



Full wwPDB EM Validation Report ⓘ

Jun 6, 2026 – 12:14 PM EDT

PDB ID : 9YRP / pdb_00009yrp
EMDB ID : EMD-73373
Title : Full-length human VPS13C in complex with calmodulin from the CryoEM composite map
Authors : Li, D.; Reinisch, K.M.
Deposited on : 2025-10-16
Resolution : 4.13 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
MolProbity : 4-5-2 with Phenix2.0
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

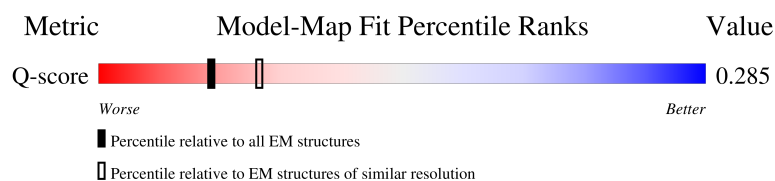
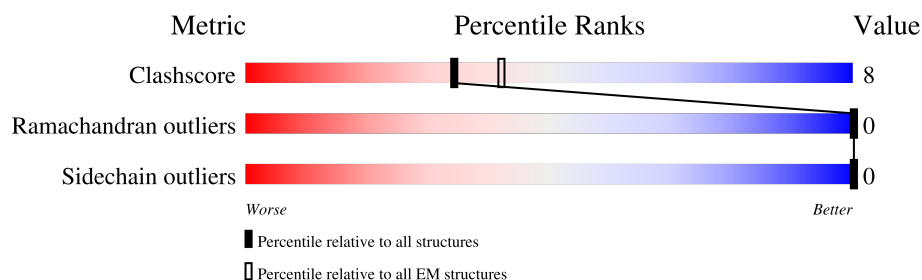
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.13 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	5607 (3.63 - 4.63)

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	149	<div> <div>52%</div> <div>91%</div> <div>8%</div> </div>
2	B	3777	<div> <div>15%</div> <div>64%</div> <div>14%</div> <div>22%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24677 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	148	Total	C	N	O	S	0	0
			1166	714	188	255	9		

- Molecule 2 is a protein called Intermembrane lipid transfer protein VPS13C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2944	Total	C	N	O	S	0	0
			23511	15092	3941	4364	114		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3754	LEU	-	expression tag	UNP Q709C8
B	3755	GLU	-	expression tag	UNP Q709C8
B	3756	ASP	-	expression tag	UNP Q709C8
B	3757	TYR	-	expression tag	UNP Q709C8
B	3758	LYS	-	expression tag	UNP Q709C8
B	3759	ASP	-	expression tag	UNP Q709C8
B	3760	HIS	-	expression tag	UNP Q709C8
B	3761	ASP	-	expression tag	UNP Q709C8
B	3762	GLY	-	expression tag	UNP Q709C8
B	3763	ASP	-	expression tag	UNP Q709C8
B	3764	TYR	-	expression tag	UNP Q709C8
B	3765	LYS	-	expression tag	UNP Q709C8
B	3766	ASP	-	expression tag	UNP Q709C8
B	3767	HIS	-	expression tag	UNP Q709C8
B	3768	ASP	-	expression tag	UNP Q709C8
B	3769	ILE	-	expression tag	UNP Q709C8
B	3770	ASP	-	expression tag	UNP Q709C8
B	3771	TYR	-	expression tag	UNP Q709C8
B	3772	LYS	-	expression tag	UNP Q709C8
B	3773	ASP	-	expression tag	UNP Q709C8
B	3774	ASP	-	expression tag	UNP Q709C8

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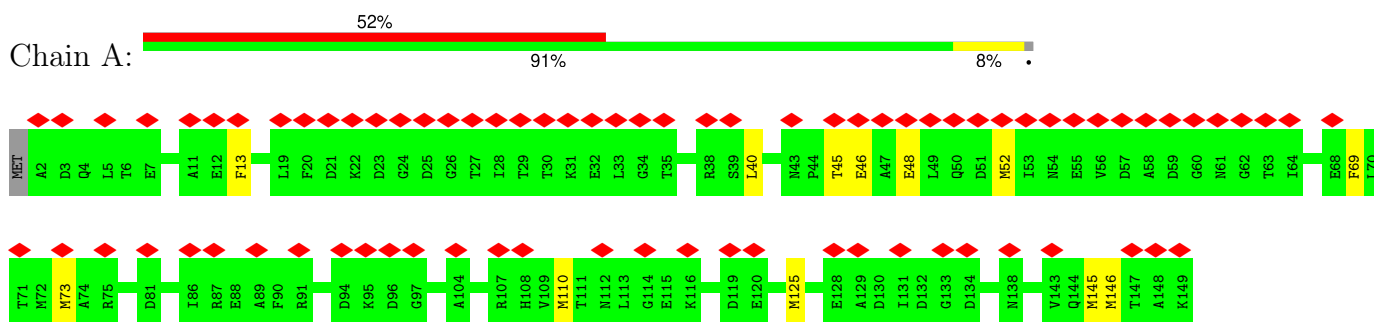
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Chain	Residue	Modelled	Actual	Comment	Reference
B	3775	ASP	-	expression tag	UNP Q709C8
B	3776	ASP	-	expression tag	UNP Q709C8
B	3777	LYS	-	expression tag	UNP Q709C8

