



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 06:57 pm BST

PDB ID : 9S55 / pdb_00009s55
EMDB ID : EMD-54590
Title : Locked-state RyR1 with ryanodine in the native membrane
Authors : Mikirtumov, V.
Deposited on : 2025-07-29
Resolution : 3.70 Å(reported)
Based on initial model : 7tzc

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:

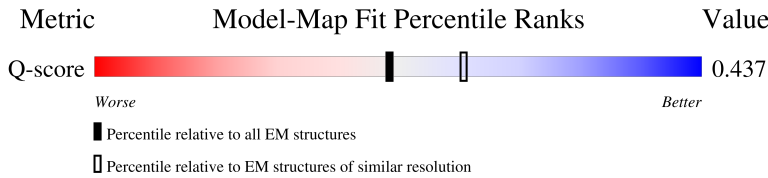
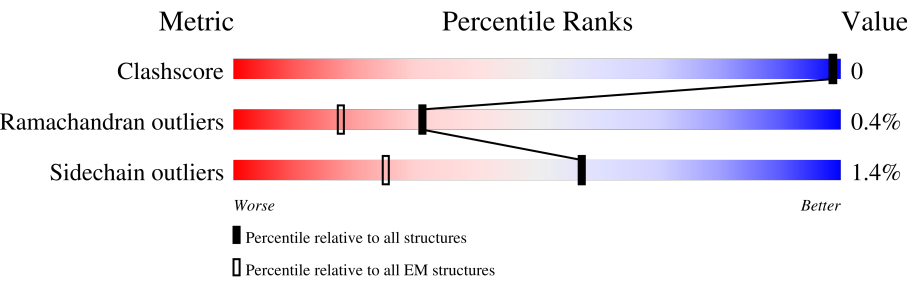
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.70 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	11569 (3.20 - 4.20)

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	
1	B	5037	
1	C	5037	
1	D	5037	

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Mol	Chain	Length	Quality of chain
2	E	108	6% 97% ..
2	F	108	7% 97% ..
2	G	108	7% 97% ..
2	H	108	6% 98% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 287008 atoms, of which 142908 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.

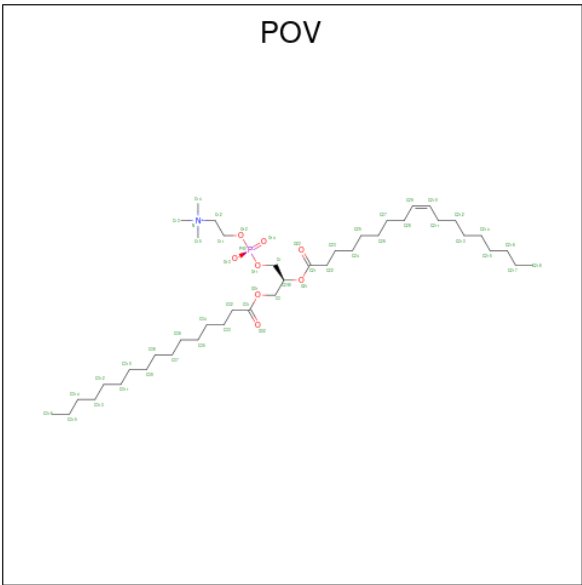
- Molecule 1 is a protein called Ryanodine receptor 1.

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 (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	B	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	B	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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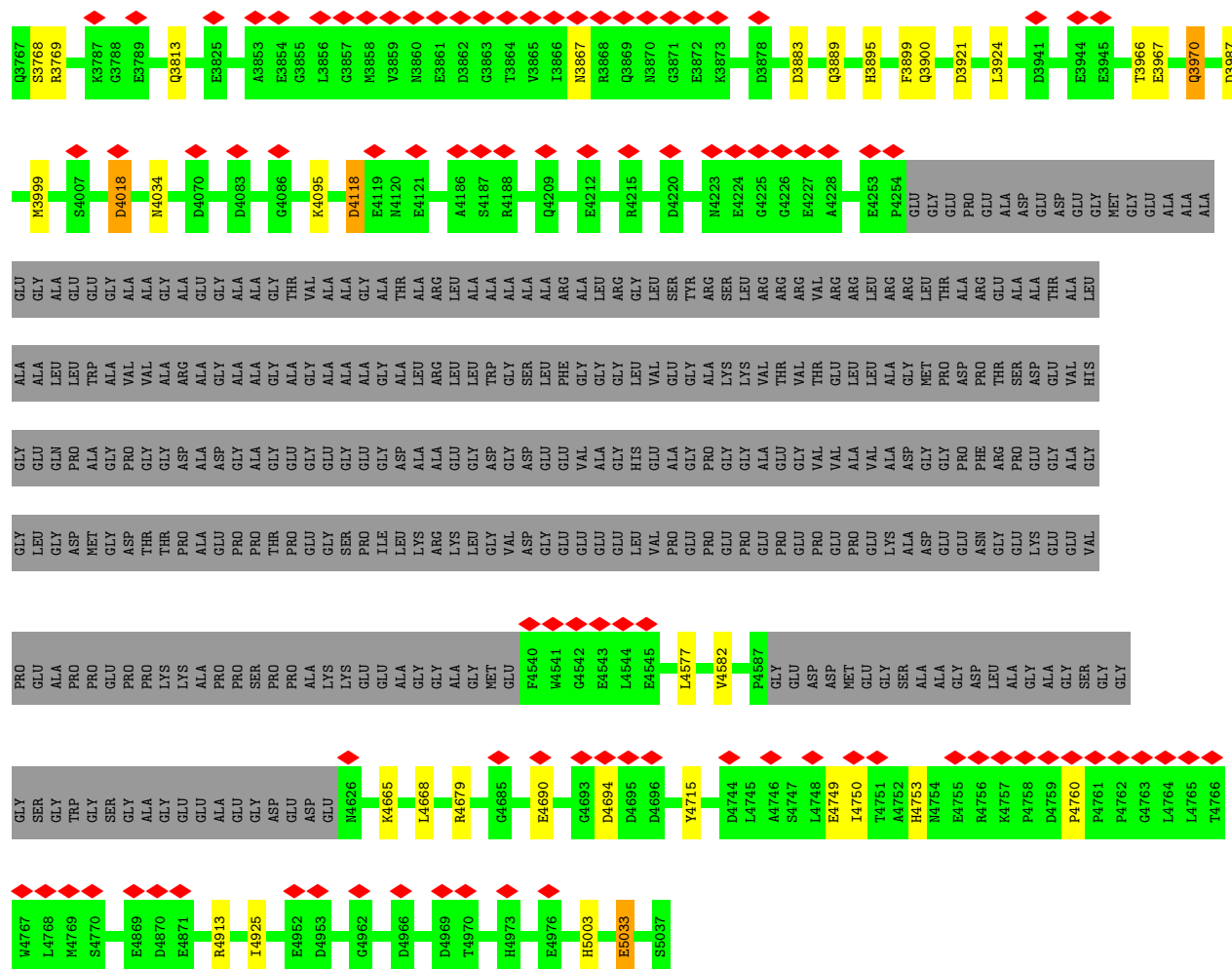
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
4	D	1	1	1	0



