.04	0.71
2:B:4960:ILE:N	2:B:4960:ILE:HD13	2.04	0.71
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.61	0.69
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.61	0.68
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.61	0.68
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.61	0.68
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.76	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.77	0.67
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.76	0.67
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.76	0.67
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.78	0.66
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.78	0.66
2:E:4231:MET:HE1	2:E:4960:ILE:HA	1.79	0.65
2:G:4231:MET:HE1	2:G:4960:ILE:HA	1.79	0.65
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.61	0.65
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.61	0.65
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.61	0.64
2:G:379:HIS:HD2	2:G:382:GLY:H	1.45	0.64
2:B:4231:MET:HE1	2:B:4960:ILE:HA	1.78	0.64
2:I:4231:MET:HE1	2:I:4960:ILE:HA	1.79	0.64
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.78	0.64
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.80	0.64
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.61	0.64
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.80	0.64
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.78	0.64
2:B:4944:ARG:HH22	2:I:4942:GLU:HA	1.63	0.63
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.80	0.63
2:I:379:HIS:HD2	2:I:382:GLY:H	1.45	0.63
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.81	0.63
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.81	0.63
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.80	0.63
2:I:4190:ILE:HD13	2:I:5026:ASP:CG	2.24	0.63
2:E:379:HIS:HD2	2:E:382:GLY:H	1.45	0.63
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.81	0.63
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.64	0.63
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.81	0.63
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.64	0.63
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.63	0.63
2:B:379:HIS:HD2	2:B:382:GLY:H	1.45	0.63
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.64	0.62
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.63	0.62
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.81	0.62
2:E:4190:ILE:HD13	2:E:5026:ASP:CG	2.24	0.62
2:B:4190:ILE:HD13	2:B:5026:ASP:CG	2.24	0.62
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.81	0.62
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.63	0.62
2:G:4982:GLU:HB3	2:G:4983:HIS:HD2	1.65	0.62
2:G:4190:ILE:HD13	2:G:5026:ASP:CG	2.24	0.62
2:E:4982:GLU:HB3	2:E:4983:HIS:HD2	1.65	0.62
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.81	0.62
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.65	0.62
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.33	0.62
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.64	0.61
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.83	0.61
2:B:4982:GLU:HB3	2:B:4983:HIS:HD2	1.65	0.61
2:I:4982:GLU:HB3	2:I:4983:HIS:HD2	1.65	0.61
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.81	0.61
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.65	0.61
2:I:4944:ARG:HH22	2:G:4942:GLU:HA	1.65	0.61
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.61
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.83	0.61
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4961:CYS:HB3	2:E:4983:HIS:HE1	1.66	0.61
2:I:4230:LYS:CG	2:I:4959:PHE:HE1	2.14	0.61
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.33	0.60
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.83	0.60
2:B:4230:LYS:CG	2:B:4959:PHE:HE1	2.14	0.60
2:G:4961:CYS:HB3	2:G:4983:HIS:HE1	1.66	0.60
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.34	0.60
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.33	0.60
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.83	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.60
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.65	0.60
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.65	0.60
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.60
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.34	0.60
2:B:4961:CYS:HB3	2:B:4983:HIS:HE1	1.65	0.60
2:E:4230:LYS:CG	2:E:4959:PHE:HE1	2.14	0.60
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.83	0.60
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.60
2:G:4230:LYS:CG	2:G:4959:PHE:HE1	2.14	0.60
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.83	0.59
2:B:4979:THR:HG22	3:B:5101:ATP:H2	1.67	0.59
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.83	0.59
2:I:4979:THR:HG22	3:I:5101:ATP:H2	1.67	0.59
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.59
2:I:4961:CYS:HB3	2:I:4983:HIS:HE1	1.65	0.59
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.85	0.59
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.83	0.59
2:B:132:ALA:HA	2:B:194:SER:HB2	1.84	0.59
2:E:4942:GLU:HA	2:G:4944:ARG:HH22	1.67	0.59
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.85	0.59
2:E:132:ALA:HA	2:E:194:SER:HB2	1.84	0.59
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.85	0.59
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.85	0.59
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.36	0.59
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.85	0.59
2:I:4190:ILE:CD1	2:I:5026:ASP:CG	2.76	0.59
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.85	0.59
2:B:4190:ILE:CD1	2:B:5026:ASP:CG	2.76	0.59
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.36	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.59
2:G:4190:ILE:CD1	2:G:5026:ASP:CG	2.76	0.59
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.35	0.59
2:E:4190:ILE:CD1	2:E:5026:ASP:CG	2.76	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.36	0.58
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.86	0.58
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.22	0.58
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.22	0.58
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.58
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.58
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.85	0.58
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.85	0.58
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.85	0.58
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.85	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.58
2:G:4979:THR:HG22	3:G:5101:ATP:H2	1.67	0.58
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.36	0.58
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.86	0.58
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.86	0.58
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.85	0.58
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.22	0.58
2:E:4979:THR:HG22	3:E:5101:ATP:H2	1.67	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.58
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.58
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.86	0.58
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.34	0.58
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.58
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.86	0.57
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.57
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.34	0.57
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.86	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.85	0.57
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.85	0.57
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.69	0.57
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.22	0.57
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.86	0.57
2:G:132:ALA:HA	2:G:194:SER:HB2	1.84	0.57
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.37	0.57
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.86	0.57
2:E:315:CYS:SG	2:E:316:PHE:N	2.78	0.57
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.87	0.57
2:I:132:ALA:HA	2:I:194:SER:HB2	1.84	0.57
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.87	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.87	0.57
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.87	0.57
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.69	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.78	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.87	0.57
2:E:4968:PHE:CZ	2:E:4978:HIS:ND1	2.73	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.87	0.57
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.86	0.56
2:I:315:CYS:SG	2:I:316:PHE:N	2.77	0.56
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.86	0.56
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.38	0.56
2:B:4968:PHE:CZ	2:B:4978:HIS:ND1	2.73	0.56
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.86	0.56
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.86	0.56
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.86	0.56
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.38	0.56
2:E:23:GLN:HB3	2:E:201:ASN:HB2	1.88	0.56
2:E:2347:GLU:O	2:E:2351:ASN:N	2.36	0.56
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.87	0.56
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.70	0.56
2:G:315:CYS:SG	2:G:316:PHE:N	2.78	0.56
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.86	0.56
2:G:4968:PHE:CZ	2:G:4978:HIS:ND1	2.73	0.56
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.56
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.86	0.56
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.70	0.56
2:G:101:LEU:HD13	2:G:150:MET:HE1	1.88	0.56
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.86	0.56
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.38	0.56
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.86	0.56
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.87	0.56
2:B:101:LEU:HD13	2:B:150:MET:HE1	1.88	0.56
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.88	0.56
2:E:101:LEU:HD13	2:E:150:MET:HE1	1.88	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.70	0.56
2:B:4190:ILE:CD1	2:B:5026:ASP:OD2	2.54	0.56
2:B:23:GLN:HB3	2:B:201:ASN:HB2	1.88	0.56
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.86	0.56
2:G:23:GLN:HB3	2:G:201:ASN:HB2	1.88	0.56
2:G:2347:GLU:O	2:G:2351:ASN:N	2.36	0.56
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.88	0.56
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.88	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.56
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.88	0.56
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.86	0.56
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.70	0.56
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.56
2:I:4968:PHE:CZ	2:I:4978:HIS:ND1	2.73	0.56
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.38	0.56
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.55
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.55
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.88	0.55
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.95	0.55
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.88	0.55
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.88	0.55
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.39	0.55
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.71	0.55
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.88	0.55
2:B:2347:GLU:O	2:B:2351:ASN:N	2.36	0.55
2:E:4190:ILE:CD1	2:E:5026:ASP:OD2	2.54	0.55
2:I:101:LEU:HD13	2:I:150:MET:HE1	1.88	0.55
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.55
2:I:2347:GLU:O	2:I:2351:ASN:N	2.36	0.55
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.88	0.55
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.95	0.55
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.71	0.55
2:I:4190:ILE:CD1	2:I:5026:ASP:OD2	2.54	0.55
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.55
2:I:23:GLN:HB3	2:I:201:ASN:HB2	1.88	0.55
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.88	0.55
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.71	0.55
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.71	0.55
2:G:4190:ILE:CD1	2:G:5026:ASP:OD2	2.54	0.55
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.88	0.55
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.88	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.55
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.89	0.55
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.88	0.55
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.90	0.55
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.89	0.55
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.95	0.55
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.88	0.55
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.89	0.54
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.87	0.54
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.80	0.54
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.88	0.54
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.89	0.54
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.89	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.41	0.54
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.88	0.54
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.81	0.54
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.88	0.54
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.95	0.54
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.54
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.89	0.54
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.90	0.54
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.88	0.54
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.41	0.54
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.90	0.54
2:E:331:VAL:HG12	2:E:333:GLY:H	1.73	0.54
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.81	0.54
2:B:111:HIS:HD2	2:B:114:SER:H	1.56	0.54
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.90	0.54
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.90	0.54
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.81	0.54
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.90	0.54
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.41	0.54
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.54
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.90	0.54
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.90	0.54
2:E:111:HIS:HD2	2:E:114:SER:H	1.56	0.54
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.90	0.54
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.70	0.54
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.90	0.54
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.41	0.54
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.39	0.54
2:G:111:HIS:HD2	2:G:114:SER:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.90	0.54
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.26	0.53
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.26	0.53
2:G:794:GLY:H	2:G:798:GLY:HA3	1.73	0.53
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.90	0.53
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.90	0.53
2:I:794:GLY:H	2:I:798:GLY:HA3	1.73	0.53
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.90	0.53
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.90	0.53
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.91	0.53
2:B:331:VAL:HG12	2:B:333:GLY:H	1.73	0.53
2:I:111:HIS:HD2	2:I:114:SER:H	1.56	0.53
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.41	0.53
2:B:794:GLY:H	2:B:798:GLY:HA3	1.73	0.53
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.89	0.53
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.91	0.53
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.90	0.53
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.90	0.53
2:B:1636:MET:HE2	2:B:1638:ALA:HB2	1.91	0.53
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.90	0.53
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.53
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.53
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.91	0.53
2:B:4942:GLU:HA	2:E:4944:ARG:HH22	1.73	0.53
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.42	0.53
2:I:313:SER:HB3	2:I:351:VAL:HB	1.91	0.53
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.26	0.53
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.42	0.53
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.74	0.53
2:E:794:GLY:H	2:E:798:GLY:HA3	1.74	0.53
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.90	0.53
2:I:331:VAL:HG12	2:I:333:GLY:H	1.73	0.53
2:G:331:VAL:HG12	2:G:333:GLY:H	1.73	0.53
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.53
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.26	0.53
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.92	0.52
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.52
2:B:2868:SER:O	2:B:2872:GLN:N	2.41	0.52
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.90	0.52
2:E:1636:MET:HE2	2:E:1638:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.43	0.52
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.52
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.75	0.52
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.82	0.52
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.39	0.52
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.75	0.52
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.42	0.52
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.75	0.52
2:E:313:SER:HB3	2:E:351:VAL:HB	1.91	0.52
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.42	0.52
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.75	0.52
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.92	0.52
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.92	0.52
2:B:313:SER:HB3	2:B:351:VAL:HB	1.91	0.52
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.90	0.52
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.91	0.52
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.92	0.52
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.52
2:I:1636:MET:HE2	2:I:1638:ALA:HB2	1.91	0.52
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.91	0.52
2:B:978:THR:HB	2:B:980:ALA:H	1.75	0.52
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.90	0.52
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.91	0.52
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.42	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.52
2:G:1636:MET:HE2	2:G:1638:ALA:HB2	1.91	0.51
2:G:4979:THR:HG22	3:G:5101:ATP:C2	2.45	0.51
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.75	0.51
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.75	0.51
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.43	0.51
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.43	0.51
1:F:27:THR:HB	1:F:100:ASP:HB3	1.93	0.51
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.43	0.51
2:B:4979:THR:HG22	3:B:5101:ATP:C2	2.45	0.51
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.82	0.51
2:G:313:SER:HB3	2:G:351:VAL:HB	1.91	0.51
2:E:485:SER:O	2:E:489:ASN:N	2.39	0.51
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.41	0.51
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.82	0.51
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.41	0.51
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.39	0.51
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.46	0.51
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.43	0.51
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.75	0.51
1:A:27:THR:HB	1:A:100:ASP:HB3	1.93	0.51
1:J:27:THR:HB	1:J:100:ASP:HB3	1.93	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.75	0.51
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.93	0.51
2:B:614:VAL:HG22	2:B:616:SER:H	1.75	0.51
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.82	0.51
2:E:4979:THR:HG22	3:E:5101:ATP:C2	2.45	0.51
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.93	0.51
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.42	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.51
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.43	0.51
2:G:614:VAL:HG22	2:G:616:SER:H	1.75	0.51
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.46	0.50
2:I:2758:PHE:O	2:I:2762:THR:N	2.45	0.50
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.45	0.50
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.93	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.45	0.50
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.45	0.50
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.50
2:I:4979:THR:HG22	3:I:5101:ATP:C2	2.45	0.50
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.94	0.50
1:H:27:THR:HB	1:H:100:ASP:HB3	1.93	0.50
2:E:978:THR:HB	2:E:980:ALA:H	1.75	0.50
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.94	0.50
2:I:614:VAL:HG22	2:I:616:SER:H	1.75	0.50
2:I:1457:UNK:N	2:I:1497:UNK:O	2.44	0.50
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.93	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.41	0.50
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.42	0.50
2:G:4239:GLU:OE2	2:G:5014:TYR:OH	2.28	0.50
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.30	0.50
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.93	0.50
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.45	0.50
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.93	0.50
2:G:2758:PHE:O	2:G:2762:THR:N	2.45	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.45	0.50
2:E:614:VAL:HG22	2:E:616:SER:H	1.75	0.50
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.42	0.50
2:E:2758:PHE:O	2:E:2762:THR:N	2.45	0.50
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.93	0.50
2:G:1457:UNK:N	2:G:1497:UNK:O	2.45	0.50
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.45	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.41	0.50
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.94	0.49
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.43	0.49
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.93	0.49
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.94	0.49
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.30	0.49
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.94	0.49
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.43	0.49
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.94	0.49
2:B:4230:LYS:CG	2:B:4959:PHE:CE1	2.95	0.49
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.30	0.49
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.94	0.49
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.94	0.49
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.94	0.49
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.93	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.45	0.49
2:I:4230:LYS:CG	2:I:4959:PHE:CE1	2.95	0.49
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.94	0.49
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.94	0.49
2:E:629:ARG:HD3	2:E:634:GLN:HG2	1.94	0.49
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.94	0.49
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.95	0.49
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.94	0.49
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.95	0.49
2:B:1457:UNK:N	2:B:1497:UNK:O	2.45	0.49
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.94	0.49
2:B:2758:PHE:O	2:B:2762:THR:N	2.45	0.49
2:I:642:THR:HG23	2:I:1613:LEU:HD12	1.95	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.49
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.95	0.49
2:B:642:THR:HG23	2:B:1613:LEU:HD12	1.95	0.49
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.95	0.49
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.45	0.49
2:E:4230:LYS:CG	2:E:4959:PHE:CE1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.46	0.49
2:I:629:ARG:HD3	2:I:634:GLN:HG2	1.94	0.49
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.41	0.49
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.45	0.49
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.95	0.49
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.95	0.49
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.94	0.49
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.94	0.49
2:G:629:ARG:HD3	2:G:634:GLN:HG2	1.94	0.49
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.45	0.49
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.31	0.49
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.46	0.49
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.94	0.49
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.94	0.48
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.95	0.48
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.48
2:G:3842:LEU:O	2:G:3929:SER:OG	2.31	0.48
2:G:4230:LYS:CG	2:G:4959:PHE:CE1	2.95	0.48
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	1.95	0.48
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.31	0.48
2:I:2868:SER:O	2:I:2872:GLN:N	2.41	0.48
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.45	0.48
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.94	0.48
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.95	0.48
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.48
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.45	0.48
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.96	0.48
2:B:629:ARG:HD3	2:B:634:GLN:HG2	1.94	0.48
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	1.95	0.48
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.93	0.48
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.46	0.48
2:B:111:HIS:CD2	2:B:114:SER:H	2.32	0.48
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	1.95	0.48
2:G:642:THR:HG23	2:G:1613:LEU:HD12	1.95	0.48
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.48
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.30	0.48
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.48
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.46	0.48
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.96	0.48
2:B:3842:LEU:O	2:B:3929:SER:OG	2.31	0.48
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3842:LEU:O	2:I:3929:SER:OG	2.31	0.48
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.95	0.48
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.96	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.48
2:B:3759:GLU:HA	2:B:3762:ARG:HE	1.78	0.48
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.45	0.48
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.94	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