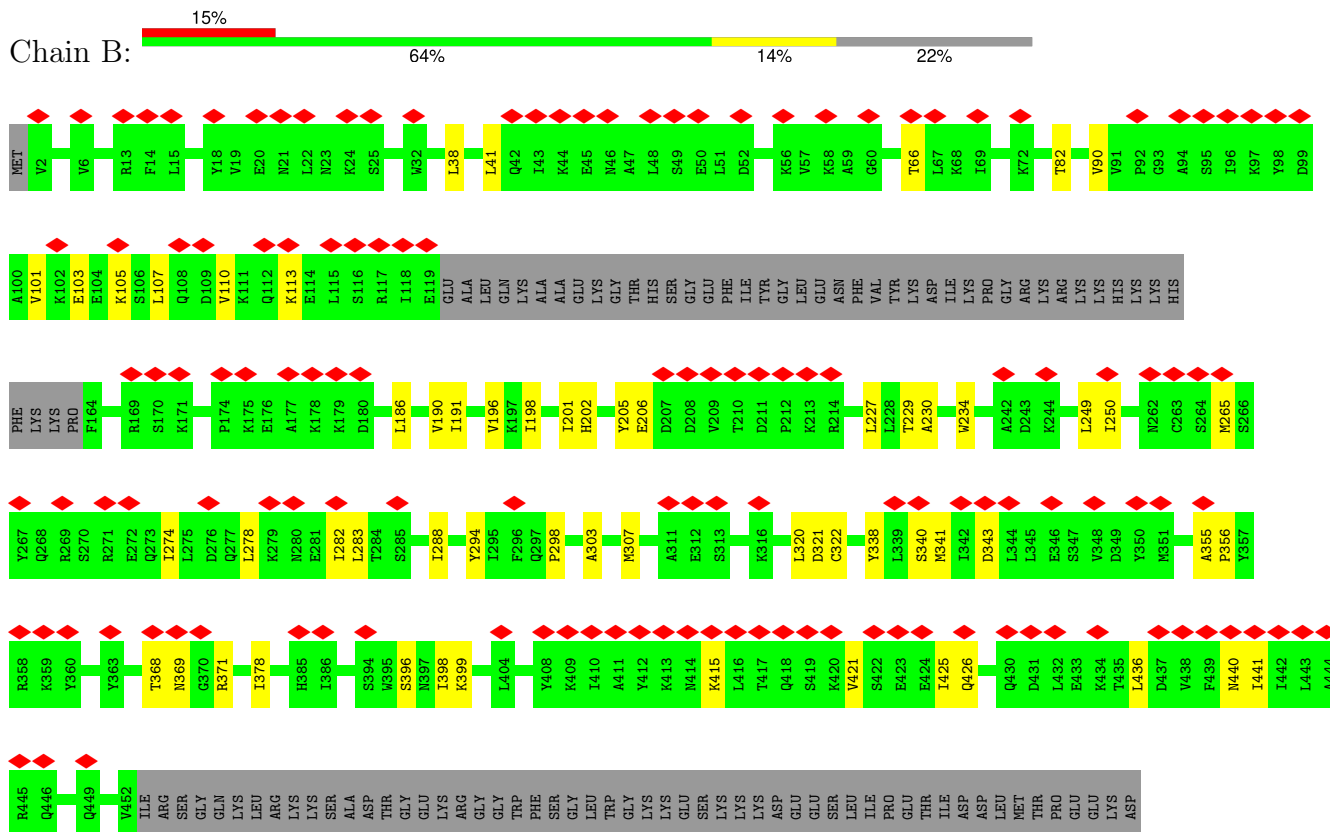
3 Residue-property plots

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: Calmodulin-1

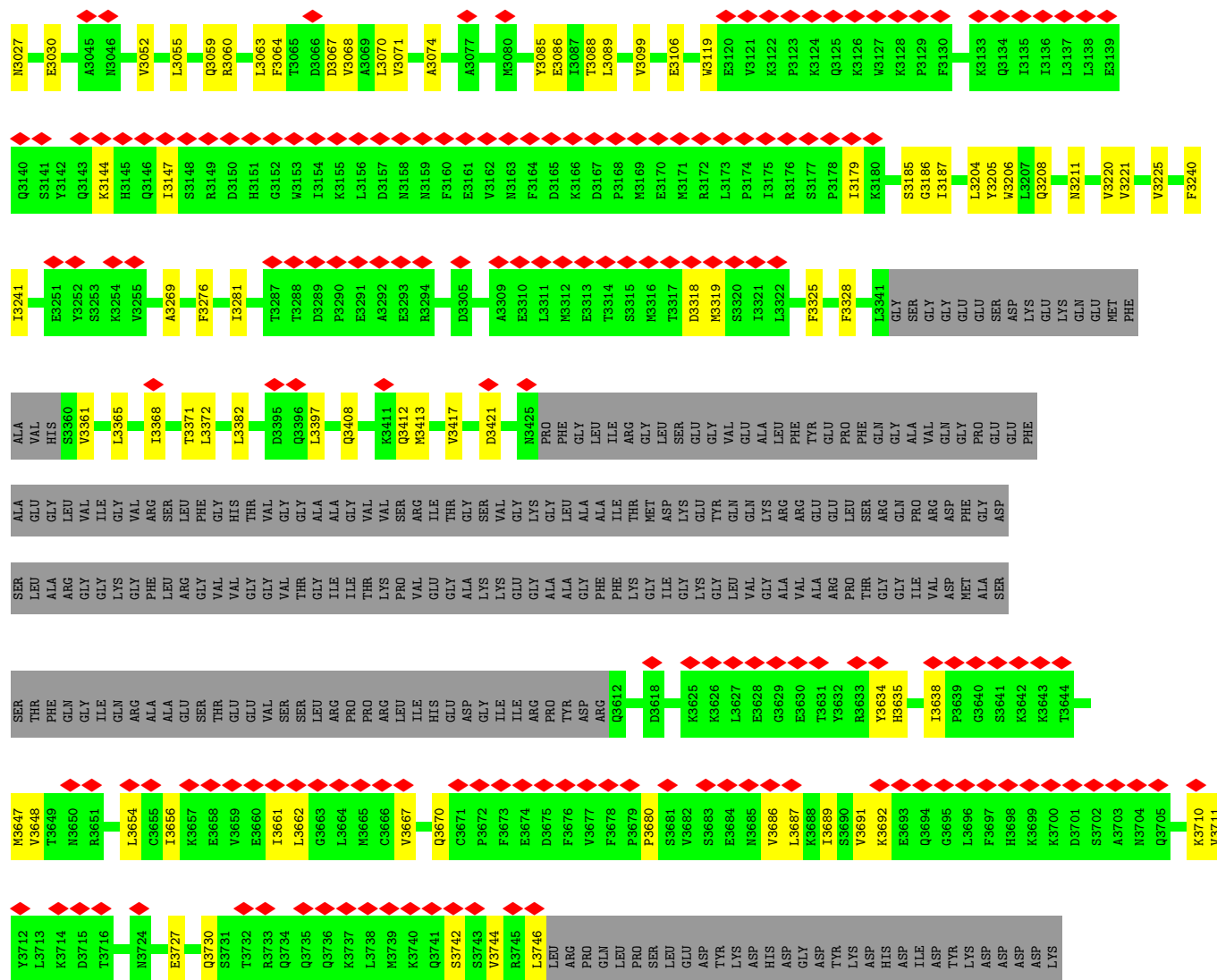


• Molecule 2: Intermembrane lipid transfer protein VPS13C





C2925	C2926	G2940	T2941	L2942	E2946	D2947	G2951	L2952	L2953	V2954	V2955	V2956	L2965	L2966	F2967	Y2970	H2971	E2972	G2973	S2974	P2975	A2977	L2978	L2979	N2980	N2981	W2985	L2988	Q2992	P2996	E2997	L3001	L3002	A3006	A3012	D3013	T3017	R3018	K3019	L3020	T3021	K3022	Y3024																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
F2797	R2798	D2799	I2800	K2806	K2807	K2808	N2809	I2810	F2811	K2812	N2813	N2814	K2815	L2818	K2841	A2844	N2845	E2848	V2853	V2866	T2867	L2868	I2874	K2877	S2878	S2879	V2884	I2887	A2888	S2889	D2890	G2891	S2892	M2893	N2896	C2906	L2907	P2908	F2909	L2914	L2918	V2923	G2924																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
T2671	L2672	R2673	N2674	L2675	L2676	P2677	V2678	S2679	L2680	L2683	G2693	P2694	A2695	I2696	L2697	S2704	R2705	L2706	E2712	L2713	V2714	L2715	I2729	E2735	S2745	T2746	E2747	T2750	L2753	V2757	L2760	R2763	L2766	S2767	W2773	L2774	L2775	N2776	K2777	T2778	T2779	R2780	V2781	L2782	E2787	A2795	D2796																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
L2567	E2568	R2569	I2570	H2580	V2581	P2582	L2583	I2592	G2593	P2594	A2595	I2596	L2597	L2598	E2599	I2609	S2610	E2613	E2614	L2615	H2616	R2617	S2618	R2619	E2620	V2621	L2625	S2633	P2636	L2637	A2643	E2647	L2648	S2649	Y2650	L2651	C2652	T2653	H2654	G2655	E2656	D2657	W2658	D2659	I2664	L2670																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
SER	GLN	GLY	ASN	LEU	SER	ILE	LEU	SER	ARG	GLN	E2484	T2491	L2492	V2493	Y2497	T2498	E2499	V2500	A2501	N2502	I2503	P2504	V2505	P2508	G2509	R2510	R2511	L2512	Y2513	D2524	S2525	V2526	L2527	V2528	Q2529	I2530	D2531	A2532	T2533	E2534	G2535	V2538	L2541	R2542	L2545	G2555	E2556	I2557	L2558	A2559	F2560	V2561	L2562	S2563	L2564	L2565	L2566	L2567	L2568	L2569	L2570	L2571	L2572	L2573	L2574	L2575	L2576	L2577	L2578	L2579	L2580	L2581	L2582	L2583	L2584	L2585	L2586	L2587	L2588	L2589	L2590	L2591	L2592	L2593	L2594	L2595	L2596	L2597	L2598	L2599	L2600	L2601	L2602	L2603	L2604	L2605	L2606	L2607	L2608	L2609	L2610	L2611	L2612	L2613	L2614	L2615	L2616	L2617	L2618	L2619	L2620	L2621	L2622	L2623	L2624	L2625	L2626	L2627	L2628	L2629	L2630	L2631	L2632	L2633	L2634	L2635	L2636	L2637	L2638	L2639	L2640	L2641	L2642	L2643	L2644	L2645	L2646	L2647	L2648	L2649	L2650	L2651	L2652	L2653	L2654	L2655	L2656	L2657	L2658	L2659	L2660	L2661	L2662	L2663	L2664	L2665	L2666	L2667	L2668	L2669	L2670	L2671	L2672	L2673	L2674	L2675	L2676	L2677	L2678	L2679	L2680	L2681	L2682	L2683	L2684	L2685	L2686	L2687	L2688	L2689	L2690	L2691	L2692	L2693	L2694	L2695	L2696	L2697	L2698	L2699	L2700	L2701	L2702	L2703	L2704	L2705	L2706	L2707	L2708	L2709	L2710	L2711	L2712	L2713	L2714	L2715	L2716	L2717	L2718	L2719	L2720	L2721	L2722	L2723	L2724	L2725	L2726	L2727	L2728	L2729	L2730	L2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	L2740	L2741	L2742	L2743	L2744	L2745	L2746	L2747	L2748	L2749	L2750	L2751	L2752	L2753	L2754	L2755	L2756	L2757	L2758	L2759	L2760	L2761	L2762	L2763	L2764	L2765	L2766	L2767	L2768	L2769	L2770	L2771	L2772	L2773	L2774	L2775	L2776	L2777	L2778	L2779	L2780	L2781	L2782	L2783	L2784	L2785	L2786	L2787	L2788	L2789	L2790	L2791	L2792	L2793	L2794	L2795	L2796	L2797	L2798	L2799	L2800	L2801	L2802	L2803	L2804	L2805	L2806	L2807	L2808	L2809	L2810	L2811	L2812	L2813	L2814	L2815	L2816	L2817	L2818	L2819	L2820	L2821	L2822	L2823	L2824	L2825	L2826	L2827	L2828	L2829	L2830	L2831	L2832	L2833	L2834	L2835	L2836	L2837	L2838	L2839	L2840	L2841	L2842	L2843	L2844	L2845	L2846	L2847	L2848	L2849	L2850	L2851	L2852	L2853	L2854	L2855	L2856	L2857	L2858	L2859	L2860	L2861	L2862	L2863	L2864	L2865	L2866	L2867	L2868	L2869	L2870	L2871	L2872	L2873	L2874	L2875	L2876	L2877	L2878	L2879	L2880	L2881	L2882	L2883	L2884	L2885	L2886	L2887	L2888	L2889	L2890	L2891	L2892	L2893	L2894	L2895	L2896	L2897	L2898	L2899	L2900	L2901	L2902	L2903	L2904	L2905	L2906	L2907	L2908	L2909	L2910	L2911	L2912	L2913	L2914	L2915	L2916	L2917	L2918	L2919	L2920	L2921	L2922	L2923	L2924	L2925	L2926	L2927	L2928	L2929	L2930	L2931	L2932	L2933	L2934	L2935	L2936	L2937	L2938	L2939	L2940	L2941	L2942	L2943	L2944	L2945	L2946	L2947	L2948	L2949	L2950	L2951	L2952	L2953	L2954	L2955	L2956	L2957	L2958	L2959	L2960	L2961	L2962	L2963	L2964	L2965	L2966	L2967	L2968	L2969	L2970	L2971	L2972	L2973	L2974	L2975	L2976	L2977	L2978	L2979	L2980	L2981	L2982	L2983	L2984	L2985	L2986	L2987	L2988	L2989	L2990	L2991	L2992	L2993	L2994	L2995	L2996	L2997	L2998	L2999	L3000	L3001	L3002	L3003	L3004	L3005	L3006	L3007	L3008	L3009	L3010	L3011	L3012	L3013	L3014	L3015	L3016	L3017	L3018	L3019	L3020	L3021	L3022	L3023	L3024	L3025	L3026	L3027	L3028	L3029	L3030	L3031	L3032	L3033	L3034	L3035	L3036	L3037	L3038	L3039	L3040	L3041	L3042	L3043	L3044	L3045	L3046	L3047	L3048	L3049	L3050	L3051	L3052	L3053	L3054	L3055	L3056	L3057	L3058	L3059	L3060	L3061	L3062	L3063	L3064	L3065	L3066	L3067	L3068	L3069	L3070	L3071	L3072	L3073	L3074	L3075	L3076	L3077	L3078	L3079	L3080	L3081	L3082	L3083	L3084	L3085	L3086	L3087	L3088	L3089	L3090	L3091	L3092	L3093	L3094	L3095	L3096	L3097	L3098	L3099	L3100	L3101	L3102	L3103	L3104	L3105	L3106	L3107	L3108	L3109	L3110	L3111	L3112	L3113	L3114	L3115	L3116	L3117	L3118	L3119	L3120	L3121	L3122	L3123	L3124	L3125	L3126	L3127	L3128	L3129	L3130	L3131	L3132	L3133	L3134	L3135	L3136	L3137	L3138	L3139	L3140	L3141	L3142	L3143	L3144	L3145	L3146	L3147	L3148	L3149	L3150	L3151	L3152	L3153	L3154	L3155	L3156	L3157	L3158	L3159	L3160	L3161	L3162	L3163	L3164	L3165	L3166	L3167	L3168	L3169	L3170	L3171	L3172	L3173	L3174	L3175	L3176	L3177	L3178	L3179	L3180	L3181	L3182	L3183	L3184	L3185	L3186	L3187	L3188	L3189	L3190	L3191	L3192	L3193	L3194	L3195	L3196	L3197	L3198	L3199	L3200	L3201	L3202	L3203	L3204	L3205	L3206	L3207	L3208	L3209	L3210	L3211	L3212	L3213	L3214	L3215	L3216	L3217	L3218	L3219	L3220	L3221	L3222	L3223	L3224	L3225	L3226	L3227	L3228	L3229	L3230	L3231	L3232	L3233	L3234	L3235	L3236	L3237	L3238	L3239	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259	L3260	L3261	L3262	L3263	L3264	L3265	L3266	L3267	L3268	L3269	L3270	L3271	L3272	L3273	L3274	L3275	L3276	L3277	L3278	L3279	L3280	L3281	L3282	L3283	L3284	L3285	L3286	L3287	L3288	L3289	L3290	L3291	L3292	L3293	L3294	L3295	L3296	L3297	L3298	L3299	L3300	L3301	L3302	L3303	L3304	L3305	L3306	L3307	L3308	L3309	L3310	L3311	L3312	L3313	L3314	L3315	L3316	L3317	L3318	L3319	L3320	L3321	L3322	L3323	L3324	L3325	L3326	L3327	L3328	L3329	L3330	L3331	L3332	L3333	L3334	L3335	L3336	L3337	L3338	L3339	L3340	L3341	L3342	L3343	L3344	L3345	L3346	L3347	L3348	L3349	L3350	L3351	L3352	L3353	L3354	L3355	L3356	L3357	L3358	L3359	L3360	L3361	L3362	L3363	L3364	L3365	L3366	L3367	L3368	L3369	L3370	L3371	L3372	L3373	L3374	L3375	L3376	L3377	L3378	L3379	L3380	L3381	L3382	L3383	L3384	L3385	L3386	L3387	L3388	L3389	L3390	L3391	L3392	L3393	L3394	L3395	L3396	L3397	L3398	L3399	L3400	L3401	L3402	L3403	L3404	L3405	L3406	L3407	L3408	L3409	L3410	L3411	L3412	L3413	L3414	L3415	L3416	L3417	L3418	L3419	L3420	L3421	L3422	L3423	L3424	L3425	L3426	L3427	L3428	L3429	L3430	L3431	L3432	L3433	L3434	L3435	L3436	L3437	L3438	L3439	L3440	L3441	L3442	L3443	L3444	L3445	L3446	L3447	L3448	L3449	L3450	L3451	L3452	L3453	L3454	L3455	L3456	L3457	L3458	L3459	L3460	L3461	L3462	L3463	L3464	L3465	L3466	L3467	L3468	L3469	L3470	L3471	L3472	L3473	L3474	L3475	L3476	L3477	L3478	L3479	L3480	L3481	L3482	L3483	L3484	L3485	L3486	L3487	L3488	L3489	L3490	L3491	L3492	L3493	L3494	L3495	L3496	L3497	L3498	L3499	L3500	L3501	L3502	L3503	L3504	L3505	L3506	L3507	L3508	L3509	L3510	L3511	L3512	L3513	L3514	L3515	L3516	L3517	L3518	L3519	L3520	L3521	L3522	L3523	L3524	L3525	L3526	L3527	L3528	L3529	L3530	L3531	L3532	L3533	L3534	L3535	L3536	L3537	L3538	L3539	L3540	L3541	L3542	L3543	L3544	L3545	L3546	L3547	L3548	L3549	L3550	L3551	L3552	L3553	L3554	L3555	L3556	L3557	L3558	L3559	L3560	L3561	L3562	L3563	L3564	L3565	L3566	L3567	L3568	L3569	L3570	L3571	L3572	L3573	L3574	L3575	L3576	L3577	L3578	L3579	L3580	L3581	L3582	L3583	L3584	L3585	L3586	L3587	L3588	L3589	L3590	L3591	L3592	L3593	L3594	L3595	L3596	L3597	L3598	L3599	L3600	L3601	L3602	L3603	L3604	L3605	L3606	L3607	L3608	L3609	L3610	L3611	L3612	L3613	L3614	L3615	L3616	L3617	L3618	L3619	L3620	L3621	L3622	L3623	L3624	L3625	L3626	L3627	L3628	L3629	L3630	L3631	L3632	L3633	L3634	L3635	L3636	L3637	L3638	L3639	L3640	L3641	L3642	L3643	L3644	L3645	L3646	L3647	L3648	L3649	L3650	L3651	L3652	L3653	L3654	L3655	L3656	L3657	L3658	L3659	L3660	L3661	L3662	L3663	L3664	L3665	L3666	L3667	L3668	L3669	L3670	L3671	L3672	L3673	L3674	L3675	L3676	L3677	L3678	L3679	L3680	L3681	L3682	L3683	L3684	L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	392473	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.408	Depositor
Minimum map value	-0.447	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	546.816, 546.816, 546.816	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.4239999, 1.4239999, 1.4239999	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.13	0/1178	0.28	0/1580
2	B	0.16	0/23945	0.35	0/32390
All	All	0.16	0/25123	0.35	0/33970