E3945	E3946	T3966	E3967	Q3970	R3984	Q3765	Q3766	Q3767	Q3768	Q3769	K3787	Q3786	E3789	E3825	A3853	E3854	G3855	L3856	G3857	M3858	N3859	N3860	E3861	D3862	G3863	T3864	V3865	E3867	L3868	E3869	V3869	E3891	L3866	N3867	Q3868	Q3869	N3870	E3871	E3872	K3873	D3876	D3883	H3895	H3896	N3897	F3898	Q3900	D3921	L3924	D3925	G3941	E3944							
L3623	L3624	S3625	K3626	Q3627	Q3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	M3638	T3639	D3666	H3667	E3682	Q3683	Q3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	H3699	E3712	K3713	S3714	K3715	L3716	E3718	D3719	H3734	L3735	E3736	GLU	GLY	ASN	GLY	GLY	ALA	GLU	GLU	GLU	GLU	GLU	H3621	K3622					
V3749	E3750	V3751	S3752	F3753	R3762	Q3765	Q3766	Q3767	Q3768	Q3769	K3787	Q3786	E3789	E3825	A3853	E3854	G3855	L3856	G3857	M3858	N3859	N3860	E3861	D3862	G3863	T3864	V3865	E3867	L3868	E3869	V3869	E3891	L3866	N3867	Q3868	Q3869	N3870	E3871	E3872	K3873	D3876	D3883	H3895	H3896	N3897	F3898	Q3900	D3921	L3924	D3925	G3941	E3944							
A3300	P3301	P3302	P3303	A3306	P3307	T3308	S3309	D3310	H3311	N3312	I3322	I3323	N3324	N3325	N3326	L3327	G3328	I3329	L3329	E3331	A3332	M3335	K3336	R3337	I3345	R3350	L3353	L3354	H3355	G3356	H3357	G3363	R3364	L3365	R3366	K3367	A3369	R3368	A3370	K3371	A3374	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384								
A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	E3397	F3398	S3399	V3400	L3401	R3402	R3403	D3404	L3405	V3406	A3407	R3414	M3428	A3429	E3433	R3436	M3437	V3438	G3439	E3440	T3444	M3445	S3446	K3447	S3448	H3449	N3450	F3451	K3452	R3453	E3454	E3455	Q3456	M3457	F3458	V3459	V3460	Q3461	L3462	E3463	L3464	M3465						
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D3544	T3545	D3546	E3547	E3548	V3549	R3550	E3551	Q3554	N3555	N3556	L3557	H3558	L3559	Q3560	G3561	K3562	S3566	R3577	G3578	L3579	F3580	Q3581	R3582	E3583	E3584	D3585	A3586	D3587	L3588	F3589	R3594	R3595	V3596	Q3597	L3603	Y3604	H3605	L3606	E3607	Q3608	F3609	E3610	H3611	F3612	Y3613	K3614	S3615	K3616	K3617	L3618	V3619	W3620	H3621	K3622					
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D3544	T3545	D3546	E3547	E3548	V3549	R3550	E3551	Q3554	N3555	N3556	L3557	H3558	L3559	Q3560	G3561	K3562	S3566	R3577	G3578	L3579	F3580	Q3581	R3582	E3583	E3584	D3585	A3586	D3587	L3588	F3589	R3594	R3595	V3596	Q3597	L3603	Y3604	H3605	L3606	E3607	Q3608	F3609	E3610	H3611	F3612	Y3613	K3614	S3615	K3616	K3617	L3618	V3619	W3620	H3621	K3622					
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V3749	E3750	V3751	S3752	F3753	R3762	Q3765	Q3766	Q3767	Q3768	Q3769	K3787	Q3786	E3789	E3825	A3853	E3854	G3855	L3856	G3857	M3858	N3859	N3860	E3861	D3862	G3863	T3864	V3865	E3867	L3868	E3869	V3869	E3891	L3866	N3867	Q3868	Q3869	N3870	E3871	E3872	K3873	D3876	D3883	H3895	H3896	N3897	F3898	Q3900	D3921	L3924	D3925	G3941	E3944							
E3945	E3946	T3966	E3967	Q3970	R3984	Q3765	Q3766	Q3767	Q3768	Q3769	K3787	Q3786	E3789	E3825	A3853	E3854	G3855	L3856	G3857	M3858	N3859	N3860	E3861	D3862	G3863	T3864	V3865	E3867	L3868	E3869	V3869	E3891	L3866	N3867	Q3868	Q3869	N3870	E3871	E3872	K3873	D3876	D3883	H3895	H3896	N3897	F3898	Q3900	D3921	L3924	D3925	G3941	E3944							
L3945	L3946	S3947	T3948	S2949	I2951	E2952	K2953	K2954	F2955	A2956	F2957	G2958	Q2961	Q2962	L2963	L2964	R2965	W2966	M2967	D2968	I2969	S2970	Q2971	E2972	F2973	I2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	I2995	K2996	F2997	F2998	A2999	I3000	K2999	GLY					
N288																																																											

