



wwPDB EM Validation Summary Report ⓘ

Jul 20, 2026 – 04:40 pm BST

PDB ID : 9S1H / pdb_00009s1h
EMDB ID : EMD-54454
Title : Apo-state RyR1 with ACP in the native membrane
Authors : Mikirtumov, V.
Deposited on : 2025-07-18
Resolution : 4.00 Å(reported)
Based on initial model : 7tzc

This is a wwPDB EM Validation Summary 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

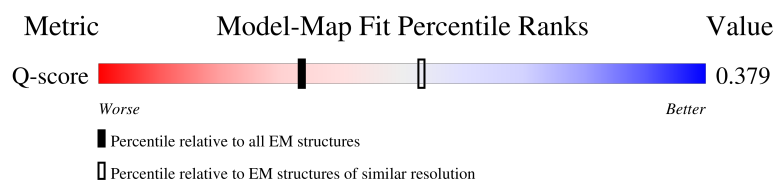
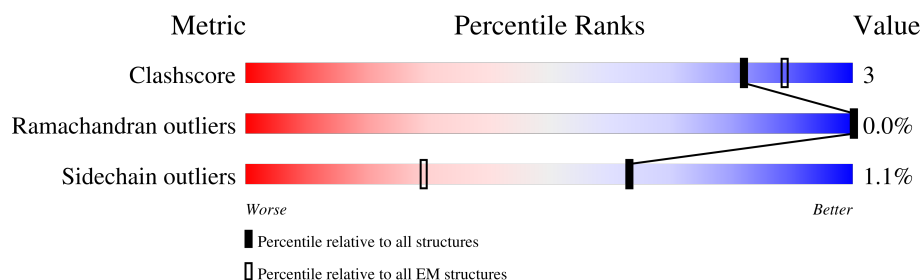
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	5037	20% 81% 6% 13%
1	B	5037	20% 81% 6% 13%
1	C	5037	20% 81% 6% 13%
1	D	5037	20% 81% 6% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	90% 8% ..
2	F	108	90% 8% ..
2	G	108	90% 8% ..
2	H	108	90% 8% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 286116 atoms, of which 142308 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

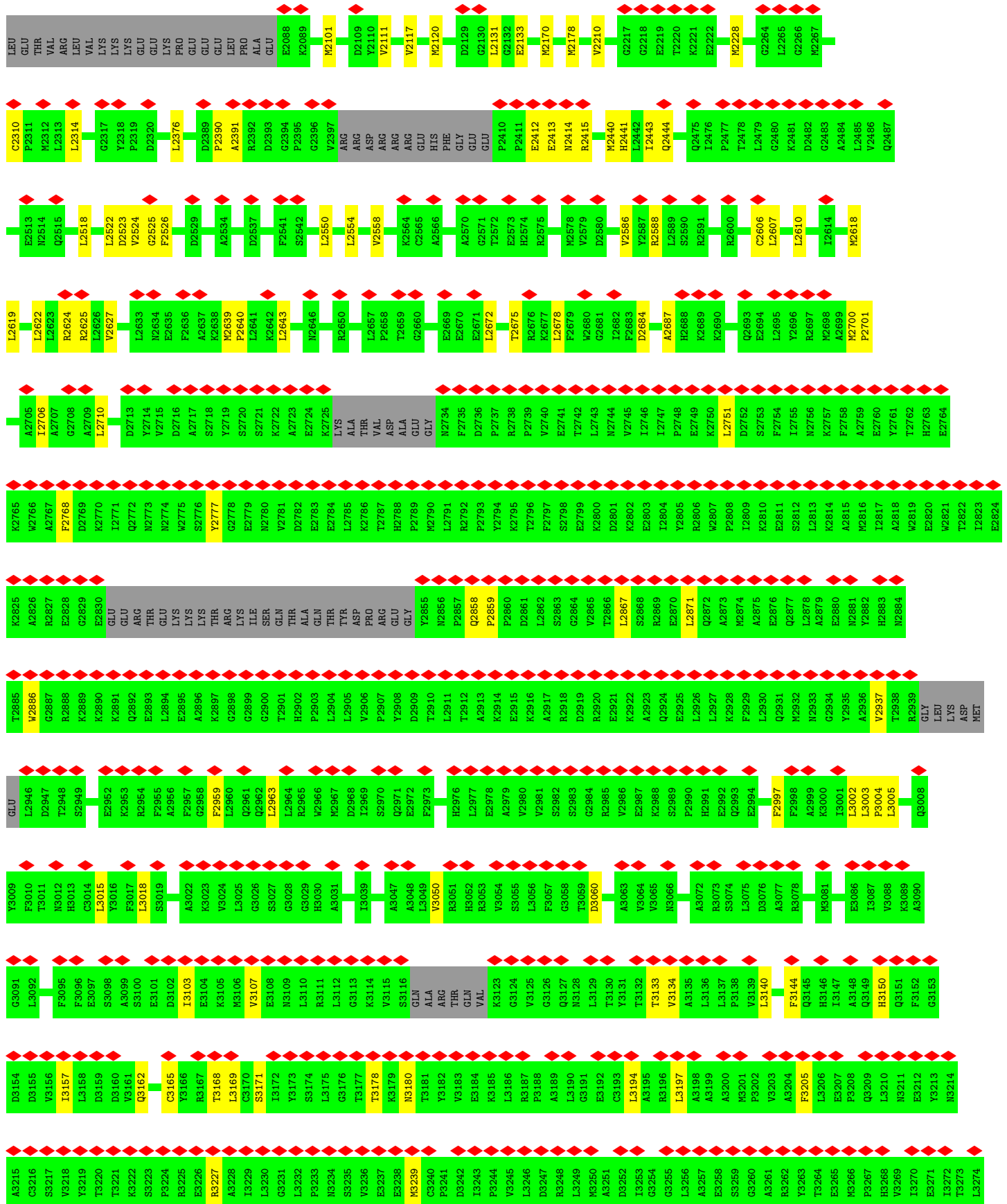
Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	F	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	G	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	H	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- # ACP

Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total 45	C 11	H 14	N 5	O 12	P 3	0
4	B	1	Total 45	C 11	H 14	N 5	O 12	P 3	0
4	C	1	Total 45	C 11	H 14	N 5	O 12	P 3	0
4	D	1	Total 45	C 11	H 14	N 5	O 12	P 3	0







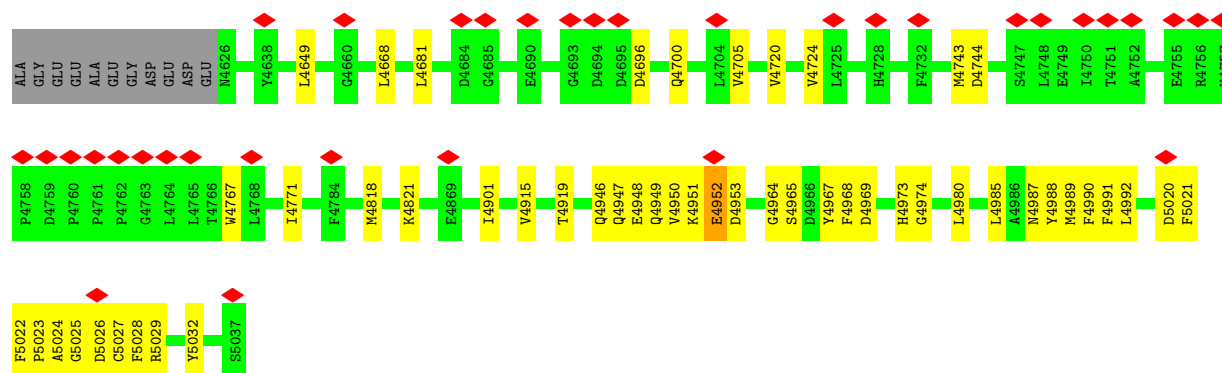


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F3144	Q3145	H3146	I3147	Q3148	Q3149	H3150	Q3151	F3152	G3153	N3154	D3155	F3156	I3157	L3158	D3159	T3160	V3161	Q3162	C3165	Y3166	R3167	T3168	L3169	G3170	V3171	E3172	Y3173	L3174	R3175	G3176	T3177	K3178	F3179	N3180	T3181	Y3182	F3183	E3184	K3185	L3186	R3187	P3188	A3189	G3190	G3191	E3192	C3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	F3202	G3260	R3262	Y3263
R3078	K3081	K3082	S3083	E3086	I3087	V3088	K3089	A3090	G3091	L3092	F3095	F3096	E3097	S3098	A3099	S3100	E3101	D3102	T3103	E3104	K3105	N3106	V3107	E3108	L3109	L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126	Q3127	L3128	L3129	E3192	T3130	L3131	T3132	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140		
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L3002	L3003	P3004																																																									

