



## wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 04:35 AM EDT

PDB ID : 5TAP  
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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

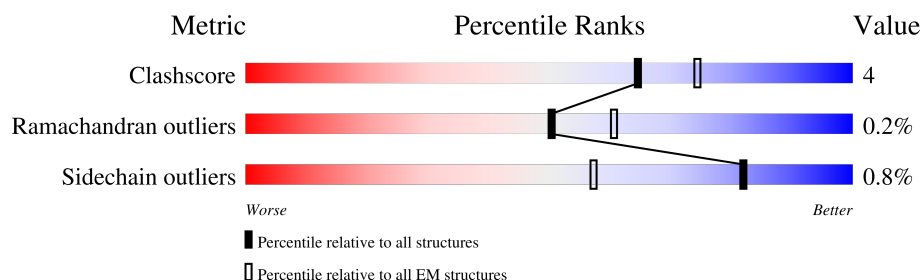
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	108	<div> <div>33%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	F	108	<div> <div>32%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	H	108	<div> <div>34%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	J	108	<div> <div>34%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	B	4416	<div> <div>35%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>
2	E	4416	<div> <div>35%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>
2	G	4416	<div> <div>35%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
2	I	4416	<div> <div>35%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>

## 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.

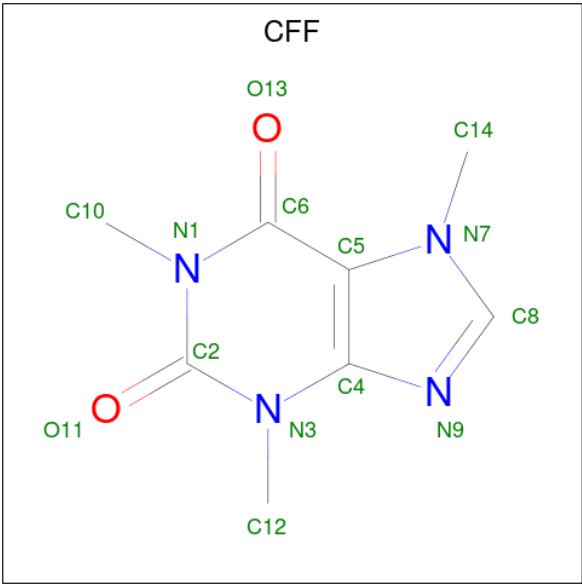
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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 (three-letter code: CFF) (formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>).



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

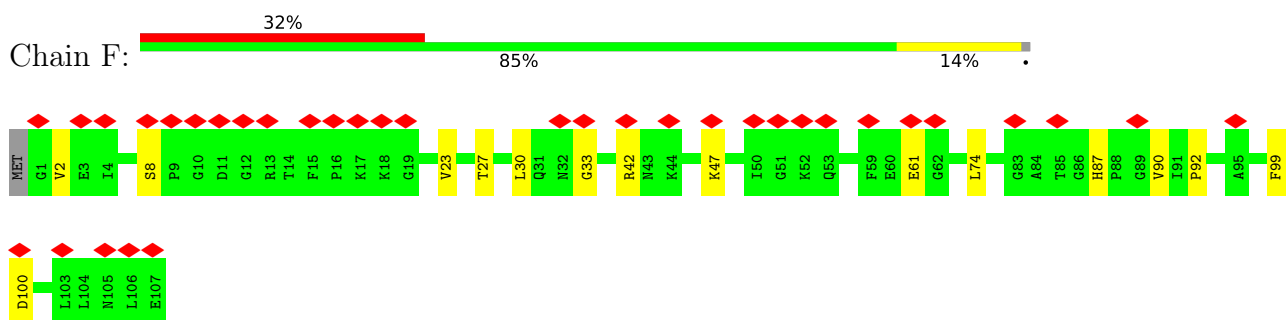
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

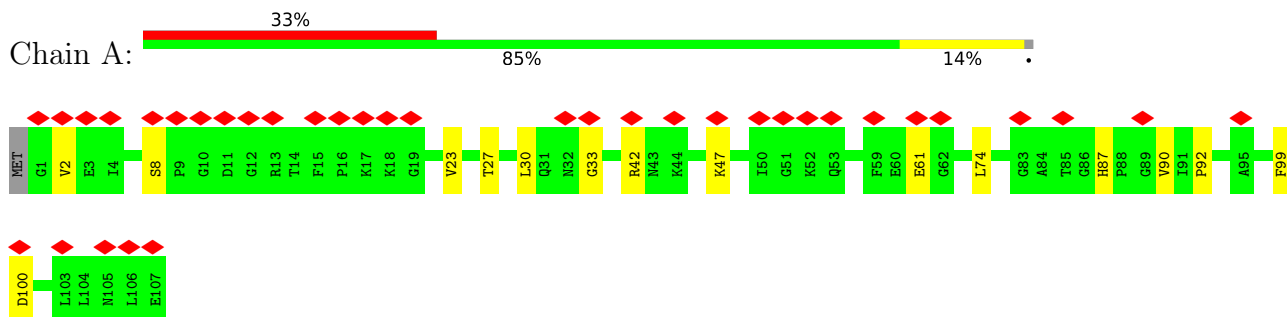
### 3 Residue-property plots [i](#)

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

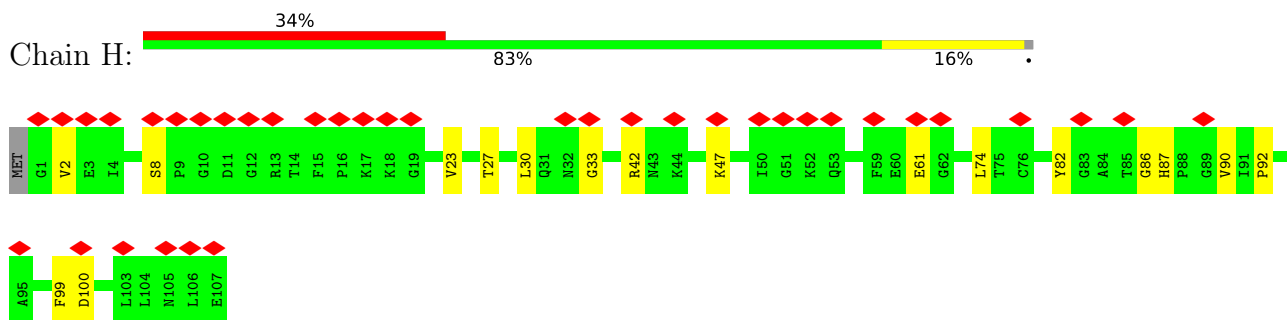
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



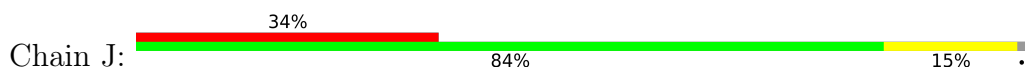
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

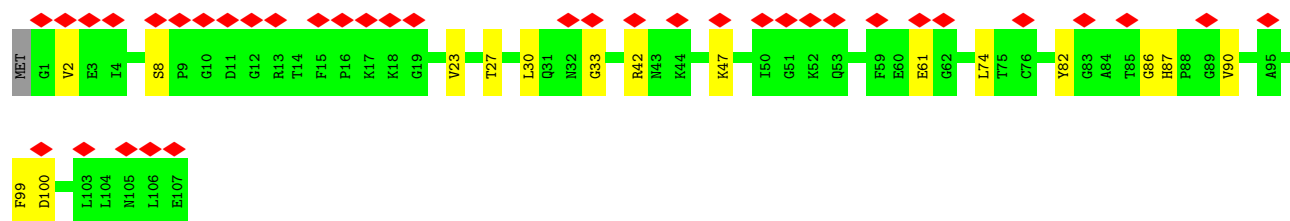


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



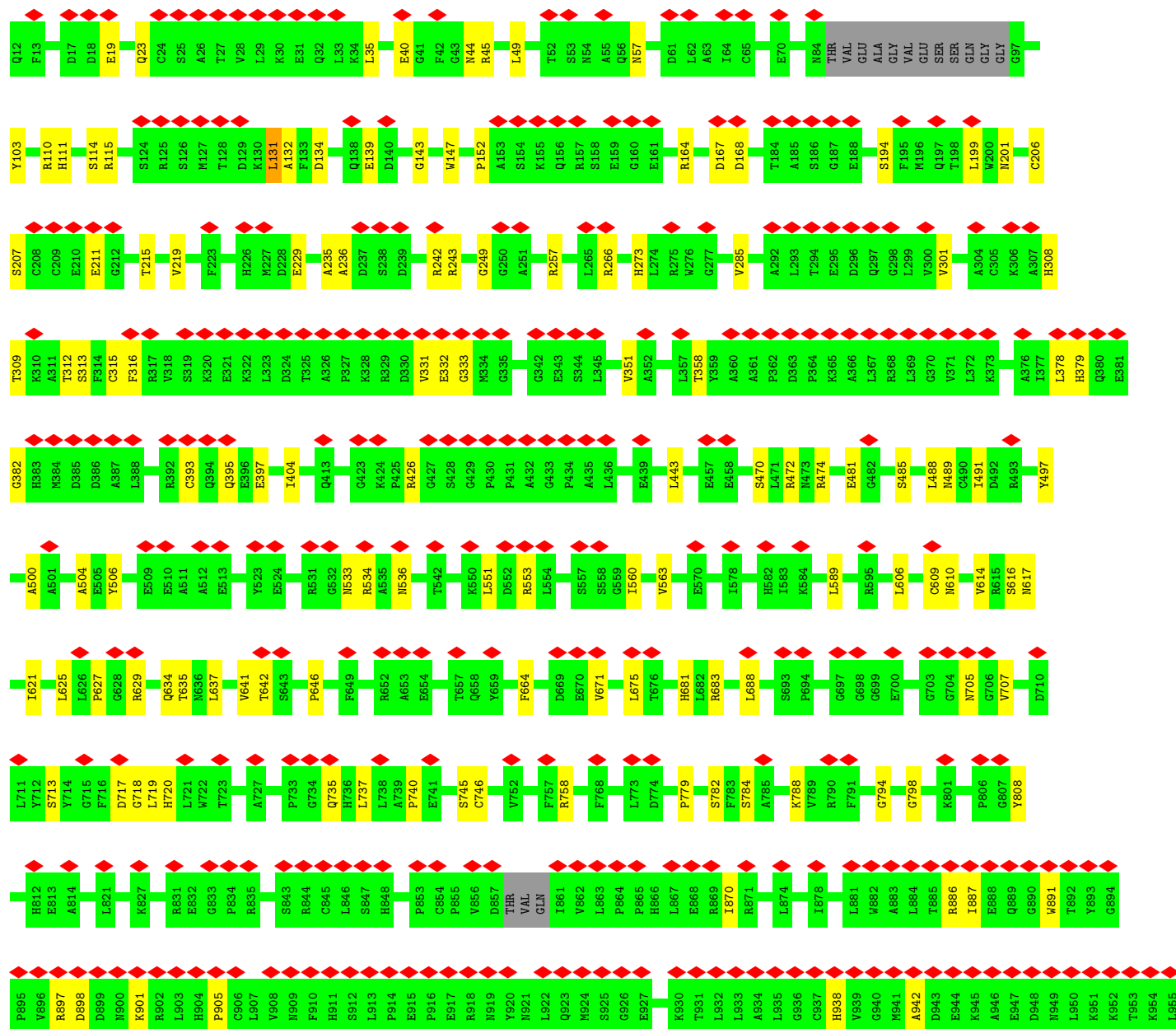
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 2: Ryanodine receptor 1