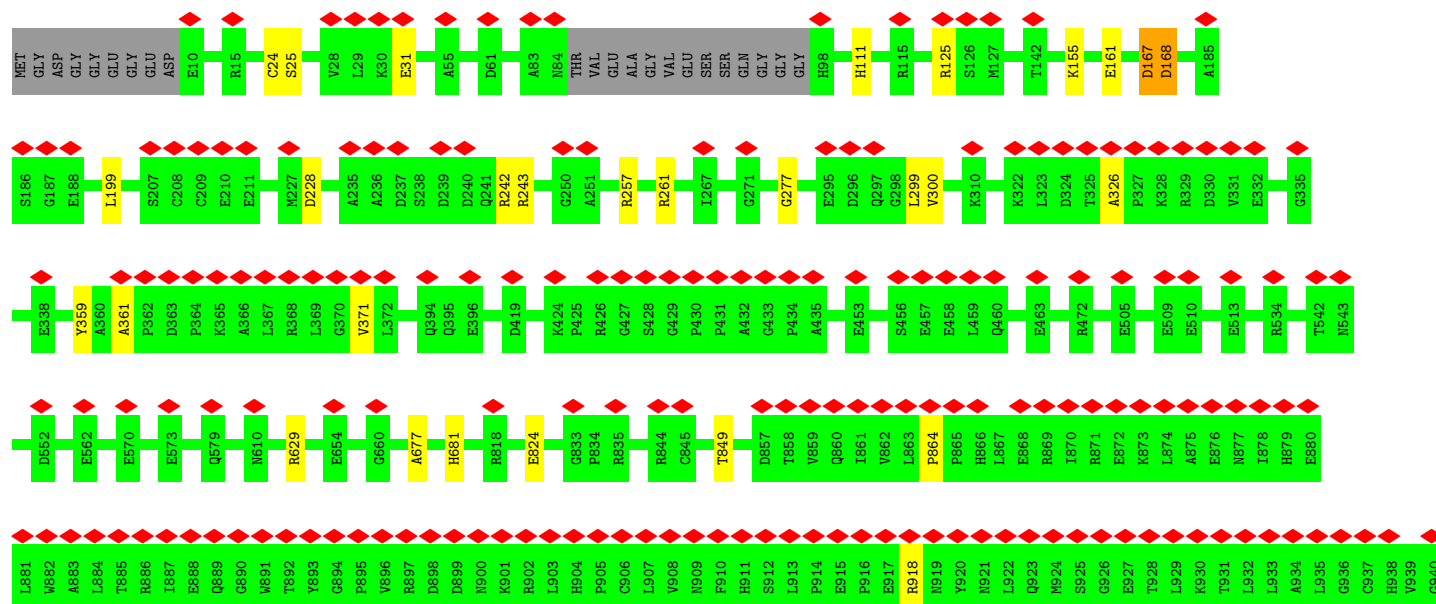


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C3635	L3557	A3479	R3310	D3310	N3234	D3159	S3083	L3018	I2951	K2891	I2771
F3636	H3558	LYS	R3396	H3311	S3235	D3160	G3084	S3019	E2952	Q2892	Q2772
R3637	L3559	ALA	D3397	L3312	V3236	S3161	F3085	P3021	K2953	E2893	I2773
M3638	Q3560	GLY	F3397	I3322	E3237	Q3162	E3086	P3020	L2954	L2894	I2774
T3639	G3561	ASP	F3398	I3323	E3238	V3163	I3087	A3022	F2955	E2895	I2775
D3666	K3562	ALA	V3400	V3324	P3241	S3164	V3088	K3023	A2956	A2896	S2776
H3667	S3566	SER	L3401	L3327	D3242	L3169	K3089	V3024	F2957	K2897	I2777
E3682	R3577	GLY	C3402	G3328	D3247	C3170	A3090	L3025	G2958	K2898	I2778
Q3683	G3578	GLY	R3403	G3329	R3248	S3171	G3091	G3026	Q2961	G2959	E2779
E3684	L3579	SER	D3404	I3329	R3249	I3172	L3092	S3027	Q2962	Q2900	I2780
E3689	P3580	ASP	L3405	E3330	L3249	Y3173	R3093	G3028	L2963	T2901	V2781
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E3686	R3582	ARG	A3407	A3332	M3250	T3178	E3097	H3030	R2965	P2903	E2783
E3687	LYS	THR	R3414	A3333	A3251	K3179	E3101	A3031	L2966	L2904	E2784
E3688	LYS	LYS	N3428	E3433	G3254	N3180	E3102	S3032	V2967	L2905	L2785
E3689	R3498	R3499	A3429	E3434	G3255	T3181	D3102	N3033	M2967	ASP	K2786
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E3691	D3501	D3501	E3433	E3436	A3257	V3183	E3104	E3035	P2907	ARG	T2787
E3692	R3502	R3502	E3437	E3437	E3258	T3179	K3105	K3036	Y2908	GLY	H2788
K3693	Y3503	Y3503	H3437	H3438	S3259	K3178	E3106	E3037	D2909	GLY	P2789
H3699	S3504	S3504	G3438	G3439	G3260	K3185	V3107	M3038	T2910	Y2855	H2790
R3595	V3505	V3505	Y3444	Y3445	A3261	L3186	E3108	I3039	L2911	N2856	L2791
V3596	Q3506	Q3506	S3446	S3447	R3262	R3187	E3109	T3040	T2912	P2857	L2792
Q3597	T3507	T3507	H3449	H3450	Y3263	P3188	N3109	S3041	A2913	Q2858	P2793
L3603	S3508	S3508	K3451	K3452	T3264	A3189	R3110	L3042	K2914	P2859	P2794
S3714	L3509	L3509	F3451	F3452	E3265	L3190	R3111	K3045	E2915	P2860	K2795
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L3716	V3511	V3511	H3449	H3450	P3267	E3192	G3113	A3047	A2917	L2862	F2797
D3717	D3529	D3529	K3451	K3452	H3268	C3193	G3114	A3048	K2918	S2863	S2798
E3718	Q3530	Q3530	E3454	E3455	I3272	A3204	V3115	L3049	D2919	G2864	E2799
D3719	M3531	M3531	E3455	E3456	M3276	E3207	S3116	V3050	R2920	T2865	K2800
E3736	L3534	L3534	Q3457	Q3458	M3276	P3208	GLN	R3051	E2921	L2867	D2801
GLY	L3535	L3535	F3458	F3459	R3283	Q3209	ALA	R3052	S2982	S2868	K2802
GLY	R3536	R3536	F3458	F3459	E3286	Q3209	THR	R3053	Q2984	E2869	E2803
GLU	R3537	R3537	F3458	F3459	E3287	L3210	GLN	V3054	Q2924	E2870	T2804
ASN	Y3613	Y3613	Q3457	Q3458	R3287	N3211	VAL	V3055	E2925	L2871	Y2805
K3614	K3614	K3614	F3458	F3459	R3287	E3212	K3123	S3056	E2926	Q2872	K2806
GLY	R3538	R3538	F3458	F3459	R3287	Y3213	G3124	L3056	K2988	L2927	Q2807
ALA	R3539	R3539	F3458	F3459	P3289	N3214	V3125	F3057	S2989	K2928	P2808
GLU	Y3540	Y3540	F3458	F3459	E3290	A3215	G3126	G3058	P2990	M2874	L2809
GLU	A3541	A3541	F3458	F3459	A3291	C3216	Q3127	T3059	H2991	A2875	K2810
GLU	K3542	K3542	Q3461	Q3462	P3292	S3217	N3128	D3060	E2992	E2876	E2811
GLU	L3543	L3543	N3462	N3463	P3293	V3218	L3129	A3061	Q2993	M2932	S2812
GLU	D3544	D3544	E3463	E3464	P3294	Y3219	T3130	P3062	E2994	K2933	L2813
GLU	T3545	T3545	I3465	I3466	A3295	T3220	Y3131	A3063	L2995	Q2934	K2814
GLU	D3546	D3546	N3466	N3467	L3296	T3221	A3135	N3066	K2996	K2935	A2815
GLU	E3547	E3547	S3468	S3469	P3297	K3222	L3136	H3069	F2997	A2936	M2816
GLU	V3549	V3549	F3469	F3470	A3298	E3226	H3146	I3070	F2998	T2937	L2817
GLU	R3550	R3550	L3470	L3471	A3300	R3227	T3147	K3073	A2999	T2938	A2818
GLU	E3551	E3551	T3471	T3472	P3301	E3227	Q3151	S3074	L2985	K2939	K2819
GLU	Q3554	Q3554	A3472	A3473	P3302	R3227	F3152	L3075	L2986	GLY	E2820
GLU	Q3554	Q3554	S3474	S3475	P3303	E3227	Q3153	D3076	K2986	LEU	E2821
GLU	Q3554	Q3554	K3475	K3476	A3306	E3227	D3154	A3077	G2867	LYS	T2822
GLU	Q3554	Q3554	S3475	S3476	V3307	E3227	D3155	R3078	R2888	ASP	L2823
GLU	Q3554	Q3554	S3475	S3476	V3307	E3227	D3155	R3078	R2888	ASP	E2824
GLU	Q3554	Q3554	S3475	S3476	V3307	E3227	D3155	R3078	R2888	ASP	K2825
GLU	Q3554	Q3554	S3475	S3476	V3307	E3227	D3155	R3078	R2888	ASP	A2826
GLU	Q3554	Q3554	S3475	S3476	V3307	E3227	D3155	R3078	R2888	ASP	K2827
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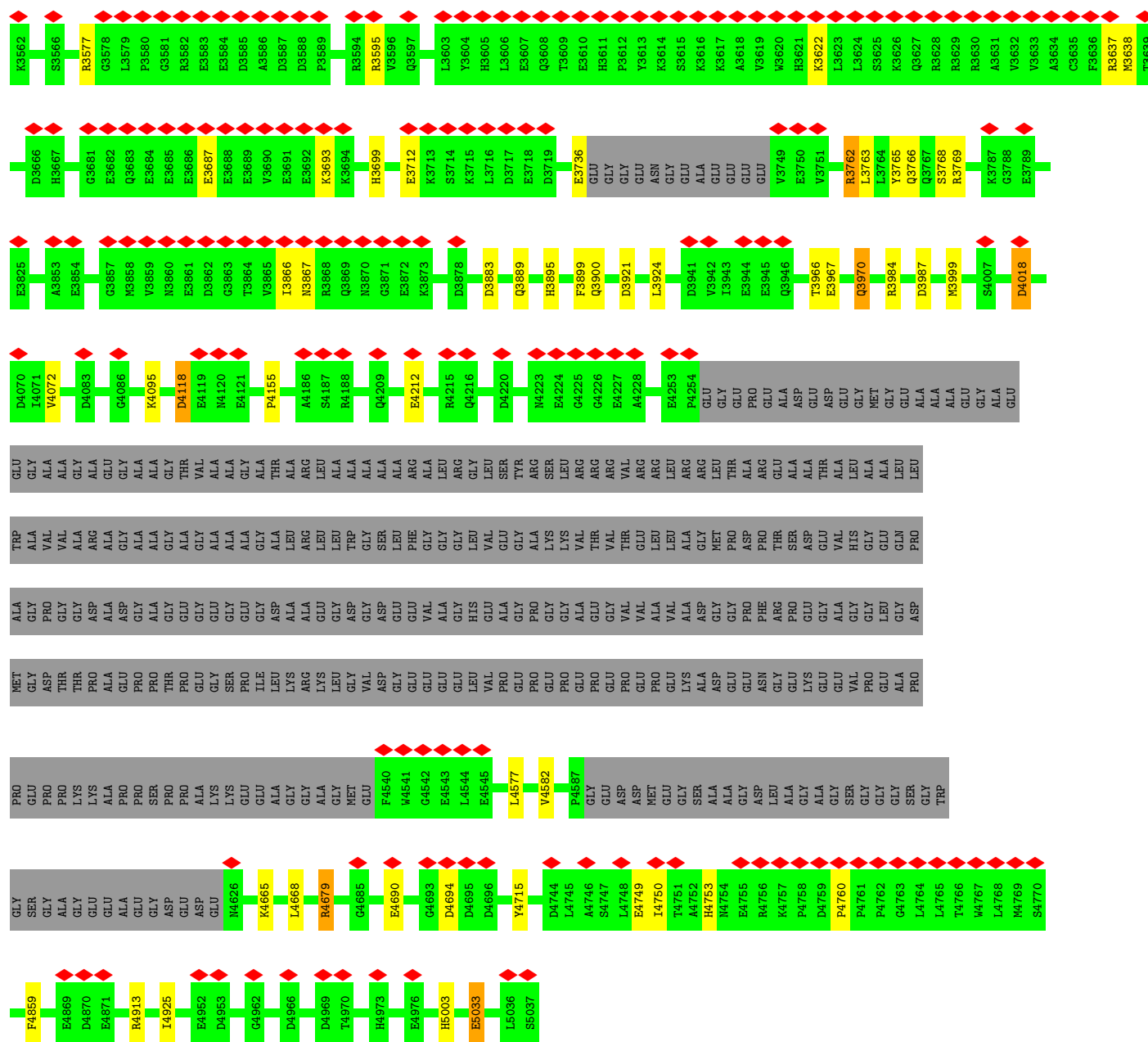
• Molecule 1: Ryanodine receptor 1

Chain C: 28% 84% 13%

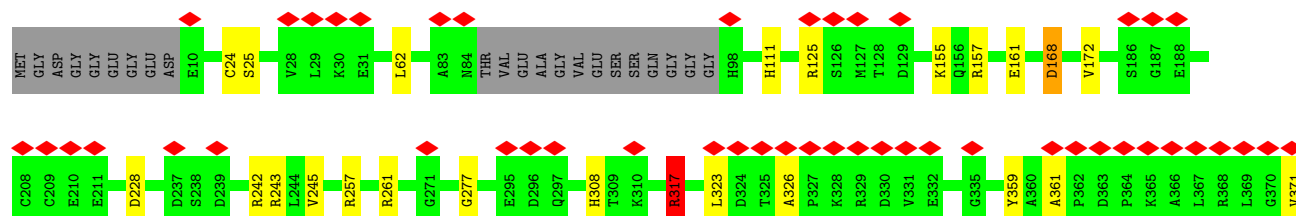
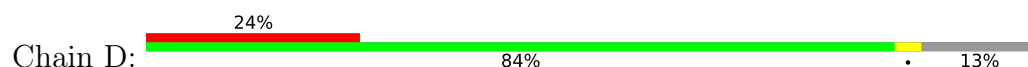