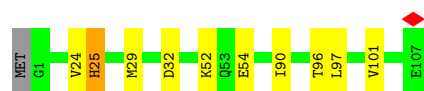


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LEU	P2319	D2523	N2634	Y2714	N2774	THR	L2894	F2955	L3018	E3097	D3159	T3220
VAL	V2524	D2524	E2635	V2715	N2775	GLU	E2895	A2956	S3019	S3098	D3160	T3221
LYS	D2376	G2525	F2526	D2716	S2776	LYS	A2896	F2957	A3022	A3099	V3161	K3222
LYS	L2376	F2526	A2637	A2717	G2777	LYS	K2897	G2958	K3023	E3101	C3162	S3223
GLU	D2389	D2529	K2638	S2718	Y2778	THR	G2898	F2959	L3024	L3102	C3165	P3224
GLU	P2390	P2390	M2639	Y2719	E2779	ARG	G2899	Q2961	V3024	Y3166	Y3166	K3225
PRO	A2391	A2534	P2640	S2720	I2779	ILE	G2900	Q2962	L3025	T3103	R3167	E3226
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GLU	D2393	D2537	K2642	K2722	V2781	GLN	H2902	L2964	S3027	K3105	T3169	A3228
LEU	G2394	P2541	V2643	A2723	E2782	THR	P2903	R2965	G3028	M3106	C3170	I3229
PRO	P2395	G2542	N2646	A2724	E2783	ALA	L2904	W2966	G3029	V3107	S3171	L3230
ALA	G2396	S2542	R2650	K2725	E2784	GLN	L2905	M2967	H3030	E3108	I3172	G3231
GLU	V2397	L2550	E2651	LYS	E2785	TYR	V2906	D2968	A3031	N3109	Y3173	G3232
	E2088	N2551	R2552	ALA	K2786	ASP	P2907	P2969	K3034	L3110	S3174	P3233
	E2089	R2552	P2553	THR	T2787	PRO	Y2908	S2970	I3039	L3111	K3175	N3234
	K2101	R2554	T2554	VAL	H2788	ARG	D2909	Q2971	A3047	G3112	G3176	S3235
	V2111	L2554	E2656	ASP	P2789	GLU	T2910	E2972	A3048	G3113	T3177	V3236
	V2117	V2558	E2671	ALA	N2790	GLY	L2911	F2973	L3049	V3114	K3178	E3237
	K2120	K2564	E2670	GLY	L2791		L2912	H2976	V3050	V3115	N3180	E3238
	D2129	C2565	E2671	N2734	P2792		K2858	L2977	R3051	S3116	T3181	N3239
	G2130	A2570	L2672	D2735	P2793		P2859	E2978	H3052	ALA	Y3182	C3240
	L2131	G2571	T2675	F2736	Y2794		K2914	A2979	R3053	ARG	V3183	P3241
	E2133	E2572	R2676	D2737	K2795		E2915	V2980	L3054	THR	G3184	D3242
	K2170	E2573	L2678	R2738	T2796		K2916	S2981	V3055	GLN	V3185	K3243
	K2178	R2574	F2679	R2739	F2797		A2917	V2982	L3056	VAL	G3123	P3244
	V2210	R2415	G2680	V2740	S2798		D2918	S2983	L3057		G3124	V3245
	G2217	M2440	G2681	E2741	E2799		R2920	G2984	F3057		Y3125	L3246
	G2218	H2441	G2682	E2742	K2800		E2921	V2985	K3058		G3126	D3247
	E2219	L2442	F2683	L2743	D2801		K2922	V2986	T3059		Q3127	R3248
	T2220	L2443	L2684	N2744	K2802		A2923	E2987	D3060		G3128	L3249
	K2221	Q2444	D2687	V2745	E2803		Q2924	K2988	A3063		L3129	K3250
	M2228	Q2475	Y2587	L2746	L2804		E2925	R2869	V3064		T3130	A3251
	G2264	I2476	R2588	P2747	Y2805		L2926	E2870	V3065		V3131	D3252
	L2265	P2477	L2589	L2751	K2806		L2927	L2871	N3066		T3132	G3253
	G2266	T2478	R2690	S2752	D2807		K2928	Q2872	A3072		V3133	G3255
	M2267	L2479	G2693	S2753	P2808		F2929	A2873	S3074		L3134	L3256
	C2310	G2480	E2694	T2754	K2809		Q2931	M2874	R3073		A3135	A3257
	P2311	K2481	L2695	T2755	E2811		L2930	E2876	S3074		L3136	E3258
	M2312	D2482	Y2696	K2756	S2812		M2932	Q2877	D3075		P3137	S3259
	L2314	G2483	R2697	N2757	L2813		Q2934	L2878	A3077		V3139	G3260
	G2317	A2484	M2698	K2757	A2815		Y2935	E2880	R3078		L3140	A3261
				F2758	N2816		A2936	N2881	I3001		F3144	R3262
				A2759	L2817		V2937	Y2882	L3002		Q3145	Y3263
				E2760	K2818		T2938	H2883	L3003		H3146	T3264
				Y2761	N2819		R2939	R2884	P3004		T3147	G3265
				T2762	E2820		GLY	T2886	S3083		A3148	M3266
				H2763	Y2821		LEU	Q2887	Q3008		I3087	Q3267
				E2764	T2822		LYS	R2888	F3009		V3088	H3268
				K2765	L2823		ASP	K2889	T3010		K3089	
				W2766	E2824		NET	R2890	N3012		A3090	
				A2767	K2825		GLU	K2891	H3013		G3091	
				F2768	A2826			Q2892	C3014		L3092	
				D2769	R2827			L2946	Y3015		F3095	
				K2770	E2828			D2947	T3016			
				I2771	G2829			T2948	Y3016			
				Q2772	E2830			S2949	K2953			
					GLU			F2952				
					GLU			K2953				