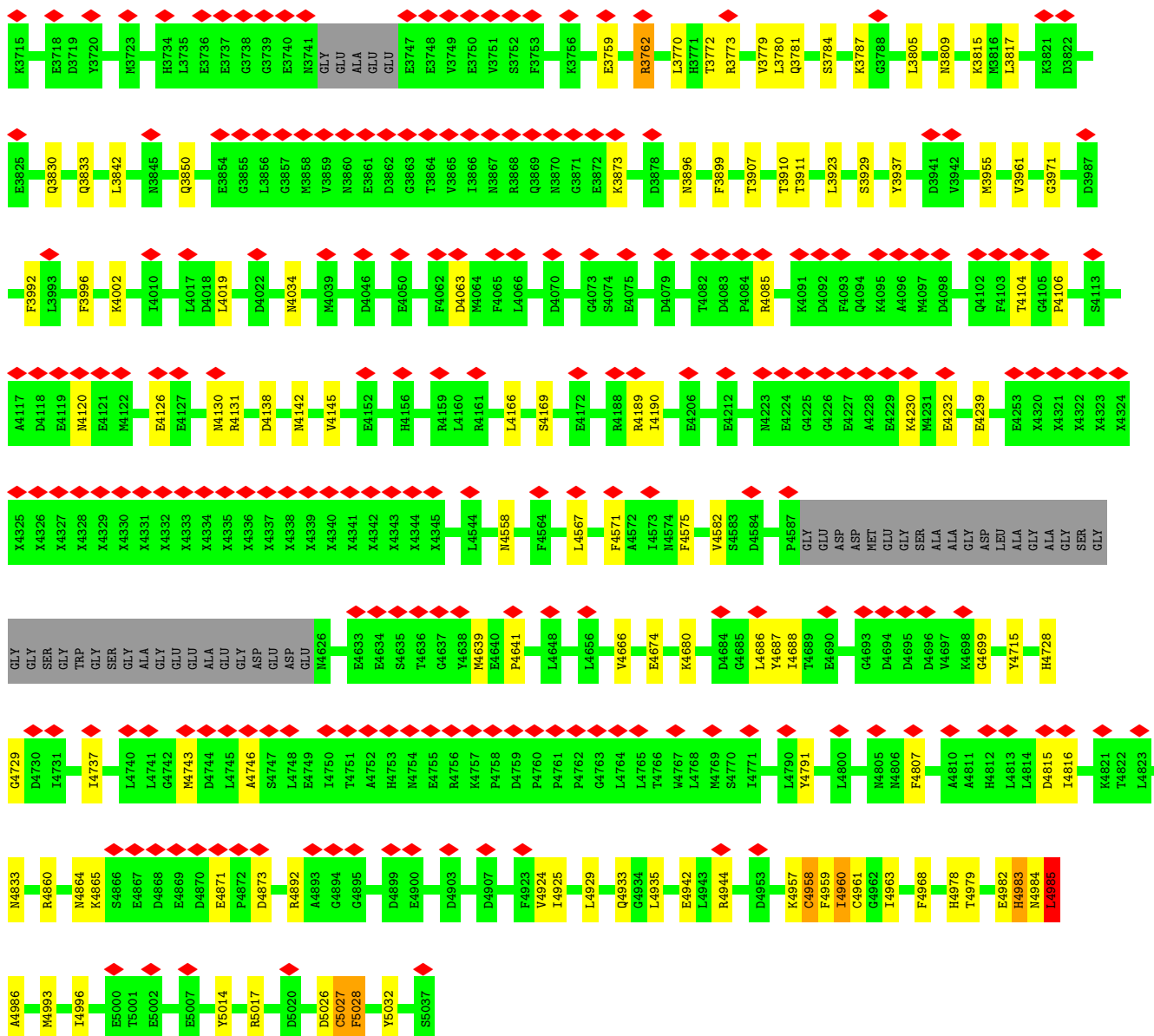
Chain B:







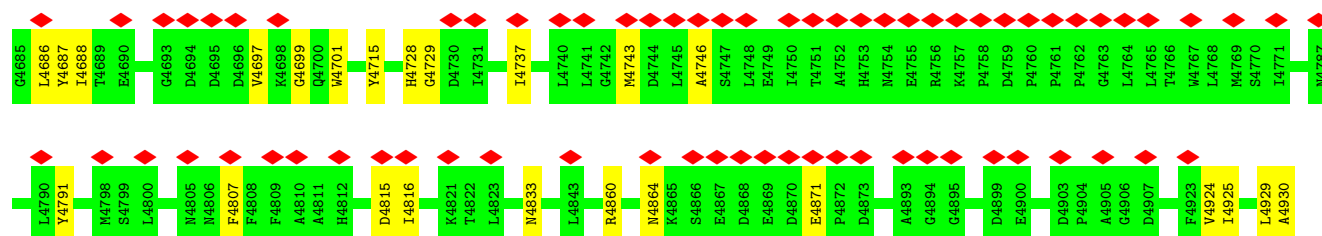




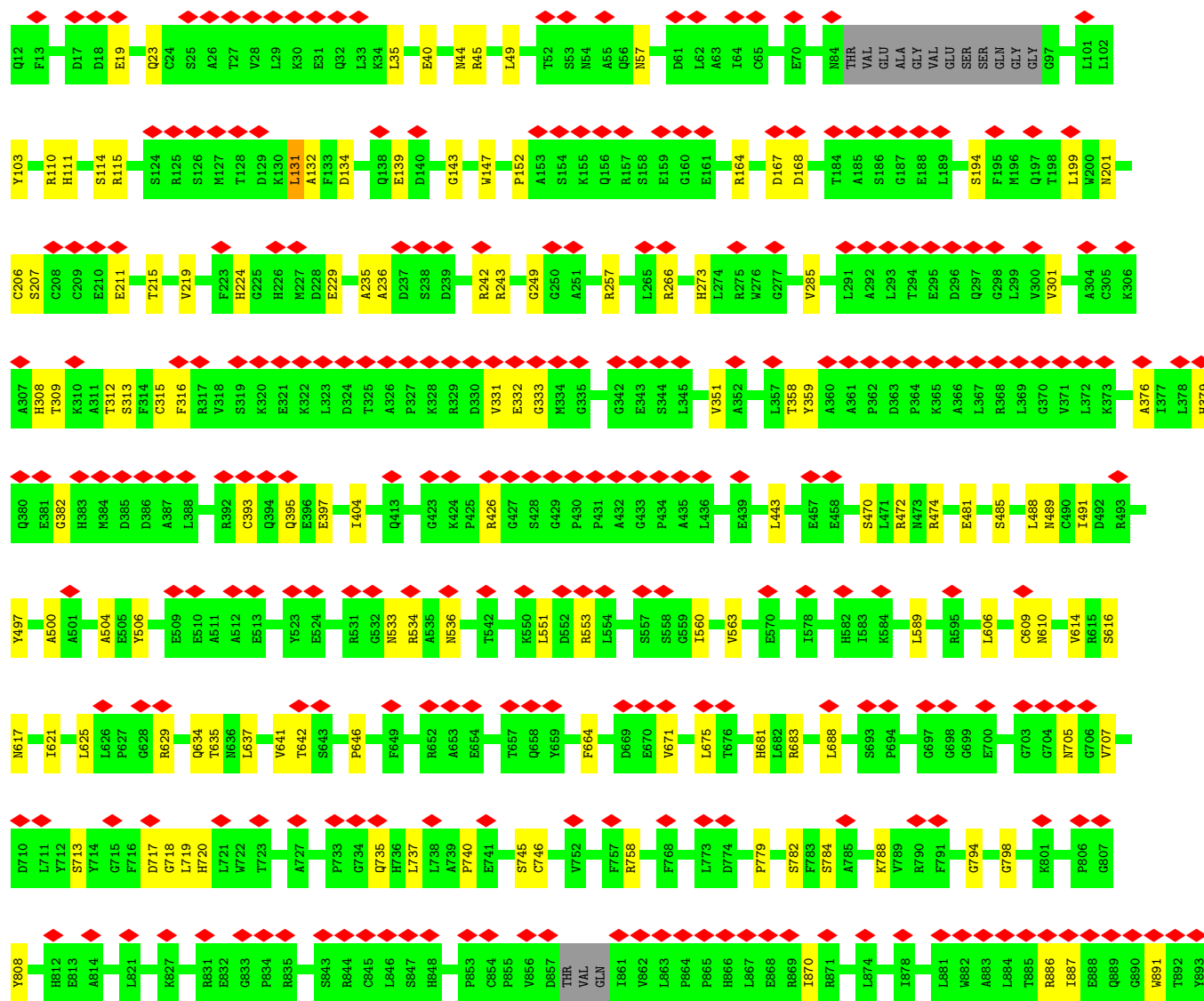
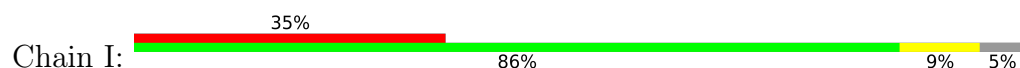