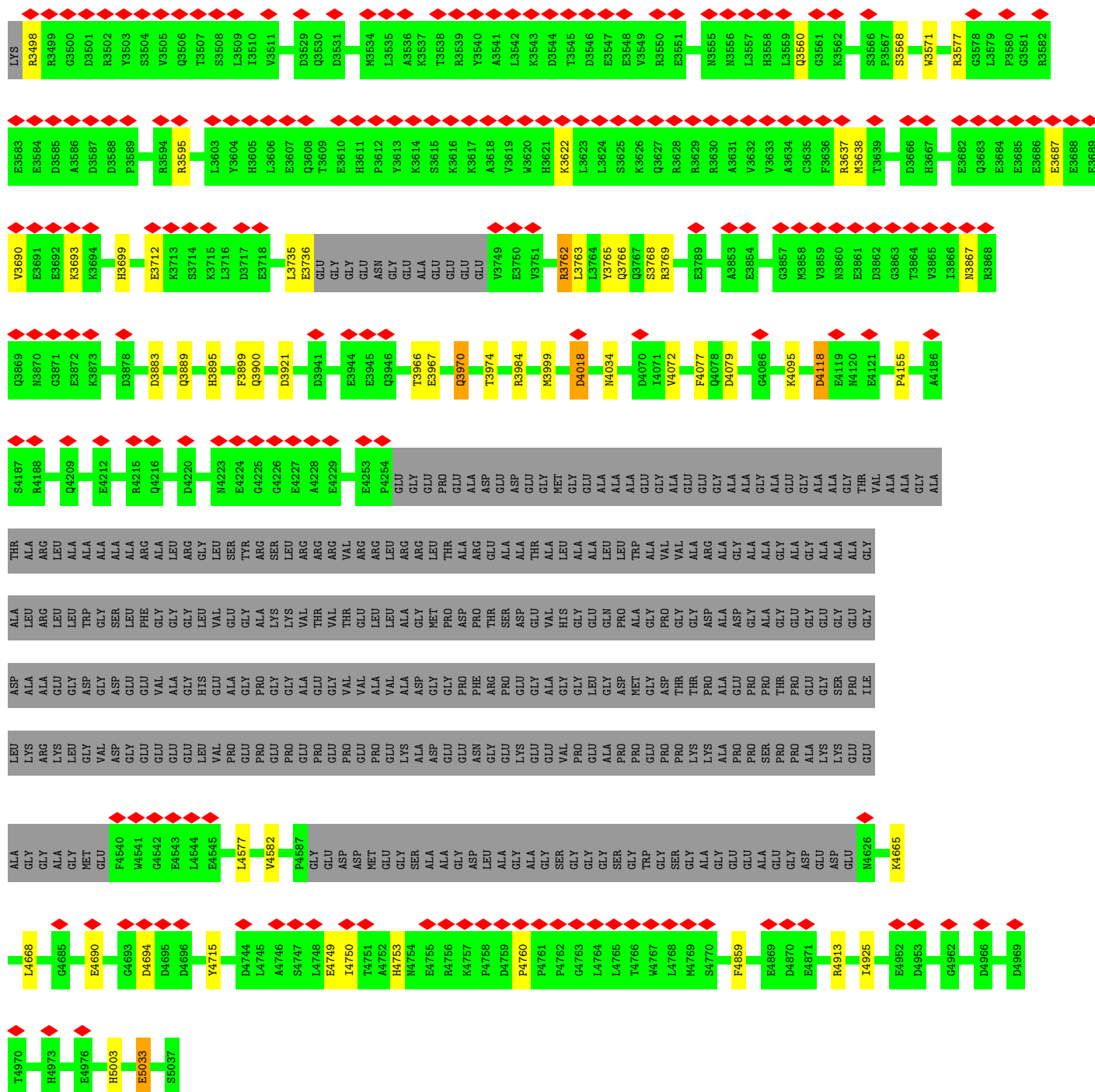


• Molecule 1: Ryanodine receptor 1

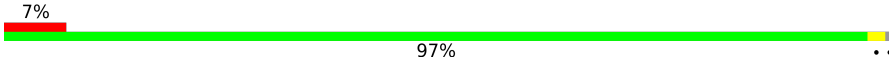




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D3330	E3331	A3332	H3335	V3346	R3350	L3353	L3354	H3355	S3356	H3357	G3363	R3366	K3367	R3368	A3369	G3370	K3371	A3374	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	G3389	G3390	L3391	L3392	L3393	V3394	R3395	D3396	E3397	F3398	S3399	V3400	L3401	C3402	R3403	D3404	L3405	Y3406	A3407																																	
Q3127	N3128	L3129	T3130	D3131	T3132	L3136	Q3151	F3152	G3153	D3154	D3155	L3158	D3159	D3160	S3164	L3169	C3170	S3171	T3177	T3178	K3179	N3180	T3181	F3182	V3183	E3184	K3185	L3186	R3187	P3188	A3189	C3193	A3204	L3210	N3211	E3212	Y3213	N3214	A3215	V3218	Y3219	T3220	T3221	K3222	S3223	P3224	K3225	E3226	R3227																																			
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F3057	G3058	T3059	D3060	A3061	P3062	A3063	N3066	R3073	S3074	L3075	D3076	A3077	R3078	N3081	K3082	S3083	G3084	P3085	E3086	I3087	V3088	K3089	A3090	G3091	L3092	R3093	S3094	E3097	E3101	D3102	I3103	E3104	K3105	M3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	K3114	V3115	S3116	ALA	ARG	THR	GLN	VAL	K3123	K3124	V3125	G3126																															
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R2541	S2542	T2543	T2544	A2547	L2548	N2551	R2552	L2553	L2554	C2555	L2556	K2564	C2565	A2566	F2567	L2568	F2569	A2570	C2571	T2572	H2574	R2575	A2576	L2577	M2578	V2579	D2580	S2581	M2582	L2583	H2584	Y2587	R2588	L2589	S2590	R2591	Q2592	R2593	S2594	L2595	T2596	K2597	A2598	Q2599	R2600	D2601	E2604	D2605	C2606	L2607	L2608	A2609	L2610																															

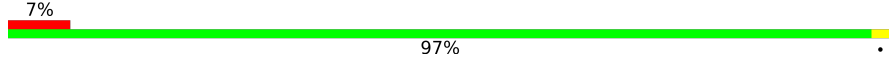


- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F:  7% 97% ..

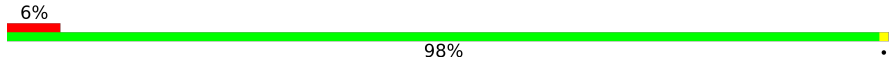


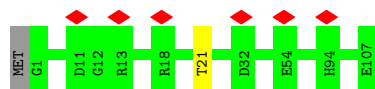
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G:  7% 97% ..



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

Chain H:  6% 98% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	157550	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 ($e^-/\text{\AA}^2$)	67.44	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	36.485	Depositor
Minimum map value	0.000	Depositor
Average map value	0.051	Depositor
Map value standard deviation	0.346	Depositor
Recommended contour level	1.39	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: POV, 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	0.81	1/35885 (0.0%)	1.33	73/48603 (0.2%)
1	B	0.80	1/35885 (0.0%)	1.33	77/48603 (0.2%)
1	C	0.80	1/35885 (0.0%)	1.33	77/48603 (0.2%)
1	D	0.80	1/35885 (0.0%)	1.35	79/48603 (0.2%)
2	E	0.82	0/851	1.38	1/1146 (0.1%)
2	F	0.81	0/851	1.37	1/1146 (0.1%)
2	G	0.81	0/851	1.37	1/1146 (0.1%)
2	H	0.81	0/851	1.37	0/1146
All	All	0.80	4/146944 (0.0%)	1.34	309/198996 (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	8
1	B	0	7
1	C	0	7
1	D	0	6
All	All	0	28

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	864	PRO	CA-C	5.52	1.54	1.51
1	D	864	PRO	CA-C	5.50	1.54	1.51
1	A	864	PRO	CA-C	5.44	1.54	1.51
1	B	864	PRO	CA-C	5.32	1.54	1.51