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1166	0	1093	10	0
2	B	23511	0	24031	394	0
All	All	24677	0	25124	401	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 8.

All (401) 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:B:1995:LEU:HB3	2:B:2028:ILE:HG22	1.65	0.78
2:B:1026:LEU:HD23	2:B:1026:LEU:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3328:PHE:CE2	2:B:3397:LEU:HD21	2.20	0.77
2:B:2202:ILE:CG2	2:B:2285:VAL:HG12	2.14	0.77
2:B:2351:LEU:HD12	2:B:2351:LEU:O	1.86	0.74
2:B:1262:VAL:HG23	2:B:1366:ILE:HD13	1.72	0.71
2:B:1618:ASN:HB2	2:B:1652:VAL:HG11	1.73	0.71
2:B:2609:ILE:HD11	2:B:2664:ILE:HG21	1.73	0.71
2:B:1538:LEU:HD23	2:B:1608:PHE:HE2	1.54	0.70
2:B:1154:VAL:O	2:B:1185:VAL:HG23	1.91	0.70
2:B:817:ILE:HG21	2:B:822:MET:SD	2.32	0.69
2:B:3225:VAL:HG22	2:B:3269:ALA:HB2	1.75	0.69
2:B:1143:HIS:HE1	2:B:1252:ILE:HG23	1.59	0.68
2:B:1264:VAL:HG22	2:B:1301:LEU:CD1	2.24	0.68
2:B:2884:VAL:HG13	2:B:2918:LEU:HD11	1.76	0.68
2:B:3654:LEU:HD13	2:B:3670:GLN:HB3	1.77	0.67
2:B:1348:LEU:HD23	2:B:1431:ILE:HD12	1.76	0.66
2:B:1271:VAL:HG13	2:B:1294:VAL:HG22	1.78	0.65
2:B:2782:LEU:HD22	2:B:2818:LEU:HD11	1.79	0.65
2:B:3328:PHE:HE2	2:B:3397:LEU:HD21	1.61	0.64
2:B:1540:LEU:HB2	2:B:1610:VAL:HG22	1.79	0.64
2:B:557:ILE:HG23	2:B:579:LEU:HD11	1.80	0.64
2:B:1833:LEU:HD23	2:B:1834:LYS:O	1.98	0.63
2:B:3204:LEU:HD23	2:B:3205:TYR:N	2.13	0.63
2:B:2000:LEU:HD23	2:B:2000:LEU:O	2.00	0.62
2:B:2556:ILE:HD12	2:B:2599:GLU:CD	2.24	0.62
2:B:1703:ILE:HG22	2:B:1705:ILE:HD11	1.81	0.61
2:B:2285:VAL:CG2	2:B:2301:ALA:HB3	2.30	0.61
2:B:2942:LEU:HD23	2:B:2976:PRO:HD3	1.82	0.61
2:B:1159:LEU:HD23	2:B:1160:ASP:N	2.16	0.61
2:B:2285:VAL:HG22	2:B:2301:ALA:HB3	1.83	0.61
1:A:145:MET:HE1	2:B:378:ILE:HD11	1.84	0.60
2:B:2314:SER:C	2:B:2315:LEU:HD12	2.26	0.60
2:B:2014:MET:HE1	2:B:2120:LEU:HD21	1.84	0.60
2:B:2207:ILE:HD11	2:B:2416:TYR:CE1	2.37	0.59
1:A:45:THR:HG22	1:A:46:GLU:H	1.68	0.59
2:B:3382:LEU:HD23	2:B:3412:GLN:OE1	2.02	0.59
2:B:1241:ILE:HG22	2:B:1273:ASN:HB3	1.85	0.59
2:B:942:LEU:HD13	2:B:959:LEU:HD12	1.85	0.59
2:B:1538:LEU:HD23	2:B:1608:PHE:CE2	2.37	0.59
2:B:38:LEU:HD21	2:B:41:LEU:HD21	1.85	0.59
2:B:2343:VAL:HG21	2:B:2385:ASN:HB3	1.84	0.58
2:B:371:ARG:O	2:B:371:ARG:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2782:LEU:CD1	2:B:2868:LEU:HD13	2.34	0.58
2:B:573:LEU:HD21	2:B:575:VAL:HG23	1.86	0.57
2:B:1298:LYS:HD2	2:B:1298:LYS:O	2.04	0.57
2:B:2132:PHE:CD2	2:B:2151:VAL:HG13	2.40	0.57
2:B:3023:THR:HG23	2:B:3027:ASN:O	2.04	0.57
2:B:573:LEU:HB3	2:B:614:THR:HG22	1.87	0.56
2:B:1262:VAL:HG23	2:B:1366:ILE:CD1	2.34	0.56
2:B:198:ILE:HG22	2:B:201:ILE:HD11	1.89	0.56
2:B:2556:ILE:HD12	2:B:2599:GLU:OE2	2.06	0.56
2:B:1874:ASP:O	2:B:1878:LEU:HD23	2.05	0.55
2:B:191:ILE:HG21	2:B:307:MET:HE2	1.89	0.55
2:B:2197:VAL:HG11	2:B:2200:PHE:CE2	2.41	0.55
2:B:2493:VAL:HG22	2:B:2499:GLU:OE1	2.07	0.55
2:B:1269:ILE:HD11	2:B:1296:LEU:HD13	1.88	0.55
2:B:3220:VAL:HG23	2:B:3220:VAL:O	2.07	0.55
2:B:3325:PHE:CZ	2:B:3397:LEU:HD22	2.41	0.55
2:B:2463:GLU:C	2:B:2464:LEU:HD12	2.32	0.55
2:B:714:LEU:HD12	2:B:759:LEU:O	2.07	0.55
2:B:1481:CYS:HB2	2:B:1494:ILE:HD11	1.89	0.54
2:B:1541:VAL:HG22	2:B:1611:PHE:CE1	2.41	0.54
2:B:1793:VAL:HG13	2:B:1795:MET:HE1	1.88	0.54
2:B:2556:ILE:HD13	2:B:2569:ARG:HH12	1.71	0.54
2:B:2202:ILE:HG21	2:B:2285:VAL:HG12	1.87	0.54
2:B:2701:VAL:HG13	2:B:2704:SER:HB3	1.89	0.54
1:A:13:PHE:CD2	1:A:73:MET:HE3	2.42	0.54
2:B:815:VAL:HB	2:B:922:LEU:HD23	1.90	0.54
2:B:990:LEU:HD11	2:B:1020:PHE:CE1	2.43	0.54
2:B:1541:VAL:HG13	2:B:1611:PHE:CE2	2.43	0.53
2:B:196:VAL:HG12	2:B:227:LEU:HB3	1.89	0.53
2:B:2729:ILE:O	2:B:2729:ILE:HG13	2.09	0.53
2:B:2527:LEU:HD23	2:B:2542:ARG:NH2	2.24	0.53
2:B:2893:MET:HE2	2:B:2893:MET:HA	1.91	0.53
2:B:3221:VAL:HG21	2:B:3276:PHE:CE2	2.44	0.52
2:B:714:LEU:HD11	2:B:758:LEU:HD21	1.89	0.52
1:A:69:PHE:O	1:A:73:MET:HG2	2.09	0.52
2:B:2980:MET:SD	2:B:3063:LEU:HD23	2.49	0.52
2:B:806:VAL:HG23	2:B:913:LEU:HA	1.90	0.52
2:B:2674:ASN:HB2	2:B:2693:LEU:HD22	1.91	0.52
2:B:2207:ILE:HD11	2:B:2416:TYR:CD1	2.44	0.52
2:B:2554:ALA:HB3	2:B:2595:ALA:HB3	1.91	0.52
2:B:2002:ASP:C	2:B:2003:LEU:HD22	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2146:MET:HA	2:B:2146:MET:HE2	1.92	0.52
2:B:3017:THR:HG22	2:B:3019:LYS:H	1.75	0.52
2:B:3654:LEU:HD13	2:B:3670:GLN:CB	2.40	0.52
2:B:3281:ILE:HD11	2:B:3361:VAL:HG21	1.92	0.52
1:A:145:MET:CE	2:B:378:ILE:HD11	2.41	0.51
2:B:2884:VAL:CG1	2:B:2918:LEU:HD11	2.39	0.51
1:A:45:THR:HG22	1:A:46:GLU:N	2.25	0.51
2:B:3086:GLU:O	2:B:3086:GLU:HG3	2.11	0.51
1:A:146:MET:HA	1:A:146:MET:HE3	1.92	0.51
2:B:2107:ALA:HB3	2:B:2136:LEU:HB3	1.93	0.51
2:B:2670:LEU:O	2:B:2701:VAL:HG12	2.11	0.51
2:B:2988:LEU:HD21	2:B:3064:PHE:CZ	2.46	0.51
2:B:3068:VAL:O	2:B:3071:VAL:HG22	2.11	0.51
2:B:3211:ASN:HB2	2:B:3221:VAL:HG23	1.93	0.51
2:B:1318:LEU:HD13	2:B:1353:VAL:HG22	1.94	0.50
2:B:2583:LEU:O	2:B:2583:LEU:HD23	2.12	0.50
2:B:2610:SER:O	2:B:2621:VAL:HG11	2.12	0.50
2:B:3021:THR:HG22	2:B:3030:GLU:HG3	1.93	0.50
2:B:320:LEU:HD21	2:B:322:CYS:HB2	1.94	0.50
2:B:2853:VAL:HG22	2:B:2868:LEU:HD23	1.94	0.50
2:B:2853:VAL:HG22	2:B:2868:LEU:CD2	2.41	0.50
2:B:1245:LEU:HB3	2:B:1269:ILE:HB	1.93	0.50
2:B:3371:THR:HG23	2:B:3371:THR:O	2.12	0.50
2:B:1191:VAL:HA	2:B:1250:ILE:HG23	1.94	0.49
2:B:1143:HIS:CE1	2:B:1252:ILE:HG23	2.45	0.49
2:B:2042:ASP:OD1	2:B:2042:ASP:C	2.55	0.49
2:B:2299:LEU:HD21	2:B:2326:VAL:CG1	2.42	0.49
2:B:2319:VAL:HG12	2:B:2320:ALA:N	2.27	0.49
2:B:2782:LEU:HD22	2:B:2818:LEU:CD1	2.43	0.49
2:B:2942:LEU:HD22	2:B:2970:TYR:CE1	2.46	0.49
2:B:2341:GLU:OE1	2:B:2388:ASN:O	2.30	0.49
2:B:1608:PHE:HB3	2:B:1624:ILE:HG12	1.93	0.49
2:B:2706:ILE:O	2:B:2706:ILE:HG13	2.12	0.49
2:B:1317:LEU:HD21	2:B:1359:ASP:HB3	1.95	0.48
2:B:2491:THR:HG22	2:B:2501:ALA:HB1	1.95	0.48
2:B:593:VAL:O	2:B:593:VAL:HG13	2.13	0.48
2:B:1029:THR:O	2:B:1033:VAL:HG23	2.13	0.48
2:B:1704:GLN:OE1	2:B:1766:ILE:HD12	2.13	0.48
2:B:2954:VAL:HG23	2:B:2967:PHE:CE1	2.49	0.48
2:B:3055:LEU:HD11	2:B:3060:ARG:NH2	2.28	0.48
2:B:2528:VAL:HG12	2:B:2541:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3240:PHE:O	2:B:3241:ILE:C	2.56	0.48
2:B:229:THR:HG22	2:B:230:ALA:N	2.29	0.48
2:B:1147:VAL:HG22	2:B:1190:ILE:HA	1.95	0.48
2:B:3328:PHE:CZ	2:B:3397:LEU:HD11	2.49	0.48
2:B:1243:ILE:HB	2:B:1271:VAL:HB	1.96	0.48
2:B:536:LEU:HD22	2:B:539:THR:OG1	2.14	0.48
2:B:2567:LEU:HD23	2:B:2567:LEU:H	1.77	0.48