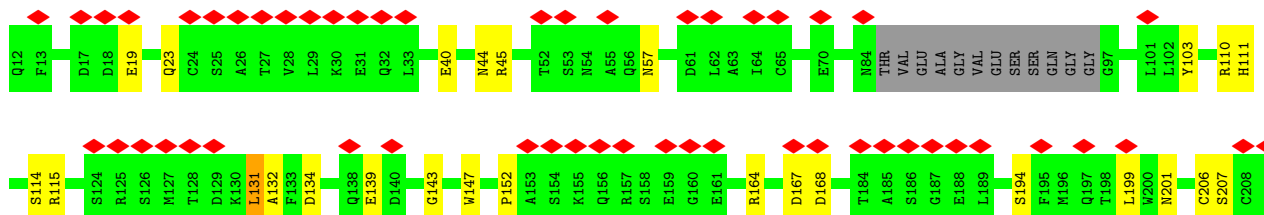
• Molecule 2: Ryanodine receptor 1

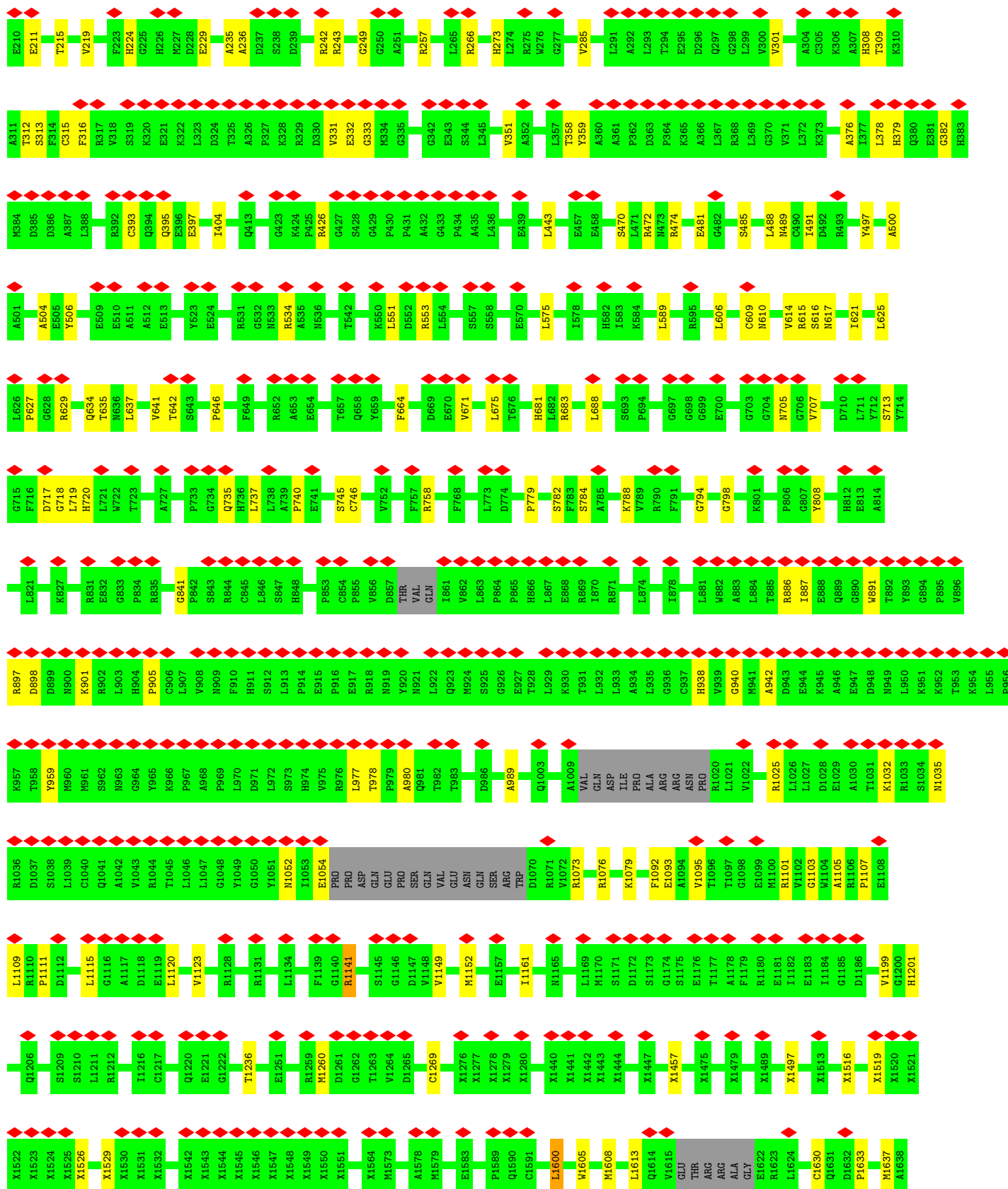




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X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3422	X3423	X3427	X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3442	X3443	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3574	X3575	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589																																																						
X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	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	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	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	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405										
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	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	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	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345
X3201	X3202	X3207	X3208	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255	X3256	X3257	X3258	X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3201	X3202	X3207	X3208	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255	X3256	X3257	X3258	X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275
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E2830	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	M2873	N2874	A2875	E2876	Q2877	L2878	A2879	E2880	Y2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	E2830	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	M2873	N2874	A2875	E2876	Q2877	L2878	A2879	E2880	Y2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889										
K2770	L2771	Q2772	N2773	N2774	N2775	S2776	Y2777	G2778	X2689	I2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	P2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	P2754	I2755	N2756	K2757	P2758	A2759	E2760	Y2761	T2762	H2763	E2764	W2765	A2767	P2769	D2769	K2770	L2771	Q2772	N2773	N2774	N2775	S2776	Y2777	G2778	X2689	I2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	P2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	P2754	I2755	N2756	K2757	P2758	A2759	E2760	Y2761	T2762	H2763	E2764	W2765	A2767	P2769	D2769								
X2674	X2675	X2676	X2677	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	P2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	P2754	I2755	N2756	K2757	P2758	A2759	E2760	Y2761	T2762	H2763	E2764	W2765	A2767	P2769	D2769	X2674	X2675	X2676	X2677	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	P2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	P2754	I2755	N2756	K2757	P2758	A2759	E2760	Y2761	T2762	H2763	E2764	W2765	A2767	P2769	D2769										
X2531	X2532	X2533	X2534	X2537	X2538	X2543	X2547	X2561	X2562	X2563	X2564	X2565	X2569	X2582	X2583	X2584	X2585	X2600	X2611	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2648	X2649	X2650	X2651	X2655	X2656	X2657	X2658	X2659	X2663	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	P2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	P2754	I2755	N2756	K2757	P2758	A2759	E2760	Y2761	T2762	H2763	E2764	W2765	A2767	P2769	D2769											
ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	GLU	N2414	R2415	V2416	R2435	P2438	H2441	K2447	G2448	E2449	I2453	D2464	L2465	L2466	I2469	I2470	S2471	L2472	P2473	L2474	O2475	I2476	P2477	T2478	L2479	X2487	X2488	X2489	X2490	I2493	X2499	X2512	X2513	X2514	X2522	X2531	X2532	X2533	X2534	X2537	X2538	X2543	X2547	X256																																																																						

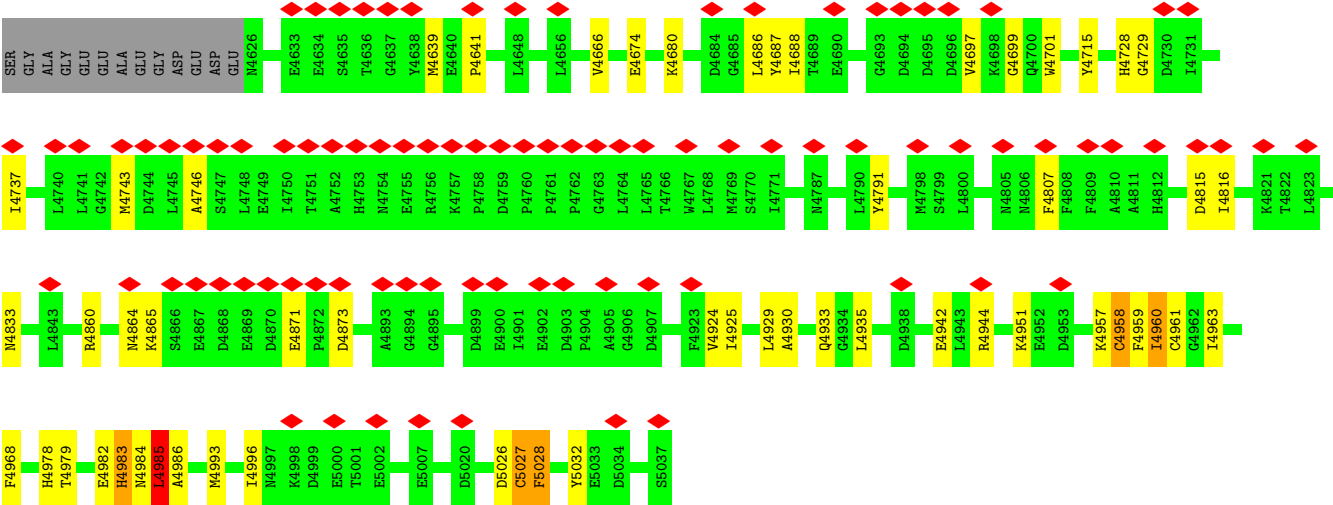








X4329	N4120	L3993	Q3830	S3714	X3588	X3526	X3405	X3344	X3274	X3200	X3050	X2951
X4330	E4121	K4002	Q3833	K3715	X3589	X3527	X3406	X3345	X3275	X3201	X3051	X2952
X4331	N4122				X3590	X3528	X3407	X3346	X3276	X3202	X3052	
X4332	E4126	Q4009	L3842	E3718	X3591	X3529	X3408	X3347	X3277		X3053	
X4333	E4127	I4010	N3845	D3719	X3592	X3530	X3409	X3348	X3278	X3207	X3057	X2964
X4334	F4128	L4017		Y3720	X3595	X3531	X3410	X3349	X3279	X3208		X2965
X4335	F4129	D4018	Q3850	M3723	X3596	X3532	X3411	X3350	X3280		X3060	X2966
X4336	N4130	L4019	E3854	H3734	X3597	X3533	X3412	X3351	X3281	X3211	X3061	X2967
X4337	R4131	D4022	Q3855	L3735		X3534	X3413	X3352	X3282	X3212	X3062	X2968
X4338	D4138		G3855	E3736	X3600	X3535	X3414	X3353	X3283	X3213	X3063	X2969
X4339		N4034	G3857	E3737	X3601	X3536	X3415	X3354	X3284	X3214	X3134	X2970
X4340	N4142	M4039	N3858	G3738	X3602	X3537	X3416	X3355	X3285	X3215	X3135	X2971
X4341	V4145		X3858	G3739	X3603	X3538		X3356	X3286	X3216	X3136	X2972
X4342	E4152	D4046	X3859	E3740	X3604	X3539	X3422	X3357	X3287	X3217	X3137	X2973
X4343	E4153		N3860	E3747	X3605	X3540	X3423	X3358	X3288	X3218	X3138	X2974
X4344	H4156		N3861	N3741	X3606	X3541		X3359	X3289	X3219	X3139	X2975
X4345		E4050	D3862	GLY	X3607	X3542	X3427	X3360	X3290	X3220	X3140	X2976
			G3863	GLU	X3608	X3543	X3432	X3361	X3291	X3221	X3141	X2995
L4544	R4159	F4062	Q3863	ALA	X3609	X3544	X3433	X3362	X3292	X3222	X3142	X2996
F4564	L4160	D4063	T3864	GLU	X3610	X3545	X3434	X3363	X3295	X3223	X3143	X2997
	R4161	F4065	V3865	GLU	X3611	X3546	X3435	X3364	X3296	X3224	X3144	X2998
L4567	L4166		L3866	E3747	X3612	X3547	X3436	X3365	X3297	X3225	X3145	X2999
			N3867	E3748	X3613	X3548	X3437	X3366	X3298	X3226	X3146	X3000
F4571	L4172	D4070	Q3868	V3749	T3639	X3549	X3438	X3369	X3299	X3227	X3147	X3001
A4572	E4177	I4071	N3869	E3750		X3550	X3439	X3370	X3300		X3148	
N4573		V4072	N3870	S3752	L3644	X3551		X3371	X3301	X3230	X3149	X3009
F4575	S4074	G4073	G3871	F3753		X3552	X3443	X3372	X3302	X3231	X3150	
	E4075	E4075	X3872		K3658	X3553		X3373	X3303	X3232	X3151	X3016
			K3873	K3756		X3554	X3450	X3374	X3304	X3233	X3152	X3017
V4582		D4079	D3877			X3555	X3451	X3375		X3234	X3153	X3018
S4583	E4206		D3878	E3759		X3556	X3452	X3376	X3308	X3235		X3019
D4584	E4212	T4082	N3896	R3762	L3663	X3557	X3453	X3377	X3309	X3236	X3158	X3020
		D4083	F3899	L3770	E3665	X3558	X3454	X3378	X3310	X3237	X3159	X3021
GLY	N4223	P4084		H3771	D3666	X3559	X3455	X3379	X3311	X3241	X3160	X3022
ASP	E4224	R4085	T3907	T3772	H3667	X3560		X3380	X3312	X3242	X3161	X3023
MET	G4225	K4091	T3910	T3773	S3668	X3561	X3459	X3381	X3313	X3243	X3162	X3024
GLU	G4226	D4092	T3911	R3773	F3668	X3562		X3382	X3314	X3244	X3163	X3025
GLY	G4227	F4093	L3923			X3563	X3463	X3383	X3315	X3245	X3170	X3026
ALA	A4228	Q4094	L3923	V3779	F3669	X3564	X3464	X3384	X3316	X3246	X3171	X3027
ALA	A4229	K4095	L3923	L3780		X3565	X3465	X3385	X3317	X3247	X3172	X3028
GLY	E4229	A4096	S3929	Q3781	D3676	X3566	X3466	X3386	X3318	X3248	X3173	X3029
ASP	K4230	M4097	Y3937	S3784	K3679	X3567	X3467	X3387	X3323	X3249	X3174	X3032
LEU	M4231	D4098		K3787	A3680	X3568	X3468	X3388	X3324	X3250	X3175	X3033
ALA	E4232			G3788	E3682	X3569	X3511	X3389	X3325	X3251	X3176	X3034
GLY		Q4102	D3941	L3805	Q3683	X3570	X3512	X3390	X3326	X3252	X3177	
ALA	E4253	F4103	V3942	L3805	E3684		X3513	X3391	X3330	X3253	X3178	X3037
GLY	X4320	T4104	K3955	N3809	E3685	X3574	X3514	X3392	X3331	X3254	X3179	X3038
SER	X4321				E3686	X3575	X3515	X3393	X3332	X3261	X3181	X3039
GLY	X4322	G4105	V3961	K3815	E3687	X3576	X3516	X3394	X3333	X3262	X3182	X3040
GLY	X4323	P4106	M3816	M3816	E3688	X3577	X3517	X3395	X3334	X3263	X3183	X3041
SER	X4324		C3971	L3817	X3688	X3578	X3518	X3396	X3335	X3264	X3184	X3042
GLY	X4325	S4113		D3822	E3689	X3579	X3519	X3397	X3336	X3265	X3190	X3043
TRP	X4326				V3690	X3580	X3520	X3397	X3337	X3266	X3191	X3044
GLY	X4327	A4117			E3691	X3581	X3521	X3398	X3338	X3267	X3192	X3045
	X4328	D4118	E4119		E3692	X3582	X3522	X3399	X3339	X3268	X3193	X3046
						X3583	X3523	X3400	X3340	X3269	X3194	X3047
					E3712	X3584	X3524	X3401	X3341	X3270	X3195	X3048
					K3713	X3585	X3525	X3402	X3342	X3271	X3196	X3049
						X3586	X3526	X3403	X3343	X3272	X3197	