All (309) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	ASP	CA-CB-CG	7.88	120.47	112.60
1	B	2629	ASP	CA-C-N	7.75	125.13	120.24
1	B	2629	ASP	C-N-CA	7.75	125.13	120.24
1	D	1690	ASP	CA-CB-CG	7.49	120.09	112.60
1	B	1690	ASP	CA-CB-CG	7.38	119.98	112.60
1	C	1690	ASP	CA-CB-CG	7.28	119.88	112.60
1	A	1690	ASP	CA-CB-CG	7.23	119.83	112.60
1	C	168	ASP	CA-CB-CG	6.93	119.53	112.60
1	D	4118	ASP	CA-CB-CG	6.78	119.38	112.60
1	B	4753	HIS	CA-CB-CG	6.77	120.57	113.80
1	C	4753	HIS	CA-CB-CG	6.77	120.57	113.80
1	D	4753	HIS	CA-CB-CG	6.71	120.51	113.80
1	A	4753	HIS	CA-CB-CG	6.67	120.47	113.80
1	D	3293	PRO	N-CA-C	6.64	118.81	110.70
1	C	3293	PRO	N-CA-C	6.61	118.76	110.70
1	B	4118	ASP	CA-CB-CG	6.55	119.15	112.60
1	D	317	ARG	CD-NE-CZ	6.49	133.49	124.40
1	A	3293	PRO	N-CA-C	6.44	118.56	110.70
1	D	168	ASP	CA-CB-CG	6.42	119.02	112.60
1	D	317	ARG	NE-CZ-NH2	6.41	124.97	119.20
1	D	228	ASP	CA-CB-CG	6.41	119.01	112.60
1	C	4118	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	167	ASP	CA-CB-CG	6.34	118.94	112.60
1	C	1229	ASN	CA-CB-CG	-6.33	106.27	112.60
1	B	2523	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	168	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	168	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	4118	ASP	CA-CB-CG	6.18	118.78	112.60
1	B	3053	ARG	NE-CZ-NH2	6.17	124.76	119.20
1	B	4018	ASP	CA-CB-CG	6.15	118.75	112.60
1	C	3595	ARG	NE-CZ-NH2	6.12	124.70	119.20
1	D	2523	ASP	CA-CB-CG	6.08	118.68	112.60
1	D	1229	ASN	CA-CB-CG	-6.08	106.52	112.60
1	A	4018	ASP	CA-CB-CG	6.07	118.67	112.60
1	D	3053	ARG	NE-CZ-NH2	6.06	124.66	119.20
1	D	3595	ARG	NE-CZ-NH2	6.06	124.65	119.20
1	A	3595	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	B	3595	ARG	NE-CZ-NH2	6.05	124.64	119.20
1	D	2001	PRO	N-CA-C	6.03	116.26	110.47
1	B	5033	GLU	N-CA-C	6.00	117.81	111.28
1	B	2026	ASP	CA-CB-CG	5.99	118.59	112.60
1	B	167	ASP	CA-CB-CG	5.96	118.56	112.60
1	D	3762	ARG	CD-NE-CZ	5.94	132.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1229	ASN	CA-CB-CG	-5.92	106.69	112.60
1	C	4859	PHE	CA-CB-CG	5.91	119.71	113.80
1	C	2523	ASP	CA-CB-CG	5.91	118.50	112.60
1	D	4018	ASP	CA-CB-CG	5.90	118.50	112.60
1	D	5033	GLU	N-CA-C	5.88	117.69	111.28
1	B	681	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	C	2001	PRO	N-CA-C	5.86	116.09	110.47
1	B	1513	ASP	CA-CB-CG	5.85	118.45	112.60
1	C	2026	ASP	CA-CB-CG	5.83	118.43	112.60
1	D	3577	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	A	1229	ASN	CA-CB-CG	-5.83	106.77	112.60
1	C	3053	ARG	NE-CZ-NH2	5.83	124.44	119.20
1	A	1513	ASP	CA-CB-CG	5.82	118.42	112.60
1	B	2001	PRO	N-CA-C	5.82	116.06	110.47
1	A	681	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	D	681	HIS	CB-CG-CD2	-5.80	123.66	131.20
1	C	681	HIS	CB-CG-CD2	-5.79	123.68	131.20
1	A	4859	PHE	CA-CB-CG	5.78	119.58	113.80
1	B	3293	PRO	N-CA-C	5.78	117.75	110.70
1	A	2523	ASP	CA-CB-CG	5.76	118.36	112.60
1	C	1017	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	A	5033	GLU	N-CA-C	5.76	117.56	111.28
1	B	4665	LYS	CA-C-N	5.75	123.86	120.24
1	B	4665	LYS	C-N-CA	5.75	123.86	120.24
1	D	2736	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	3900	GLN	OE1-CD-NE2	-5.75	116.86	122.60
1	A	2026	ASP	CA-CB-CG	5.74	118.34	112.60
1	C	5033	GLU	N-CA-C	5.74	117.54	111.28
1	C	3900	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	A	2452	ARG	NE-CZ-NH2	5.72	124.35	119.20
1	C	1000	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	C	1090	PHE	CA-CB-CG	5.71	119.50	113.80
1	A	1017	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	D	1090	PHE	CA-CB-CG	5.70	119.50	113.80
1	D	4690	GLU	N-CA-C	5.70	118.70	111.69
1	A	4690	GLU	N-CA-C	5.68	118.68	111.69
1	C	1513	ASP	CA-CB-CG	5.67	118.27	112.60
1	D	2026	ASP	CA-CB-CG	5.65	118.25	112.60
1	B	4690	GLU	N-CA-C	5.64	118.63	111.69
1	D	3900	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	B	1017	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	C	4665	LYS	CA-C-N	5.62	123.78	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4665	LYS	C-N-CA	5.62	123.78	120.24
1	A	4665	LYS	CA-C-N	5.61	123.78	120.24
1	A	4665	LYS	C-N-CA	5.61	123.78	120.24
1	A	3984	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	B	1090	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	1000	ARG	NE-CZ-NH2	5.58	124.23	119.20
1	D	4859	PHE	CA-CB-CG	5.58	119.38	113.80
1	C	4690	GLU	N-CA-C	5.58	118.55	111.69
1	C	4018	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	1000	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	D	1000	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	D	4665	LYS	CA-C-N	5.57	123.75	120.24
1	D	4665	LYS	C-N-CA	5.57	123.75	120.24
1	A	1090	PHE	CA-CB-CG	5.56	119.36	113.80
1	C	2452	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	D	3974	THR	N-CA-C	5.55	117.33	111.28
1	C	2333	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	2333	ASP	CA-CB-CG	5.54	118.14	112.60
1	D	1513	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	2452	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	B	3053	ARG	CD-NE-CZ	5.51	132.12	124.40
1	D	4925	ILE	N-CA-C	5.51	115.71	110.53
1	D	2104	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	B	261	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	D	261	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	3053	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	D	326	ALA	N-CA-C	5.49	113.16	108.22
1	D	2738	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	A	3900	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	C	2104	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	B	2333	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	2738	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	D	2452	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	C	2738	ARG	NE-CZ-NH2	5.43	124.08	119.20
1	B	1743	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	D	1743	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	B	2736	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	2738	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	D	1249	PRO	N-CA-CB	5.41	106.22	103.19
1	C	4925	ILE	N-CA-C	5.40	115.61	110.53
1	D	3053	ARG	CD-NE-CZ	5.40	131.96	124.40
1	A	1249	PRO	N-CA-CB	5.39	106.21	103.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1249	PRO	N-CA-CB	5.39	106.21	103.19
1	A	326	ALA	N-CA-C	5.38	113.06	108.22
1	A	1201	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	D	2629	ASP	CA-C-N	5.37	123.63	120.24
1	D	2629	ASP	C-N-CA	5.37	123.63	120.24
1	B	2104	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	C	3272	ILE	CB-CA-C	5.37	116.17	110.91
1	D	1201	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	C	1025	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	A	4925	ILE	N-CA-C	5.36	115.57	110.53
1	B	1025	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	C	3987	ASP	CA-CB-CG	-5.35	107.25	112.60
1	B	4925	ILE	N-CA-C	5.35	115.56	110.53
1	B	3093	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	C	261	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	A	2104	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	A	1025	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	B	2109	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	1017	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	261	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	D	2333	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	3687	GLU	N-CA-C	5.32	119.36	112.86
1	A	1743	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	3498	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	C	3883	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	5003	HIS	CA-CB-CG	5.32	119.12	113.80
1	C	243	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	B	3883	ASP	CA-CB-CG	5.30	117.90	112.60
1	D	3498	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	2001	PRO	N-CA-C	5.30	115.56	110.47
1	B	3498	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	C	3498	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	2736	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	243	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	3093	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	3560	GLN	CA-C-N	5.29	126.20	120.44
1	B	3560	GLN	C-N-CA	5.29	126.20	120.44
1	C	326	ALA	N-CA-C	5.29	112.98	108.22