2:B:1247:ALA:HB1	2:B:1266:LEU:HB3	1.95	0.48
2:B:1778:ILE:HD12	2:B:1819:THR:HG21	1.96	0.48
2:B:2906:CYS:C	2:B:2907:LEU:HD22	2.39	0.48
2:B:3319:MET:N	2:B:3319:MET:HE2	2.29	0.48
2:B:1950:TYR:HA	2:B:1968:GLN:HA	1.96	0.47
2:B:283:LEU:HD12	2:B:288:ILE:HA	1.96	0.47
2:B:2992:GLN:HE22	2:B:3012:ALA:H	1.61	0.47
2:B:1090:LEU:HB3	2:B:1112:LEU:HB3	1.96	0.47
2:B:234:TRP:HD1	2:B:249:LEU:HD21	1.79	0.47
2:B:3088:THR:HG22	2:B:3089:LEU:N	2.30	0.47
2:B:282:ILE:HG22	2:B:282:ILE:O	2.14	0.47
2:B:2299:LEU:HD21	2:B:2326:VAL:HG13	1.97	0.47
2:B:2513:TYR:HA	2:B:2652:CYS:HB2	1.96	0.47
2:B:2637:LEU:HD23	2:B:2637:LEU:O	2.15	0.47
2:B:2678:TYR:HB2	2:B:2715:LEU:HD11	1.96	0.47
2:B:2874:ILE:HD13	2:B:2965:ILE:HB	1.95	0.47
2:B:3635:HIS:HB3	2:B:3647:MET:HG3	1.97	0.47
2:B:695:LYS:HB3	2:B:696:PRO:CD	2.45	0.47
2:B:1261:ALA:O	2:B:1303:ARG:HA	2.15	0.47
2:B:1541:VAL:HG22	2:B:1611:PHE:CZ	2.49	0.47
2:B:338:TYR:O	2:B:341:MET:HG3	2.15	0.47
2:B:2757:VAL:HG12	2:B:2766:LEU:CD2	2.45	0.47
2:B:913:LEU:HD23	2:B:946:ALA:HB3	1.97	0.47
2:B:1029:THR:HG21	2:B:1099:ASN:CG	2.39	0.47
2:B:2527:LEU:HD23	2:B:2542:ARG:CZ	2.45	0.47
2:B:3019:LYS:HE3	2:B:3030:GLU:HB3	1.98	0.47
2:B:2512:LEU:HD11	2:B:2525:SER:HB3	1.97	0.46
2:B:3656:ILE:HD12	2:B:3667:VAL:HA	1.97	0.46
2:B:3692:LYS:HD2	2:B:3692:LYS:C	2.41	0.46
2:B:956:VAL:HG23	2:B:956:VAL:O	2.15	0.46
2:B:340:SER:O	2:B:343:ASP:OD1	2.33	0.46
2:B:2285:VAL:O	2:B:2285:VAL:HG23	2.14	0.46
2:B:2814:ASN:O	2:B:2815:LYS:HB2	2.14	0.46
2:B:3281:ILE:CD1	2:B:3361:VAL:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1539:ASP:C	2:B:1540:LEU:HD12	2.41	0.46
2:B:690:LEU:HD11	2:B:692:ILE:CG1	2.46	0.46
2:B:1181:LEU:HB2	2:B:1239:VAL:HG13	1.98	0.46
2:B:2014:MET:HE1	2:B:2120:LEU:HD11	1.97	0.46
2:B:415:LYS:NZ	2:B:421:VAL:HG13	2.31	0.46
2:B:1149:ILE:HG23	2:B:1149:ILE:O	2.16	0.46
2:B:1767:ILE:HG23	2:B:1767:ILE:O	2.16	0.46
2:B:2112:PRO:HD2	2:B:2132:PHE:O	2.16	0.46
2:B:2542:ARG:NH1	2:B:2546:GLN:HG3	2.30	0.46
2:B:2650:TYR:HA	2:B:3744:VAL:HG13	1.96	0.46
2:B:2676:LEU:HD11	2:B:2753:LEU:HD13	1.97	0.46
2:B:2781:VAL:O	2:B:2781:VAL:HG23	2.15	0.46
2:B:3067:ASP:HB2	2:B:3070:LEU:HD12	1.98	0.46
2:B:1187:CYS:HA	2:B:1246:LYS:O	2.16	0.46
2:B:2503:ILE:HG13	2:B:2503:ILE:O	2.16	0.46
2:B:2774:LEU:HD23	2:B:2866:VAL:HB	1.98	0.46
2:B:1700:VAL:HG12	2:B:1701:GLY:O	2.16	0.46
2:B:2648:LEU:HD12	2:B:2651:ILE:HD11	1.97	0.46
2:B:2200:PHE:HD2	2:B:2280:VAL:HG11	1.80	0.46
2:B:723:LEU:C	2:B:723:LEU:HD23	2.41	0.45
2:B:1154:VAL:HG12	2:B:1155:PHE:HD1	1.80	0.45
2:B:2497:TYR:OH	2:B:2583:LEU:HD22	2.15	0.45
2:B:2531:ASP:OD2	2:B:2538:VAL:HB	2.16	0.45
2:B:2592:ILE:HD11	2:B:2625:LEU:HD22	1.99	0.45
2:B:2750:THR:HG23	2:B:2806:LYS:HE2	1.98	0.45
2:B:206:GLU:HB3	2:B:265:MET:HE3	1.98	0.45
2:B:368:THR:O	2:B:369:ASN:CG	2.59	0.45
2:B:529:ALA:O	2:B:530:HIS:CG	2.70	0.45
2:B:1859:ILE:HD12	2:B:1936:LEU:HD11	1.98	0.45
2:B:2501:ALA:O	2:B:2502:ASN:OD1	2.33	0.45
2:B:2583:LEU:HD23	2:B:2583:LEU:C	2.42	0.45
2:B:2782:LEU:HD12	2:B:2868:LEU:HD13	1.98	0.45
2:B:2953:LEU:HD23	2:B:2953:LEU:H	1.81	0.45
2:B:925:THR:HG21	2:B:931:GLU:HA	1.98	0.45
2:B:1464:LYS:HG2	2:B:1465:THR:H	1.81	0.45
2:B:2014:MET:HA	2:B:2051:CYS:HB3	1.98	0.45
2:B:2291:LEU:C	2:B:2291:LEU:HD23	2.41	0.45
2:B:2524:ASP:HB3	2:B:2583:LEU:HD21	1.99	0.45
2:B:2553:ILE:HD12	2:B:2594:PRO:HB2	1.99	0.45
2:B:3106:GLU:O	2:B:3106:GLU:HG2	2.16	0.45
2:B:3689:ILE:HG22	2:B:3691:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:LYS:HZ3	2:B:421:VAL:HG13	1.81	0.45
2:B:954:THR:HG23	2:B:954:THR:O	2.15	0.45
2:B:1454:VAL:HG13	2:B:1477:ILE:CD1	2.46	0.45
2:B:2545:LEU:O	2:B:2581:VAL:HG22	2.17	0.45
2:B:202:HIS:HE2	2:B:278:LEU:HD22	1.81	0.45
2:B:1292:MET:N	2:B:1292:MET:HE2	2.32	0.45
2:B:2422:ALA:O	2:B:2423:PRO:C	2.60	0.45
2:B:2942:LEU:HD22	2:B:2970:TYR:CZ	2.51	0.45
2:B:1454:VAL:HG13	2:B:1474:LEU:HD11	1.98	0.45
2:B:2651:ILE:HD12	2:B:3744:VAL:O	2.17	0.45
2:B:1185:VAL:CG1	2:B:1245:LEU:HB2	2.46	0.45
2:B:1950:TYR:O	2:B:2063:PHE:CZ	2.70	0.45
2:B:2198:LYS:HG3	2:B:2199:GLU:N	2.32	0.45
2:B:2985:TRP:HB2	2:B:3024:TYR:OH	2.16	0.45
2:B:3661:ILE:HG13	2:B:3662:LEU:H	1.81	0.45
2:B:2906:CYS:O	2:B:2907:LEU:HD22	2.17	0.45
2:B:1547:LEU:O	2:B:1551:MET:HG2	2.18	0.44
2:B:2338:PRO:HB2	2:B:2341:GLU:HG3	1.99	0.44
2:B:2680:LEU:HD21	2:B:2713:LEU:HD22	1.98	0.44
2:B:3023:THR:HA	2:B:3027:ASN:O	2.17	0.44
2:B:369:ASN:OD1	2:B:369:ASN:O	2.36	0.44
2:B:573:LEU:HD23	2:B:573:LEU:C	2.43	0.44
2:B:778:MET:CG	2:B:778:MET:O	2.65	0.44
2:B:798:ASP:HB3	2:B:801:MET:HE3	1.97	0.44
2:B:2775:ILE:HD11	2:B:2867:THR:HG22	1.99	0.44
2:B:110:VAL:O	2:B:113:LYS:HG3	2.17	0.44
2:B:1761:LYS:HE3	2:B:1783:LEU:HD12	2.00	0.44
2:B:1830:ILE:HG23	2:B:1830:ILE:O	2.18	0.44
2:B:2354:ASP:OD1	2:B:2355:VAL:N	2.51	0.44
2:B:2815:LYS:HE3	2:B:3421:ASP:HB2	1.99	0.44
2:B:3206:TRP:O	2:B:3208:GLN:N	2.51	0.44
2:B:3365:LEU:HD11	2:B:3372:LEU:H	1.81	0.44
2:B:3413:MET:O	2:B:3417:VAL:HG12	2.17	0.44
2:B:3661:ILE:HG13	2:B:3662:LEU:N	2.33	0.44
2:B:2064:PHE:O	2:B:2068:VAL:HG12	2.17	0.44
2:B:2527:LEU:HD11	2:B:2648:LEU:HD22	1.99	0.44
2:B:2556:ILE:HD13	2:B:2569:ARG:NH1	2.33	0.44
2:B:753:ILE:HG22	2:B:756:VAL:CG2	2.48	0.44
2:B:1766:ILE:HG12	2:B:1778:ILE:HG12	2.00	0.44
2:B:2505:VAL:HG12	2:B:2505:VAL:O	2.17	0.44
2:B:229:THR:HG22	2:B:230:ALA:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:765:GLU:OE1	2:B:769:LYS:HA	2.18	0.44
2:B:795:VAL:HG12	2:B:801:MET:SD	2.57	0.44
2:B:2773:TRP:HB3	2:B:2800:ILE:HG21	2.00	0.44
2:B:191:ILE:HG21	2:B:307:MET:CE	2.47	0.43
2:B:250:ILE:HB	2:B:303:ALA:HB3	1.99	0.43
2:B:2782:LEU:HD22	2:B:2818:LEU:CG	2.48	0.43
2:B:283:LEU:HD22	2:B:298:PRO:CG	2.48	0.43
2:B:695:LYS:HB3	2:B:696:PRO:HD2	2.00	0.43
2:B:758:LEU:O	2:B:759:LEU:HD12	2.18	0.43
2:B:2782:LEU:HB3	2:B:2818:LEU:HD11	2.00	0.43
2:B:2887:ILE:HD13	2:B:2893:MET:HE1	2.00	0.43
1:A:40:LEU:HD22	2:B:398:ILE:HG23	1.99	0.43
2:B:758:LEU:C	2:B:759:LEU:HD12	2.44	0.43
2:B:2841:LYS:HG2	2:B:2848:GLU:OE2	2.19	0.43
2:B:2887:ILE:HG23	2:B:2892:SER:O	2.18	0.43
2:B:1334:SER:HG	2:B:1335:TRP:CD1	2.36	0.43
2:B:2207:ILE:HD12	2:B:2414:PHE:CE2	2.53	0.43
2:B:2158:ALA:H	2:B:2173:VAL:HG23	1.82	0.43
2:B:1454:VAL:HG13	2:B:1477:ILE:HD11	2.01	0.43
2:B:1535:PHE:HB3	2:B:1605:LEU:HA	2.01	0.43
2:B:1872:GLU:HB2	2:B:2063:PHE:CE1	2.53	0.43
2:B:3185:SER:O	2:B:3186:GLY:C	2.62	0.43
2:B:3318:ASP:C	2:B:3319:MET:HE2	2.44	0.43
2:B:355:ALA:N	2:B:356:PRO:HD2	2.33	0.43