2:I:3759:GLU:HA	2:I:3762:ARG:HE	1.78	0.48
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	1.95	0.48
2:G:111:HIS:CD2	2:G:114:SER:H	2.32	0.48
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.46	0.48
2:B:4984:ASN:C	2:B:4986:ALA:H	2.22	0.48
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.31	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.32	0.48
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.79	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:I:4984:ASN:C	2:I:4986:ALA:H	2.22	0.48
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.79	0.47
2:I:4954:MET:HE3	3:I:5101:ATP:H1'	1.96	0.47
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.94	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.47
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.31	0.47
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.96	0.47
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.79	0.47
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.79	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
2:G:4741:LEU:HB2	2:G:4743:MET:HE2	1.96	0.47
2:G:4954:MET:HE3	3:G:5101:ATP:H1'	1.96	0.47
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.96	0.47
2:B:4741:LEU:HB2	2:B:4743:MET:HE2	1.96	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.47
2:E:3759:GLU:HA	2:E:3762:ARG:HE	1.78	0.47
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.28	0.47
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.46	0.47
2:E:642:THR:HG23	2:E:1613:LEU:HD12	1.95	0.47
2:E:3842:LEU:O	2:E:3929:SER:OG	2.31	0.47
2:I:4741:LEU:HB2	2:I:4743:MET:HE2	1.96	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.39	0.47
2:G:3759:GLU:HA	2:G:3762:ARG:HE	1.78	0.47
2:E:111:HIS:CD2	2:E:114:SER:H	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.96	0.47
2:E:4741:LEU:HB2	2:E:4743:MET:HE2	1.96	0.47
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.79	0.47
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.79	0.47
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.79	0.47
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.79	0.47
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.96	0.47
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.96	0.47
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.96	0.47
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.96	0.47
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.97	0.47
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.97	0.47
2:E:4954:MET:HE3	3:E:5101:ATP:H1'	1.96	0.47
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.96	0.47
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.97	0.47
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.47
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.97	0.47
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.79	0.47
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.97	0.47
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.47	0.47
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.97	0.47
2:G:4984:ASN:C	2:G:4986:ALA:H	2.22	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.47
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.97	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:3676:ASP:HA	2:B:3679:LYS:HB3	1.97	0.47
2:B:4954:MET:HE3	3:B:5101:ATP:H1'	1.96	0.47
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.97	0.47
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.96	0.47
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.96	0.47
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.96	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.47
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.28	0.47
2:E:4984:ASN:C	2:E:4986:ALA:H	2.22	0.47
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.79	0.47
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.96	0.47
2:I:3676:ASP:HA	2:I:3679:LYS:HB3	1.97	0.47
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.79	0.47
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.79	0.46
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.96	0.46
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.79	0.46
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.79	0.46
2:I:4239:GLU:OE2	2:I:5014:TYR:OH	2.28	0.46
2:G:395:GLN:HG3	2:G:397:GLU:H	1.80	0.46
2:B:1738:LEU:HB3	2:B:2146:PRO:HG3	1.97	0.46
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.97	0.46
2:E:395:GLN:HG3	2:E:397:GLU:H	1.80	0.46
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.97	0.46
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.97	0.46
2:G:3676:ASP:HA	2:G:3679:LYS:HB3	1.97	0.46
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.79	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.96	0.46
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.97	0.46
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.98	0.46
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.97	0.46
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.97	0.46
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	1.98	0.46
2:B:134:ASP:OD1	2:B:134:ASP:N	2.48	0.46
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.98	0.46
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.96	0.46
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.49	0.46
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.49	0.46
2:G:1738:LEU:HB3	2:G:2146:PRO:HG3	1.97	0.46
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.98	0.46
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.98	0.46
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.96	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.46	0.46
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.97	0.46
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.97	0.46
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.96	0.46
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.97	0.46
2:B:485:SER:O	2:B:489:ASN:N	2.39	0.46
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.97	0.46
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.98	0.46
2:E:1738:LEU:HB3	2:E:2146:PRO:HG3	1.97	0.46
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	1.98	0.46
2:I:1738:LEU:HB3	2:I:2146:PRO:HG3	1.97	0.46
2:E:134:ASP:N	2:E:134:ASP:OD1	2.48	0.46
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.98	0.46
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.47	0.46
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.81	0.45
2:B:395:GLN:HG3	2:B:397:GLU:H	1.80	0.45
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.49	0.45
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.98	0.45
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.79	0.45
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.97	0.45
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	1.98	0.45
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.98	0.45
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.81	0.45
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.43	0.45
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.98	0.45
2:B:621:ILE:O	2:B:625:LEU:N	2.48	0.45
2:I:395:GLN:HG3	2:I:397:GLU:H	1.80	0.45
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	1.98	0.45
2:G:134:ASP:OD1	2:G:134:ASP:N	2.48	0.45
2:G:236:ALA:HA	2:G:242:ARG:HD2	1.98	0.45
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.98	0.45
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.97	0.45
2:B:2780:ASN:O	2:B:2787:THR:OG1	2.31	0.45
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.98	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.49	0.45
2:B:236:ALA:HA	2:B:242:ARG:HD2	1.98	0.45
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.27	0.45
2:E:3676:ASP:HA	2:E:3679:LYS:HB3	1.97	0.45
2:B:4963:ILE:HD13	2:B:5027:CYS:SG	2.57	0.45
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.97	0.45
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	1.98	0.45
2:I:4963:ILE:HD13	2:I:5027:CYS:SG	2.57	0.45
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.45
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.34	0.45
2:E:940:GLY:O	2:E:1052:ASN:N	2.49	0.45
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.99	0.45
2:I:236:ALA:HA	2:I:242:ARG:HD2	1.98	0.45
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	1.98	0.45
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.70	0.45
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.99	0.45
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.99	0.45
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.99	0.45
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.99	0.45
2:B:4571:PHE:O	2:B:4575:PHE:N	2.50	0.45
2:B:4729:GLY:HA2	2:B:4737:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.99	0.45
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.45
2:E:4571:PHE:O	2:E:4575:PHE:N	2.50	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.52	0.45
2:B:1516:UNK:N	2:B:1529:UNK:O	2.50	0.45
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.99	0.45
2:E:236:ALA:HA	2:E:242:ARG:HD2	1.98	0.45
2:E:309:THR:O	2:E:313:SER:OG	2.35	0.45
2:E:4963:ILE:HD13	2:E:5027:CYS:SG	2.57	0.45
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.34	0.45
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.98	0.45
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.99	0.44
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.98	0.44
2:B:4239:GLU:OE2	2:B:5014:TYR:OH	2.28	0.44
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.98	0.44
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.99	0.44
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.99	0.44
2:G:1516:UNK:N	2:G:1529:UNK:O	2.50	0.44
2:G:4729:GLY:HA2	2:G:4737:ILE:HG13	1.99	0.44
2:B:3910:THR:HG23	2:B:3911:THR:HG23	2.00	0.44
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.00	0.44
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.49	0.44
2:E:164:ARG:N	2:E:167:ASP:OD2	2.51	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.52	0.44
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.34	0.44
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.49	0.44
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	2.00	0.44
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.81	0.44
2:I:4142:ASN:HA	2:I:4145:VAL:HG12	2.00	0.44
2:G:3365:UNK:O	2:G:3369:UNK:N	2.51	0.44
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.99	0.44
2:G:4963:ILE:HD13	2:G:5027:CYS:SG	2.57	0.44
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.00	0.44
2:E:3910:THR:HG23	2:E:3911:THR:HG23	2.00	0.44
2:I:164:ARG:N	2:I:167:ASP:OD2	2.51	0.44
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.98	0.44
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.99	0.44
2:G:309:THR:O	2:G:313:SER:OG	2.35	0.44
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	2.00	0.44
2:G:4142:ASN:HA	2:G:4145:VAL:HG12	2.00	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.99	0.44
2:E:2780:ASN:O	2:E:2787:THR:OG1	2.31	0.44
2:I:134:ASP:OD1	2:I:134:ASP:N	2.49	0.44
2:I:266:ARG:NH1	2:I:332:GLU:OE2	2.51	0.44
2:I:309:THR:O	2:I:313:SER:OG	2.35	0.44
2:I:1516:UNK:N	2:I:1529:UNK:O	2.50	0.44
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.44
2:G:164:ARG:N	2:G:167:ASP:OD2	2.51	0.44
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.99	0.44
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.81	0.44
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.98	0.44
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.44
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.99	0.44
2:E:1516:UNK:N	2:E:1529:UNK:O	2.50	0.44
2:E:2159:LEU:HD22	2:E:2201:LEU:HD23	1.99	0.44
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.44
2:B:897:ARG:HB2	2:B:905:PRO:HG3	2.00	0.44
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	2.00	0.44
2:E:621:ILE:O	2:E:625:LEU:N	2.48	0.44
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	2.00	0.44
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.00	0.44
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	2.00	0.44
2:G:5028:PHE:O	2:G:5028:PHE:CG	2.70	0.44
2:B:2159:LEU:HD22	2:B:2201:LEU:HD23	1.99	0.44
2:E:3365:UNK:O	2:E:3369:UNK:N	2.51	0.44
2:I:224:HIS:N	2:I:229:GLU:O	2.46	0.44
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.00	0.44
2:I:2159:LEU:HD22	2:I:2201:LEU:HD23	1.99	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.51	0.44
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.44
2:G:897:ARG:HB2	2:G:905:PRO:HG3	2.00	0.44
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.83	0.43
2:E:4729:GLY:HA2	2:E:4737:ILE:HG13	1.99	0.43
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.70	0.43
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.99	0.43
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.50	0.43
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.43
2:G:497:TYR:HB3	2:G:500:ALA:HB2	2.00	0.43
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.00	0.43
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.00	0.43
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.43
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	1.98	0.43
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.00	0.43
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.84	0.43
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	2.00	0.43
2:E:4142:ASN:HA	2:E:4145:VAL:HG12	2.00	0.43
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.00	0.43
2:G:266:ARG:NH1	2:G:332:GLU:OE2	2.51	0.43
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.84	0.43
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.52	0.43
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.43
2:E:497:TYR:HB3	2:E:500:ALA:HB2	2.00	0.43
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.00	0.43
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	1.98	0.43
2:E:4697:VAL:O	2:E:4701:TRP:N	2.50	0.43
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.99	0.43
2:G:621:ILE:O	2:G:625:LEU:N	2.48	0.43
2:G:4571:PHE:O	2:G:4575:PHE:N	2.50	0.43
2:B:309:THR:O	2:B:313:SER:OG	2.35	0.43
2:B:4933:GLN:HG2	2:I:4930:ALA:HB2	2.00	0.43
2:B:5028:PHE:O	2:B:5028:PHE:CG	2.70	0.43
2:E:243:ARG:NH1	2:E:301:VAL:O	2.46	0.43
2:E:266:ARG:NH1	2:E:332:GLU:OE2	2.51	0.43
2:E:897:ARG:HB2	2:E:905:PRO:HG3	2.00	0.43
2:I:897:ARG:HB2	2:I:905:PRO:HG3	2.00	0.43
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.99	0.43
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.52	0.43
1:J:23:VAL:HG22	1:J:47:LYS:HG2	2.01	0.43
2:B:497:TYR:HB3	2:B:500:ALA:HB2	2.00	0.43
2:E:5028:PHE:O	2:E:5028:PHE:CG	2.70	0.43
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.00	0.43
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.84	0.43
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.00	0.43
1:A:23:VAL:HG22	1:A:47:LYS:HG2	2.01	0.43
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	2.00	0.43
2:I:4960:ILE:N	2:I:4960:ILE:CD1	2.73	0.43
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.50	0.43
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.00	0.43
2:B:4892:ARG:NH2	2:I:4898:GLY:O	2.52	0.43
2:G:4982:GLU:HB3	2:G:4983:HIS:H	1.67	0.43
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:I:4571:PHE:O	2:I:4575:PHE:N	2.50	0.43
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.00	0.43
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	2.00	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.00	0.43
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.52	0.43
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.43
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.01	0.43
2:I:497:TYR:HB3	2:I:500:ALA:HB2	2.00	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.00	0.42
2:E:2103:VAL:O	2:E:2107:GLN:N	2.46	0.42
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.51	0.42
1:F:23:VAL:HG22	1:F:47:LYS:HG2	2.01	0.42
1:F:30:LEU:HD23	1:F:33:GLY:HA3	2.01	0.42
2:B:266:ARG:NH1	2:B:332:GLU:OE2	2.51	0.42
2:I:4729:GLY:HA2	2:I:4737:ILE:HG13	1.99	0.42
1:H:30:LEU:HD23	1:H:33:GLY:HA3	2.01	0.42
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.52	0.42
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.02	0.42
2:E:4982:GLU:HB3	2:E:4983:HIS:H	1.67	0.42
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.52	0.42
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	2.00	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:B:164:ARG:N	2:B:167:ASP:OD2	2.51	0.42
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.00	0.42
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.50	0.42
2:I:485:SER:O	2:I:489:ASN:N	2.39	0.42
2:G:224:HIS:N	2:G:229:GLU:O	2.46	0.42
2:G:243:ARG:NH1	2:G:301:VAL:O	2.46	0.42
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.50	0.42
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.52	0.42
2:G:2159:LEU:HD22	2:G:2201:LEU:HD23	1.99	0.42
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.52	0.42
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.47	0.42
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	2.02	0.42
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.02	0.42
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.01	0.42
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.51	0.42
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.42
2:B:4558:ASN:OD1	2:B:4558:ASN:N	2.51	0.42
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4190:ILE:HD13	2:I:5026:ASP:OD2	2.19	0.42
1:A:30:LEU:HD23	1:A:33:GLY:HA3	2.01	0.42
1:H:23:VAL:HG22	1:H:47:LYS:HG2	2.01	0.42
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.53	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.51	0.42
1:J:30:LEU:HD23	1:J:33:GLY:HA3	2.01	0.42
2:B:3992:PHE:O	2:B:3996:PHE:N	2.42	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.42
2:E:4984:ASN:C	2:E:4986:ALA:N	2.78	0.42
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.01	0.42
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.02	0.42
2:G:4984:ASN:C	2:G:4986:ALA:N	2.78	0.42
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.53	0.42
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	2.02	0.42
2:I:621:ILE:O	2:I:625:LEU:N	2.48	0.42
2:B:206:CYS:SG	2:B:207:SER:N	2.93	0.41
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.02	0.41
2:B:4984:ASN:C	2:B:4986:ALA:N	2.78	0.41
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.02	0.41
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.02	0.41
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.02	0.41
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.51	0.41
2:B:4230:LYS:CD	2:B:4959:PHE:CE1	2.83	0.41
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.02	0.41
2:E:3781:GLN:HA	2:E:3784:SER:HB3	2.02	0.41
2:E:4189:ARG:NH1	2:E:5032:TYR:OH	2.53	0.41
2:I:940:GLY:O	2:I:1052:ASN:N	2.49	0.41
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.53	0.41
2:G:358:THR:HG21	2:G:382:GLY:HA2	2.02	0.41
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.49	0.41
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.53	0.41
2:G:2212:VAL:O	2:G:2216:GLY:N	2.45	0.41
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.02	0.41
2:B:4958:CYS:O	2:B:4958:CYS:SG	2.79	0.41
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.94	0.41
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.41
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.41
2:E:215:THR:HG22	2:E:273:HIS:HA	2.03	0.41
2:E:359:TYR:HA	2:E:376:ALA:HA	2.02	0.41
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.41	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.03	0.41
2:B:215:THR:HG22	2:B:273:HIS:HA	2.03	0.41
2:E:206:CYS:SG	2:E:207:SER:N	2.93	0.41
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.86	0.41
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.92	0.41
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	2.03	0.41
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	2.02	0.41
2:I:4984:ASN:C	2:I:4986:ALA:N	2.78	0.41
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.47	0.41
2:G:1671:ARG:NH2	2:G:1713:ASP:HB3	2.36	0.41
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.28	0.41
2:B:1671:ARG:NH2	2:B:1713:ASP:HB3	2.36	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.41
2:B:4189:ARG:NH1	2:B:5032:TYR:OH	2.53	0.41
2:E:1595:LEU:HD23	2:E:1595:LEU:HA	1.96	0.41
2:I:358:THR:HG21	2:I:382:GLY:HA2	2.02	0.41
2:I:707:VAL:HG23	2:I:713:SER:HB2	2.03	0.41
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.52	0.41
2:G:206:CYS:SG	2:G:207:SER:N	2.93	0.41
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.54	0.41
2:G:2339:VAL:HG12	2:G:2345:SER:H	1.86	0.41
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.41
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.03	0.41
2:E:358:THR:HG21	2:E:382:GLY:HA2	2.02	0.41
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	2.02	0.41
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.03	0.41
2:I:215:THR:HG22	2:I:273:HIS:HA	2.03	0.41
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.70	0.41
2:G:378:LEU:HD23	2:G:378:LEU:HA	1.88	0.41
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.94	0.41
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.02	0.41
2:B:168:ASP:HB3	2:B:199:LEU:HD22	2.02	0.41
2:B:2339:VAL:HG12	2:B:2345:SER:H	1.85	0.41
2:B:4865:LYS:HB2	2:B:4873:ASP:HB3	2.03	0.41
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.53	0.41
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.53	0.41
2:I:243:ARG:NH1	2:I:301:VAL:O	2.46	0.41
2:G:359:TYR:HA	2:G:376:ALA:HA	2.02	0.41
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	2.03	0.41
2:G:940:GLY:O	2:G:1052:ASN:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.86	0.41
1:J:82:TYR:O	1:J:86:GLY:N	2.54	0.41
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.01	0.41
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	2.03	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.56	0.41
2:B:3781:GLN:HA	2:B:3784:SER:HB3	2.02	0.41
2:E:224:HIS:N	2:E:229:GLU:O	2.46	0.41
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.01	0.41
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.54	0.41
2:E:2339:VAL:HG12	2:E:2345:SER:H	1.86	0.41
2:I:168:ASP:HB3	2:I:199:LEU:HD22	2.02	0.41
2:I:359:TYR:HA	2:I:376:ALA:HA	2.02	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.86	0.41
2:I:1671:ARG:NH2	2:I:1713:ASP:HB3	2.36	0.41
2:I:2543:UNK:O	2:I:2547:UNK:N	2.54	0.41
2:I:4958:CYS:O	2:I:4958:CYS:SG	2.79	0.41
2:I:4982:GLU:N	2:I:4982:GLU:OE1	2.54	0.41
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.03	0.41
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.56	0.41
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	2.02	0.41
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.35	0.41
2:G:4951:LYS:HE2	2:G:4951:LYS:HB3	1.96	0.41
2:B:378:LEU:HD23	2:B:378:LEU:HA	1.88	0.41
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.94	0.41
2:B:2305:CYS:O	2:B:2324:ASN:ND2	2.54	0.41
2:E:168:ASP:HB3	2:E:199:LEU:HD22	2.03	0.41
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.49	0.41
2:E:2543:UNK:O	2:E:2547:UNK:N	2.54	0.41
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.86	0.41
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.41	0.41
2:I:2880:GLU:O	2:I:2884:ASN:N	2.53	0.41
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.86	0.41
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	2.03	0.41
2:G:4697:VAL:O	2:G:4701:TRP:N	2.50	0.41
2:G:4958:CYS:O	2:G:4958:CYS:SG	2.79	0.41
2:B:358:THR:HG21	2:B:382:GLY:HA2	2.02	0.40
2:B:707:VAL:HG23	2:B:713:SER:HB2	2.03	0.40
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	2.03	0.40
2:B:4968:PHE:CZ	2:B:4978:HIS:HE1	2.37	0.40
2:B:4982:GLU:OE1	2:B:4982:GLU:N	2.54	0.40
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:206:CYS:SG	2:I:207:SER:N	2.93	0.40
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	2.03	0.40
2:I:4933:GLN:HG2	2:G:4930:ALA:HB2	2.03	0.40
2:I:4982:GLU:HB3	2:I:4983:HIS:H	1.67	0.40
2:G:215:THR:HG22	2:G:273:HIS:HA	2.03	0.40
2:G:575:LEU:HD22	2:G:609:CYS:HB3	2.03	0.40
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	2.03	0.40
1:H:82:TYR:O	1:H:86:GLY:N	2.54	0.40
1:H:92:PRO:HD3	2:G:627:PRO:HB2	2.02	0.40
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.86	0.40
2:B:1865:MET:SD	2:B:1865:MET:N	2.95	0.40
2:B:4138:ASP:N	2:B:4138:ASP:OD1	2.52	0.40
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.02	0.40
2:E:4930:ALA:HB2	2:G:4933:GLN:HG2	2.03	0.40
2:I:1865:MET:N	2:I:1865:MET:SD	2.94	0.40
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.04	0.40
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	2.03	0.40
2:G:168:ASP:HB3	2:G:199:LEU:HD22	2.02	0.40
2:B:870:ILE:HD12	2:B:870:ILE:HA	1.92	0.40
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.40
2:E:378:LEU:HD23	2:E:378:LEU:HA	1.88	0.40
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	2.03	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.36	0.40
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.56	0.40
2:E:3992:PHE:O	2:E:3996:PHE:N	2.42	0.40
2:E:4982:GLU:OE1	2:E:4982:GLU:N	2.54	0.40
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.94	0.40
2:I:560:ILE:HA	2:I:563:VAL:HG12	2.04	0.40
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.54	0.40
2:I:2339:VAL:HG12	2:I:2345:SER:H	1.86	0.40
2:I:3781:GLN:HA	2:I:3784:SER:HB3	2.02	0.40
2:I:4697:VAL:O	2:I:4701:TRP:N	2.50	0.40
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.04	0.40
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.79	0.40
2:G:4865:LYS:HB2	2:G:4873:ASP:HB3	2.03	0.40
2:B:560:ILE:HA	2:B:563:VAL:HG12	2.04	0.40
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	2.03	0.40
2:B:2543:UNK:O	2:B:2547:UNK:N	2.54	0.40
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.02	0.40
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.04	0.40
2:E:2212:VAL:O	2:E:2216:GLY:N	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3992:PHE:O	2:I:3996:PHE:N	2.42	0.40
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	2.02	0.40
2:G:4189:ARG:NH1	2:G:5032:TYR:OH	2.53	0.40
2:B:2212:VAL:O	2:B:2216:GLY:N	2.45	0.40
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.54	0.40
2:B:2880:GLU:O	2:B:2884:ASN:N	2.53	0.40
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.04	0.40
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.03	0.40
2:E:2145:SER:HB2	2:E:3647:HIS:CE1	2.57	0.40
2:E:2305:CYS:O	2:E:2324:ASN:ND2	2.55	0.40
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	2.03	0.40
2:I:2305:CYS:O	2:I:2324:ASN:ND2	2.54	0.40
2:I:2780:ASN:O	2:I:2787:THR:OG1	2.31	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%)	2906 (90%)	323 (10%)	6 (0%)	43	77
2	E	3235/4416 (73%)	2908 (90%)	321 (10%)	6 (0%)	43	77
2	G	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	43	77
2	I	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	43	77
All	All	13360/18096 (74%)	12010 (90%)	1326 (10%)	24 (0%)	44	77