1	C	3577	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	3577	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	3883	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	3093	ARG	NE-CZ-NH2	5.27	123.95	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2000	SER	CA-C-N	5.27	123.51	119.66
1	A	2000	SER	C-N-CA	5.27	123.51	119.66
1	B	3687	GLU	N-CA-C	5.27	119.55	113.38
1	D	1022	VAL	CB-CA-C	5.27	114.50	109.33
1	C	5003	HIS	CA-CB-CG	5.27	119.07	113.80
1	A	3687	GLU	N-CA-C	5.26	119.54	113.38
1	C	824	GLU	N-CA-C	5.26	114.36	108.25
1	D	111	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	B	3577	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	C	4750	ILE	N-CA-C	5.26	115.98	110.62
1	D	1478	ASP	CA-CB-CG	5.26	117.86	112.60
2	G	88	PRO	N-CA-CB	5.26	105.86	102.92
1	A	3560	GLN	CA-C-N	5.25	126.17	120.44
1	A	3560	GLN	C-N-CA	5.25	126.17	120.44
1	C	2629	ASP	CA-C-N	5.25	123.55	120.24
1	C	2629	ASP	C-N-CA	5.25	123.55	120.24
1	B	3987	ASP	CA-CB-CG	-5.25	107.35	112.60
1	B	1249	PRO	N-CA-CB	5.25	106.13	103.19
1	C	111	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	B	4750	ILE	N-CA-C	5.24	115.96	110.62
1	A	243	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	B	111	HIS	CB-CG-CD2	-5.22	124.41	131.20
1	C	242	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	C	1743	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	D	824	GLU	N-CA-C	5.22	114.31	108.25
1	D	3560	GLN	CA-C-N	5.21	126.12	120.44
1	D	3560	GLN	C-N-CA	5.21	126.12	120.44
1	B	326	ALA	N-CA-C	5.21	112.91	108.22
1	C	1201	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	B	824	GLU	N-CA-C	5.21	114.29	108.25
1	A	824	GLU	N-CA-C	5.20	114.29	108.25
1	A	1658	ASP	CA-CB-CG	5.20	117.80	112.60
1	D	3984	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	D	3883	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	1658	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	2037	ASP	CA-CB-CG	5.20	117.80	112.60
1	D	4750	ILE	N-CA-C	5.20	115.92	110.62
1	A	4750	ILE	N-CA-C	5.19	115.92	110.62
1	C	3560	GLN	CA-C-N	5.19	126.10	120.44
1	C	3560	GLN	C-N-CA	5.19	126.10	120.44
1	B	2037	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	1201	HIS	CB-CG-CD2	-5.18	124.47	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	125	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	A	1275	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	D	1719	HIS	N-CA-C	5.18	119.81	112.93
1	A	1752	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	B	1275	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	D	3637	ARG	N-CA-C	5.17	118.64	111.71
1	A	2037	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	2629	ASP	CA-C-N	5.17	123.50	120.24
1	A	2629	ASP	C-N-CA	5.17	123.50	120.24
1	B	4760	PRO	N-CA-CB	5.17	105.91	103.22
1	D	5003	HIS	CA-CB-CG	5.17	118.97	113.80
1	C	3687	GLU	N-CA-C	5.17	119.42	113.38
1	B	1478	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	111	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	D	3093	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	B	3152	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	3987	ASP	CA-CB-CG	-5.15	107.45	112.60
1	C	1719	HIS	N-CA-C	5.15	119.78	112.93
1	D	257	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	A	2109	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	1658	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	243	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	D	242	ARG	NE-CZ-NH2	5.14	123.83	119.20
2	E	88	PRO	N-CA-CB	5.14	105.80	102.92
1	A	3152	PHE	CA-CB-CG	5.13	118.94	113.80
1	C	125	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	D	3699	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	C	1478	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	4760	PRO	N-CA-CB	5.12	105.89	103.22
1	D	2000	SER	CA-C-N	5.12	123.40	119.66
1	D	2000	SER	C-N-CA	5.12	123.40	119.66
1	B	3699	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	D	1658	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	3895	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	D	1275	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A	3699	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	B	1813	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	5003	HIS	CA-CB-CG	5.11	118.91	113.80
1	C	3889	GLN	OE1-CD-NE2	-5.11	117.50	122.60
1	A	1719	HIS	N-CA-C	5.10	119.72	112.93
1	B	1719	HIS	N-CA-C	5.10	119.72	112.93
1	D	1752	ARG	NE-CZ-NH2	5.10	123.79	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1087	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	C	3699	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	D	308	HIS	CB-CG-CD2	-5.10	124.58	131.20
1	A	3897	ASN	N-CA-C	5.09	116.83	111.28
1	A	242	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	1478	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	3970	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	C	1275	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	D	3970	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	B	3895	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	C	2000	SER	CA-C-N	5.08	123.37	119.66
1	C	2000	SER	C-N-CA	5.08	123.37	119.66
1	C	1752	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	C	1808	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	B	2000	SER	CA-C-N	5.08	123.37	119.66
1	B	2000	SER	C-N-CA	5.08	123.37	119.66
1	B	3889	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	B	1087	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	A	1813	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	C	3970	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	D	4760	PRO	N-CA-CB	5.07	105.86	103.22
1	B	242	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	D	3895	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	A	1434	TYR	N-CA-C	5.07	117.09	109.23
1	A	3921	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	257	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	A	2676	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	C	3053	ARG	CD-NE-CZ	5.06	131.49	124.40
1	C	3637	ARG	N-CA-C	5.06	118.49	111.71
1	D	1813	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	C	2109	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	3152	PHE	CA-CB-CG	5.06	118.86	113.80
1	D	2109	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	3895	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	B	257	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	C	3366	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	D	3152	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	257	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	D	1087	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	B	3813	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	B	125	ARG	NE-CZ-NH2	5.04	123.74	119.20
2	F	88	PRO	N-CA-CB	5.04	105.74	102.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2037	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	1828	ASP	N-CA-C	5.03	116.80	109.30
1	B	368	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	B	1752	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	D	3889	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	C	228	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	386	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	918	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	D	1964	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	B	308	HIS	CB-CG-CD2	-5.01	124.68	131.20
1	B	1808	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A	3970	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	C	3984	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	C	918	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1049	TYR	Sidechain
1	A	157	ARG	Sidechain
1	A	2794	TYR	Sidechain
1	A	3436	ARG	Sidechain
1	A	3762	ARG	Sidechain
1	A	3769	ARG	Sidechain
1	A	4715	TYR	Sidechain
1	A	4913	ARG	Sidechain
1	B	1049	TYR	Sidechain
1	B	157	ARG	Sidechain
1	B	3762	ARG	Sidechain
1	B	3769	ARG	Sidechain
1	B	4715	TYR	Sidechain
1	B	4913	ARG	Sidechain
1	B	629	ARG	Sidechain
1	C	1049	TYR	Sidechain
1	C	3436	ARG	Sidechain
1	C	3762	ARG	Sidechain
1	C	3769	ARG	Sidechain
1	C	4715	TYR	Sidechain
1	C	4913	ARG	Sidechain
1	C	629	ARG	Sidechain
1	D	1049	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	157	ARG	Sidechain
1	D	3436	ARG	Sidechain
1	D	3769	ARG	Sidechain
1	D	4715	TYR	Sidechain
1	D	4913	ARG	Sidechain