2:B:2031:SER:O	2:B:2041:ILE:HA	2.18	0.43
2:B:2375:PRO:HB2	2:B:3085:TYR:HA	2.01	0.43
2:B:2557:ILE:O	2:B:2570:ILE:HG12	2.19	0.43
2:B:3634:TYR:O	2:B:3648:VAL:HG22	2.19	0.43
2:B:274:ILE:O	2:B:278:LEU:HG	2.19	0.43
2:B:1134:VAL:HB	2:B:1147:VAL:HB	2.01	0.43
2:B:2974:SER:N	2:B:3059:GLN:OE1	2.52	0.43
2:B:3382:LEU:HD22	2:B:3408:GLN:HB3	2.00	0.43
2:B:283:LEU:HD13	2:B:294:TYR:HE2	1.84	0.43
2:B:1650:MET:HE1	2:B:1652:VAL:HG22	2.00	0.43
2:B:2542:ARG:HD2	2:B:2580:HIS:ND1	2.34	0.43
2:B:3742:SER:O	2:B:3746:LEU:HG	2.19	0.43
2:B:752:GLU:HB3	2:B:754:LYS:HE3	2.00	0.42
2:B:1542:LEU:HD12	2:B:1612:VAL:HG22	1.99	0.42
2:B:2062:ASP:OD1	2:B:2063:PHE:N	2.51	0.42
2:B:2177:CYS:SG	2:B:2197:VAL:HG13	2.59	0.42
2:B:425:ILE:HG23	2:B:426:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:948:MET:HB2	2:B:953:LEU:HD13	2.02	0.42
2:B:1291:ARG:C	2:B:1292:MET:HE2	2.44	0.42
2:B:941:GLN:HB2	2:B:960:LYS:HB2	2.00	0.42
2:B:964:LEU:O	2:B:964:LEU:HG	2.19	0.42
2:B:1495:ILE:CG2	2:B:1538:LEU:HD11	2.48	0.42
2:B:2673:ARG:HB3	2:B:2767:SER:HA	2.01	0.42
2:B:600:ILE:HG22	2:B:600:ILE:O	2.19	0.42
2:B:2018:LYS:HB3	2:B:2047:LYS:HB3	2.01	0.42
2:B:2200:PHE:CD2	2:B:2280:VAL:HG11	2.54	0.42
2:B:3099:VAL:HA	2:B:3106:GLU:HA	2.02	0.42
2:B:1758:ILE:CG2	2:B:1760:LEU:HG	2.49	0.42
2:B:2636:PRO:HB2	2:B:2705:ARG:NH2	2.35	0.42
2:B:3052:VAL:HG11	2:B:3074:ALA:HB2	2.01	0.42
2:B:2501:ALA:O	2:B:2502:ASN:C	2.63	0.42
2:B:2981:ASN:HB3	2:B:3001:LEU:HD22	2.02	0.42
2:B:553:LEU:HD23	2:B:585:THR:O	2.20	0.42
2:B:1292:MET:HB2	2:B:1327:VAL:HB	2.01	0.42
2:B:1536:ALA:O	2:B:1606:ASN:HB3	2.18	0.42
2:B:1825:LEU:HG	2:B:1826:PRO:HD2	2.01	0.42
2:B:2546:GLN:HB2	2:B:2663:ILE:HG12	2.02	0.42
2:B:3365:LEU:HA	2:B:3368:ILE:HD12	2.02	0.42
2:B:3680:PRO:HB2	2:B:3687:LEU:HD11	2.01	0.42
1:A:110:MET:HE1	1:A:125:MET:SD	2.59	0.42
2:B:616:PRO:HD3	2:B:622:ASP:O	2.20	0.42
2:B:1951:ASN:HA	2:B:2063:PHE:CE1	2.55	0.42
2:B:2182:GLU:O	2:B:2193:ILE:HA	2.20	0.42
2:B:2735:GLU:HA	2:B:2757:VAL:HG22	2.01	0.42
2:B:2760:ILE:O	2:B:2760:ILE:HG13	2.20	0.42
2:B:283:LEU:HD22	2:B:298:PRO:HG2	2.01	0.42
2:B:702:PRO:HG3	2:B:707:HIS:HB2	2.00	0.42
2:B:817:ILE:HG21	2:B:822:MET:CE	2.49	0.42
2:B:928:GLN:C	2:B:929:LYS:HD3	2.44	0.42
2:B:1020:PHE:HD2	2:B:1090:LEU:HG	1.84	0.42
2:B:2202:ILE:HG23	2:B:2285:VAL:HG12	1.98	0.42
2:B:2389:ILE:HG22	2:B:2390:THR:N	2.35	0.42
2:B:2392:SER:HA	2:B:3099:VAL:O	2.20	0.42
2:B:321:ASP:OD1	2:B:321:ASP:C	2.63	0.42
2:B:369:ASN:OD1	2:B:369:ASN:C	2.62	0.42
2:B:1183:LEU:O	2:B:1243:ILE:HA	2.20	0.42
2:B:3013:ASP:OD1	2:B:3013:ASP:O	2.37	0.42
2:B:810:LEU:C	2:B:810:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2213:LEU:HD12	2:B:2410:THR:HG22	2.02	0.41
2:B:3144:LYS:HA	2:B:3147:ILE:HG12	2.02	0.41
2:B:3686:VAL:HG11	2:B:3710:LYS:HG3	2.02	0.41
2:B:227:LEU:HD13	2:B:250:ILE:HG13	2.02	0.41
2:B:234:TRP:CD1	2:B:249:LEU:HD21	2.54	0.41
2:B:2343:VAL:HG21	2:B:2385:ASN:CB	2.50	0.41
2:B:2813:LYS:HB2	2:B:2815:LYS:HZ3	1.85	0.41
2:B:2956:VAL:HG13	2:B:2956:VAL:O	2.19	0.41
2:B:3638:ILE:CD1	2:B:3711:VAL:HG13	2.50	0.41
2:B:761:ALA:HB1	2:B:772:PHE:CD1	2.55	0.41
2:B:1264:VAL:HG22	2:B:1301:LEU:HD13	2.01	0.41
2:B:1670:PHE:CB	2:B:1700:VAL:HG22	2.49	0.41
2:B:2023:ASN:OD1	2:B:2024:ASN:N	2.53	0.41
2:B:2508:PRO:HA	2:B:2530:ILE:HB	2.02	0.41
2:B:2570:ILE:HD12	2:B:2582:PRO:HD2	2.02	0.41
2:B:630:GLN:O	2:B:632:VAL:HG23	2.19	0.41
2:B:1130:GLU:C	2:B:1154:VAL:HG23	2.45	0.41
2:B:1251:VAL:HG12	2:B:1253:PRO:HD3	2.02	0.41
2:B:1318:LEU:HD12	2:B:1352:ASN:O	2.20	0.41
2:B:1537:SER:HA	2:B:1607:ALA:O	2.20	0.41
2:B:1995:LEU:O	2:B:2027:MET:N	2.53	0.41
2:B:2387:MET:HE2	2:B:2387:MET:HB3	1.99	0.41
2:B:436:LEU:HD23	2:B:441:ILE:HG13	2.02	0.41
2:B:623:GLN:O	2:B:688:LEU:HD12	2.20	0.41
2:B:1999:THR:HG22	2:B:2013:ARG:NH1	2.34	0.41
2:B:2621:VAL:HB	2:B:2643:ALA:HB3	2.03	0.41
2:B:2779:THR:O	2:B:2795:ALA:HB1	2.20	0.41
2:B:186:LEU:O	2:B:190:VAL:HG23	2.19	0.41
2:B:436:LEU:HD21	2:B:440:ASN:HB2	2.01	0.41
2:B:1872:GLU:HB3	2:B:1952:ASN:HA	2.01	0.41
2:B:940:THR:OG1	2:B:961:LYS:HB2	2.21	0.41
2:B:1190:ILE:O	2:B:1250:ILE:HG12	2.20	0.41
2:B:1474:LEU:HB3	2:B:1506:LEU:HG	2.03	0.41
2:B:1673:GLN:O	2:B:1696:LEU:HD12	2.20	0.41
2:B:1988:SER:HA	2:B:2034:GLN:O	2.20	0.41
2:B:2813:LYS:HB2	2:B:2815:LYS:NZ	2.35	0.41
2:B:3654:LEU:HD12	2:B:3656:ILE:HD11	2.03	0.41
2:B:1116:LEU:HD22	2:B:1125:LEU:HD22	2.03	0.41
2:B:1181:LEU:HD13	2:B:1239:VAL:HG11	2.01	0.41
2:B:1596:VAL:HG22	2:B:1635:PRO:HG3	2.03	0.41
2:B:2377:MET:O	2:B:3085:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2649:SER:O	2:B:2650:TYR:HD1	2.04	0.41
2:B:2671:THR:HG21	2:B:2763:ARG:NH2	2.35	0.41
2:B:3328:PHE:CE2	2:B:3397:LEU:HD11	2.56	0.41
2:B:101:VAL:O	2:B:105:LYS:HD3	2.20	0.41
2:B:760:PHE:HE2	2:B:762:ARG:HE	1.68	0.41
2:B:811:PRO:O	2:B:918:LYS:HB2	2.21	0.41
2:B:1262:VAL:HG22	2:B:1303:ARG:HH12	1.85	0.41
2:B:1456:GLN:HB2	2:B:1475:LYS:CB	2.50	0.41
2:B:2049:TYR:O	2:B:2049:TYR:CG	2.73	0.41
2:B:2126:PRO:HB2	2:B:2211:THR:HG23	2.02	0.41
2:B:103:GLU:O	2:B:107:LEU:HG	2.21	0.41
2:B:396:SER:O	2:B:399:LYS:HG2	2.21	0.41
2:B:1289:ILE:HG23	2:B:1328:ASN:OD1	2.21	0.41
2:B:1778:ILE:CD1	2:B:1819:THR:HG21	2.51	0.41
2:B:2179:LEU:HD12	2:B:2179:LEU:O	2.20	0.41
2:B:2197:VAL:HB	2:B:2280:VAL:HG22	2.03	0.41
2:B:3002:LEU:HD12	2:B:3002:LEU:O	2.20	0.41
2:B:1020:PHE:CD2	2:B:1090:LEU:HG	2.56	0.40
2:B:1802:PRO:HG3	2:B:1850:TRP:CH2	2.56	0.40
2:B:3119:TRP:CE3	2:B:3179:ILE:HD12	2.56	0.40
2:B:90:VAL:HG23	2:B:205:TYR:CD1	2.56	0.40
2:B:1302:TYR:C	2:B:1303:ARG:HE	2.29	0.40
2:B:2343:VAL:HG12	2:B:2344:GLU:HG3	2.02	0.40
2:B:2351:LEU:HD12	2:B:2353:LEU:CD1	2.52	0.40
2:B:3727:GLU:HA	2:B:3730:GLN:HG2	2.03	0.40
2:B:798:ASP:HB3	2:B:801:MET:HG2	2.04	0.40
2:B:3186:GLY:O	2:B:3187:ILE:C	2.64	0.40
1:A:48:GLU:O	1:A:52:MET:HG2	2.22	0.40
2:B:66:THR:HB	2:B:82:THR:OG1	2.21	0.40
2:B:2874:ILE:HG12	2:B:2909:PHE:HB2	2.02	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	146/149 (98%)	145 (99%)	1 (1%)	0	100	100
2	B	2892/3777 (77%)	2667 (92%)	225 (8%)	0	100	100
All	All	3038/3926 (77%)	2812 (93%)	226 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	126/127 (99%)	126 (100%)	0	100	100
2	B	2671/3385 (79%)	2671 (100%)	0	100	100
All	All	2797/3512 (80%)	2797 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
2	B	385	HIS
2	B	566	GLN
2	B	615	ASN
2	B	651	ASN
2	B	658	GLN
2	B	927	GLN
2	B	1119	GLN
2	B	1370	ASN
2	B	1709	HIS
2	B	2327	HIS
2	B	2348	GLN
2	B	2358	ASN