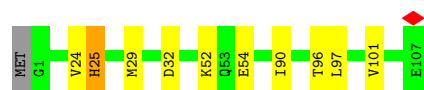
PRO	THR	ASP	PRO	GLY	VAL	ALA	T4200	S4007	D3719	A3601	A3536	A3472	R3403	F3341	Y3280
PRO	THR	THR	ALA	GLY	VAL	ALA	M4201	S4008	D3727	V3602	K3537	A3473	D3404	A3342	L3281
LYS	ASP	ARG	ALA	ALA	ARG	GLY	R4202	S4009	E3736	L3603	T3538	D3473	L3405	Q3343	P3282
ALA	ALA	ALA	Q4204	GLY	GLY	GLY	Q4204	Q4009	GLY	H3605	R3539	S3474	Y3406	P3344	R3283
PRO	PRO	GLY	E4212	ALA	ALA	ALA	E4212	L4012	GLY	L3606	Y3540	S3475	A3407	I3345	W3284
PRO	PRO	ALA	R4215	ALA	ALA	ALA	R4215	D4046	GLY	L3607	A3541	S3476	L3408	Y3346	W3285
THR	THR	GLY	Q4216	THR	THR	THR	Q4216	Q4046	GLY	E3607	L3542	K3477	L3411	S3347	E3286
GLU	GLU	ALA	F4217	ALA	ALA	ALA	F4217	I4058	GLY	Q3608	K3543	M3478	L3412	R3348	R3287
ALA	ALA	ALA	I4218	ALA	ALA	ALA	I4218	K4069	ASN	L3609	T3544	A3479	L3413	R3349	P3289
PRO	PRO	GLY	F4219	ALA	ALA	ALA	F4219	D4070	GLY	E3610	T3545	L3414	I3413	R3350	F3289
ILE	ILE	GLY	V4220	ALA	ALA	ALA	V4220	V4071	ALA	H3611	D3546	Y3415	R3414	P3351	E3290
LEU	LEU	ALA	V4221	THR	THR	THR	V4221	V4072	GLY	P3612	E3547	Y3416	ASP	E3352	A3291
LYS	LYS	ALA	M4222	ALA	ALA	ALA	M4222	W4072	GLY	Y3613	E3548	V3417	L3353	L3353	P3292
ALA	ALA	ALA	V4223	ALA	ALA	ALA	V4223	E4075	GLY	K3614	V3549	N3418	L3354	P3293	P3293
ARG	ARG	ARG	E4224	LEU	LEU	LEU	E4224	V3749	GLY	S3615	R3550	GLY	Y3415	H3355	A3295
LEU	LEU	ALA	G4225	ALA	ALA	ALA	G4225	E3750	GLY	K3616	E3551	GLY	V3416	S3356	P3294
ALA	ALA	ALA	Q4226	ALA	ALA	ALA	Q4226	V3751	GLY	A3617	F3552	GLY	ASP	H3357	L3296
ASP	ASP	ALA	E4227	ALA	ALA	ALA	E4227	S3752	GLY	K3618	L3553	GLY	H3422	F3358	P3297
ALA	ALA	ALA	A4228	ALA	ALA	ALA	A4228	R4085	GLY	A3619	F3554	GLY	W3423	P3297	A3298
GLY	GLY	GLY	E4229	ARG	ARG	ARG	E4229	V3794	GLY	W3620	Q3554	GLY	E3426	G3298	G3298
GLY	GLY	VAL	F4234	ALA	ALA	ALA	F4234	L3835	GLY	H3621	N3555	GLY	P3427	G3299	A3299
GLY	GLY	ALA	V4235	LEU	LEU	LEU	V4235	V3841	GLY	L3622	N3556	GLY	N3428	A3300	A3300
LEU	LEU	ALA	S4236	GLY	GLY	GLY	S4236	L3844	GLY	L3623	L3557	GLY	A3429	L3365	P3301
VAL	VAL	VAL	F4237	LEU	LEU	LEU	F4237	L3844	GLY	L3624	H3558	GLY	N3430	R3366	P3302
PRO	PRO	ALA	D4240	GLY	GLY	GLY	D4240	S4115	GLY	S3625	L3559	GLY	A3431	R3367	P3303
GLY	GLY	GLY	E4244	ALA	ALA	ALA	E4244	E4116	GLY	K3626	Q3560	GLY	L3434	R3368	C3304
PRO	PRO	PRO	A4248	LEU	LEU	LEU	A4248	M4120	GLY	Q3627	G3561	GLY	P3435	A3369	T3305
GLY	GLY	GLY	E4253	LEU	LEU	LEU	E4253	E4121	GLY	R3628	R3562	GLY	R3436	A3306	A3306
GLY	GLY	GLY	P4254	ARG	ARG	ARG	P4254	M4122	GLY	L3629	V3563	GLY	M3437	V3307	V3307
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	I4123	GLY	R3630	E3564	GLY	V3438	T3308	T3308
ALA	ALA	ALA	GLY	ARG	ARG	ARG	GLY	M4124	GLY	R3631	G3565	GLY	S3309	S3309	S3309
ALA	ALA	ALA	GLY	ARG	ARG	ARG	GLY	A4129	GLY	A3632	S3666	GLY	A3374	D3310	D3310
ASP	ASP	ASP	GLY	ARG	ARG	ARG	GLY	H4153	GLY	V3633	R3570	GLY	E3376	H3311	H3311
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	L4153	GLY	A3634	K3577	GLY	E3377	L3312	L3312
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	L4178	GLY	C3635	M3573	GLY	Q3378	N3313	N3313
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	G4179	GLY	L3663	R3577	GLY	R3447	S3314	S3314
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	R4180	GLY	T3664	R3577	GLY	S3446	L3315	L3315
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	I4181	GLY	E3665	G3578	GLY	S3448	L3316	L3316
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	E4182	GLY	D3666	L3579	GLY	H3449	G3317	G3317
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	I4183	GLY	H3667	P3580	GLY	N3450	N3318	N3318
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	M4184	GLY	E3667	Q3581	GLY	K3451	I3319	I3319
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	E4185	GLY	G3681	R3582	GLY	F3452	L3320	L3320
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	A4186	GLY	E3682	R3582	GLY	K3452	R3321	R3321
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	E4186	GLY	Q3683	R3583	GLY	R3453	I3322	I3322
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	R4189	GLY	Q3684	E3584	GLY	E3454	N3325	N3325
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	I4190	GLY	E3685	E3584	GLY	E3455	H3326	H3326
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	E4191	GLY	E3686	D3585	GLY	Q3456	L3327	L3327
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	R4192	GLY	E3687	A3586	GLY	N3457	G3328	G3328
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	E4196	GLY	E3687	D3587	GLY	F3458	I3329	I3329
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	I4197	GLY	E3688	D3588	GLY	V3459	D3330	D3330
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	S4198	GLY	E3689	P3589	GLY	V3460	L3332	L3332
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	E4199	GLY	V3690	E3590	GLY	Q3461	D3331	D3331
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	A3997	GLY	E3691	K3591	GLY	N3462	A3332	A3332
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	A3997	GLY	E3692	L3592	GLY	I3464	T3333	T3333
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	A3997	GLY	E3692	V3593	GLY	D3334	W3334	W3334
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	A3997	GLY	E3692	R3594	GLY	N3465	H3335	H3335
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	A3997	GLY	E3692	R3595	GLY	N3466	K3336	K3336
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GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	A3997	GLY	E3692	E3598	GLY	F3469	A3339	A3339
GLY	GLY	GLY	GLY	ARG	ARG	ARG	GLY	A3997	GLY	E3692	V3599	GLY	L3401	L3340	L3340
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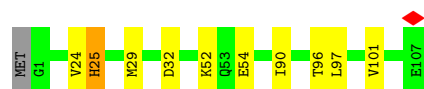
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	27861	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 ($e^-/\text{\AA}^2$)	59.9	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.429	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.046	Depositor
Map value standard deviation	0.265	Depositor
Recommended contour level	0.977	Depositor
Map size (Å)	409.80002, 409.80002, 409.80002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.366, 1.366, 1.366	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	23/35885 (0.1%)	0.56	109/48603 (0.2%)
1	B	0.43	23/35885 (0.1%)	0.56	108/48603 (0.2%)
1	C	0.43	23/35885 (0.1%)	0.56	107/48603 (0.2%)
1	D	0.43	24/35885 (0.1%)	0.56	123/48603 (0.3%)
2	E	0.30	1/851 (0.1%)	0.46	2/1146 (0.2%)
2	F	0.30	1/851 (0.1%)	0.46	2/1146 (0.2%)
2	G	0.31	1/851 (0.1%)	0.46	2/1146 (0.2%)
2	H	0.30	1/851 (0.1%)	0.46	2/1146 (0.2%)
All	All	0.42	97/146944 (0.1%)	0.56	455/198996 (0.2%)

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
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
All	All	0	5

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4973	HIS	CE1-NE2	-8.83	1.23	1.32
1	C	4973	HIS	CE1-NE2	-8.83	1.23	1.32
1	A	4973	HIS	CE1-NE2	-8.78	1.23	1.32
1	D	4973	HIS	CE1-NE2	-8.75	1.23	1.32
1	B	4192	ARG	CZ-NH2	-8.33	1.22	1.33

The worst 5 of 455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4220	ASP	CA-CB-CG	7.78	120.38	112.60
1	B	4220	ASP	CA-CB-CG	7.73	120.33	112.60
1	A	4220	ASP	CA-CB-CG	7.70	120.30	112.60
1	C	4220	ASP	CA-CB-CG	7.70	120.30	112.60
1	D	4969	ASP	CA-CB-CG	7.36	119.96	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4215	ARG	Sidechain
2	E	25	HIS	Sidechain
2	F	25	HIS	Sidechain
2	G	25	HIS	Sidechain
2	H	25	HIS	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35088	34734	34715	173	0
1	B	35088	34734	34715	183	0
1	C	35088	34734	34715	182	0
1	D	35088	34734	34715	177	0
2	E	832	829	831	5	0
2	F	832	829	831	6	0
2	G	832	829	831	5	0
2	H	832	829	831	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	14	14	0	0
4	B	31	14	14	0	0
4	C	31	14	14	1	0
4	D	31	14	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	143808	142308	142240	723	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 3.

The worst 5 of 723 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)
1:B:589:LEU:HD22	1:B:599:VAL:HG21	1.66	0.76
1:D:589:LEU:HD22	1:D:599:VAL:HG21	1.66	0.76
1:C:589:LEU:HD22	1:C:599:VAL:HG21	1.66	0.76
1:A:589:LEU:HD22	1:A:599:VAL:HG21	1.66	0.75
1:B:2675:THR:HG21	1:B:2710:LEU:HD21	1.69	0.74

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	4376/5037 (87%)	4201 (96%)	173 (4%)	2 (0%)	100	100
1	B	4376/5037 (87%)	4200 (96%)	174 (4%)	2 (0%)	100	100
1	C	4376/5037 (87%)	4201 (96%)	173 (4%)	2 (0%)	100	100
1	D	4376/5037 (87%)	4201 (96%)	173 (4%)	2 (0%)	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17924/20580 (87%)	17208 (96%)	708 (4%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	850	ASP
1	B	850	ASP
1	C	850	ASP
1	D	850	ASP
1	A	3623	LEU

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	3827/4276 (90%)	3785 (99%)	42 (1%)	65	74
1	B	3827/4276 (90%)	3784 (99%)	43 (1%)	65	74
1	C	3827/4276 (90%)	3785 (99%)	42 (1%)	65	74
1	D	3827/4276 (90%)	3785 (99%)	42 (1%)	65	74
2	E	89/90 (99%)	88 (99%)	1 (1%)	65	74
2	F	89/90 (99%)	88 (99%)	1 (1%)	65	74
2	G	89/90 (99%)	88 (99%)	1 (1%)	65	74
2	H	89/90 (99%)	88 (99%)	1 (1%)	65	74
All	All	15664/17464 (90%)	15491 (99%)	173 (1%)	63	74