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG
2	B	4985	LEU
2	E	1708	ARG
2	E	4985	LEU
2	I	1708	ARG
2	I	4985	LEU
2	G	1708	ARG
2	G	4985	LEU
2	B	1840	PRO
2	E	1840	PRO
2	I	1840	PRO
2	G	1840	PRO
2	B	4641	PRO
2	E	4641	PRO
2	I	4641	PRO
2	G	4641	PRO
2	B	1932	PRO
2	E	1932	PRO
2	I	1932	PRO
2	G	1932	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
2	G	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
2	I	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
All	All	10324/12444 (83%)	10268 (100%)	56 (0%)	78	81

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	719	LEU
2	B	978	THR
2	B	1600	LEU
2	B	1676	LEU
2	B	2339	VAL
2	B	3663	LEU
2	B	3805	LEU
2	B	4166	LEU
2	B	4957	LYS
2	B	4958	CYS
2	B	4960	ILE
2	B	4983	HIS
2	B	5027	CYS
2	E	131	LEU
2	E	719	LEU
2	E	978	THR
2	E	1600	LEU
2	E	1676	LEU
2	E	2339	VAL
2	E	3663	LEU
2	E	3805	LEU
2	E	4166	LEU
2	E	4957	LYS
2	E	4958	CYS
2	E	4960	ILE
2	E	4983	HIS
2	E	5027	CYS
2	I	131	LEU
2	I	719	LEU
2	I	978	THR
2	I	1600	LEU
2	I	1676	LEU

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Mol	Chain	Res	Type
2	I	2339	VAL
2	I	3663	LEU
2	I	3805	LEU
2	I	4166	LEU
2	I	4957	LYS
2	I	4958	CYS
2	I	4960	ILE
2	I	4983	HIS
2	I	5027	CYS
2	G	131	LEU
2	G	719	LEU
2	G	978	THR
2	G	1600	LEU
2	G	1676	LEU
2	G	2339	VAL
2	G	3663	LEU
2	G	3805	LEU
2	G	4166	LEU
2	G	4957	LYS
2	G	4958	CYS
2	G	4960	ILE
2	G	4983	HIS
2	G	5027	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (250) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	32	ASN
1	F	43	ASN
1	F	87	HIS
1	A	32	ASN
1	A	43	ASN
1	A	87	HIS
1	H	32	ASN
1	H	43	ASN
1	H	87	HIS
1	J	32	ASN
1	J	43	ASN
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	224	HIS

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Mol	Chain	Res	Type
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	412	ASN
2	B	489	ASN
2	B	520	ASN
2	B	582	HIS
2	B	725	HIS
2	B	765	GLN
2	B	838	HIS
2	B	877	ASN
2	B	1041	GLN
2	B	1274	HIS
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	1949	GLN
2	B	1970	GLN
2	B	2005	GLN
2	B	2041	HIS
2	B	2127	GLN
2	B	2194	HIS
2	B	2324	ASN
2	B	2349	ASN
2	B	2763	HIS
2	B	2772	GLN
2	B	2773	ASN
2	B	3704	HIS
2	B	3809	ASN
2	B	3814	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3994	HIS
2	B	4034	ASN