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Mol	Chain	Res	Type
2	B	2522	HIS
2	B	2529	GLN
2	B	2546	GLN
2	B	2600	HIS
2	B	2719	GLN
2	B	3143	GLN
2	B	3145	HIS
2	B	3223	HIS
2	B	3301	GLN
2	B	3336	HIS
2	B	3404	HIS
2	B	3705	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

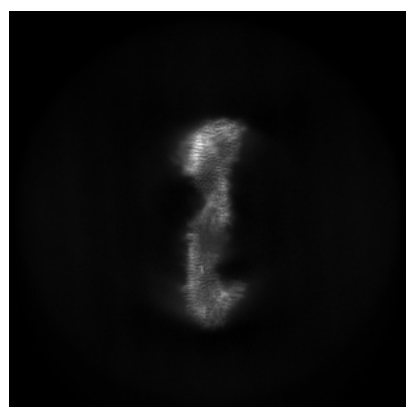
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73373. These allow visual inspection of the internal detail of the map and identification of artifacts.

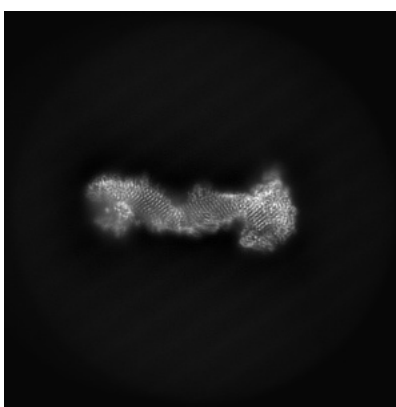
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

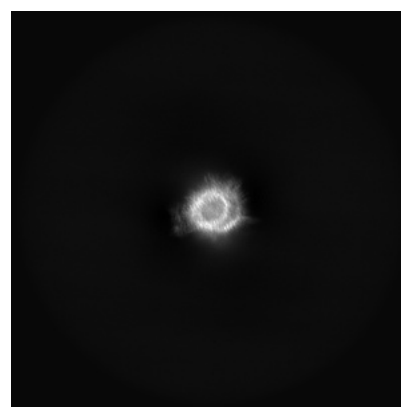
6.1.1 Primary map



X



Y



Z

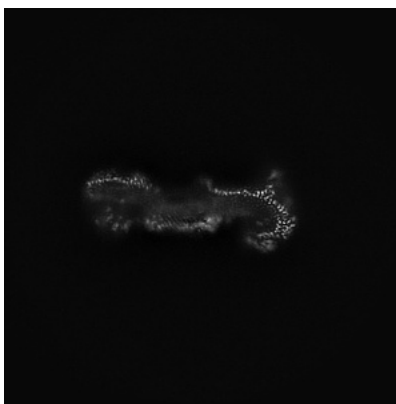
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

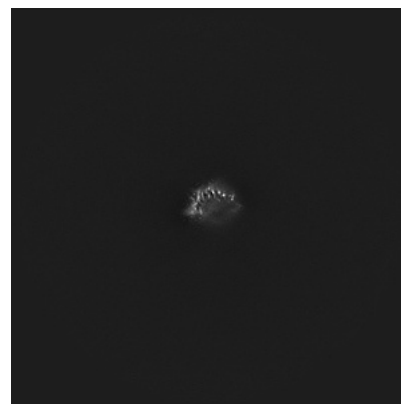
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

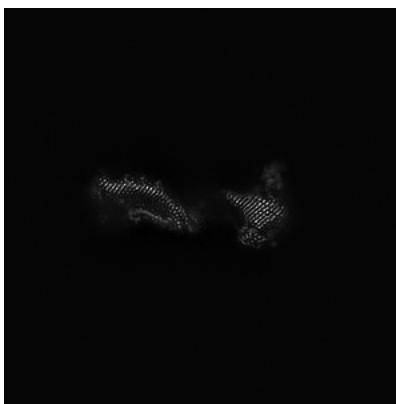
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