## 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: ATP, ZN, CFF

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.32	0/834	0.51	0/1123
1	F	0.32	0/834	0.51	0/1123
1	H	0.32	0/834	0.51	0/1123
1	J	0.32	0/834	0.51	0/1123
2	B	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	E	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	G	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	I	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
All	All	0.31	4/105048 (0.0%)	0.54	36/142628 (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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2476	ILE	C-N	5.37	1.44	1.34
2	B	2476	ILE	C-N	5.34	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2476	ILE	C-N	5.33	1.44	1.34
2	G	2476	ILE	C-N	5.30	1.44	1.34

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	8.29	134.37	115.30
2	G	131	LEU	CA-CB-CG	8.28	134.35	115.30
2	B	131	LEU	CA-CB-CG	8.27	134.32	115.30
2	E	131	LEU	CA-CB-CG	8.27	134.32	115.30
2	G	1600	LEU	CA-CB-CG	7.05	131.52	115.30

There are no chirality outliers.

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	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	236	0
2	E	29499	0	24749	235	0
2	G	29499	0	24749	231	0
2	I	29499	0	24749	233	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	31	0	12	2	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	949	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.

The worst 5 of 949 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

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	47	81
2	E	3235/4416 (73%)	2908 (90%)	321 (10%)	6 (0%)	47	81
2	G	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	47	81
2	I	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	47	81
All	All	13360/18096 (74%)	12010 (90%)	1326 (10%)	24 (0%)	50	81

5 of 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

### 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%)	2472 (99%)	21 (1%)	81	89
2	E	2493/3022 (82%)	2472 (99%)	21 (1%)	81	89
2	G	2493/3022 (82%)	2472 (99%)	21 (1%)	81	89
2	I	2493/3022 (82%)	2472 (99%)	21 (1%)	81	89
All	All	10324/12444 (83%)	10240 (99%)	84 (1%)	82	89

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	4166	LEU
2	G	3762	ARG
2	I	4958	CYS
2	G	553	ARG
2	G	4085	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	4034	ASN
2	G	3946	GLN
2	I	1598	GLN
2	G	3896	ASN
2	G	1598	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	I	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.34	5 (16%)
4	CFF	E	5102	-	8,15,15	2.57	3 (37%)	8,23,23	1.43	2 (25%)
4	CFF	G	5102	-	8,15,15	2.59	3 (37%)	8,23,23	1.43	2 (25%)
3	ATP	G	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.35	5 (16%)
3	ATP	B	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.35	5 (16%)
4	CFF	B	5102	-	8,15,15	2.58	3 (37%)	8,23,23	1.42	2 (25%)
3	ATP	E	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.35	5 (16%)
4	CFF	I	5102	-	8,15,15	2.59	3 (37%)	8,23,23	1.41	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	I	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	B	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5102	CFF	C5-C4	-4.82	1.33	1.39
4	I	5102	CFF	C5-C4	-4.82	1.33	1.39
4	E	5102	CFF	C5-C4	-4.81	1.33	1.39
4	B	5102	CFF	C5-C4	-4.81	1.33	1.39
4	I	5102	CFF	C6-N1	-4.19	1.32	1.38

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5101	ATP	N3-C2-N1	-3.25	123.60	128.68
3	E	5101	ATP	N3-C2-N1	-3.23	123.62	128.68
3	B	5101	ATP	N3-C2-N1	-3.22	123.64	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5101	ATP	N3-C2-N1	-3.19	123.69	128.68
3	I	5101	ATP	PB-O3B-PG	-2.90	122.87	132.83

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

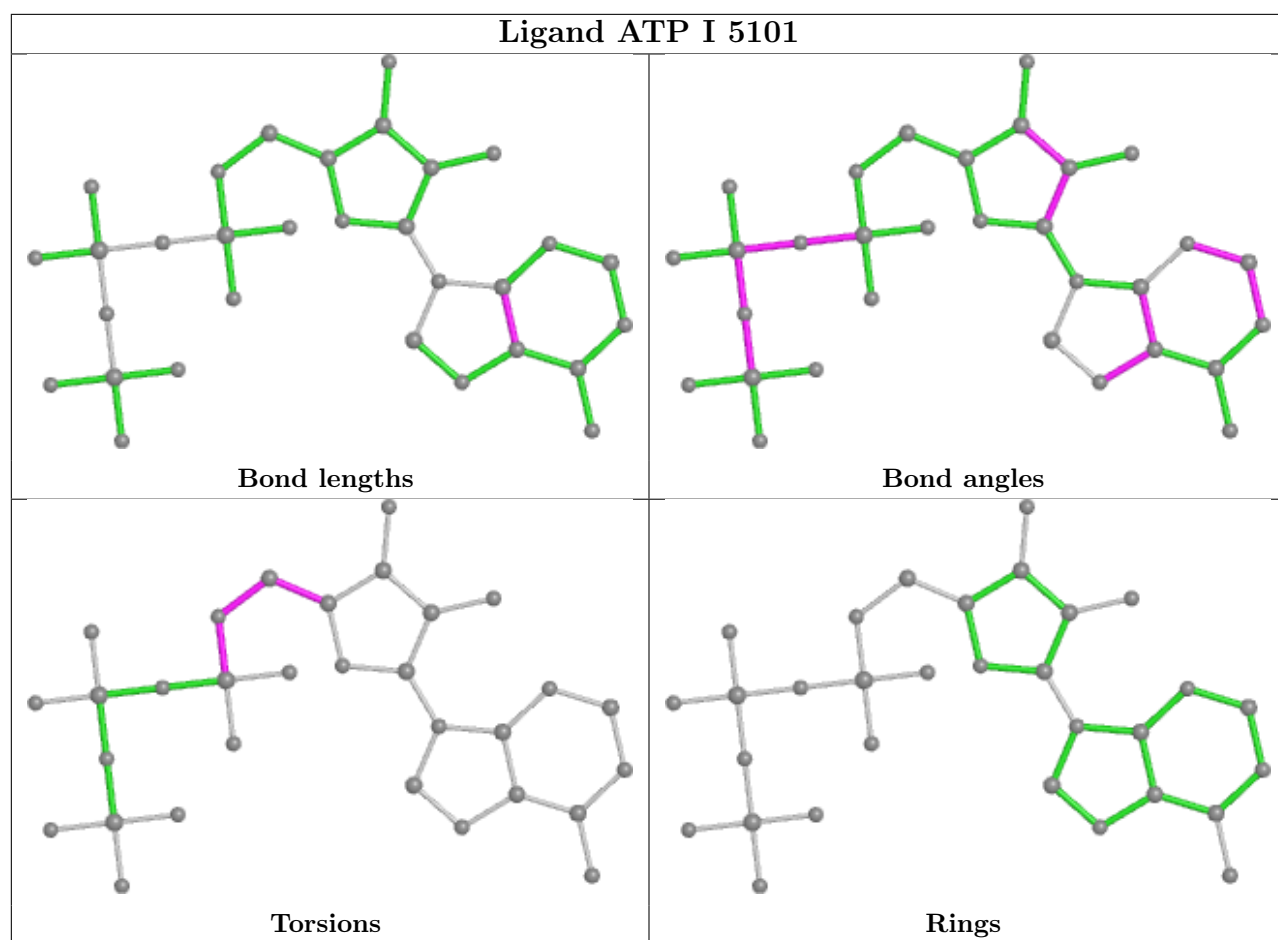
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	O4'-C4'-C5'-O5'

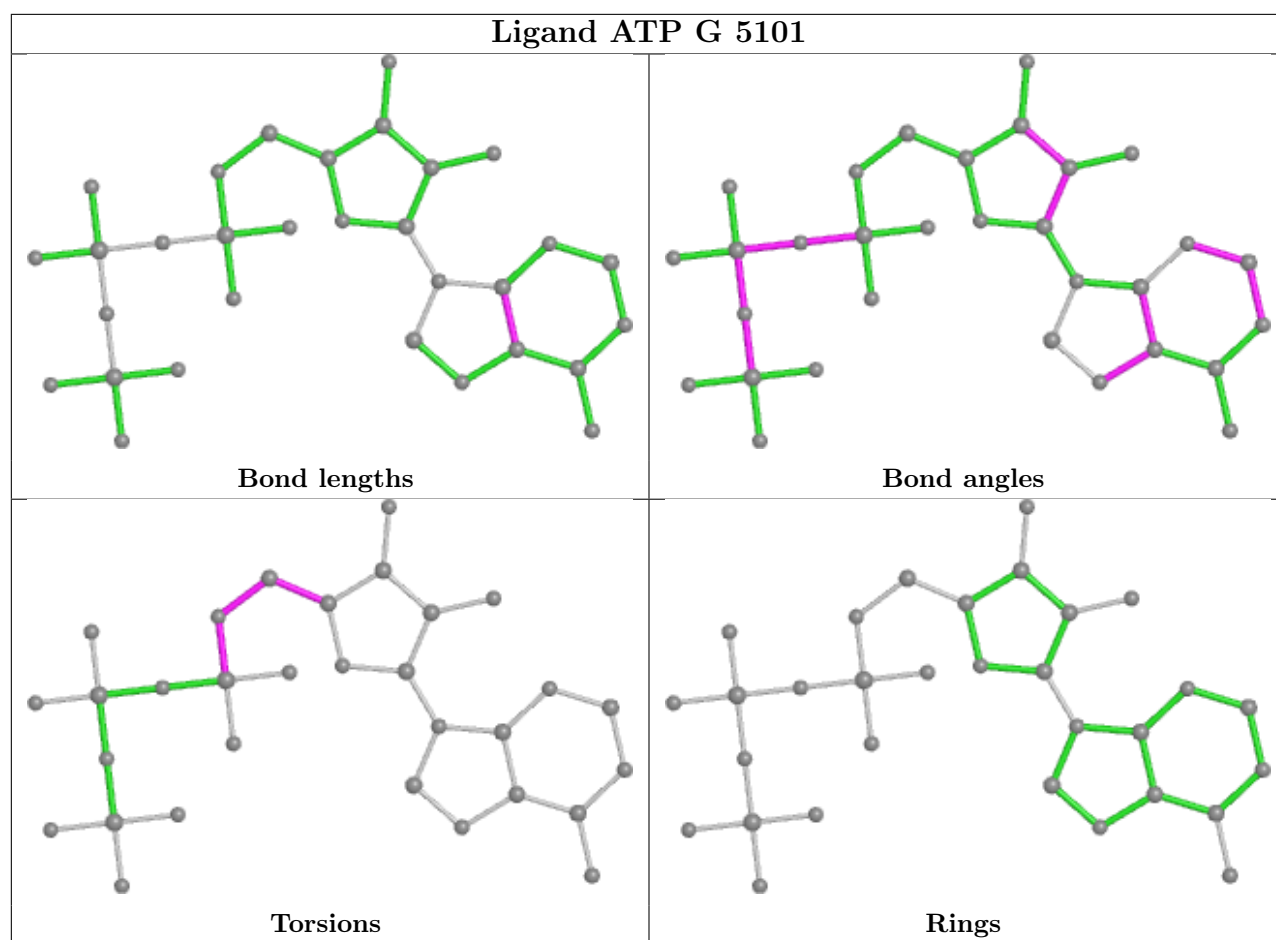
There are no ring outliers.