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4046	ASP
1	D	1923	GLU
1	C	4183	ILE
1	D	359	TYR
1	D	2937	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2284	ASN
1	C	4833	ASN
1	C	2688	HIS
1	C	3927	GLN
1	D	405	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ACP	D	5102	-	30,33,33	1.30	4 (13%)	45,52,52	1.35	7 (15%)
4	ACP	B	5102	-	30,33,33	1.30	4 (13%)	45,52,52	1.30	6 (13%)
4	ACP	A	5102	-	30,33,33	1.28	3 (10%)	45,52,52	1.34	8 (17%)
4	ACP	C	5101	-	30,33,33	1.30	4 (13%)	45,52,52	1.32	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACP	D	5102	-	-	6/19/38/38	0/3/3/3
4	ACP	B	5102	-	-	2/19/38/38	0/3/3/3
4	ACP	A	5102	-	-	9/19/38/38	0/3/3/3
4	ACP	C	5101	-	-	7/19/38/38	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5102	ACP	PB-O2B	-3.32	1.48	1.56
4	B	5102	ACP	PB-O2B	-3.26	1.48	1.56
4	C	5101	ACP	PB-O2B	-3.12	1.49	1.56
4	D	5102	ACP	PB-O2B	-3.07	1.49	1.56
4	B	5102	ACP	PG-O3G	-2.94	1.48	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5102	ACP	O1G-PG-C3B	3.48	118.74	111.24
4	A	5102	ACP	C5-C4-N3	-3.37	122.35	126.75
4	C	5101	ACP	O1G-PG-C3B	3.25	118.24	111.24
4	D	5102	ACP	PB-O3A-PA	-3.09	122.75	132.56
4	C	5101	ACP	C5-C4-N3	-3.09	122.72	126.75

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5102	ACP	PB-C3B-PG-O1G
4	A	5102	ACP	PB-C3B-PG-O2G
4	A	5102	ACP	PB-C3B-PG-O3G
4	A	5102	ACP	C4'-C5'-O5'-PA
4	C	5101	ACP	PB-C3B-PG-O1G

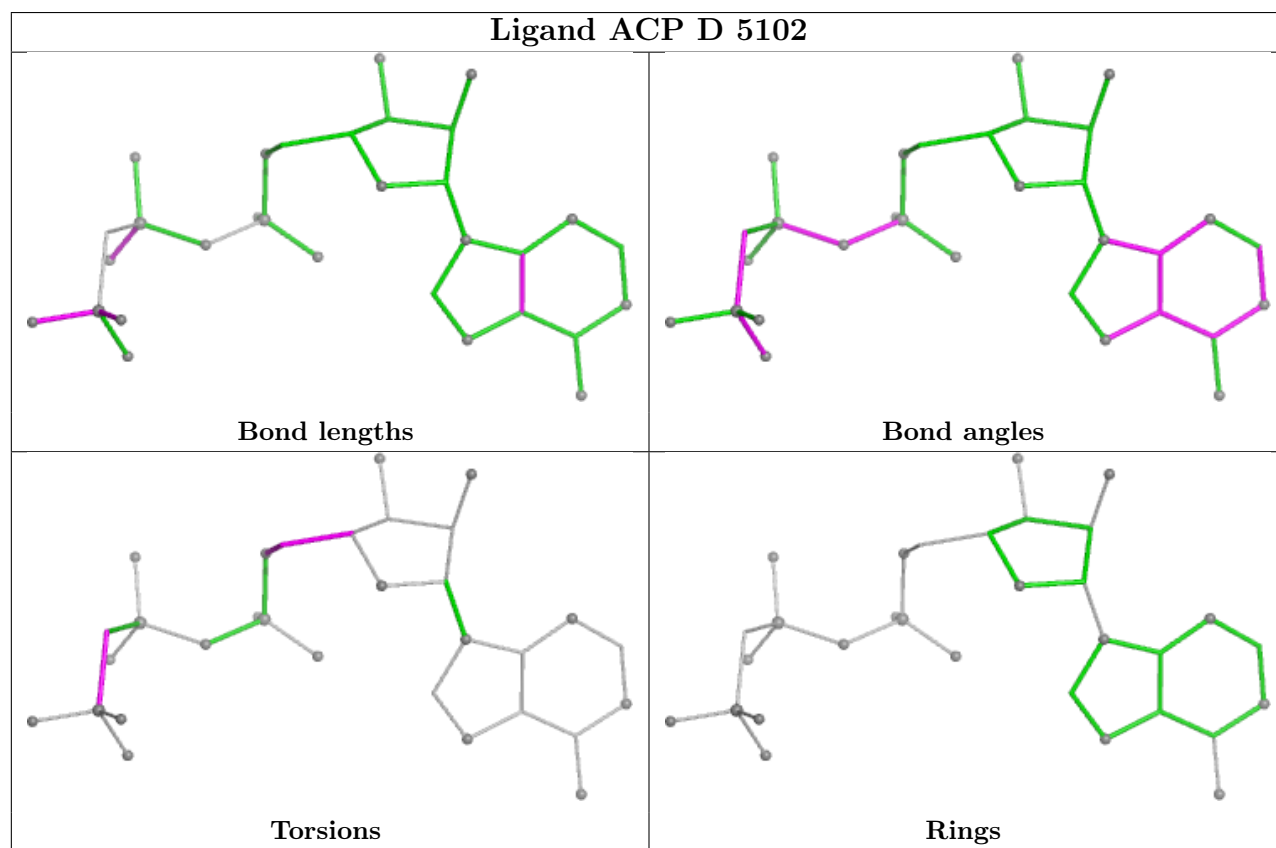
There are no ring outliers.

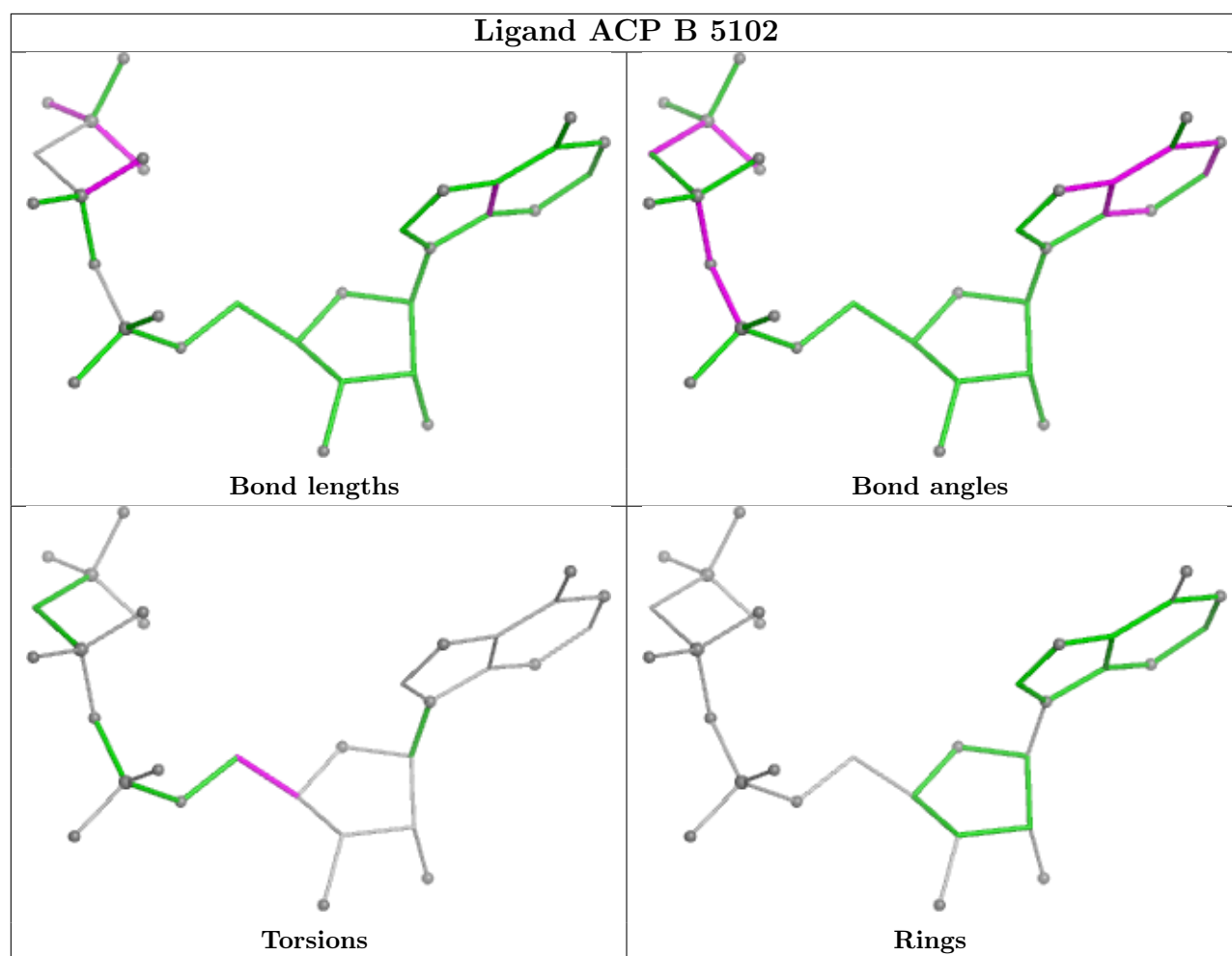
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5102	ACP	1	0
4	C	5101	ACP	1	0