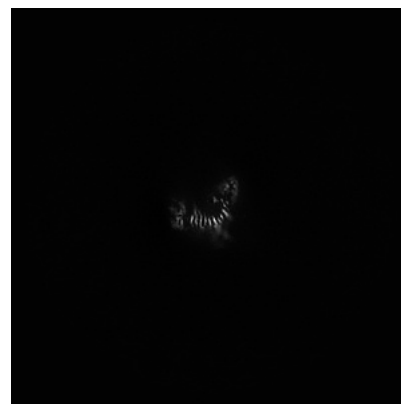
6.3.1 Primary map



X Index: 206



Y Index: 179



Z Index: 245

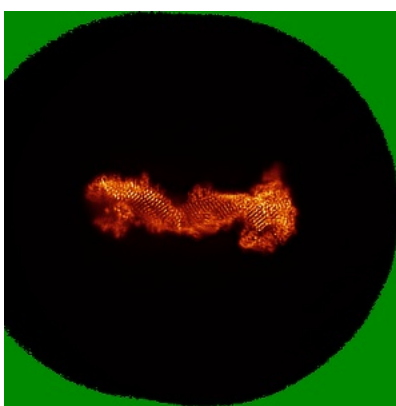
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y



Z

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 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

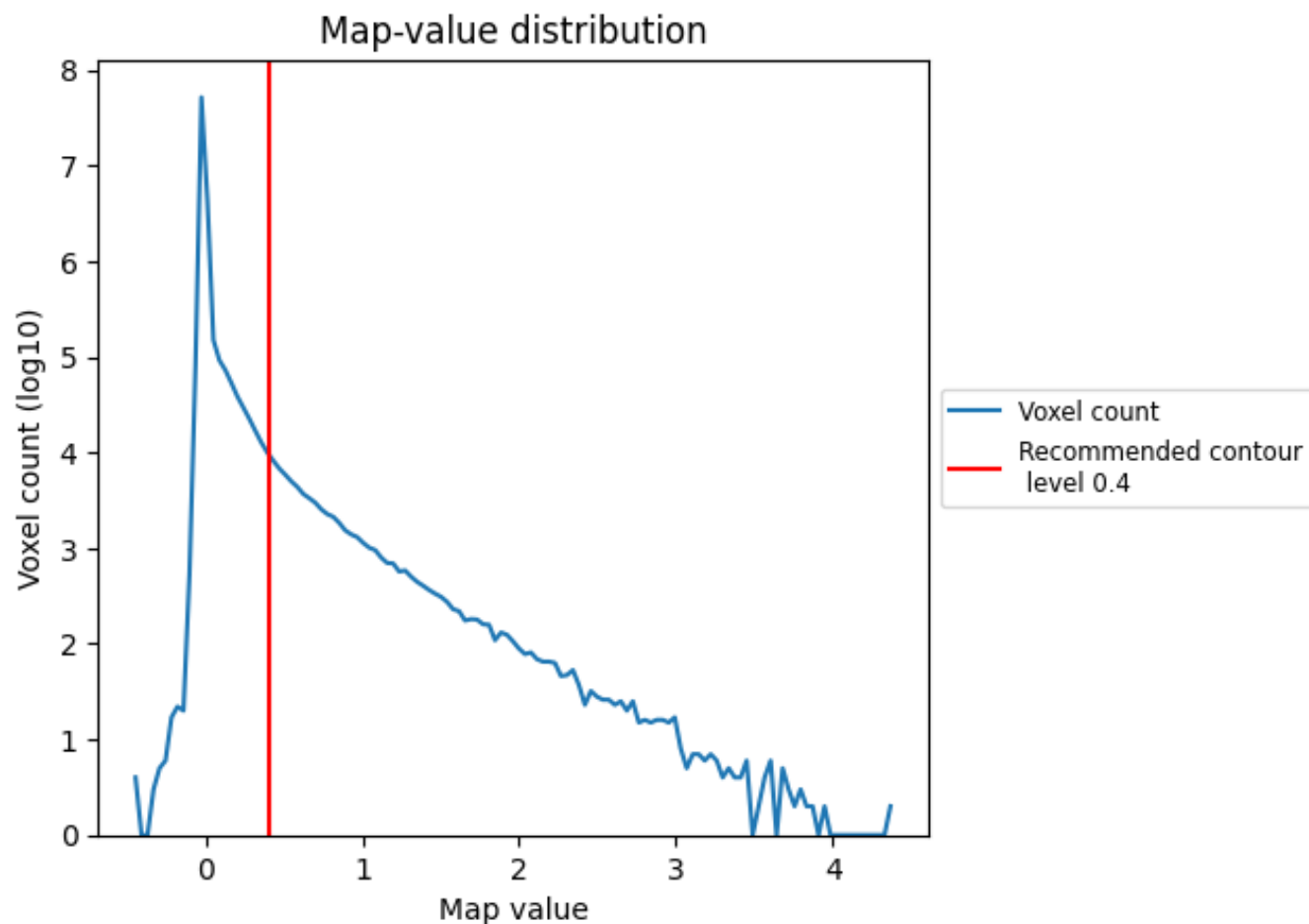
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

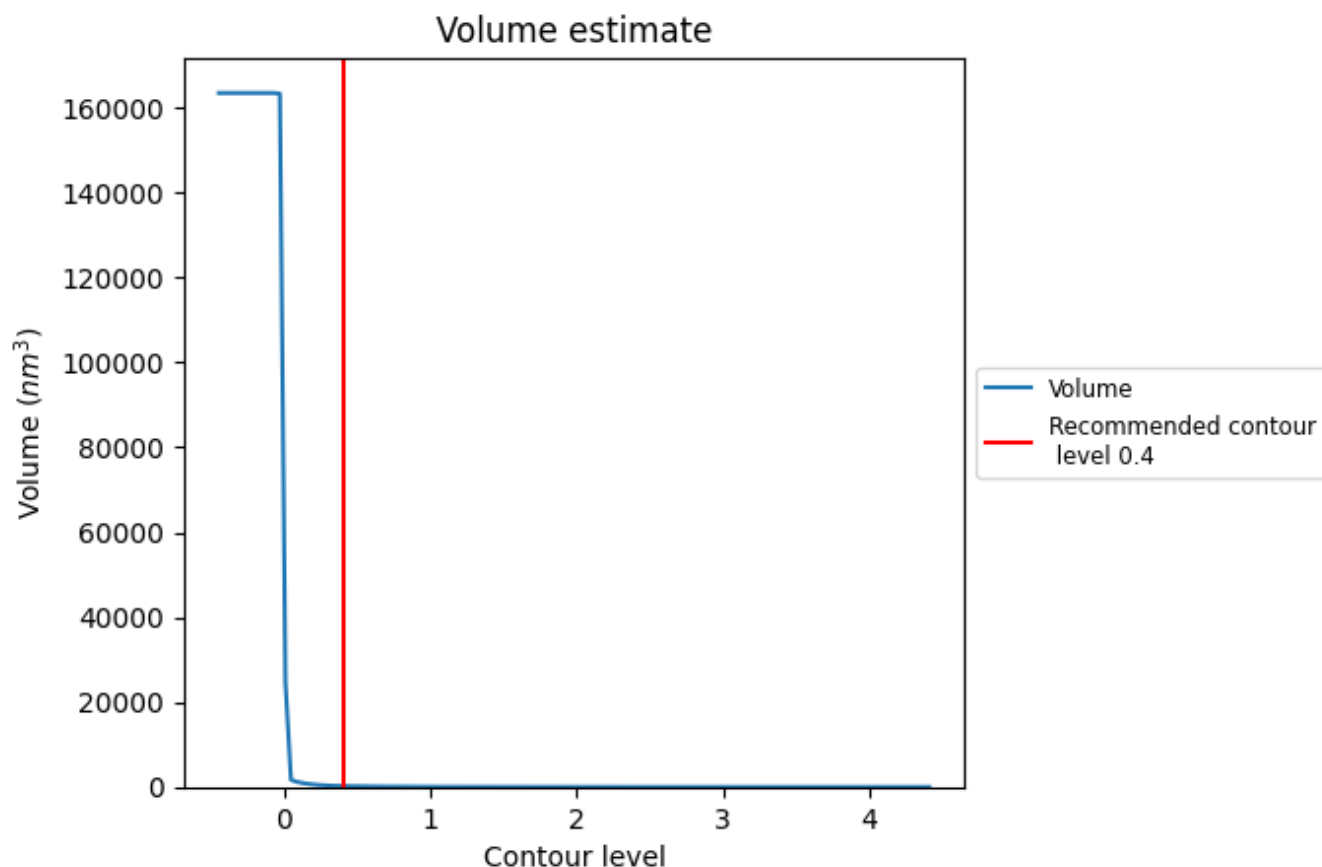
This section contains the results of statistical analysis of the map.

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.

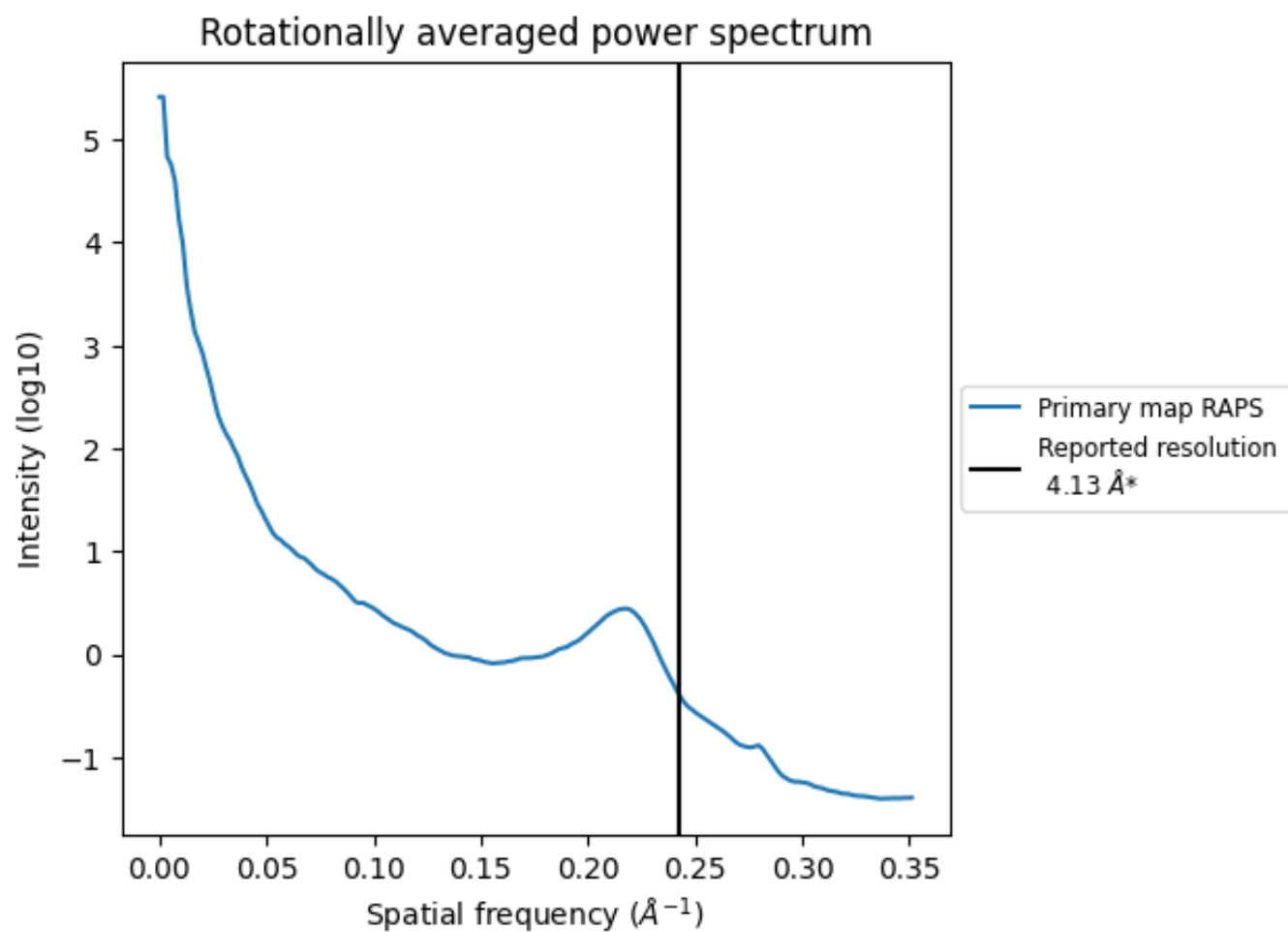
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm^3 ; this corresponds to an approximate mass of 192 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 0.242 \AA^{-1}