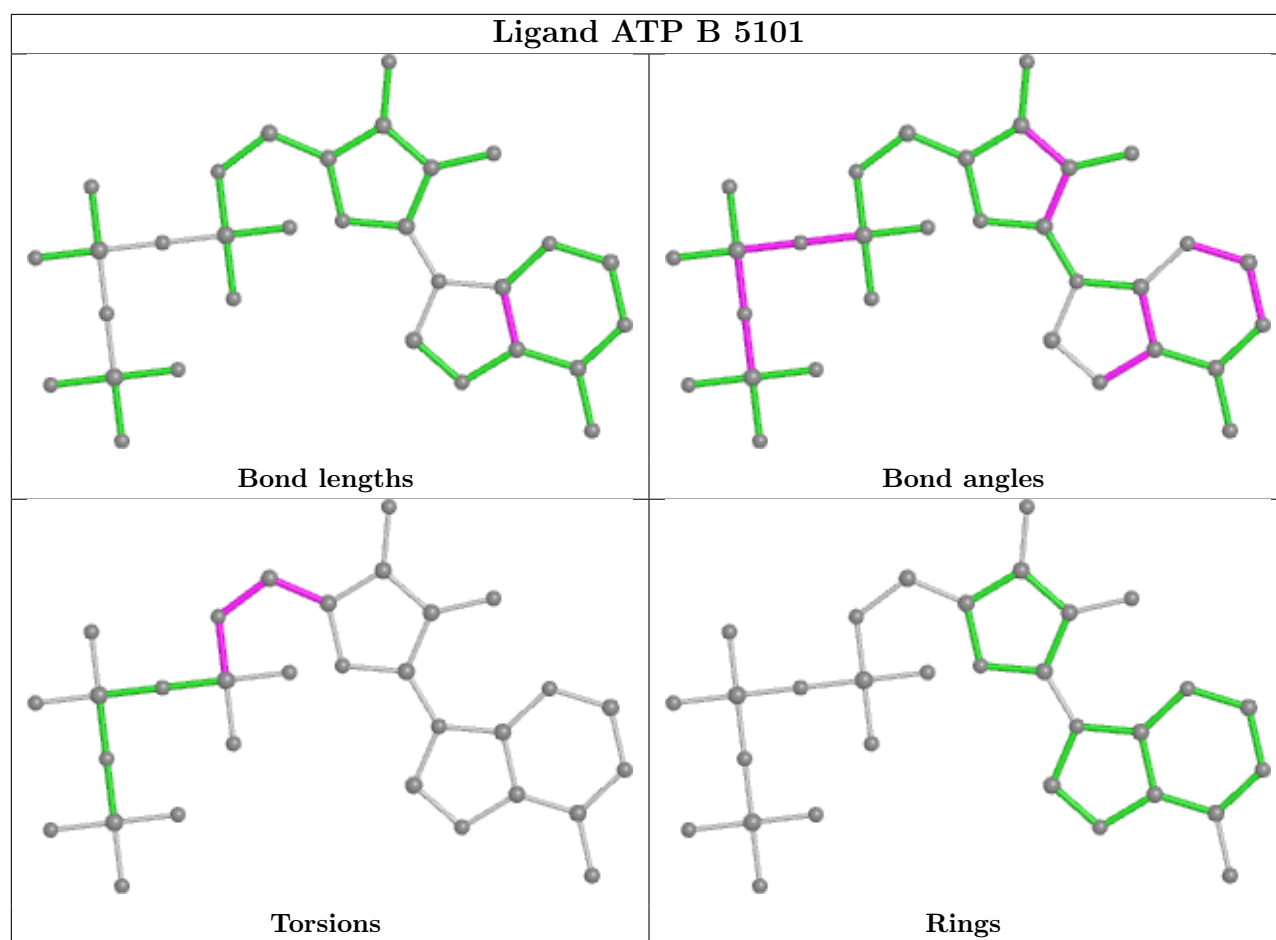
4 monomers are involved in 8 short contacts:

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

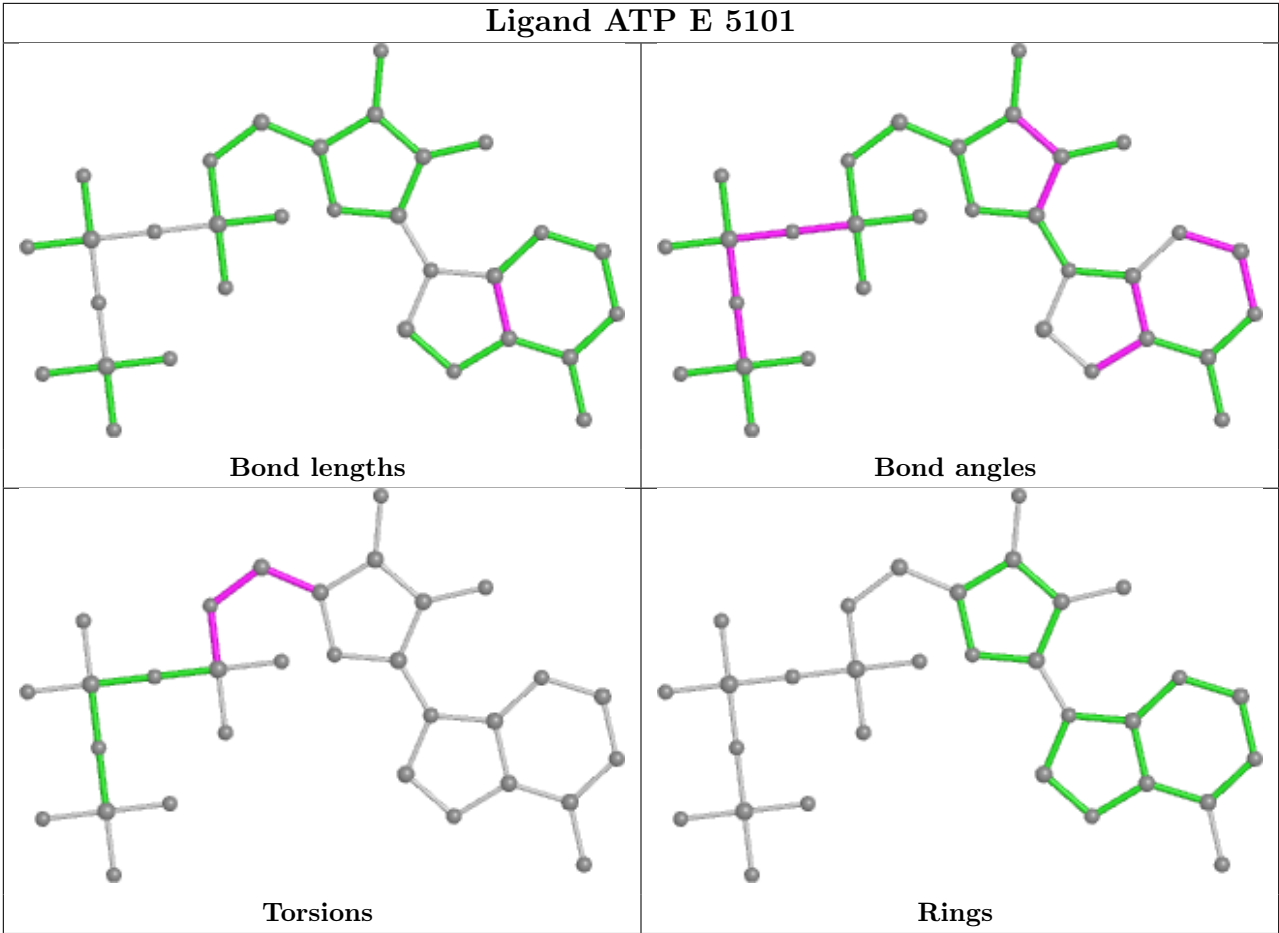
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

The worst 5 of 56 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

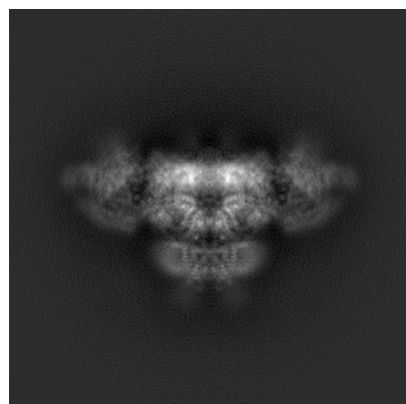
## 6 Map visualisation [i](#)

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.

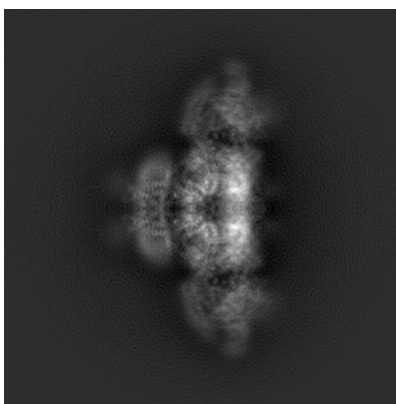
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