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	35088	34734	34715	8	0
1	B	35088	34734	34715	9	0
1	C	35088	34734	34715	8	0
1	D	35088	34734	34715	12	0
2	E	832	829	831	0	0
2	F	832	829	831	0	0
2	G	832	829	831	0	0
2	H	832	829	831	0	0
3	A	104	164	164	0	0
3	B	104	164	164	0	0
3	C	104	164	164	0	0
3	D	104	164	164	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	144100	142908	142840	37	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 0.

All (37) 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:A:3966:THR:CG2	1:A:3970:GLN:HE21	2.17	0.57
1:C:3966:THR:CG2	1:C:3970:GLN:HE21	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3966:THR:CG2	1:D:3970:GLN:HE21	2.18	0.57
1:B:3966:THR:CG2	1:B:3970:GLN:HE21	2.19	0.55
1:A:3765:TYR:CD1	1:A:3765:TYR:C	2.90	0.50
1:D:3999:MET:HA	1:D:3999:MET:HE2	1.94	0.49
1:B:3999:MET:HA	1:B:3999:MET:HE2	1.96	0.47
1:D:3762:ARG:O	1:D:3766:GLN:HG3	2.15	0.47
1:B:3762:ARG:O	1:B:3766:GLN:HG3	2.15	0.47
1:C:3999:MET:HE2	1:C:3999:MET:HA	1.96	0.47
1:C:3762:ARG:O	1:C:3766:GLN:HG3	2.16	0.46
1:A:3762:ARG:O	1:A:3766:GLN:HG3	2.16	0.45
1:A:3999:MET:HA	1:A:3999:MET:HE2	1.98	0.45
1:C:4679:ARG:HH21	1:C:4679:ARG:HG2	1.83	0.43
1:B:299:LEU:HD23	1:B:300:VAL:N	2.34	0.43
1:B:2170:MET:HG3	1:B:2214:VAL:HG12	2.00	0.43
1:A:3924:LEU:HD11	1:A:3984:ARG:NH2	2.33	0.42
1:C:2170:MET:HG3	1:C:2214:VAL:HG12	2.01	0.42
1:D:24:CYS:SG	1:D:25:SER:N	2.92	0.42
1:D:1773:PRO:HA	1:D:2153:MET:HE1	2.02	0.42
1:C:3765:TYR:O	1:C:3765:TYR:CG	2.73	0.42
1:B:4679:ARG:HG2	1:B:4679:ARG:HH21	1.85	0.42
1:C:299:LEU:HD23	1:C:300:VAL:N	2.35	0.42
1:D:4077:PHE:CD1	1:D:4077:PHE:C	2.98	0.41
1:A:24:CYS:SG	1:A:25:SER:N	2.93	0.41
1:A:299:LEU:HD23	1:A:300:VAL:N	2.35	0.41
1:B:2813:LEU:HD13	1:B:2813:LEU:C	2.45	0.41
1:D:2813:LEU:C	1:D:2813:LEU:HD13	2.45	0.41
1:D:3568:SER:HA	1:D:3571:TRP:CD1	2.56	0.41
1:B:2089:LYS:HA	1:B:2089:LYS:HE2	2.03	0.41
1:D:317:ARG:CG	1:D:317:ARG:HH21	2.34	0.41
1:D:2089:LYS:HA	1:D:2089:LYS:HE2	2.03	0.41
1:D:3765:TYR:O	1:D:3765:TYR:CD2	2.74	0.41
1:D:3765:TYR:O	1:D:3765:TYR:CG	2.72	0.40
1:B:3765:TYR:CD2	1:B:3765:TYR:O	2.75	0.40
1:C:24:CYS:SG	1:C:25:SER:N	2.94	0.40
1:A:4679:ARG:HG2	1:A:4679:ARG:HH21	1.86	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	4376/5037 (87%)	4164 (95%)	199 (4%)	13 (0%)	36	65
1	B	4376/5037 (87%)	4166 (95%)	193 (4%)	17 (0%)	30	60
1	C	4376/5037 (87%)	4162 (95%)	197 (4%)	17 (0%)	30	60
1	D	4376/5037 (87%)	4160 (95%)	199 (4%)	17 (0%)	30	60
2	E	105/108 (97%)	100 (95%)	5 (5%)	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%)	100 (95%)	5 (5%)	0	100	100
All	All	17924/20580 (87%)	17054 (95%)	806 (4%)	64 (0%)	31	60

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3693	LYS
1	D	3693	LYS
1	A	849	THR
1	A	2663	ASN
1	A	3622	LYS
1	B	849	THR
1	B	2663	ASN
1	B	3622	LYS
1	B	3693	LYS
1	C	2663	ASN
1	C	3622	LYS
1	C	3693	LYS
1	C	3867	ASN
1	D	2663	ASN
1	D	3622	LYS
1	D	3867	ASN
1	A	2413	GLU

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Mol	Chain	Res	Type
1	B	2342	ASN
1	C	2342	ASN
1	C	2413	GLU
1	D	2413	GLU
1	B	1050	GLY
1	B	2413	GLU
1	B	2718	SER
1	B	3867	ASN
1	C	1923	GLU
1	C	4694	ASP
1	D	277	GLY
1	D	677	ALA
1	D	2343	GLY
1	D	4072	VAL
1	A	276	TRP
1	A	677	ALA
1	A	1050	GLY
1	B	677	ALA
1	B	1923	GLU
1	B	3613	TYR
1	B	4694	ASP
1	C	677	ALA
1	C	1050	GLY
1	C	4072	VAL
1	C	4155	PRO
1	D	849	THR
1	D	4694	ASP
1	A	361	ALA
1	A	2343	GLY
1	C	849	THR
1	D	1050	GLY
1	D	2594	SER
1	B	361	ALA
1	D	4155	PRO
1	A	371	VAL
1	B	277	GLY
1	C	361	ALA
1	C	371	VAL
1	D	361	ALA
1	A	277	GLY
1	B	371	VAL
1	C	277	GLY

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Mol	Chain	Res	Type
1	C	3866	ILE
1	D	371	VAL
1	A	4155	PRO
1	B	3690	VAL
1	D	3690	VAL

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%)	3780 (99%)	47 (1%)	63	72
1	B	3827/4276 (90%)	3777 (99%)	50 (1%)	61	71
1	C	3827/4276 (90%)	3774 (99%)	53 (1%)	59	70
1	D	3827/4276 (90%)	3767 (98%)	60 (2%)	55	68
2	E	89/90 (99%)	88 (99%)	1 (1%)	65	73
2	F	89/90 (99%)	88 (99%)	1 (1%)	65	73
2	G	89/90 (99%)	88 (99%)	1 (1%)	65	73
2	H	89/90 (99%)	88 (99%)	1 (1%)	65	73
All	All	15664/17464 (90%)	15450 (99%)	214 (1%)	57	70

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LYS
1	A	161	GLU
1	A	168	ASP
1	A	359	TYR
1	A	385	ASP
1	A	974	HIS
1	A	1021	LEU
1	A	1041	GLN
1	A	1251	GLU
1	A	1281	ASN

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Mol	Chain	Res	Type
1	A	1435	TYR
1	A	1480	GLN
1	A	1552	VAL
1	A	1690	ASP
1	A	1769	THR
1	A	1990	GLU
1	A	2026	ASP
1	A	2149	VAL
1	A	2157	GLU
1	A	2275	VAL
1	A	2307	LEU
1	A	2358	ILE
1	A	2663	ASN
1	A	2754	PHE
1	A	3053	ARG
1	A	3219	TYR
1	A	3258	GLU
1	A	3272	ILE
1	A	3308	THR
1	A	3414	ARG
1	A	3456	GLN
1	A	3638	MET
1	A	3712	GLU
1	A	3736	GLU
1	A	3768	SER
1	A	3899	PHE
1	A	3921	ASP
1	A	3924	LEU
1	A	3967	GLU
1	A	4018	ASP
1	A	4095	LYS
1	A	4118	ASP
1	A	4577	LEU
1	A	4582	VAL
1	A	4668	LEU
1	A	4749	GLU
1	A	5033	GLU
1	B	155	LYS
1	B	161	GLU
1	B	168	ASP
1	B	359	TYR
1	B	953	THR

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Mol	Chain	Res	Type
1	B	974	HIS
1	B	1021	LEU
1	B	1041	GLN
1	B	1251	GLU
1	B	1281	ASN
1	B	1435	TYR
1	B	1480	GLN
1	B	1552	VAL
1	B	1690	ASP
1	B	1769	THR
1	B	1990	GLU
1	B	2026	ASP
1	B	2149	VAL
1	B	2157	GLU
1	B	2275	VAL
1	B	2307	LEU
1	B	2358	ILE
1	B	2663	ASN
1	B	2667	THR
1	B	2754	PHE
1	B	2884	ASN
1	B	3037	GLU
1	B	3219	TYR
1	B	3258	GLU
1	B	3272	ILE
1	B	3308	THR
1	B	3456	GLN
1	B	3638	MET
1	B	3712	GLU
1	B	3736	GLU
1	B	3763	LEU
1	B	3768	SER
1	B	3899	PHE
1	B	3921	ASP
1	B	3924	LEU
1	B	3967	GLU
1	B	4018	ASP
1	B	4034	ASN
1	B	4095	LYS
1	B	4118	ASP
1	B	4577	LEU
1	B	4582	VAL

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Mol	Chain	Res	Type
1	B	4668	LEU
1	B	4749	GLU
1	B	5033	GLU
1	C	31	GLU
1	C	155	LYS
1	C	161	GLU
1	C	167	ASP
1	C	168	ASP
1	C	199	LEU
1	C	359	TYR
1	C	953	THR
1	C	974	HIS
1	C	1021	LEU
1	C	1041	GLN
1	C	1251	GLU
1	C	1281	ASN
1	C	1435	TYR
1	C	1480	GLN
1	C	1552	VAL
1	C	1690	ASP
1	C	1769	THR
1	C	1990	GLU
1	C	2026	ASP
1	C	2149	VAL
1	C	2157	GLU
1	C	2275	VAL
1	C	2307	LEU
1	C	2358	ILE
1	C	2620	GLN
1	C	2663	ASN
1	C	2754	PHE
1	C	3037	GLU
1	C	3219	TYR
1	C	3258	GLU
1	C	3308	THR
1	C	3414	ARG
1	C	3456	GLN
1	C	3638	MET
1	C	3712	GLU
1	C	3736	GLU
1	C	3763	LEU
1	C	3768	SER