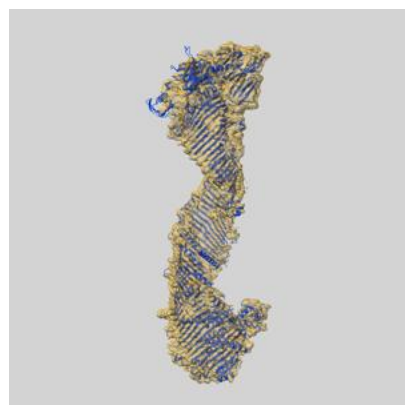
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

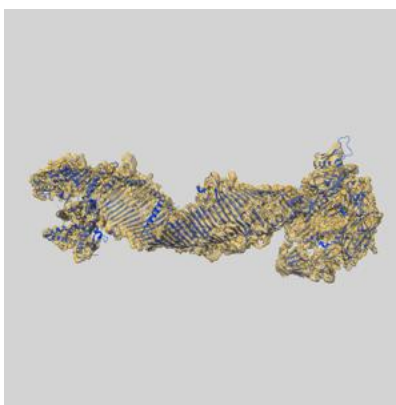
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73373 and PDB model 9YRP. Per-residue inclusion information can be found in section [3](#) on page [5](#).

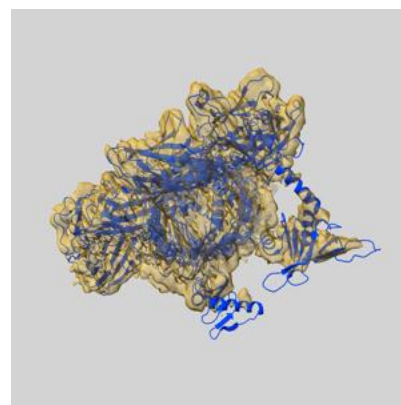
9.1 Map-model overlay [i](#)



X



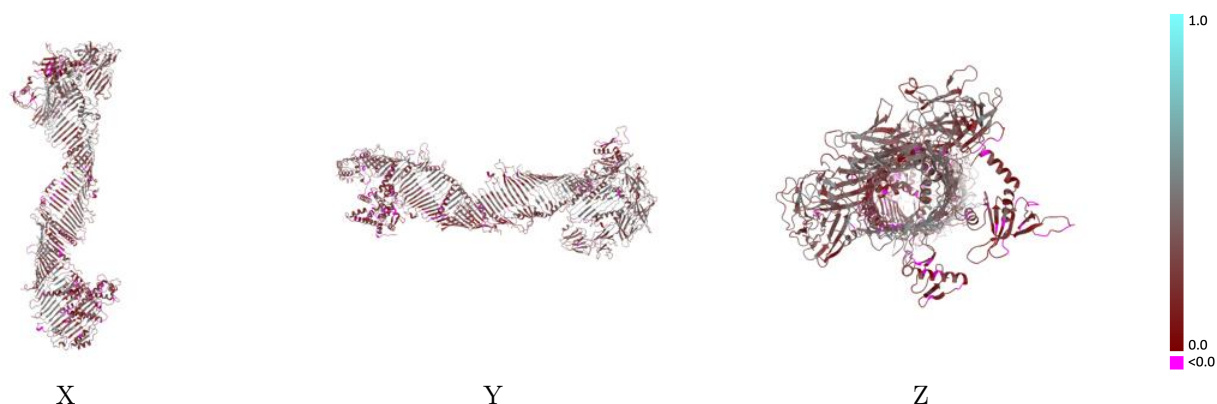
Y



Z

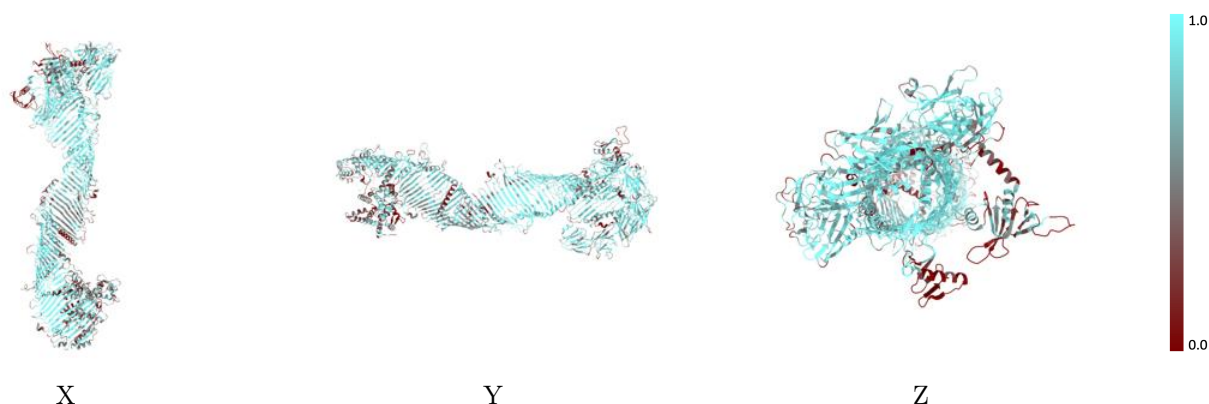
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



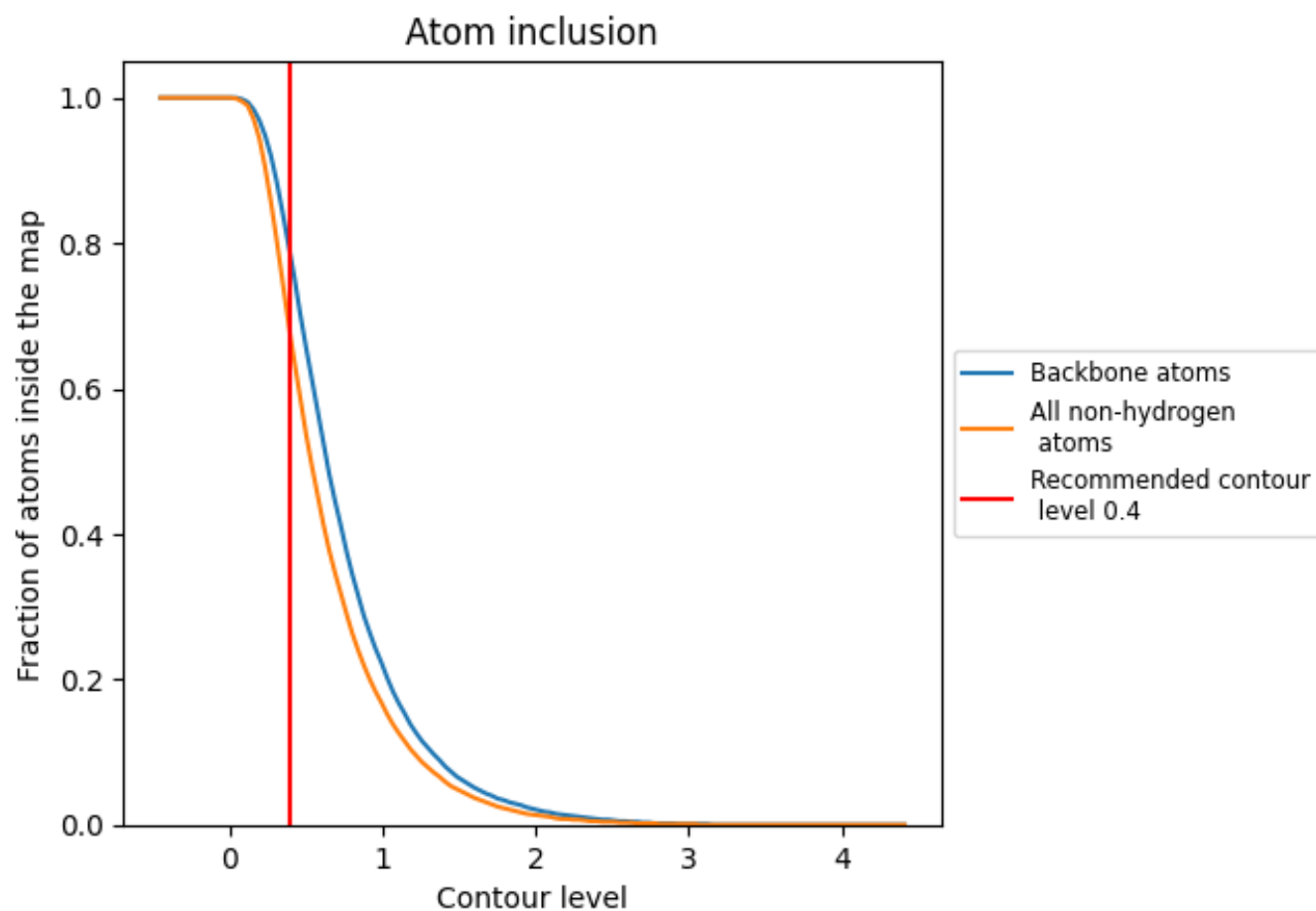
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6720	<div></div> 0.2850
A	<div></div> 0.4110	<div></div> 0.1850
B	<div></div> 0.6850	<div></div> 0.2900