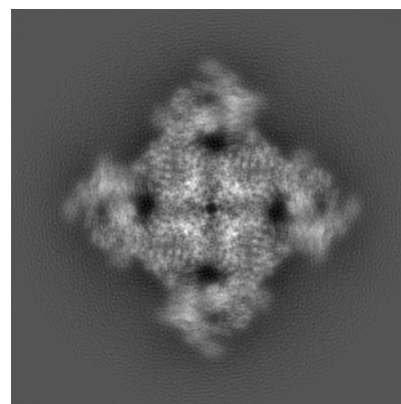
#### 6.1.1 Primary map



X

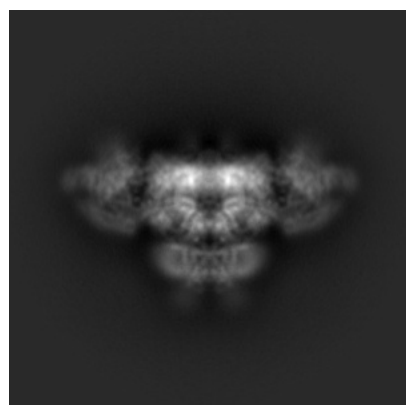


Y

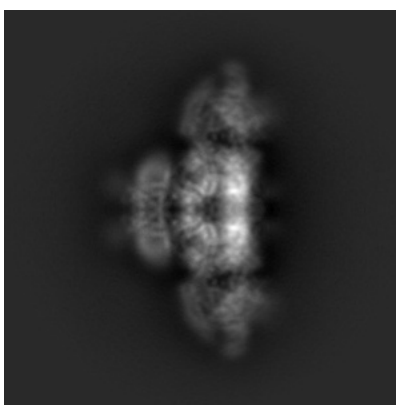


Z

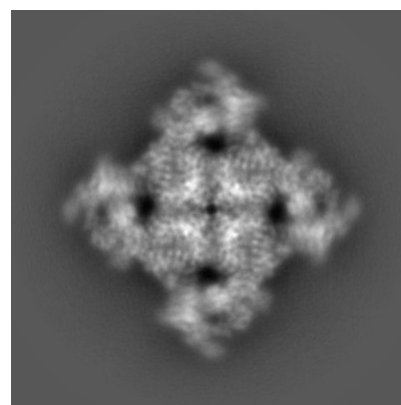
#### 6.1.2 Raw map



X



Y

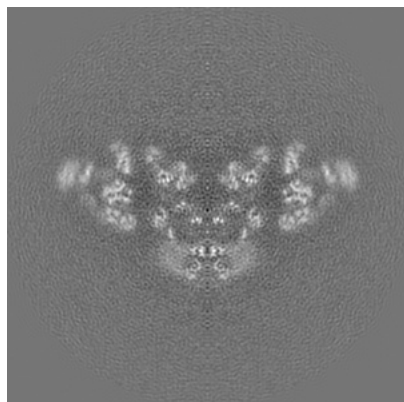


Z

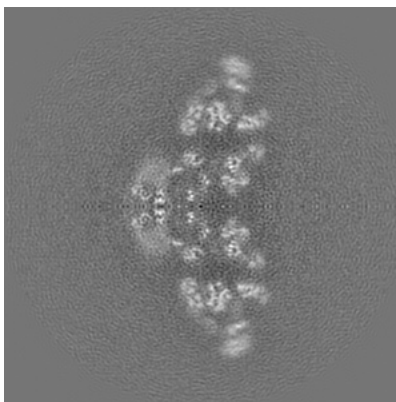
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

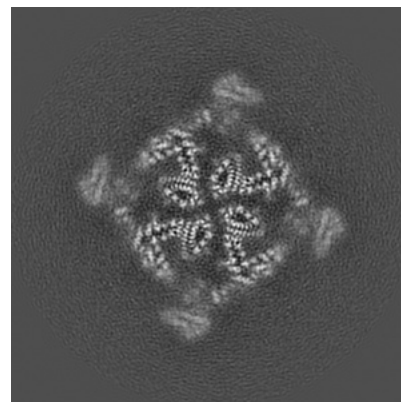
### 6.2.1 Primary map



X Index: 200

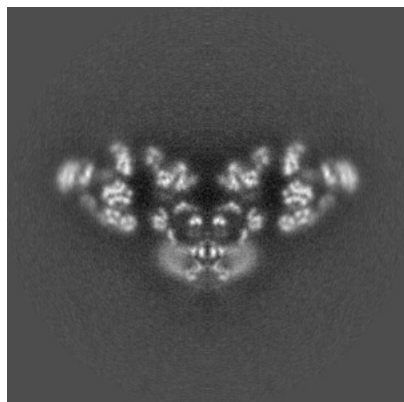


Y Index: 200

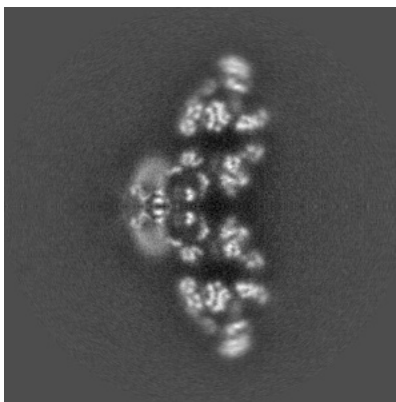


Z Index: 200

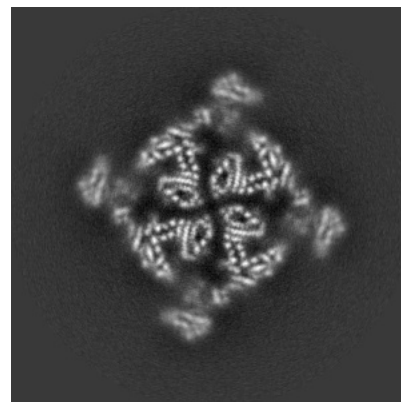
### 6.2.2 Raw map



X Index: 200



Y Index: 200

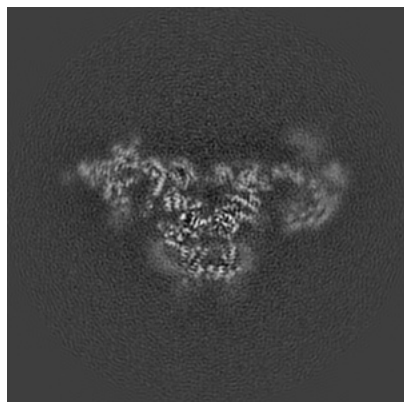


Z Index: 200

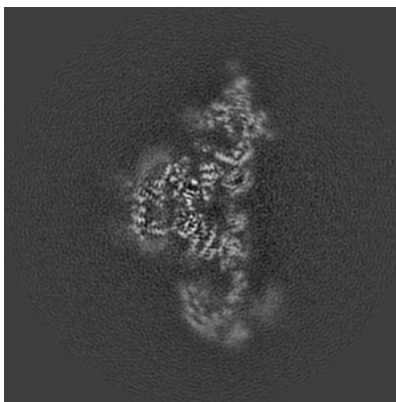
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

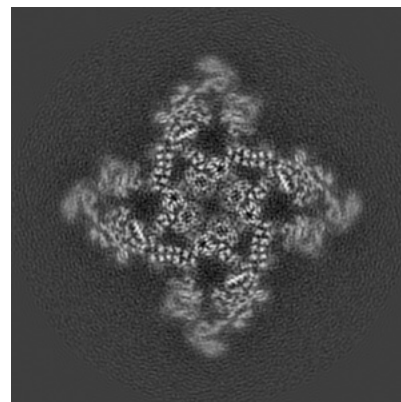
### 6.3.1 Primary map



X Index: 216

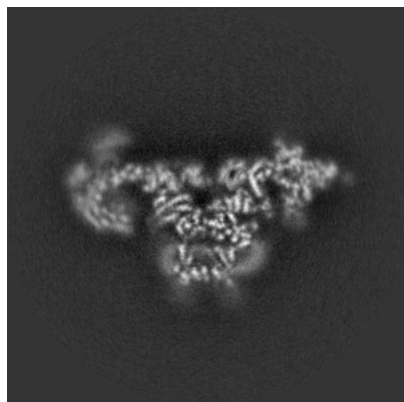


Y Index: 216

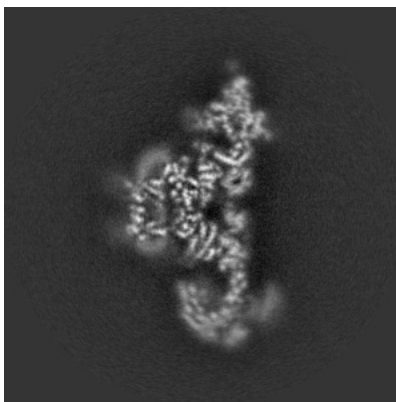


Z Index: 227

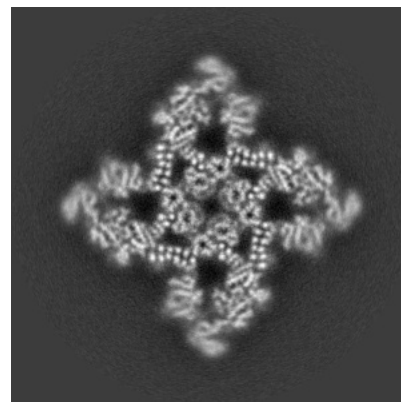
### 6.3.2 Raw map



X Index: 183



Y Index: 217

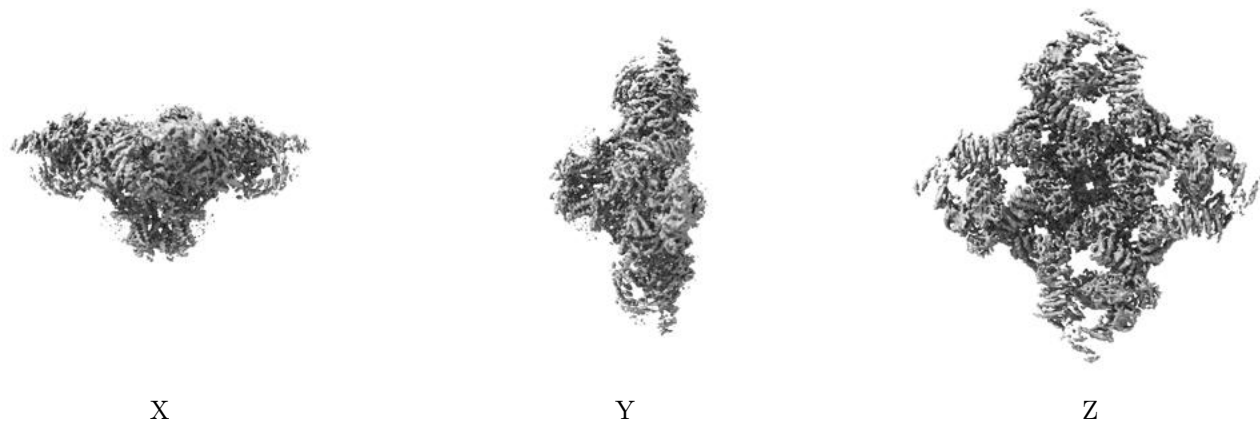


Z Index: 227

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



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

### 6.4.2 Raw map



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

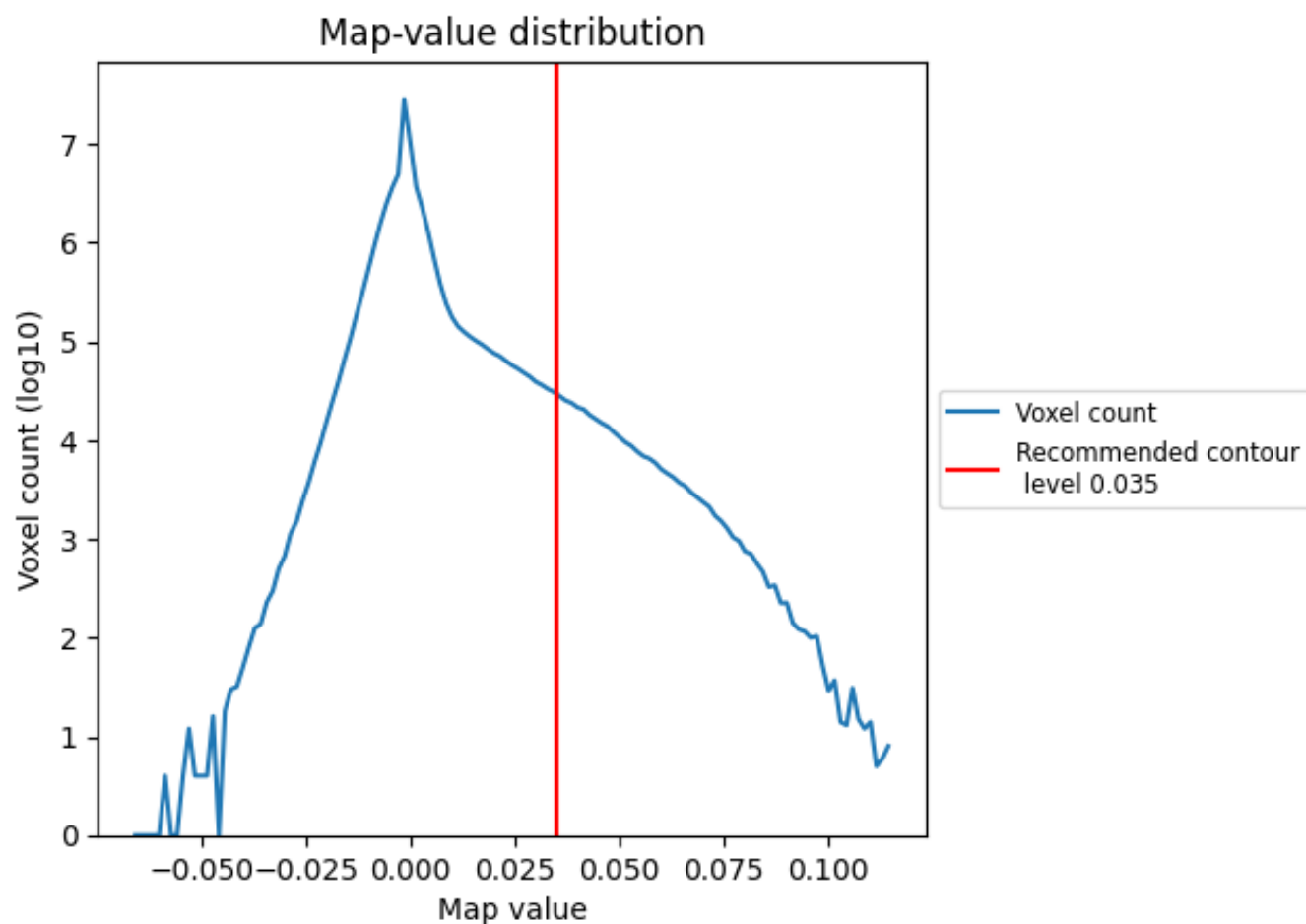
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