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Mol	Chain	Res	Type
2	B	4054	ASN
2	B	4109	GLN
2	B	4133	GLN
2	B	4246	GLN
2	B	4691	GLN
2	B	4728	HIS
2	B	4776	GLN
2	B	4803	HIS
2	B	4806	ASN
2	B	4947	GLN
2	B	4973	HIS
2	B	4983	HIS
2	B	4987	ASN
2	B	5006	GLN
2	B	5031	GLN
2	E	57	ASN
2	E	111	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	412	ASN
2	E	489	ASN
2	E	520	ASN
2	E	582	HIS
2	E	725	HIS
2	E	765	GLN
2	E	838	HIS
2	E	877	ASN
2	E	1041	GLN
2	E	1274	HIS
2	E	1665	HIS
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1760	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	1949	GLN
2	E	1970	GLN

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Mol	Chain	Res	Type
2	E	2005	GLN
2	E	2041	HIS
2	E	2127	GLN
2	E	2194	HIS
2	E	2324	ASN
2	E	2349	ASN
2	E	2763	HIS
2	E	2772	GLN
2	E	2773	ASN
2	E	3704	HIS
2	E	3809	ASN
2	E	3814	GLN
2	E	3830	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3994	HIS
2	E	4034	ASN
2	E	4054	ASN
2	E	4109	GLN
2	E	4133	GLN
2	E	4246	GLN
2	E	4728	HIS
2	E	4803	HIS
2	E	4806	ASN
2	E	4947	GLN
2	E	4973	HIS
2	E	4983	HIS
2	E	4987	ASN
2	E	5006	GLN
2	E	5031	GLN
2	I	57	ASN
2	I	111	HIS
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	412	ASN
2	I	489	ASN
2	I	520	ASN

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Mol	Chain	Res	Type
2	I	582	HIS
2	I	725	HIS
2	I	765	GLN
2	I	838	HIS
2	I	877	ASN
2	I	1665	HIS
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	1949	GLN
2	I	1970	GLN
2	I	2005	GLN
2	I	2041	HIS
2	I	2127	GLN
2	I	2194	HIS
2	I	2324	ASN
2	I	2349	ASN
2	I	2763	HIS
2	I	2772	GLN
2	I	3704	HIS
2	I	3809	ASN
2	I	3814	GLN
2	I	3830	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3994	HIS
2	I	4034	ASN
2	I	4054	ASN
2	I	4109	GLN
2	I	4133	GLN
2	I	4246	GLN
2	I	4691	GLN
2	I	4728	HIS
2	I	4803	HIS
2	I	4806	ASN

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Mol	Chain	Res	Type
2	I	4947	GLN
2	I	4973	HIS
2	I	4983	HIS
2	I	4987	ASN
2	I	5006	GLN
2	I	5031	GLN
2	G	57	ASN
2	G	111	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	412	ASN
2	G	489	ASN
2	G	520	ASN
2	G	582	HIS
2	G	725	HIS
2	G	765	GLN
2	G	838	HIS
2	G	877	ASN
2	G	1220	GLN
2	G	1274	HIS
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	1949	GLN
2	G	2005	GLN
2	G	2041	HIS
2	G	2127	GLN
2	G	2194	HIS
2	G	2260	ASN
2	G	2324	ASN
2	G	2349	ASN
2	G	2763	HIS
2	G	2772	GLN
2	G	2773	ASN

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Mol	Chain	Res	Type
2	G	3704	HIS
2	G	3809	ASN
2	G	3814	GLN
2	G	3830	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3994	HIS
2	G	4034	ASN
2	G	4054	ASN
2	G	4109	GLN
2	G	4133	GLN
2	G	4246	GLN
2	G	4691	GLN
2	G	4728	HIS
2	G	4776	GLN
2	G	4803	HIS
2	G	4806	ASN
2	G	4947	GLN
2	G	4973	HIS
2	G	4983	HIS
2	G	4987	ASN
2	G	5006	GLN
2	G	5031	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CFF	B	5102	-	15,15,15	1.92	4 (26%)	23,23,23	2.86	11 (47%)
3	ATP	E	5101	-	32,33,33	1.36	5 (15%)	48,52,52	1.79	9 (18%)
4	CFF	I	5102	-	15,15,15	1.92	4 (26%)	23,23,23	2.86	11 (47%)
4	CFF	E	5102	-	15,15,15	1.91	4 (26%)	23,23,23	2.85	11 (47%)
4	CFF	G	5102	-	15,15,15	1.91	4 (26%)	23,23,23	2.85	11 (47%)
3	ATP	I	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.77	9 (18%)
3	ATP	B	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.78	9 (18%)
3	ATP	G	5101	-	32,33,33	1.35	5 (15%)	48,52,52	1.79	9 (18%)

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
4	CFF	B	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	B	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	G	5101	-	-	5/22/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5101	ATP	C5-C4	4.10	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	ATP	C5-C4	4.05	1.46	1.39
3	G	5101	ATP	C5-C4	4.05	1.46	1.39
3	I	5101	ATP	C5-C4	4.03	1.46	1.39
4	I	5102	CFF	C6-N1	-3.95	1.32	1.40
4	B	5102	CFF	C6-N1	-3.91	1.32	1.40
4	G	5102	CFF	C6-N1	-3.91	1.32	1.40
4	E	5102	CFF	C6-N1	-3.90	1.32	1.40
4	E	5102	CFF	C4-N3	-2.83	1.33	1.38
3	E	5101	ATP	C5-N7	-2.81	1.34	1.39
3	G	5101	ATP	C5-N7	-2.81	1.34	1.39
3	B	5101	ATP	C5-N7	-2.81	1.34	1.39
3	I	5101	ATP	C5-N7	-2.81	1.34	1.39
4	B	5102	CFF	C4-N3	-2.80	1.33	1.38
4	I	5102	CFF	C4-N3	-2.80	1.33	1.38
4	G	5102	CFF	C4-N3	-2.78	1.33	1.38
4	B	5102	CFF	C5-N7	-2.31	1.34	1.38
4	E	5102	CFF	C5-N7	-2.31	1.34	1.38
4	G	5102	CFF	C5-N7	-2.31	1.34	1.38
4	I	5102	CFF	C5-N7	-2.29	1.34	1.38
4	G	5102	CFF	O13-C6	-2.22	1.18	1.23
4	B	5102	CFF	O13-C6	-2.21	1.18	1.23
4	I	5102	CFF	O13-C6	-2.21	1.18	1.23
3	G	5101	ATP	C4-N9	-2.20	1.33	1.37
3	E	5101	ATP	C4-N9	-2.19	1.33	1.37
3	B	5101	ATP	C5-C6	2.19	1.47	1.41
3	I	5101	ATP	C5-C6	2.19	1.47	1.41
3	B	5101	ATP	C4-N9	-2.18	1.33	1.37
3	E	5101	ATP	C5-C6	2.18	1.47	1.41
3	G	5101	ATP	C5-C6	2.18	1.47	1.41
4	E	5102	CFF	O13-C6	-2.17	1.18	1.23
3	I	5101	ATP	C4-N9	-2.14	1.33	1.37
3	E	5101	ATP	C8-N7	2.09	1.35	1.31
3	I	5101	ATP	C8-N7	2.09	1.35	1.31
3	B	5101	ATP	C8-N7	2.06	1.35	1.31
3	G	5101	ATP	C8-N7	2.06	1.35	1.31

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5102	CFF	C14-N7-C8	-7.58	112.09	126.28
4	I	5102	CFF	C14-N7-C8	-7.58	112.09	126.28
4	E	5102	CFF	C14-N7-C8	-7.57	112.11	126.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C14-N7-C8	-7.56	112.14	126.28
3	E	5101	ATP	C5-C4-N3	-5.94	118.53	126.72
3	B	5101	ATP	C5-C4-N3	-5.92	118.56	126.72
3	G	5101	ATP	C5-C4-N3	-5.92	118.56	126.72
3	I	5101	ATP	C5-C4-N3	-5.90	118.59	126.72
3	E	5101	ATP	N3-C4-N9	5.05	135.75	127.17
3	B	5101	ATP	N3-C4-N9	5.02	135.70	127.17
3	G	5101	ATP	N3-C4-N9	5.00	135.67	127.17
3	I	5101	ATP	N3-C4-N9	4.99	135.66	127.17
4	I	5102	CFF	C14-N7-C5	4.95	139.56	127.77
4	B	5102	CFF	C14-N7-C5	4.94	139.52	127.77
4	E	5102	CFF	C14-N7-C5	4.92	139.47	127.77
4	G	5102	CFF	C14-N7-C5	4.92	139.47	127.77
4	E	5102	CFF	C5-C6-N1	4.69	120.64	112.06
4	G	5102	CFF	C5-C6-N1	4.68	120.64	112.06
4	B	5102	CFF	C5-C6-N1	4.66	120.60	112.06
4	I	5102	CFF	C5-C6-N1	4.66	120.59	112.06
3	E	5101	ATP	C2-N3-C4	3.70	120.86	111.83
3	G	5101	ATP	C2-N3-C4	3.68	120.83	111.83
3	B	5101	ATP	C2-N3-C4	3.68	120.82	111.83
3	I	5101	ATP	C2-N3-C4	3.66	120.78	111.83
4	G	5102	CFF	C6-N1-C2	-3.64	119.74	125.66
4	E	5102	CFF	C6-N1-C2	-3.63	119.77	125.66
4	B	5102	CFF	C6-N1-C2	-3.62	119.77	125.66
4	I	5102	CFF	C6-N1-C2	-3.62	119.78	125.66
3	E	5101	ATP	C4-N9-C8	3.34	109.25	105.74
3	G	5101	ATP	C4-N9-C8	3.30	109.20	105.74
3	G	5101	ATP	N3-C2-N1	-3.29	123.60	128.58
3	B	5101	ATP	C4-N9-C8	3.29	109.19	105.74
3	E	5101	ATP	N3-C2-N1	-3.28	123.62	128.58
3	B	5101	ATP	N3-C2-N1	-3.26	123.64	128.58
3	I	5101	ATP	C4-N9-C8	3.25	109.15	105.74
3	I	5101	ATP	N3-C2-N1	-3.23	123.69	128.58
4	I	5102	CFF	N3-C4-N9	3.14	131.21	126.27
4	B	5102	CFF	N3-C4-N9	3.12	131.17	126.27
4	G	5102	CFF	N3-C4-N9	3.09	131.13	126.27
4	E	5102	CFF	N3-C4-N9	3.09	131.12	126.27
4	E	5102	CFF	N7-C8-N9	-3.07	107.92	113.48
4	B	5102	CFF	N7-C8-N9	-3.07	107.92	113.48
4	I	5102	CFF	N7-C8-N9	-3.06	107.94	113.48
4	G	5102	CFF	N7-C8-N9	-3.05	107.95	113.48
3	G	5101	ATP	C4-C5-N7	-3.05	107.10	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5101	ATP	C4-C5-N7	-3.03	107.11	110.58
3	B	5101	ATP	C4-C5-N7	-3.01	107.14	110.58
3	I	5101	ATP	C4-C5-N7	-2.98	107.18	110.58
4	B	5102	CFF	O13-C6-C5	-2.88	120.49	126.38
4	I	5102	CFF	O13-C6-C5	-2.88	120.49	126.38
4	G	5102	CFF	O13-C6-C5	-2.88	120.49	126.38
4	E	5102	CFF	O13-C6-C5	-2.87	120.50	126.38
4	E	5102	CFF	C6-C5-C4	-2.86	119.31	122.92
4	G	5102	CFF	C6-C5-C4	-2.83	119.36	122.92
4	B	5102	CFF	C6-C5-C4	-2.83	119.36	122.92
4	I	5102	CFF	C6-C5-C4	-2.79	119.40	122.92
3	G	5101	ATP	C5-N7-C8	2.66	107.62	103.45
3	E	5101	ATP	C5-N7-C8	2.63	107.59	103.45
3	B	5101	ATP	C5-N7-C8	2.63	107.58	103.45
3	I	5101	ATP	C5-N7-C8	2.61	107.55	103.45
3	G	5101	ATP	N9-C8-N7	-2.55	110.31	113.94
3	E	5101	ATP	N9-C8-N7	-2.53	110.34	113.94
3	B	5101	ATP	N9-C8-N7	-2.53	110.35	113.94
3	I	5101	ATP	N9-C8-N7	-2.50	110.39	113.94
4	G	5102	CFF	C10-N1-C2	2.41	121.53	117.33
4	B	5102	CFF	C10-N1-C2	2.41	121.53	117.33
4	E	5102	CFF	C10-N1-C2	2.41	121.53	117.33
4	B	5102	CFF	C12-N3-C4	-2.40	117.21	120.75
4	G	5102	CFF	C12-N3-C4	-2.40	117.22	120.75
4	I	5102	CFF	C10-N1-C2	2.39	121.50	117.33
4	I	5102	CFF	C12-N3-C4	-2.39	117.22	120.75
4	G	5102	CFF	C12-N3-C2	2.39	121.50	117.33
4	B	5102	CFF	C12-N3-C2	2.37	121.46	117.33
4	E	5102	CFF	C12-N3-C4	-2.36	117.26	120.75
4	I	5102	CFF	C12-N3-C2	2.36	121.45	117.33
4	E	5102	CFF	C12-N3-C2	2.35	121.43	117.33
3	G	5101	ATP	O4'-C1'-N9	2.07	112.06	108.09
3	E	5101	ATP	O4'-C1'-N9	2.06	112.05	108.09
3	B	5101	ATP	O4'-C1'-N9	2.06	112.04	108.09
3	I	5101	ATP	O4'-C1'-N9	2.05	112.03	108.09