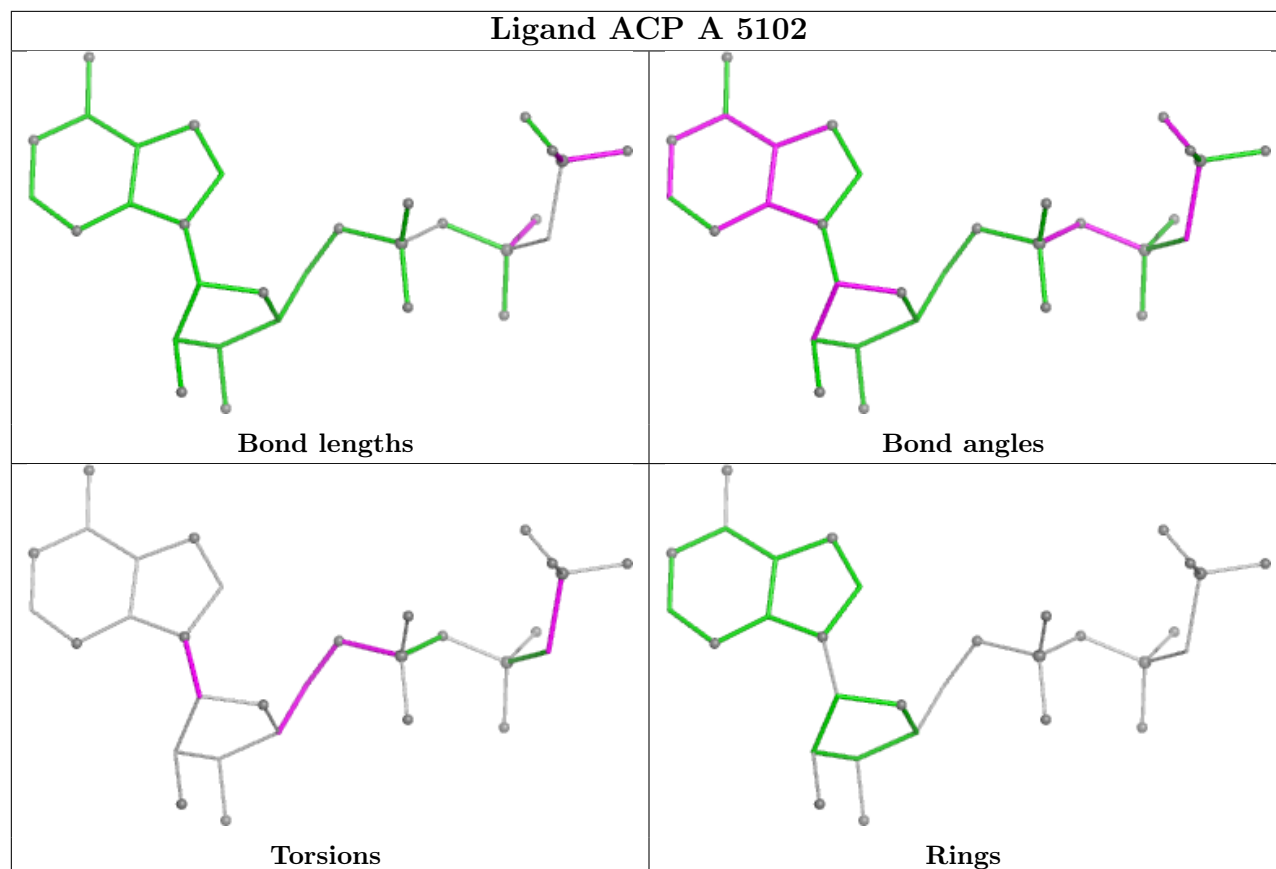
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

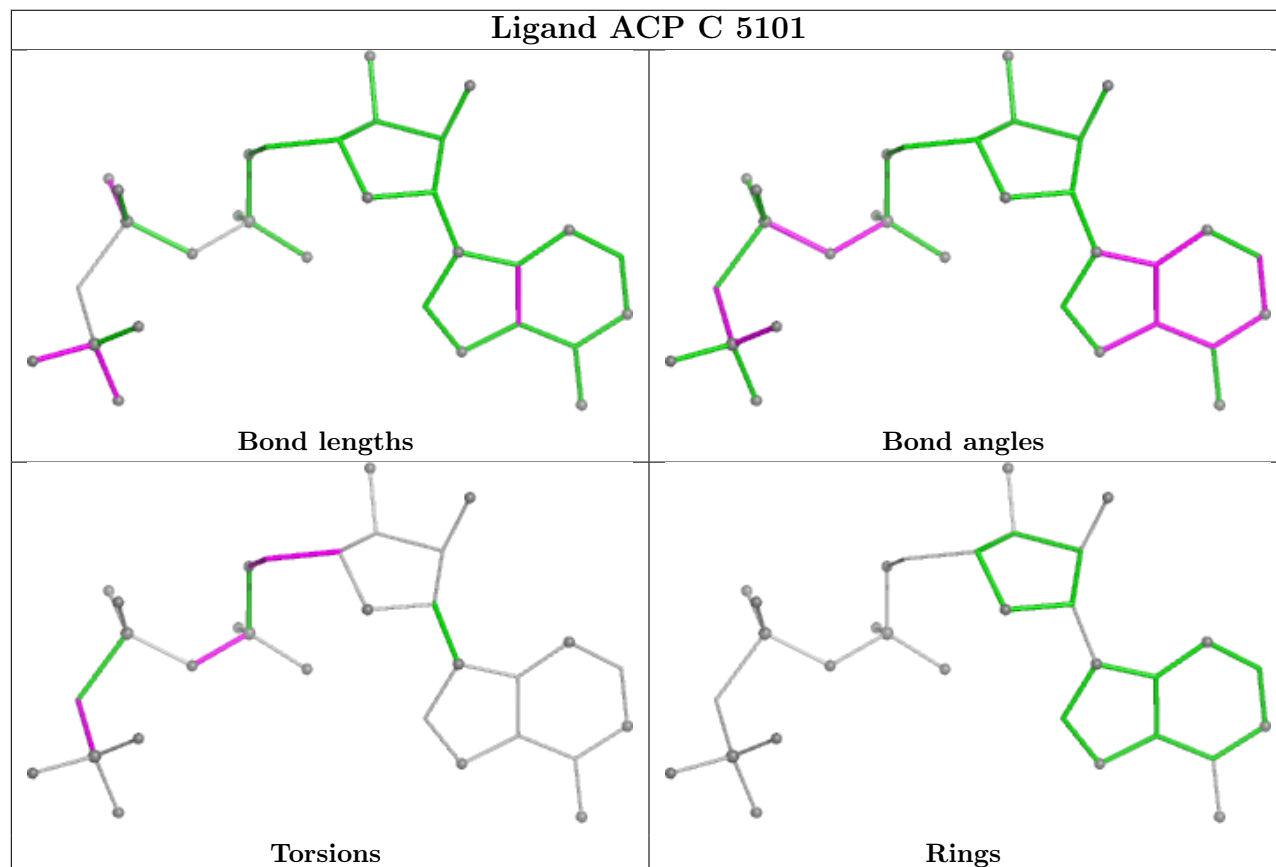




Ligand ACP A 5102



Ligand ACP C 5101



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.

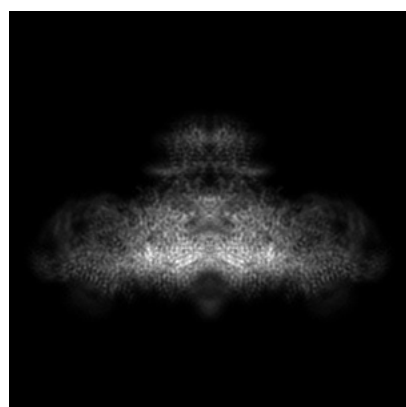
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54454. These allow visual inspection of the internal detail of the map and identification of artifacts.