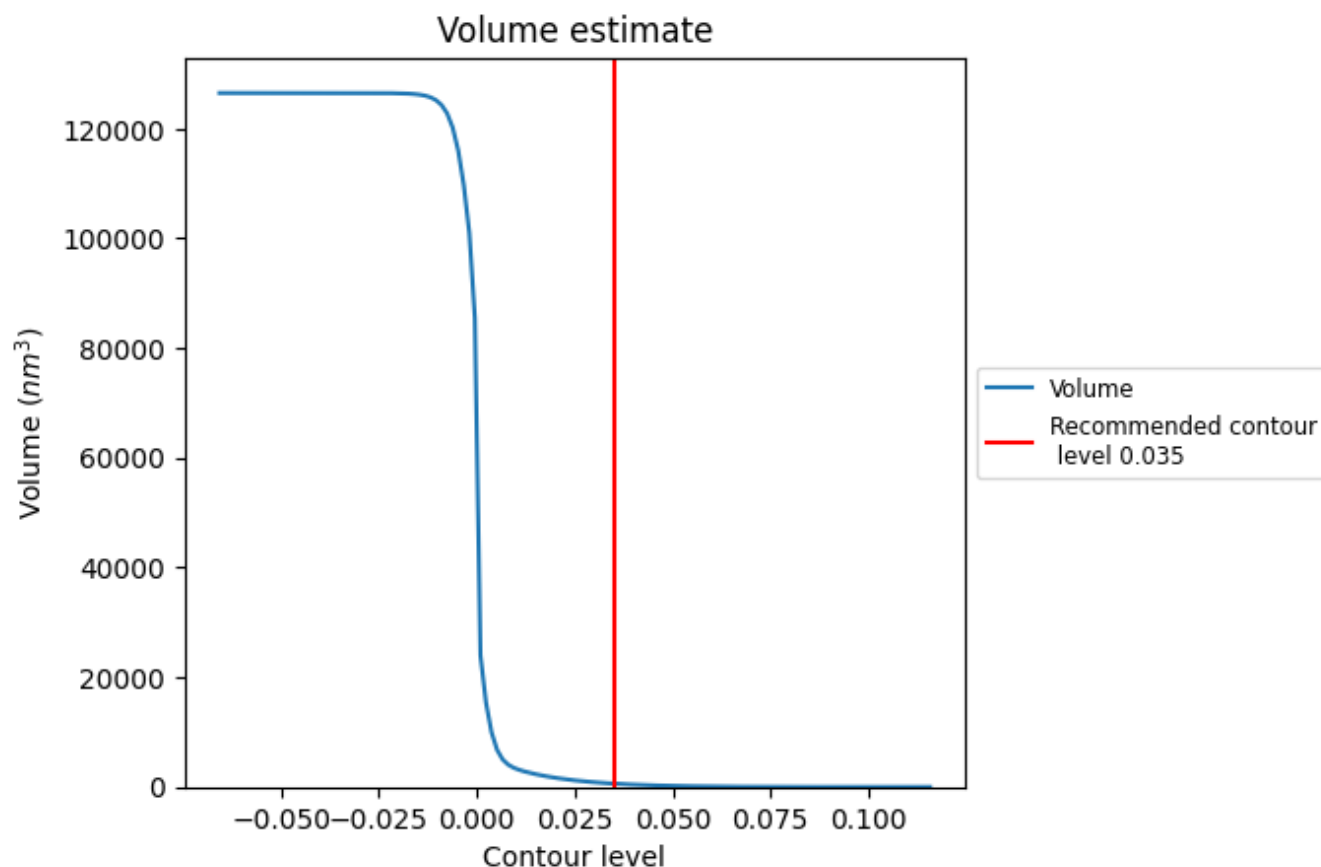
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

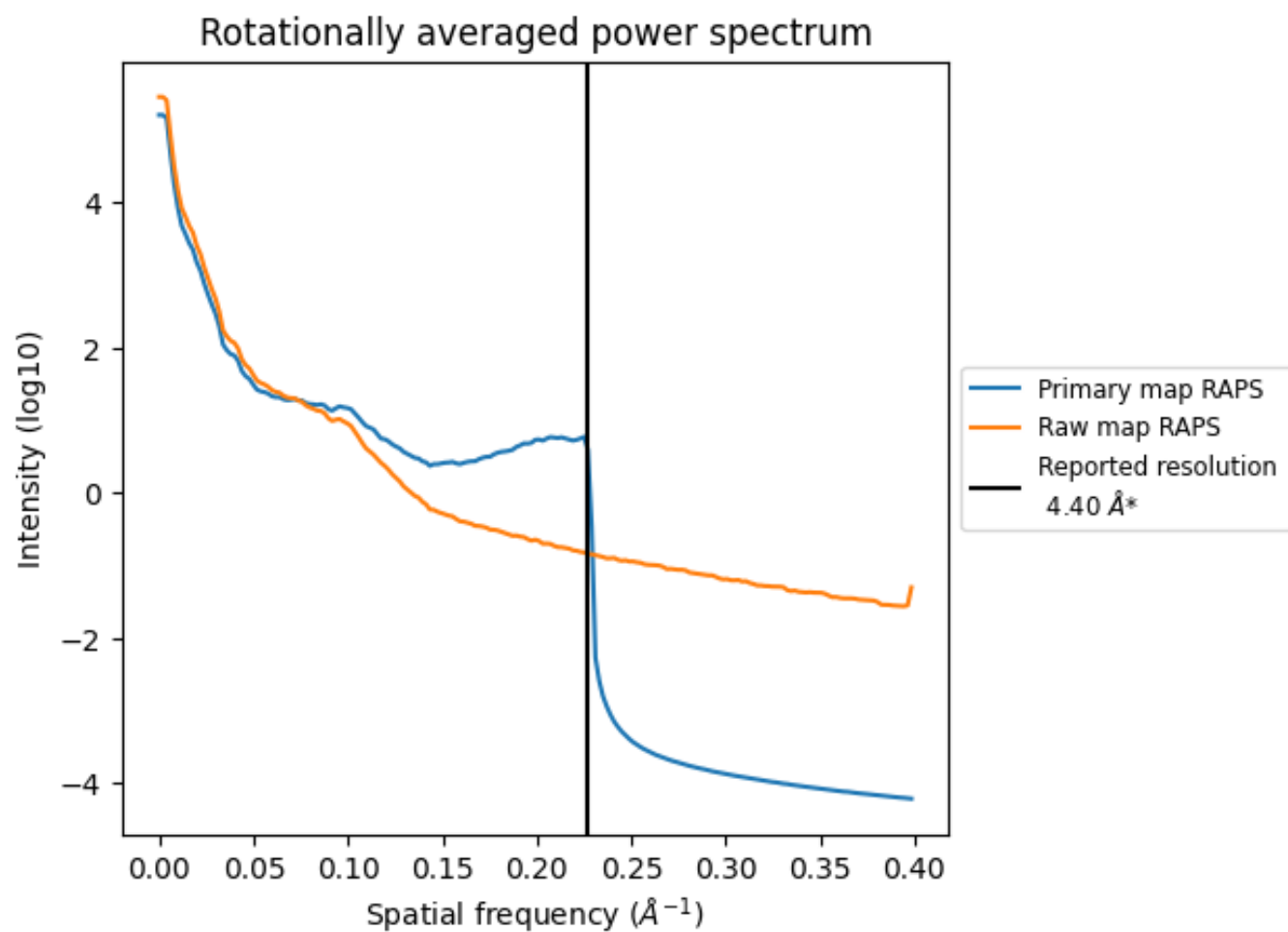


The volume at the recommended contour level is 610 nm<sup>3</sup>; this corresponds to an approximate mass of 551 kDa.

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 [i](#)