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O3A

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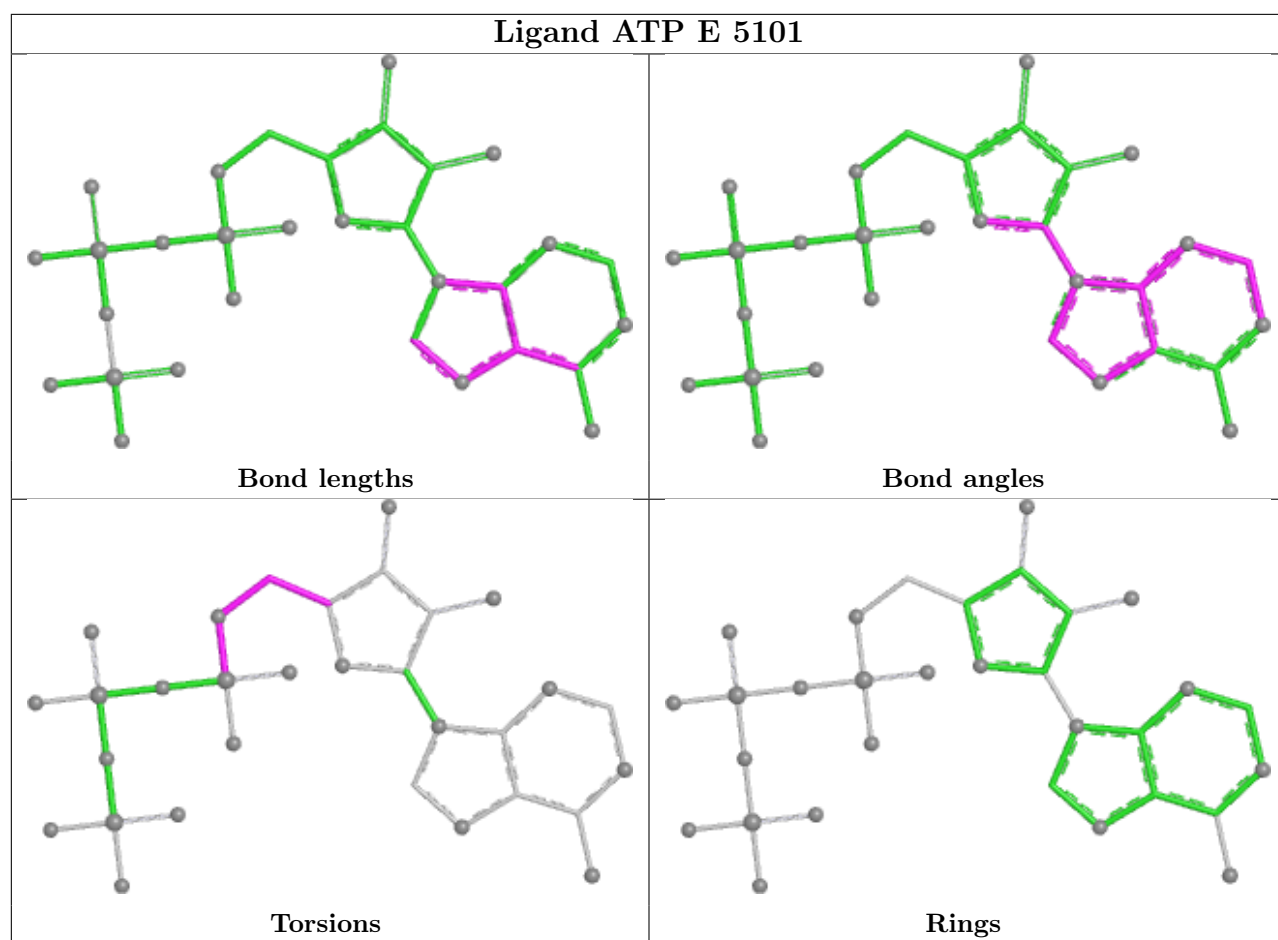
Mol	Chain	Res	Type	Atoms
3	I	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	B	5101	ATP	C3'-C4'-C5'-O5'
3	E	5101	ATP	O4'-C4'-C5'-O5'
3	E	5101	ATP	C3'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	C3'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	C3'-C4'-C5'-O5'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

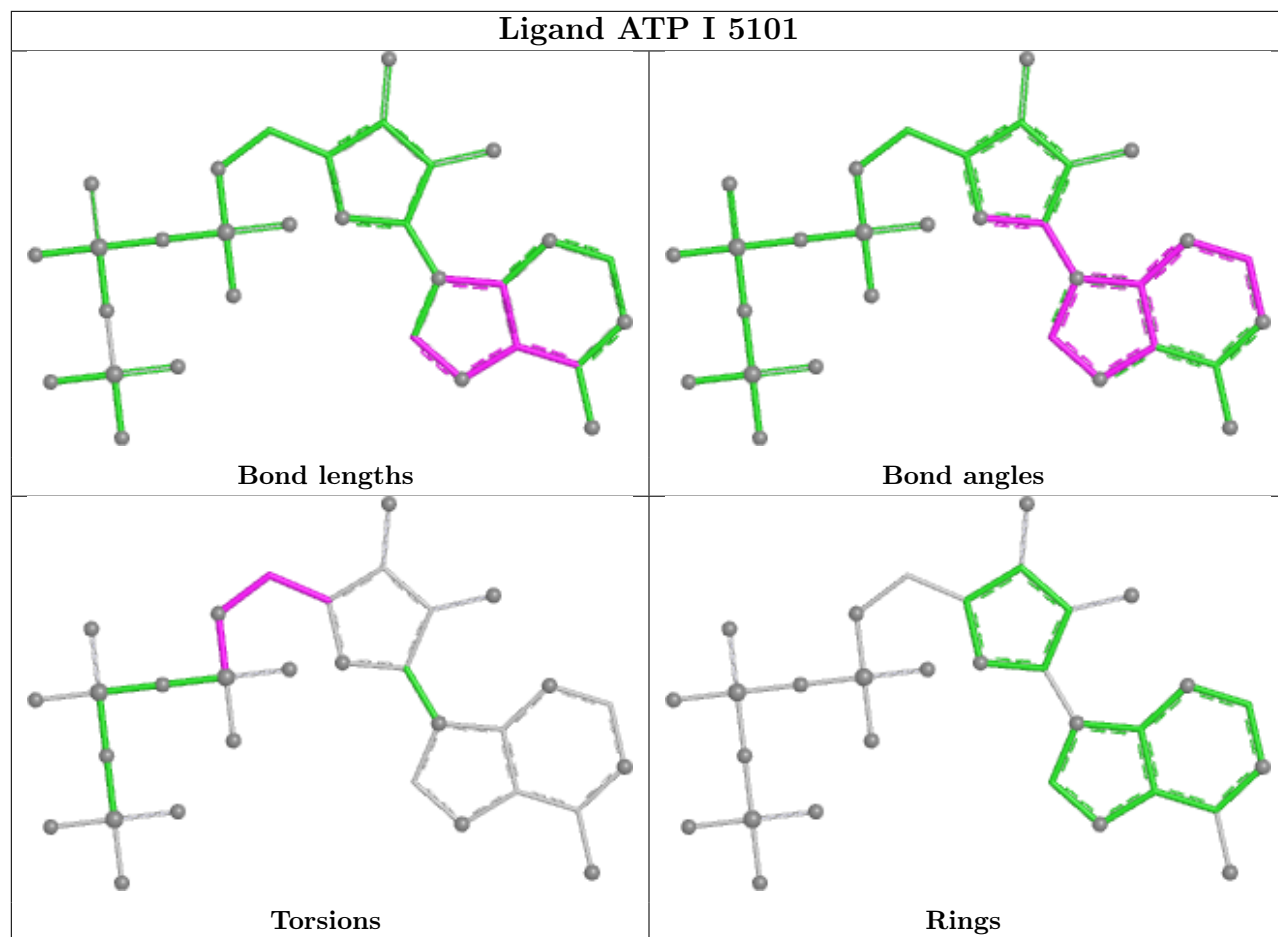
There are no ring outliers.

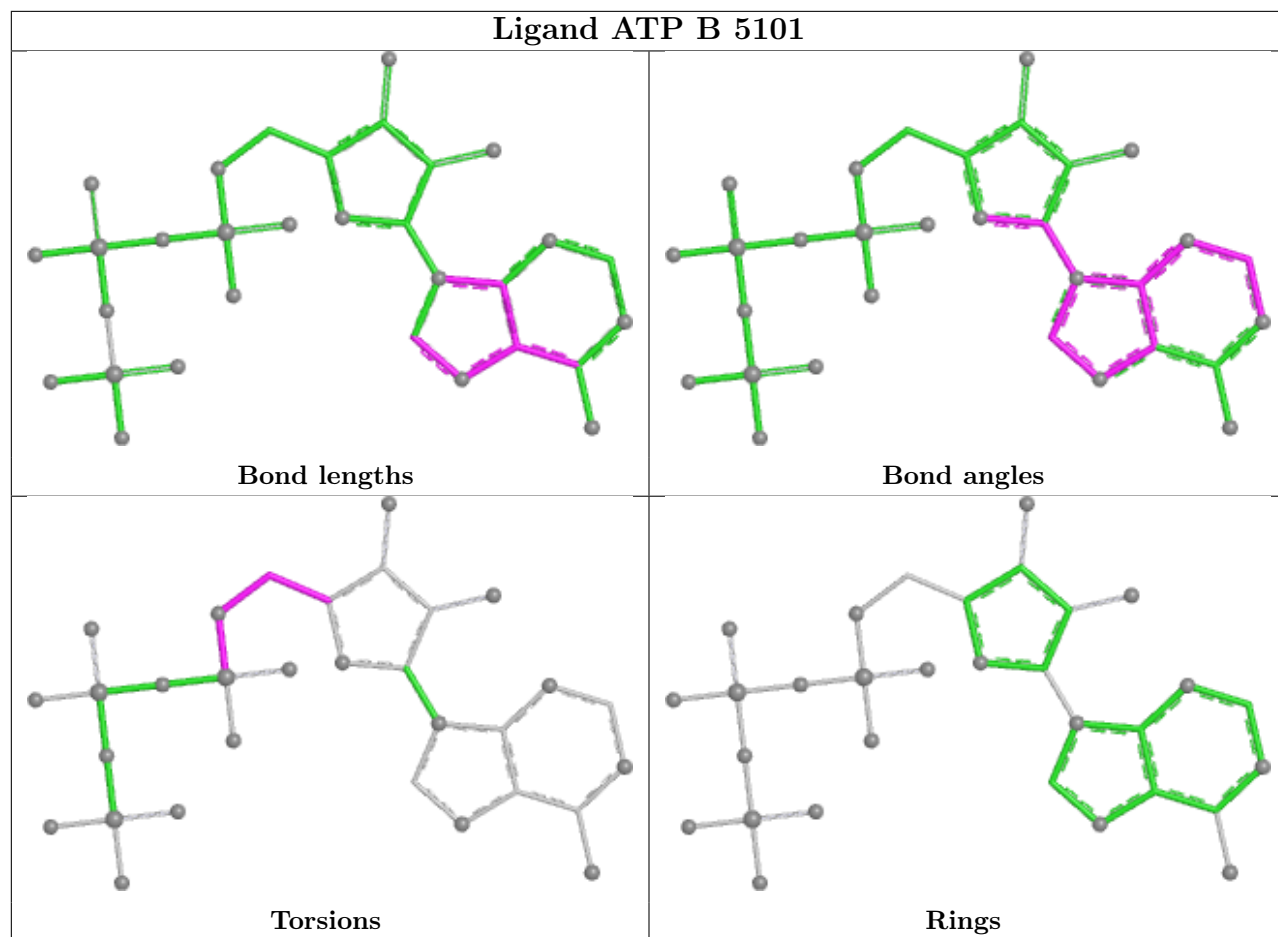
4 monomers are involved in 12 short contacts:

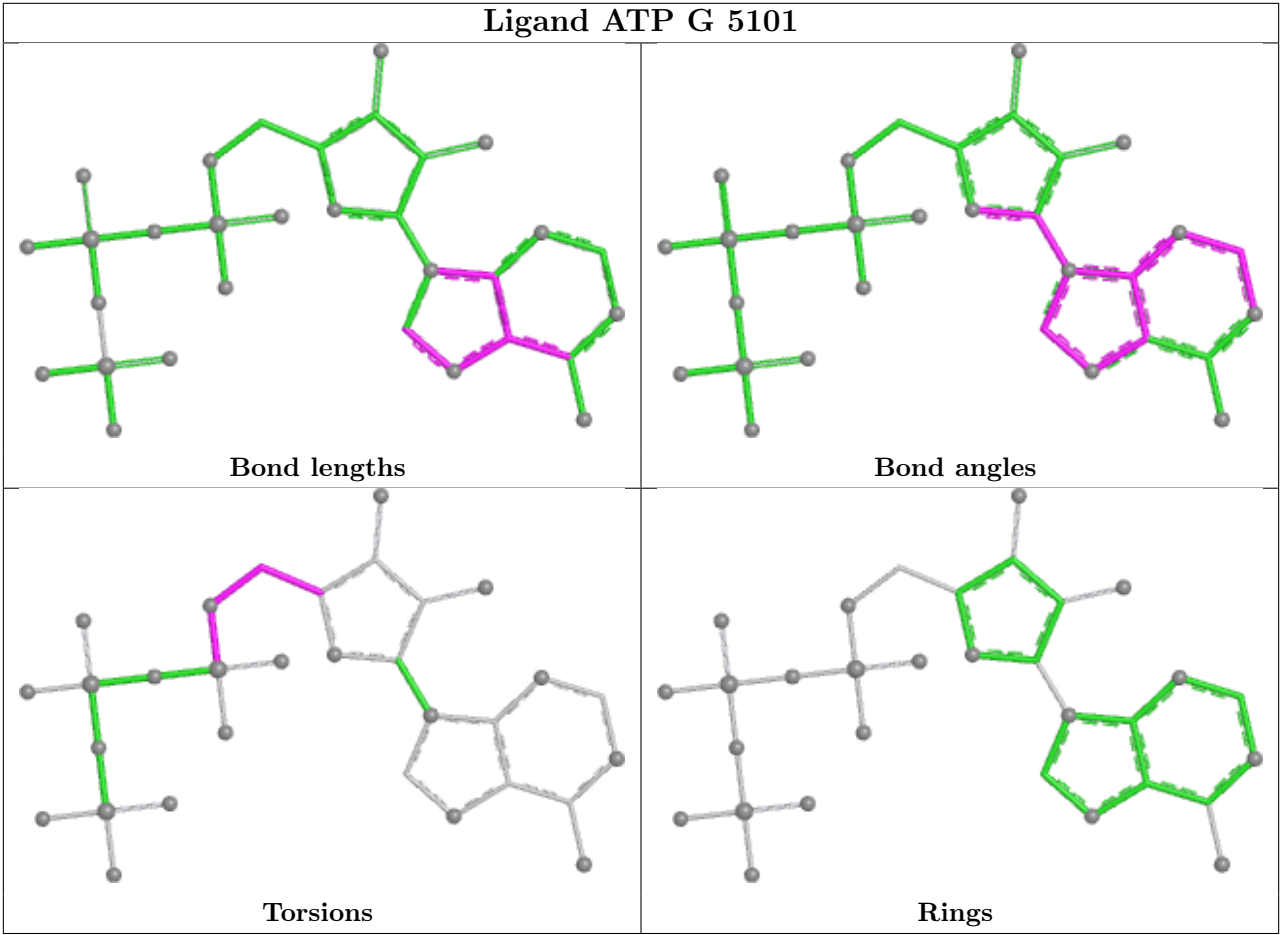
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	3	0
3	I	5101	ATP	3	0
3	B	5101	ATP	3	0
3	G	5101	ATP	3	0