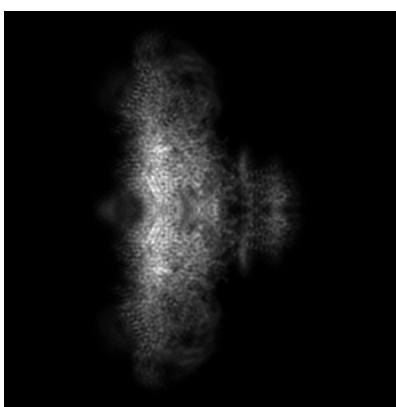
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

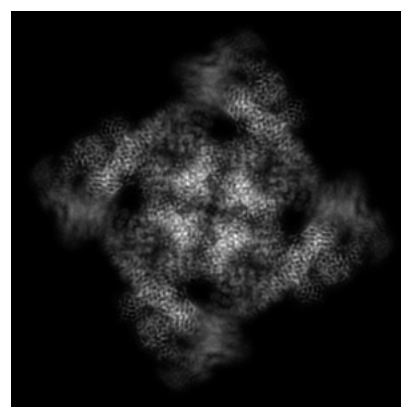
6.1.1 Primary map



X



Y

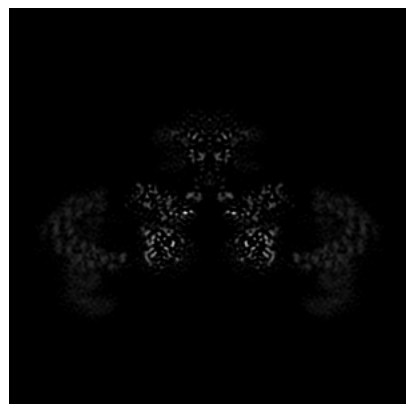


Z

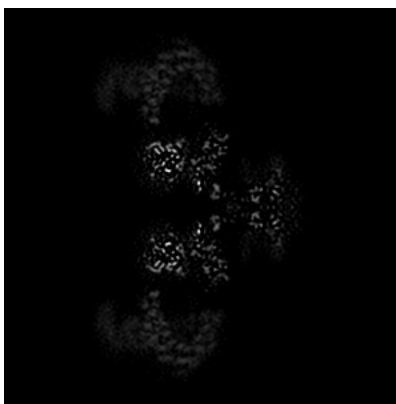
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

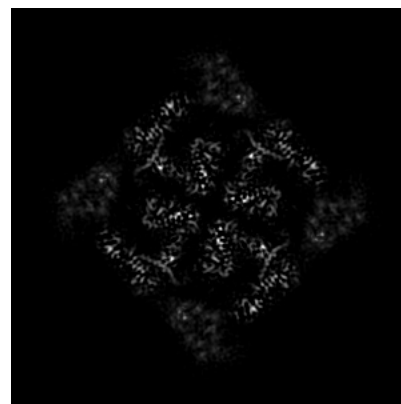
6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

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: 174



Y Index: 126

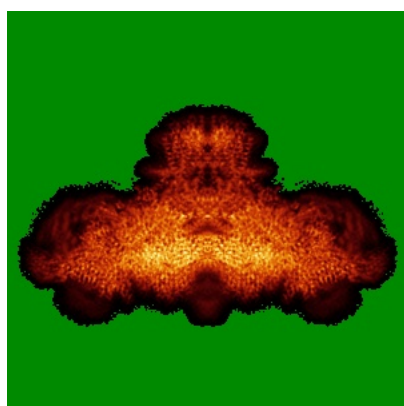


Z Index: 116

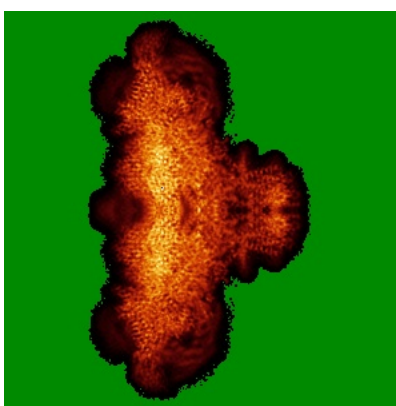
The images above show the largest variance slices of the map in three orthogonal directions.

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

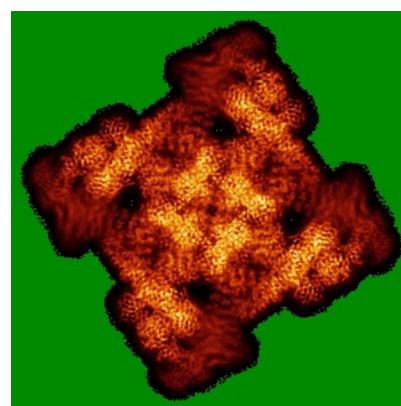
6.4.1 Primary map



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

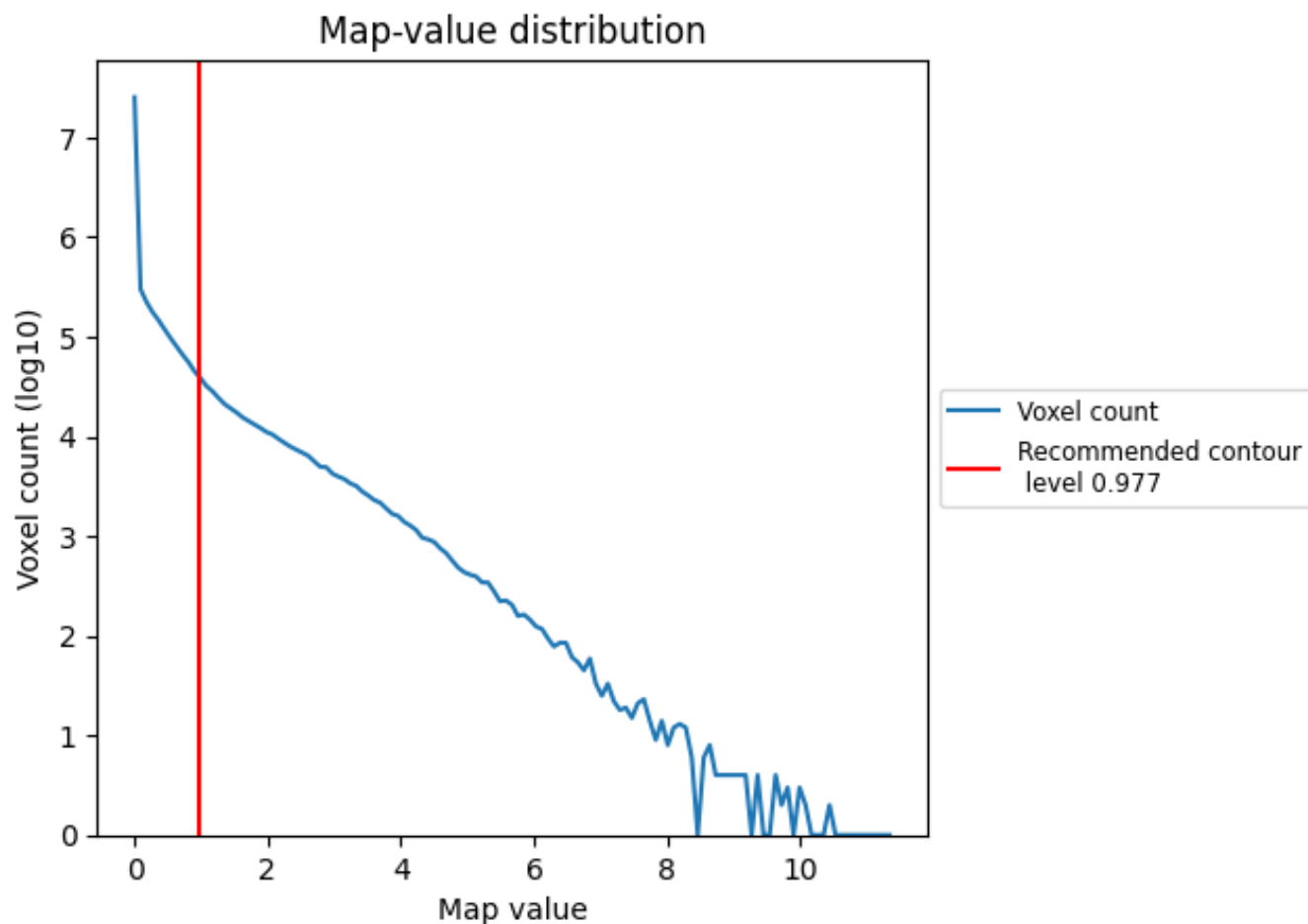
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