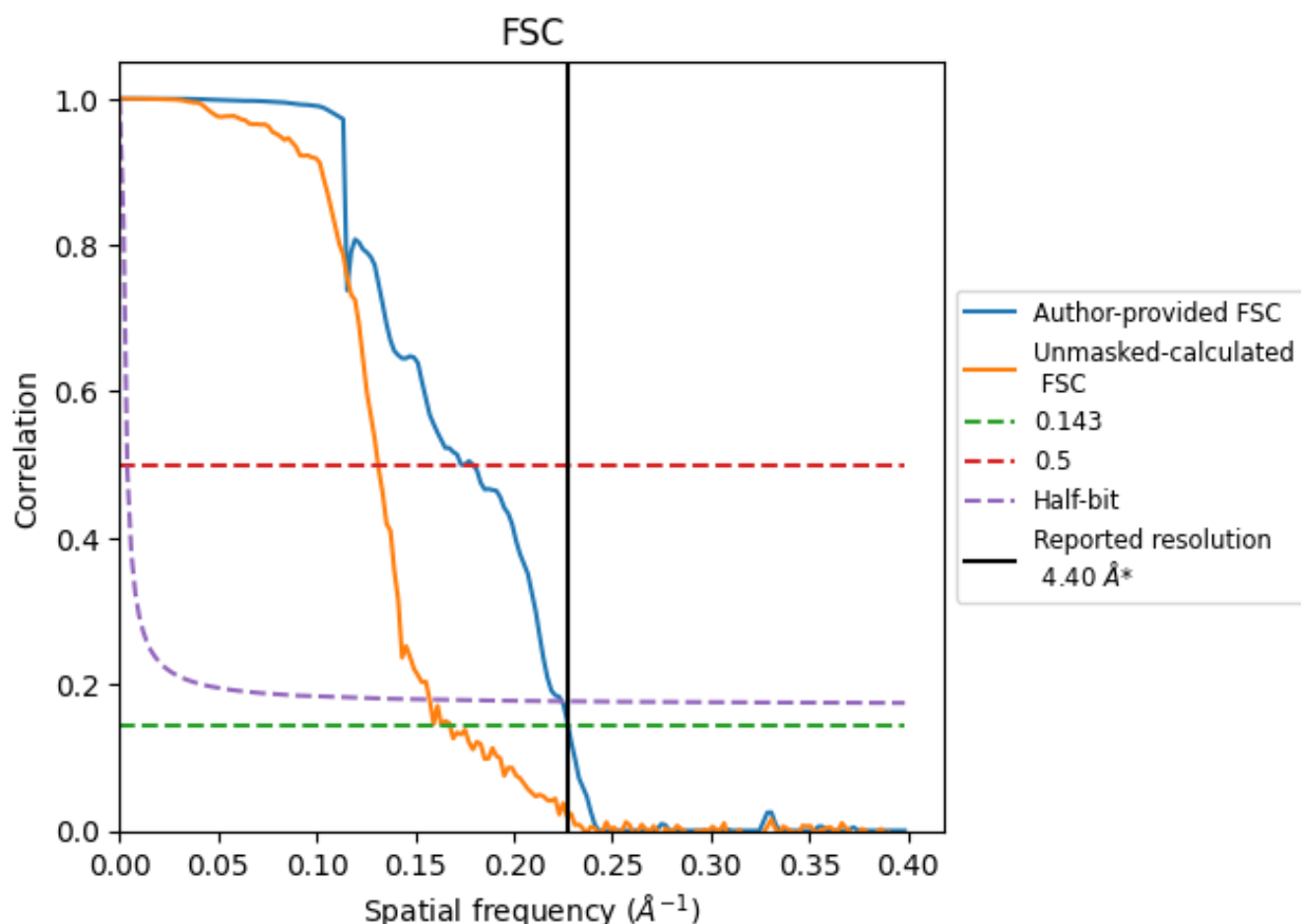


\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

## 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 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

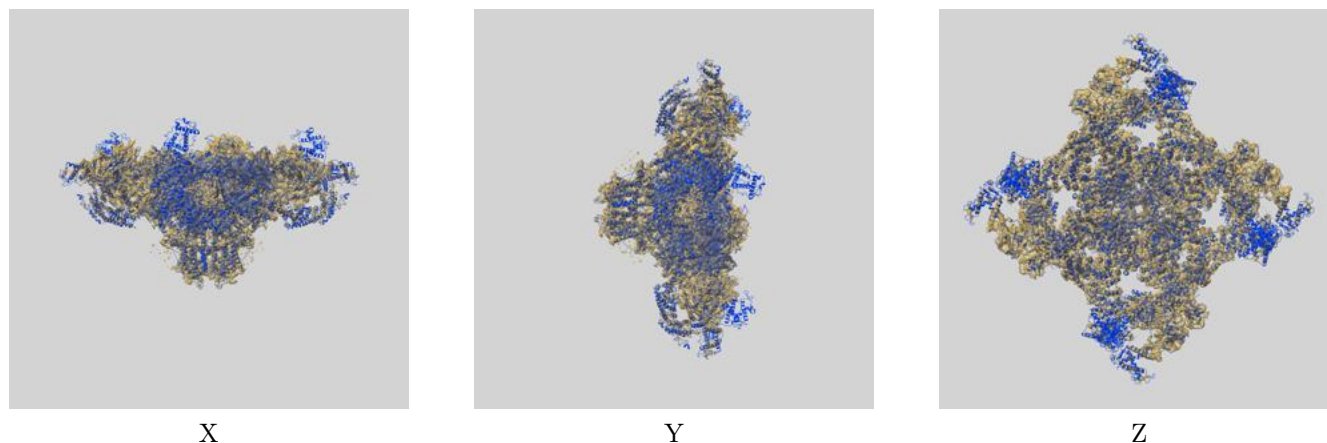
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.39	5.58	4.46
Unmasked-calculated*	5.96	7.62	6.36

\*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](#)

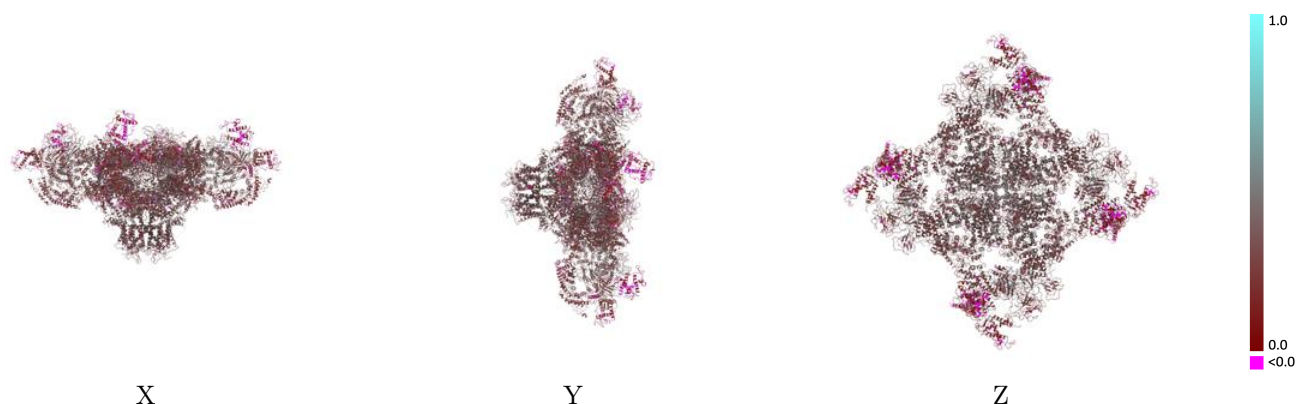
This section contains information regarding the fit between EMDB map EMD-8381 and PDB model 5TAP. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



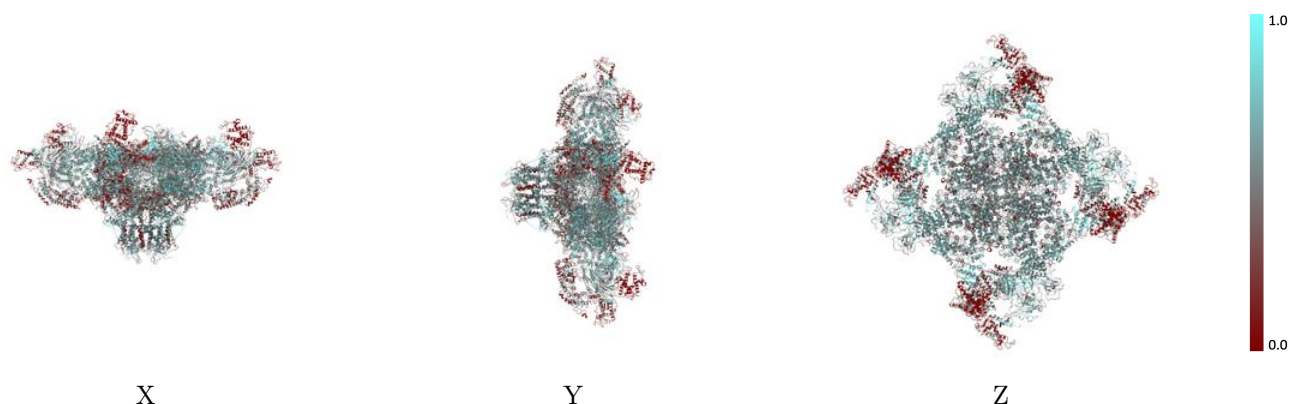
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



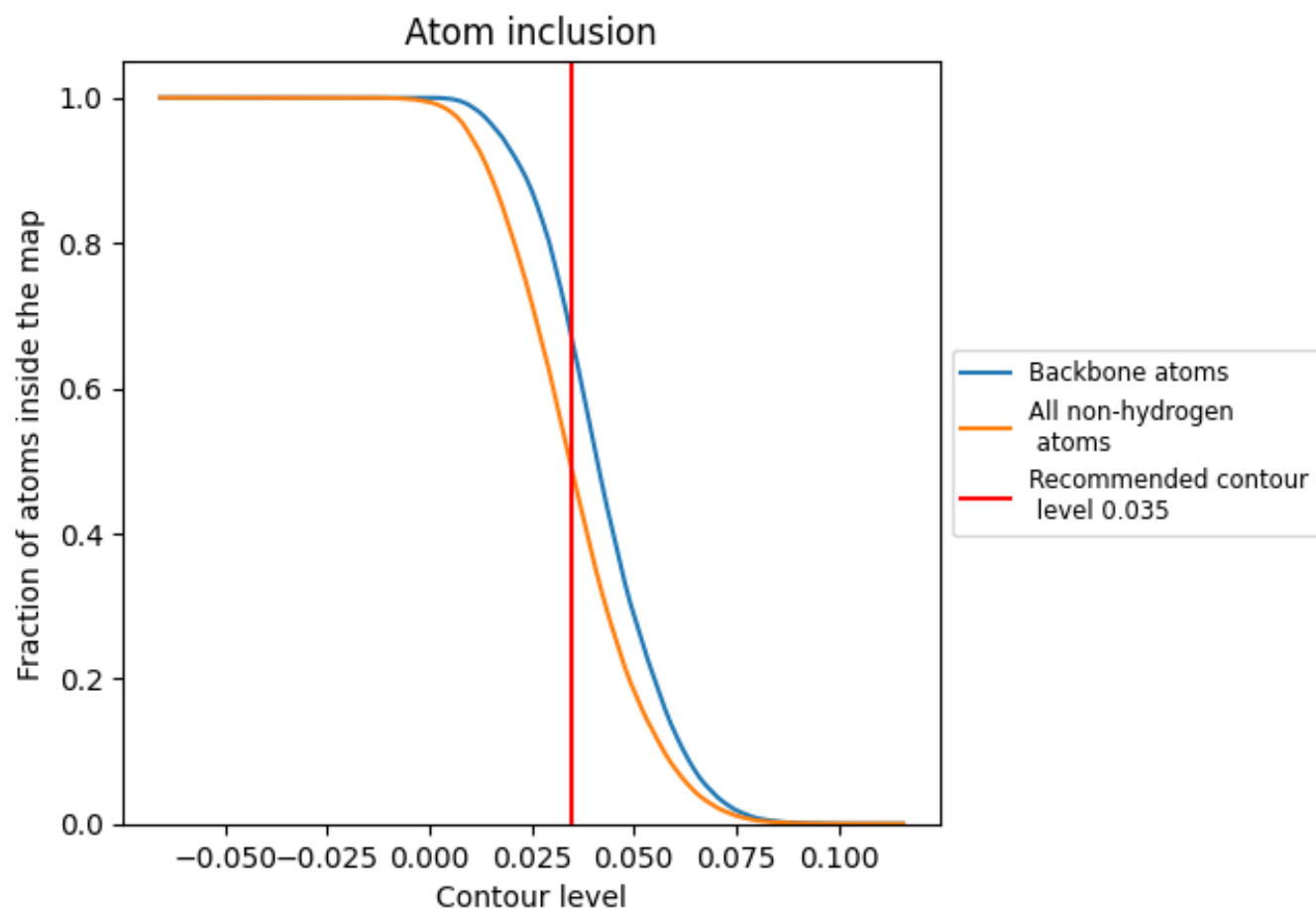
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div><div></div></div> 0.4836	<div><div></div></div> 0.2940
A	<div><div></div></div> 0.4901	<div><div></div></div> 0.3030
B	<div><div></div></div> 0.4838	<div><div></div></div> 0.2940
E	<div><div></div></div> 0.4839	<div><div></div></div> 0.2930
F	<div><div></div></div> 0.4938	<div><div></div></div> 0.3070
G	<div><div></div></div> 0.4833	<div><div></div></div> 0.2930
H	<div><div></div></div> 0.4888	<div><div></div></div> 0.3040
I	<div><div></div></div> 0.4826	<div><div></div></div> 0.2930
J	<div><div></div></div> 0.4901	<div><div></div></div> 0.3020

1.0

0.0

<0.0