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	E	14
2	I	14
2	G	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	74.00
1	E	4345:UNK	C	4540:PHE	N	74.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	74.00
1	G	4345:UNK	C	4540:PHE	N	74.00
1	B	3613:UNK	C	3639:THR	N	43.80
1	E	3613:UNK	C	3639:THR	N	43.80
1	I	3613:UNK	C	3639:THR	N	43.80
1	G	3613:UNK	C	3639:THR	N	43.80
1	B	4253:GLU	C	4320:UNK	N	26.28
1	E	4253:GLU	C	4320:UNK	N	26.28
1	I	4253:GLU	C	4320:UNK	N	26.28
1	G	4253:GLU	C	4320:UNK	N	26.28
1	G	3163:UNK	C	3170:UNK	N	16.13
1	B	3163:UNK	C	3170:UNK	N	16.12
1	E	3163:UNK	C	3170:UNK	N	16.12
1	I	3163:UNK	C	3170:UNK	N	16.12
1	B	3063:UNK	C	3134:UNK	N	15.30
1	E	3063:UNK	C	3134:UNK	N	15.30
1	I	3063:UNK	C	3134:UNK	N	15.30
1	G	3063:UNK	C	3134:UNK	N	15.30
1	B	3468:UNK	C	3511:UNK	N	14.89
1	E	3468:UNK	C	3511:UNK	N	14.89
1	I	3468:UNK	C	3511:UNK	N	14.89
1	G	3468:UNK	C	3511:UNK	N	14.89
1	B	2703:UNK	C	2734:ASN	N	13.90
1	E	2703:UNK	C	2734:ASN	N	13.90
1	I	2703:UNK	C	2734:ASN	N	13.90
1	G	2703:UNK	C	2734:ASN	N	13.90
1	B	3236:UNK	C	3241:UNK	N	13.63
1	E	3236:UNK	C	3241:UNK	N	13.63
1	I	3236:UNK	C	3241:UNK	N	13.63
1	G	3236:UNK	C	3241:UNK	N	13.63
1	B	2976:UNK	C	2995:UNK	N	12.77
1	E	2976:UNK	C	2995:UNK	N	12.77
1	I	2976:UNK	C	2995:UNK	N	12.77
1	G	2976:UNK	C	2995:UNK	N	12.77
1	B	1564:UNK	C	1573:MET	N	12.33
1	E	1564:UNK	C	1573:MET	N	12.33
1	I	1564:UNK	C	1573:MET	N	12.33
1	G	1564:UNK	C	1573:MET	N	12.33
1	B	3254:UNK	C	3261:UNK	N	8.26
1	E	3254:UNK	C	3261:UNK	N	8.26
1	I	3254:UNK	C	3261:UNK	N	8.26
1	G	3254:UNK	C	3261:UNK	N	8.26

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	1297:UNK	C	1430:UNK	N	6.06
1	G	1297:UNK	C	1430:UNK	N	6.06
1	B	1297:UNK	C	1430:UNK	N	6.05
1	I	1297:UNK	C	1430:UNK	N	6.05
1	B	2939:ARG	C	2942:UNK	N	3.63
1	E	2939:ARG	C	2942:UNK	N	3.63
1	I	2939:ARG	C	2942:UNK	N	3.63
1	G	2939:ARG	C	2942:UNK	N	3.63
1	B	2479:LEU	C	2487:UNK	N	3.24
1	E	2479:LEU	C	2487:UNK	N	3.24
1	I	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24

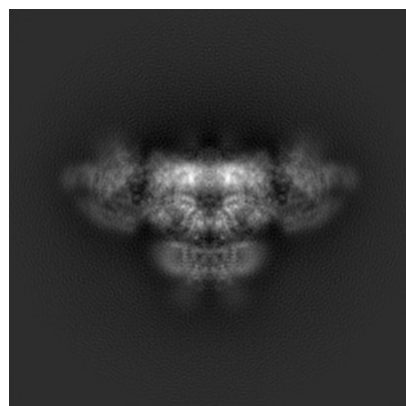
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8381. These allow visual inspection of the internal detail of the map and identification of artifacts.

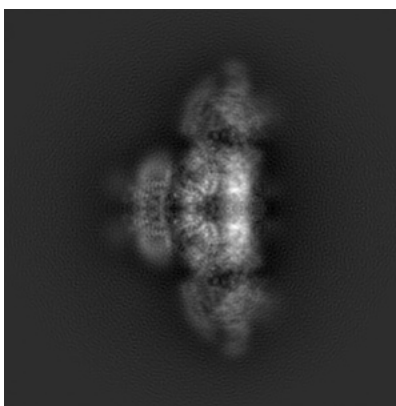
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

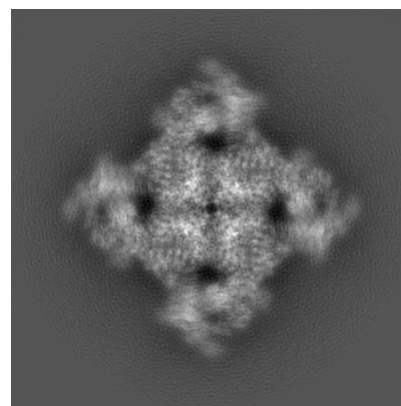
6.1.1 Primary map



X



Y

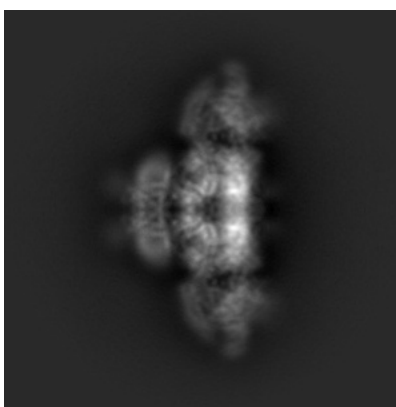


Z

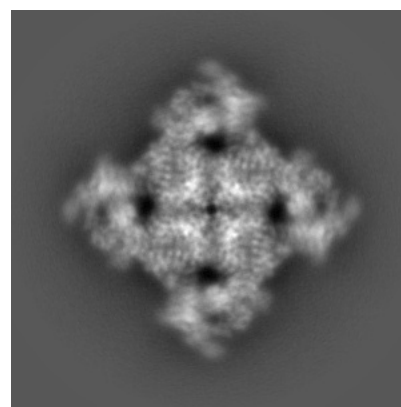
6.1.2 Raw map



X



Y

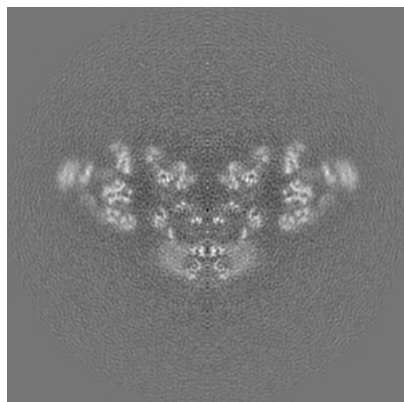


Z

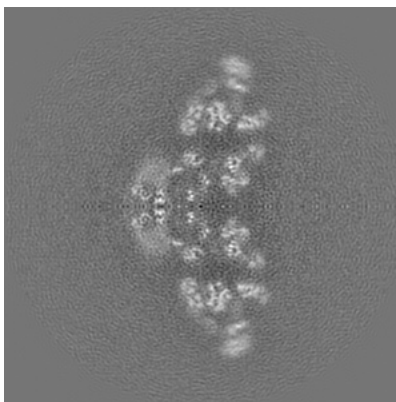
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

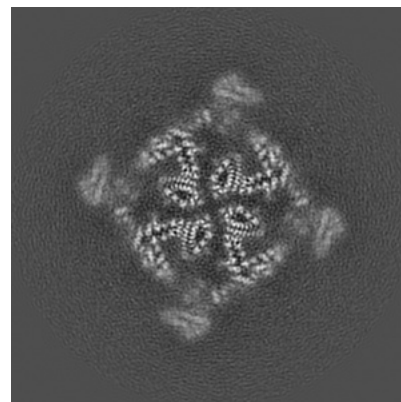
6.2.1 Primary map



X Index: 200

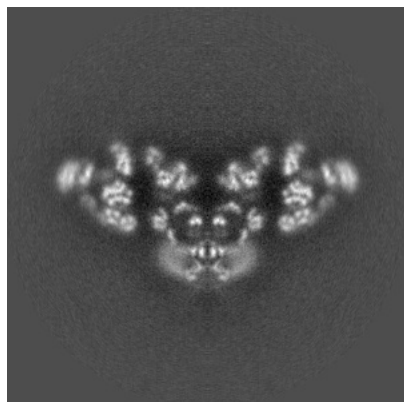


Y Index: 200

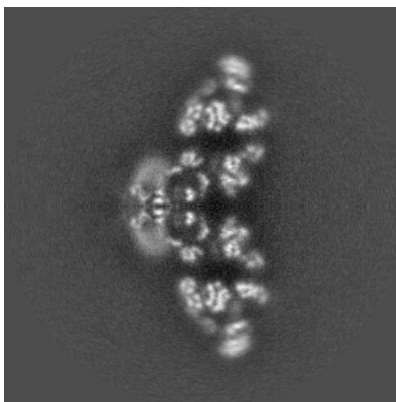


Z Index: 200

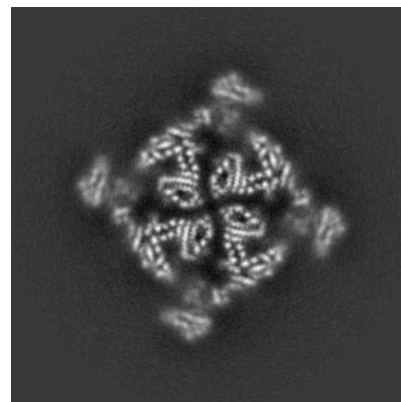
6.2.2 Raw map



X Index: 200



Y Index: 200

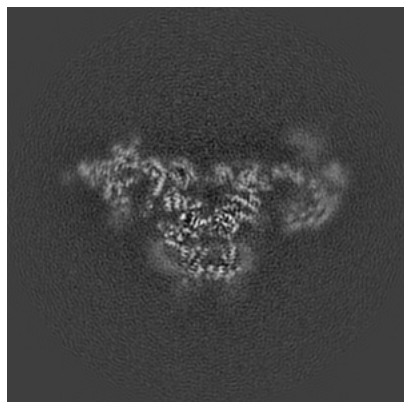


Z Index: 200

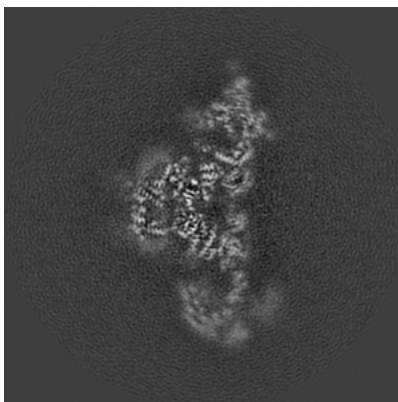
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

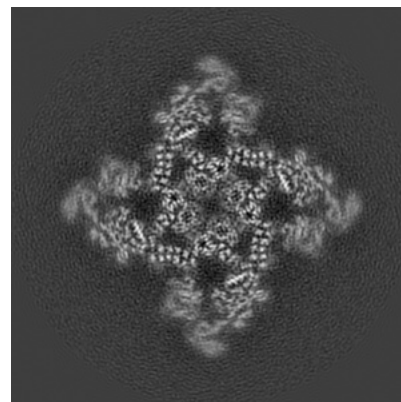
6.3.1 Primary map



X Index: 216

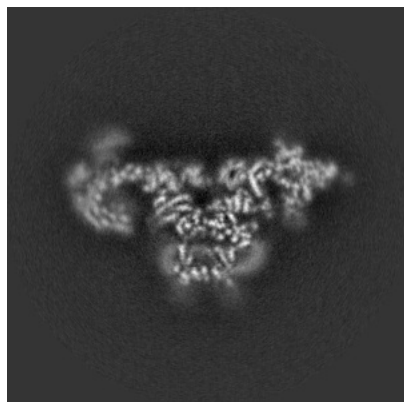


Y Index: 216

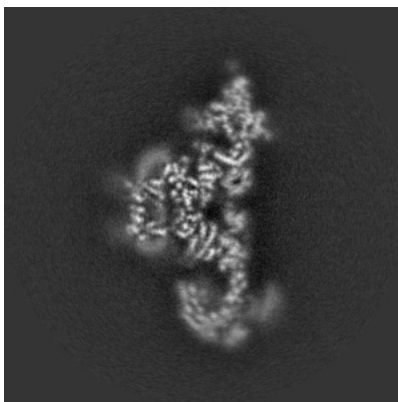


Z Index: 227

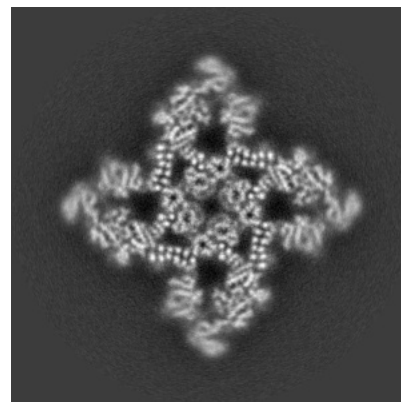
6.3.2 Raw map



X Index: 183



Y Index: 217

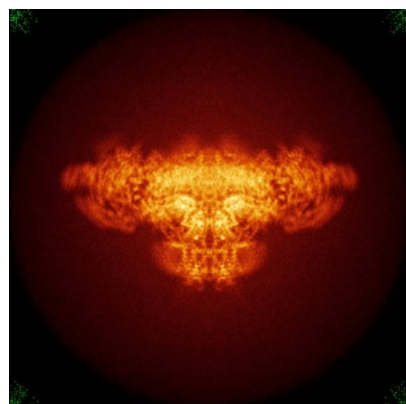


Z Index: 227

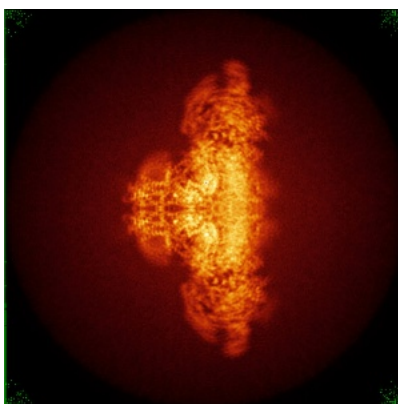
The images above show the largest variance slices of the map in three orthogonal directions.