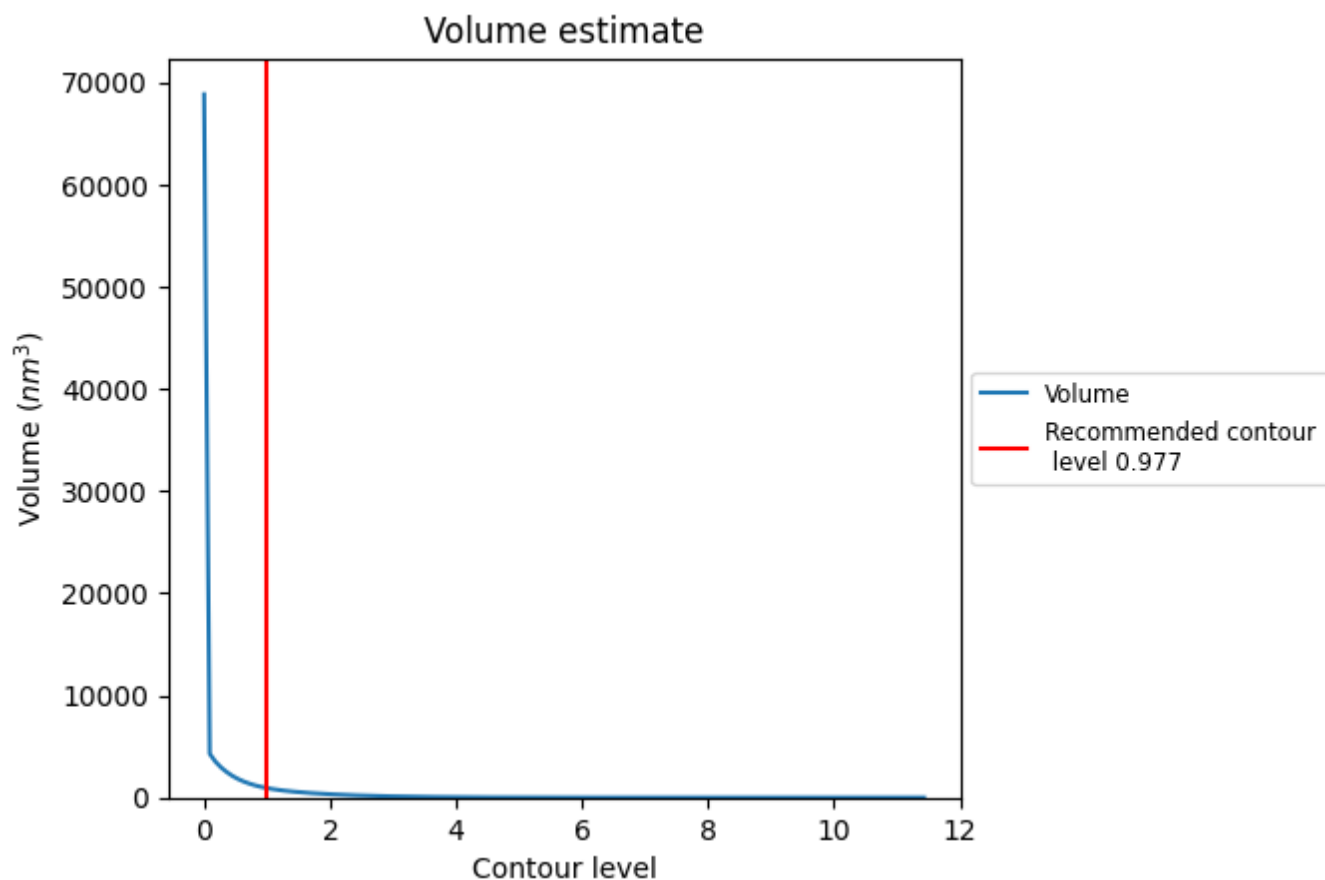
This section contains the results of statistical analysis of the map.

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.

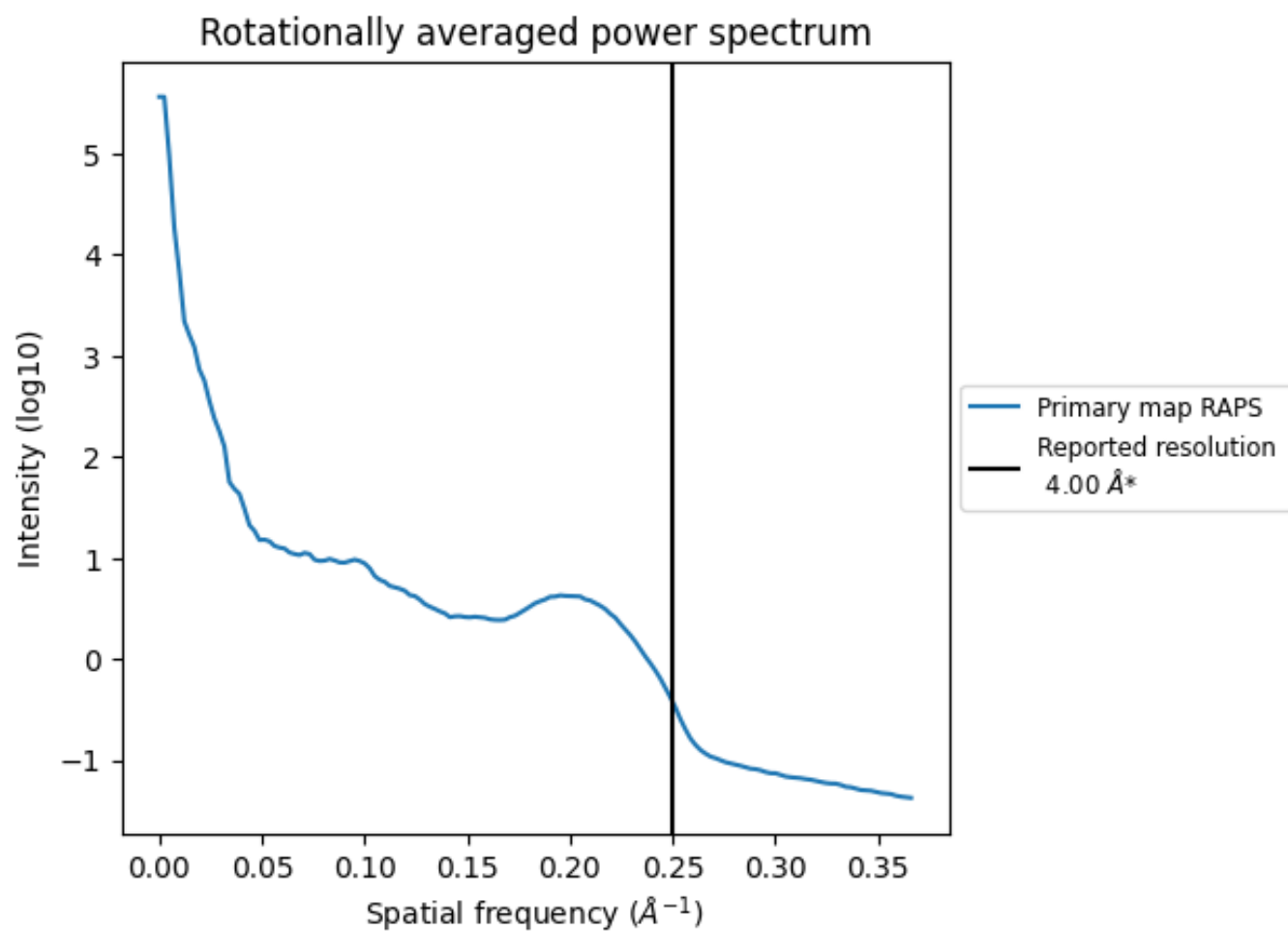
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 952 nm^3 ; this corresponds to an approximate mass of 860 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 0.250 Å⁻¹

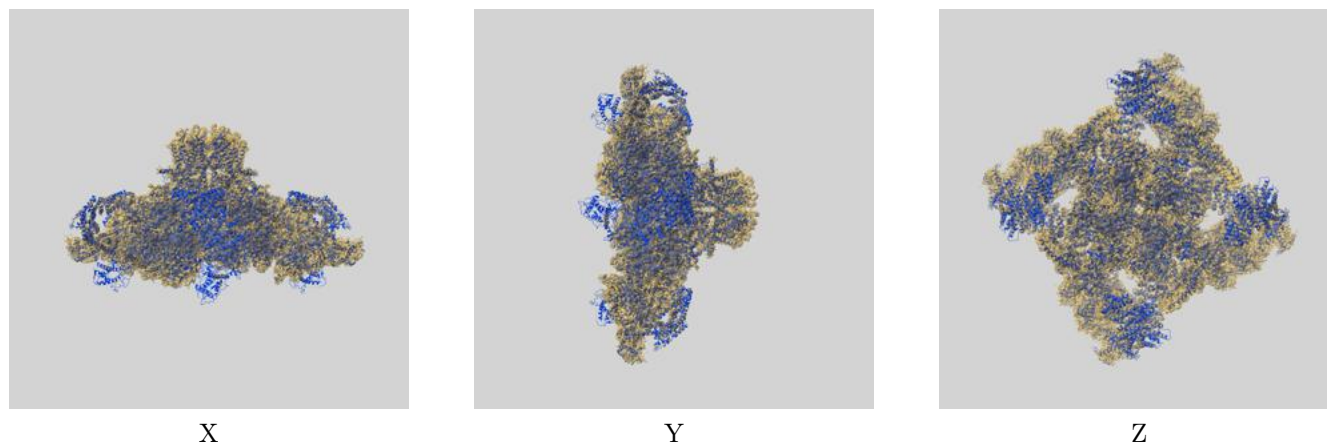
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

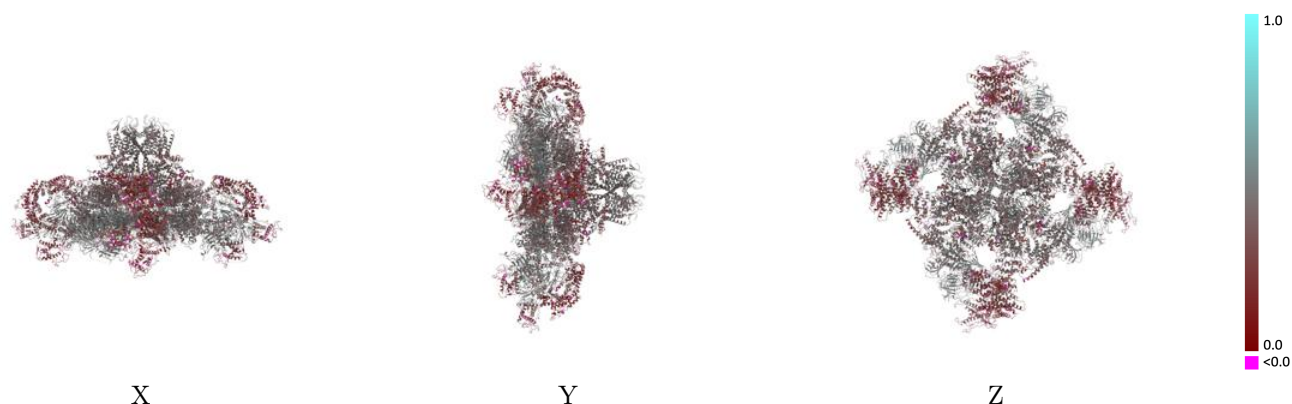
This section contains information regarding the fit between EMDB map EMD-54454 and PDB model 9S1H. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



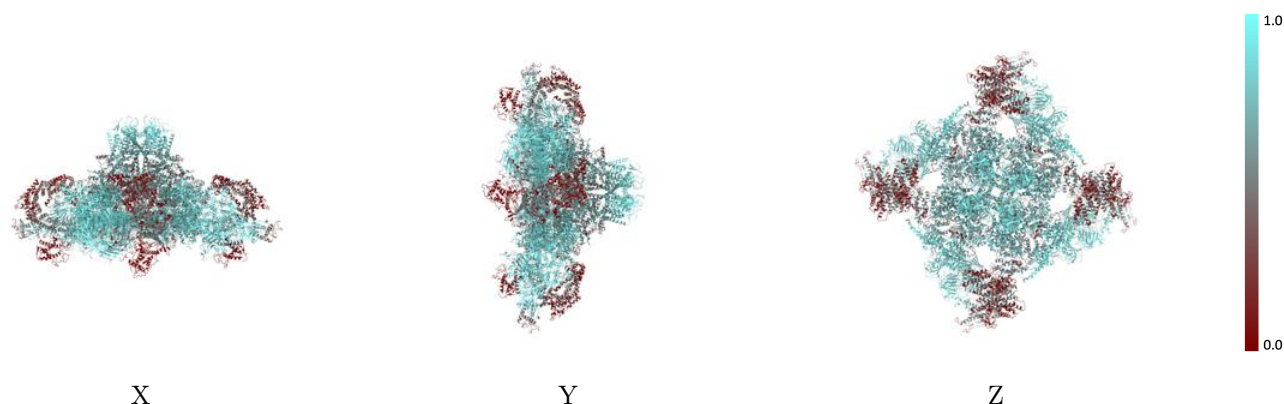
The images above show the 3D surface view of the map at the recommended contour level 0.977 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



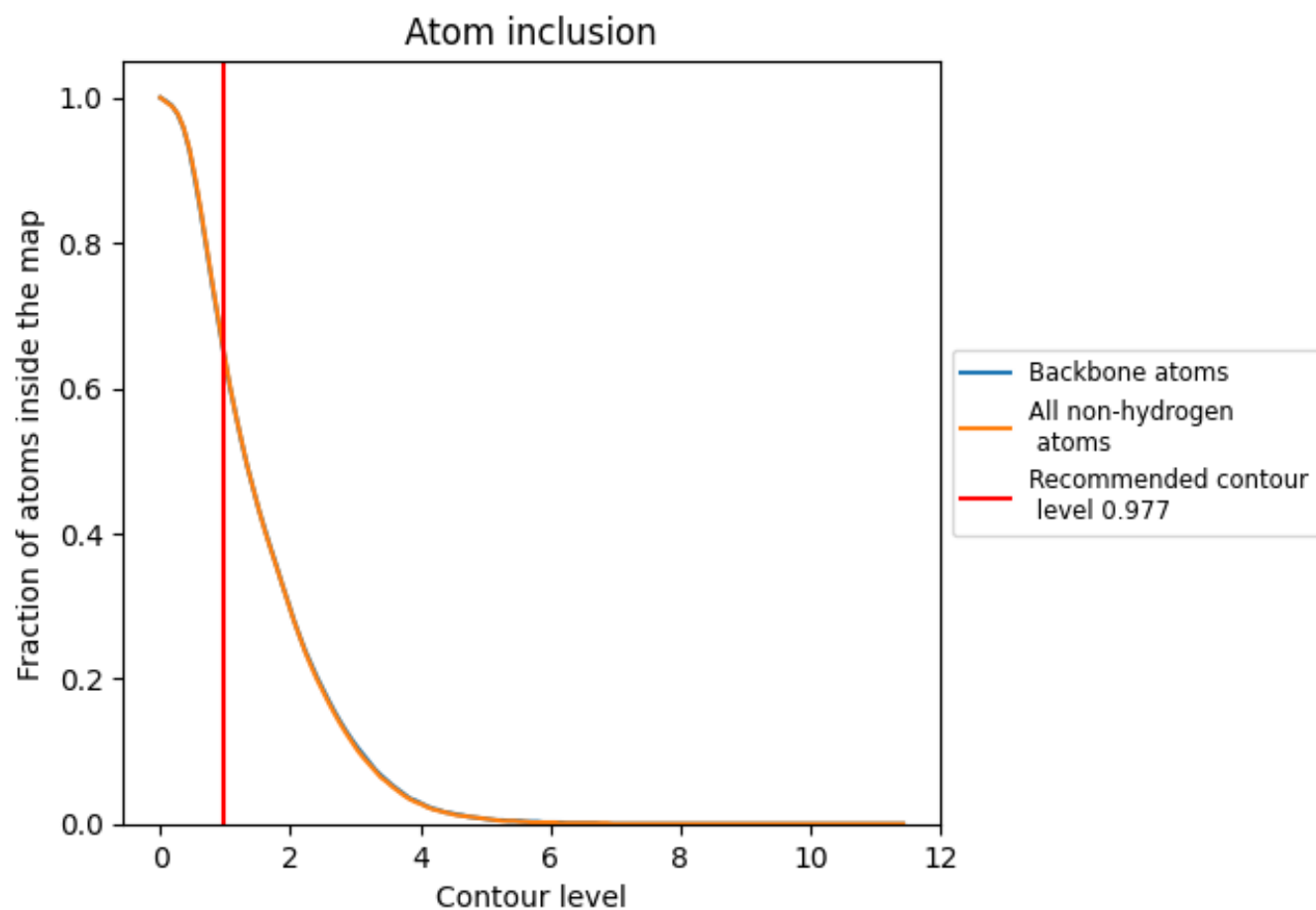
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.977).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 65% 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 (0.977) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6500	0.3790
A	0.6480	0.3770
B	0.6470	0.3780
C	0.6480	0.3770
D	0.6580	0.3750
E	0.8650	0.4620
F	0.8650	0.4630
G	0.8650	0.4660
H	0.8760	0.4590