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

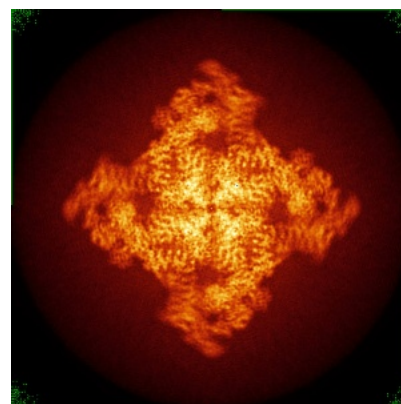
6.4.1 Primary map



X

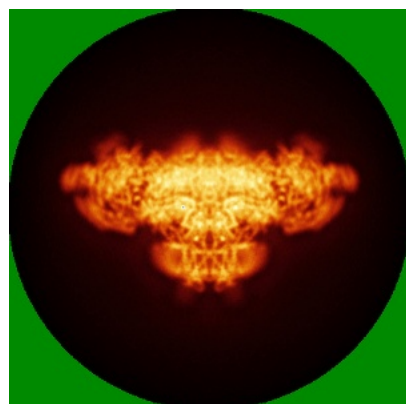


Y

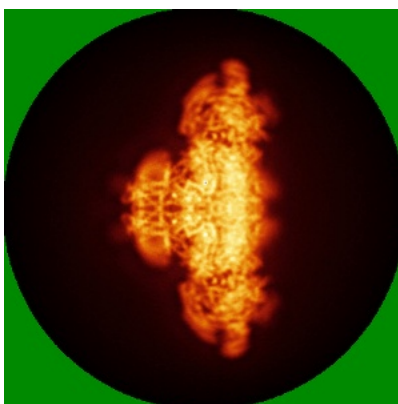


Z

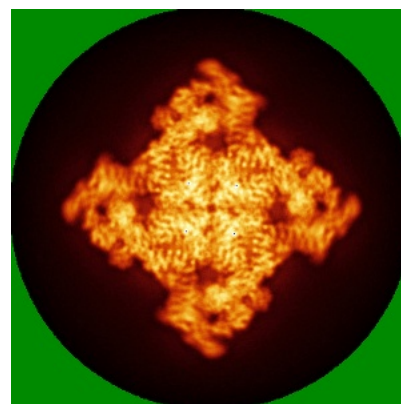
6.4.2 Raw map



X



Y

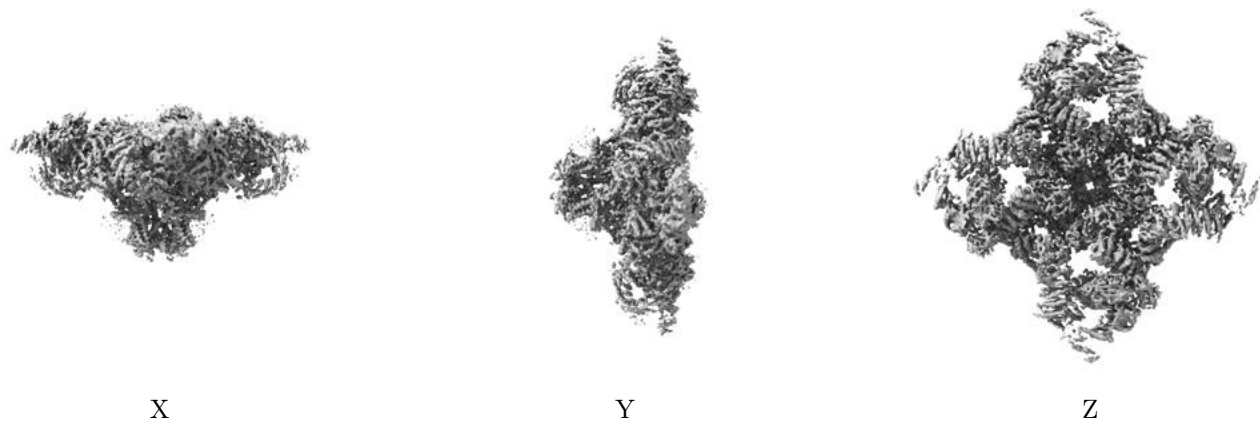


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

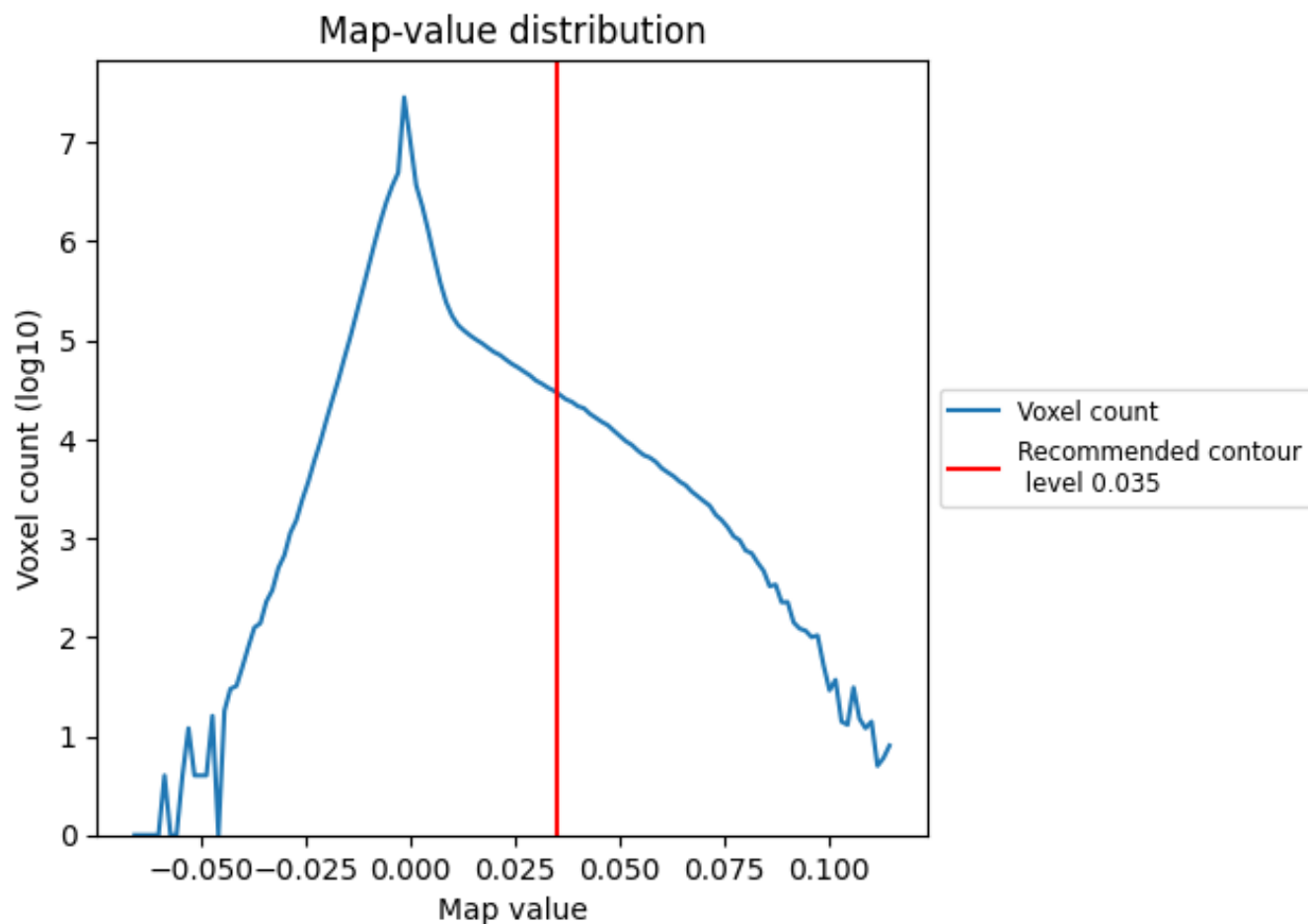
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

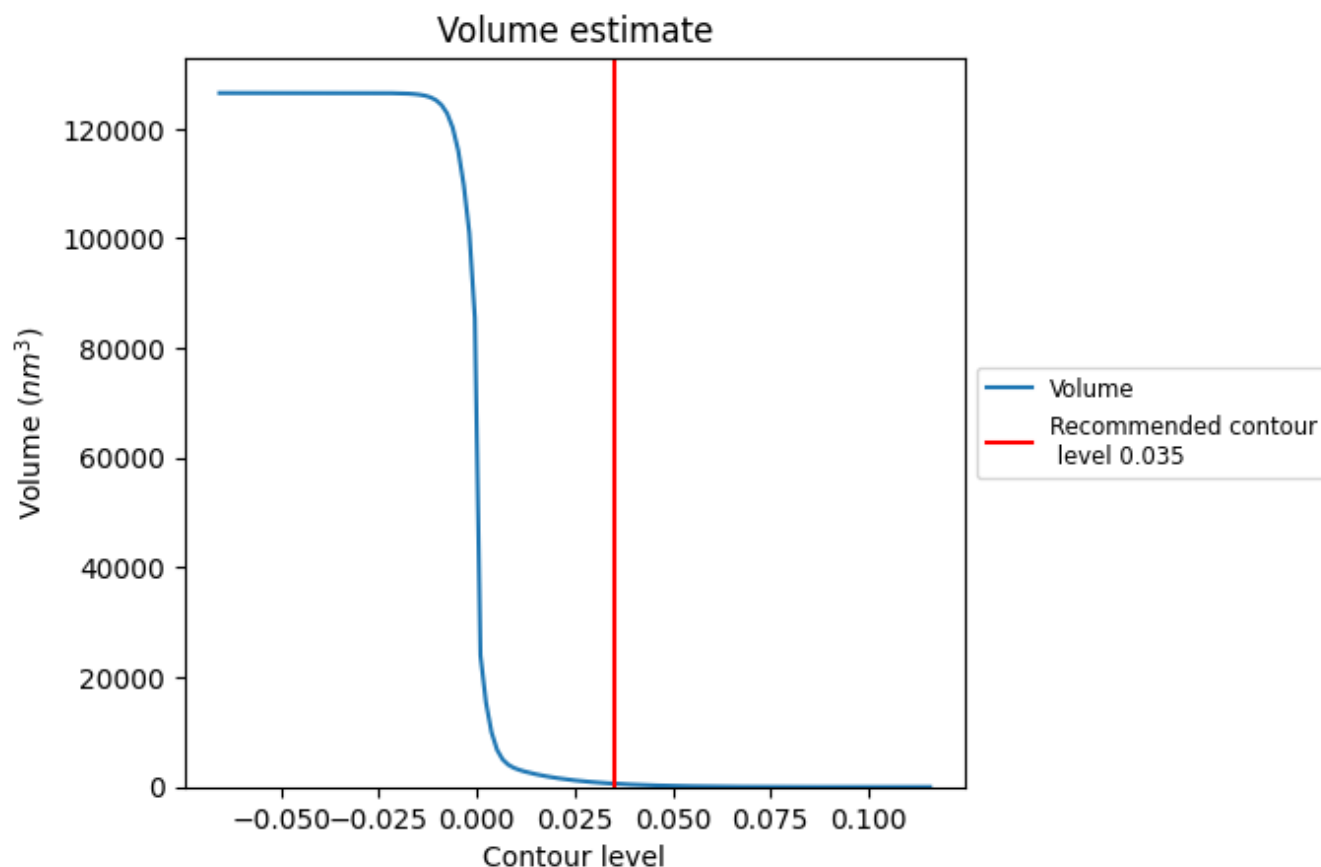
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

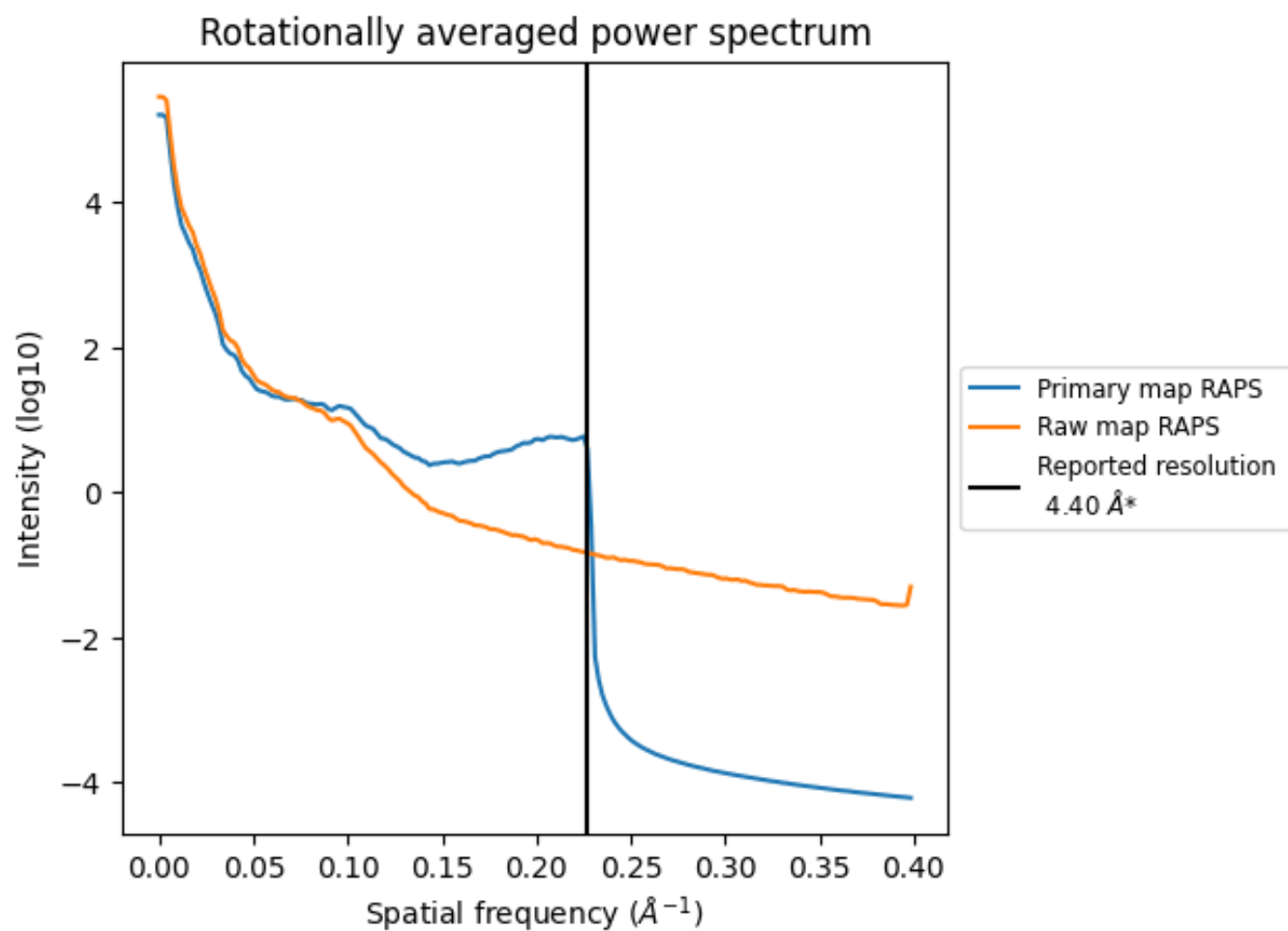
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 610 nm³; this corresponds to an approximate mass of 551 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 ⓘ

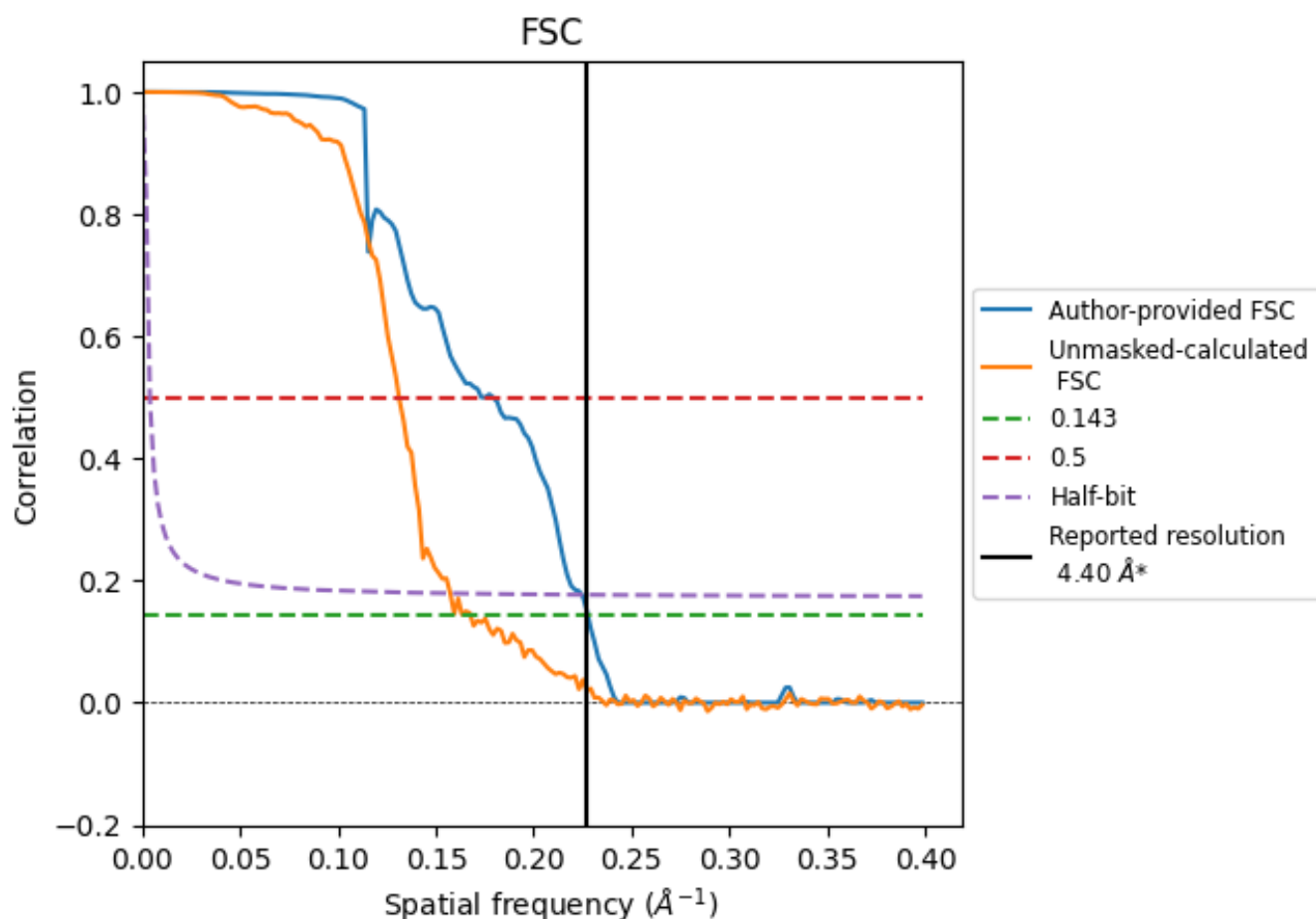


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

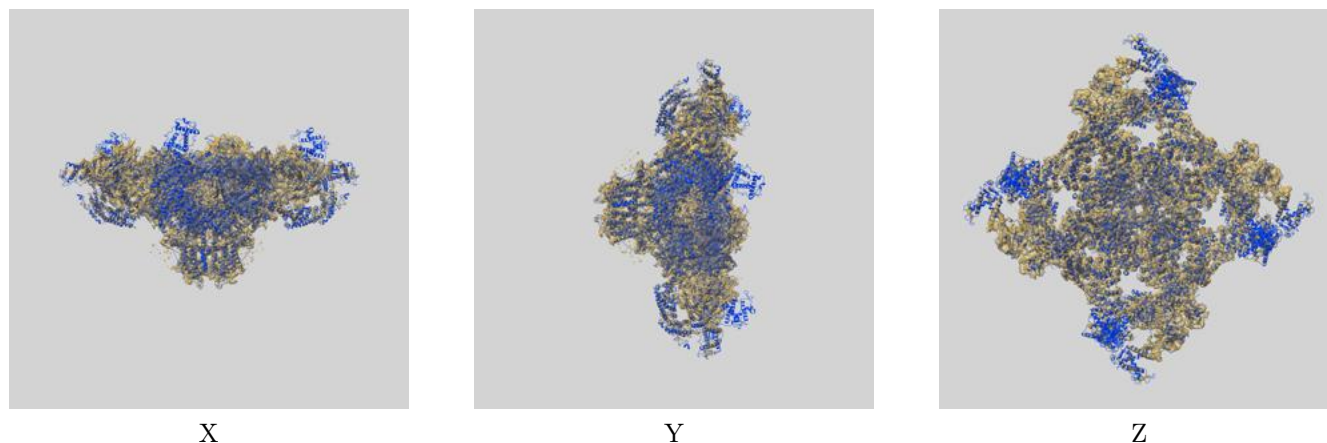
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.39	5.58	4.46
Unmasked-calculated*	5.96	7.62	6.36

*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 5.96 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

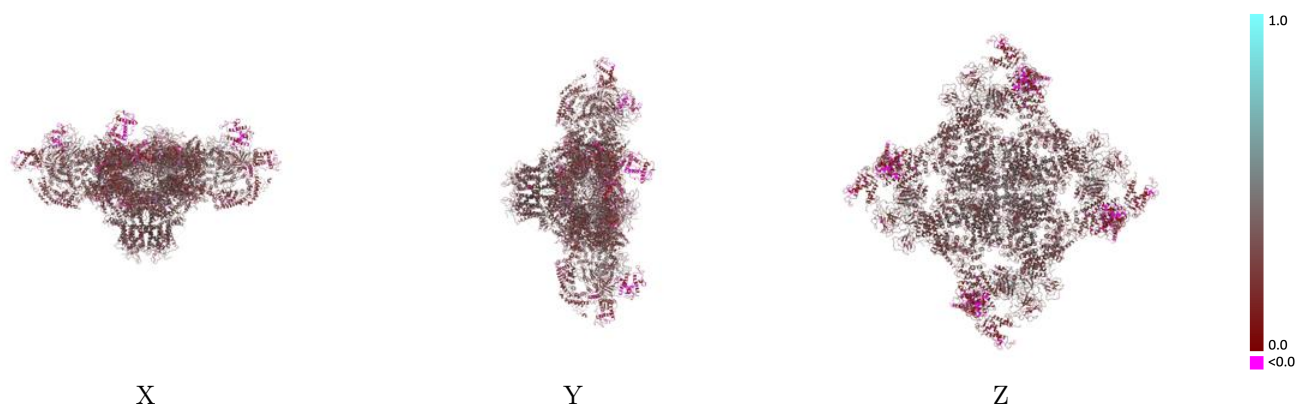
This section contains information regarding the fit between EMDB map EMD-8381 and PDB model 5TAP. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



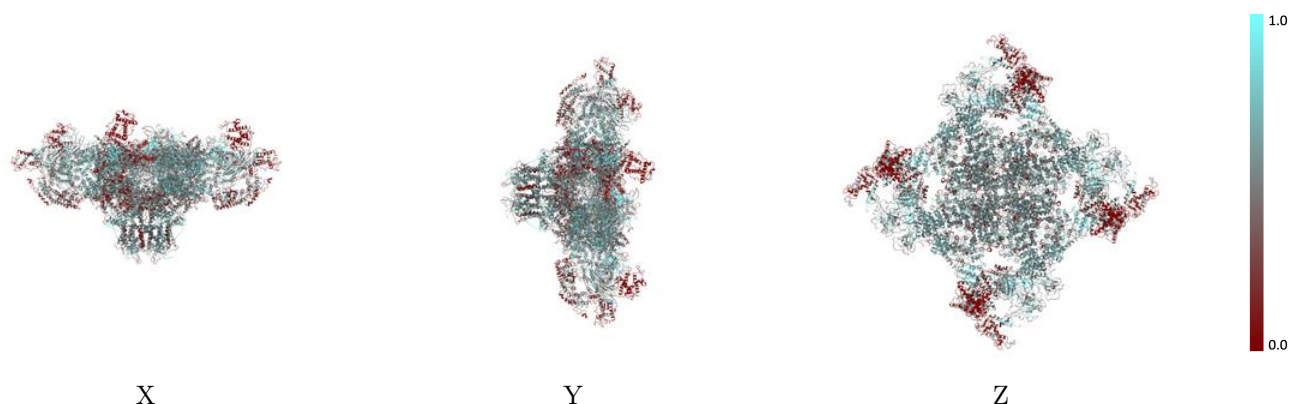
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



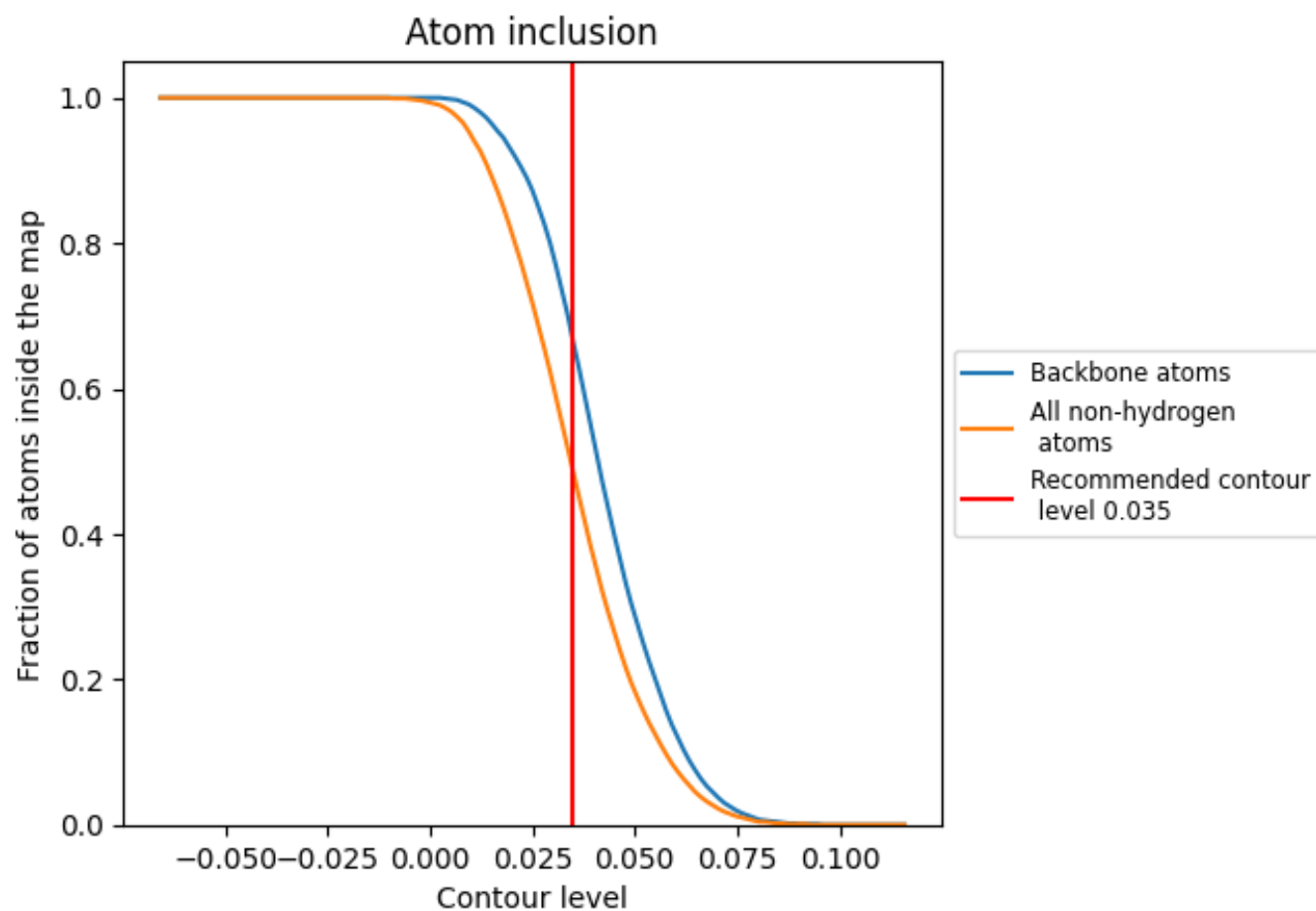
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4840	0.2940
A	0.4900	0.3030
B	0.4840	0.2940
E	0.4840	0.2930
F	0.4940	0.3070
G	0.4830	0.2930
H	0.4890	0.3040
I	0.4830	0.2930
J	0.4900	0.3020

1.0

0.0

<0.0