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Mol	Chain	Res	Type
1	C	3899	PHE
1	C	3921	ASP
1	C	3924	LEU
1	C	3967	GLU
1	C	4018	ASP
1	C	4095	LYS
1	C	4118	ASP
1	C	4212	GLU
1	C	4577	LEU
1	C	4582	VAL
1	C	4668	LEU
1	C	4679	ARG
1	C	4749	GLU
1	C	5033	GLU
1	D	62	LEU
1	D	155	LYS
1	D	161	GLU
1	D	168	ASP
1	D	172	VAL
1	D	245	VAL
1	D	317	ARG
1	D	323	LEU
1	D	359	TYR
1	D	380	GLN
1	D	576	ASN
1	D	870	ILE
1	D	950	LEU
1	D	1021	LEU
1	D	1251	GLU
1	D	1281	ASN
1	D	1435	TYR
1	D	1480	GLN
1	D	1690	ASP
1	D	1769	THR
1	D	1990	GLU
1	D	2026	ASP
1	D	2149	VAL
1	D	2153	MET
1	D	2156	LEU
1	D	2162	ILE
1	D	2275	VAL
1	D	2307	LEU

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Mol	Chain	Res	Type
1	D	2356	LEU
1	D	2358	ILE
1	D	2620	GLN
1	D	2663	ASN
1	D	2754	PHE
1	D	2884	ASN
1	D	3037	GLU
1	D	3219	TYR
1	D	3258	GLU
1	D	3272	ILE
1	D	3308	THR
1	D	3346	VAL
1	D	3456	GLN
1	D	3638	MET
1	D	3712	GLU
1	D	3735	LEU
1	D	3736	GLU
1	D	3763	LEU
1	D	3768	SER
1	D	3899	PHE
1	D	3921	ASP
1	D	3967	GLU
1	D	4018	ASP
1	D	4034	ASN
1	D	4079	ASP
1	D	4095	LYS
1	D	4118	ASP
1	D	4577	LEU
1	D	4582	VAL
1	D	4668	LEU
1	D	4749	GLU
1	D	5033	GLU
2	E	21	THR
2	F	21	THR
2	G	21	THR
2	H	21	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (179) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	151	HIS

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Mol	Chain	Res	Type
1	A	190	GLN
1	A	218	HIS
1	A	297	GLN
1	A	383	HIS
1	A	579	GLN
1	A	581	ASN
1	A	705	ASN
1	A	963	ASN
1	A	1011	GLN
1	A	1201	HIS
1	A	1220	GLN
1	A	1460	HIS
1	A	1482	ASN
1	A	1571	ASN
1	A	1663	HIS
1	A	1688	HIS
1	A	1928	GLN
1	A	1949	GLN
1	A	1973	GLN
1	A	2005	GLN
1	A	2095	GLN
1	A	2100	HIS
1	A	2204	HIS
1	A	2284	ASN
1	A	2763	HIS
1	A	2773	ASN
1	A	2931	GLN
1	A	2993	GLN
1	A	3069	HIS
1	A	3109	ASN
1	A	3127	GLN
1	A	3268	HIS
1	A	3418	ASN
1	A	3621	HIS
1	A	3667	HIS
1	A	3860	ASN
1	A	3970	GLN
1	A	4009	GLN
1	A	4034	ASN
1	A	4753	HIS
1	A	4754	ASN
1	B	57	ASN

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Mol	Chain	Res	Type
1	B	151	HIS
1	B	218	HIS
1	B	383	HIS
1	B	489	ASN
1	B	579	GLN
1	B	581	ASN
1	B	681	HIS
1	B	705	ASN
1	B	963	ASN
1	B	974	HIS
1	B	1011	GLN
1	B	1201	HIS
1	B	1220	GLN
1	B	1460	HIS
1	B	1571	ASN
1	B	1660	GLN
1	B	1663	HIS
1	B	1679	ASN
1	B	1928	GLN
1	B	1949	GLN
1	B	1973	GLN
1	B	2005	GLN
1	B	2095	GLN
1	B	2100	HIS
1	B	2204	HIS
1	B	2487	GLN
1	B	2763	HIS
1	B	2773	ASN
1	B	2931	GLN
1	B	2976	HIS
1	B	2993	GLN
1	B	3069	HIS
1	B	3109	ASN
1	B	3128	ASN
1	B	3162	GLN
1	B	3268	HIS
1	B	3418	ASN
1	B	3621	HIS
1	B	3647	HIS
1	B	3927	GLN
1	B	3970	GLN
1	B	4009	GLN

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Mol	Chain	Res	Type
1	B	4753	HIS
1	B	4754	ASN
1	C	57	ASN
1	C	156	GLN
1	C	218	HIS
1	C	383	HIS
1	C	489	ASN
1	C	536	ASN
1	C	579	GLN
1	C	581	ASN
1	C	705	ASN
1	C	963	ASN
1	C	974	HIS
1	C	1011	GLN
1	C	1201	HIS
1	C	1220	GLN
1	C	1460	HIS
1	C	1571	ASN
1	C	1660	GLN
1	C	1663	HIS
1	C	1679	ASN
1	C	1928	GLN
1	C	1973	GLN
1	C	2005	GLN
1	C	2095	GLN
1	C	2100	HIS
1	C	2204	HIS
1	C	2487	GLN
1	C	2763	HIS
1	C	2773	ASN
1	C	2931	GLN
1	C	2993	GLN
1	C	3069	HIS
1	C	3109	ASN
1	C	3128	ASN
1	C	3268	HIS
1	C	3418	ASN
1	C	3647	HIS
1	C	3667	HIS
1	C	3860	ASN
1	C	3970	GLN
1	C	4034	ASN

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Mol	Chain	Res	Type
1	C	4753	HIS
1	C	4754	ASN
1	D	57	ASN
1	D	203	ASN
1	D	218	HIS
1	D	297	GLN
1	D	349	GLN
1	D	383	HIS
1	D	475	GLN
1	D	489	ASN
1	D	533	ASN
1	D	579	GLN
1	D	581	ASN
1	D	593	HIS
1	D	681	HIS
1	D	705	ASN
1	D	765	GLN
1	D	963	ASN
1	D	1201	HIS
1	D	1220	GLN
1	D	1296	GLN
1	D	1299	GLN
1	D	1460	HIS
1	D	1545	ASN
1	D	1563	GLN
1	D	1663	HIS
1	D	1679	ASN
1	D	1928	GLN
1	D	1949	GLN
1	D	1973	GLN
1	D	2005	GLN
1	D	2095	GLN
1	D	2100	HIS
1	D	2204	HIS
1	D	2773	ASN
1	D	2774	ASN
1	D	2993	GLN
1	D	3069	HIS
1	D	3109	ASN
1	D	3162	GLN
1	D	3211	ASN
1	D	3268	HIS

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Mol	Chain	Res	Type
1	D	3418	ASN
1	D	3605	HIS
1	D	3647	HIS
1	D	3667	HIS
1	D	3897	ASN
1	D	3927	GLN
1	D	3970	GLN
1	D	4753	HIS
1	D	4754	ASN

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 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	POV	C	5102	-	51,51,51	0.71	0	57,59,59	0.45	0
3	POV	A	5102	-	51,51,51	0.72	0	57,59,59	0.47	0
3	POV	D	5101	-	51,51,51	0.71	1 (1%)	57,59,59	0.76	2 (3%)
3	POV	B	5101	-	51,51,51	0.69	0	57,59,59	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	C	5101	-	51,51,51	0.71	1 (1%)	57,59,59	0.74	2 (3%)
3	POV	B	5102	-	51,51,51	0.73	1 (1%)	57,59,59	0.79	2 (3%)
3	POV	D	5102	-	51,51,51	0.73	0	57,59,59	0.47	0
3	POV	A	5101	-	51,51,51	0.74	1 (1%)	57,59,59	0.76	2 (3%)

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	POV	C	5102	-	-	5/55/55/55	-
3	POV	A	5102	-	-	8/55/55/55	-
3	POV	D	5101	-	-	17/55/55/55	-
3	POV	B	5101	-	-	11/55/55/55	-
3	POV	C	5101	-	-	14/55/55/55	-
3	POV	B	5102	-	-	12/55/55/55	-
3	POV	D	5102	-	-	7/55/55/55	-
3	POV	A	5101	-	-	17/55/55/55	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5101	POV	C3-C2	2.21	1.57	1.50
3	B	5102	POV	C3-C2	2.18	1.57	1.50
3	C	5101	POV	C3-C2	2.17	1.57	1.50
3	D	5101	POV	C3-C2	2.15	1.57	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5102	POV	C2-O21-C21	4.17	128.05	117.79
3	A	5101	POV	C2-O21-C21	3.97	127.56	117.79
3	D	5101	POV	C2-O21-C21	3.93	127.46	117.79
3	C	5101	POV	C2-O21-C21	3.73	126.98	117.79
3	A	5101	POV	O21-C21-C22	2.40	116.68	111.50
3	D	5101	POV	O21-C21-C22	2.38	116.64	111.50
3	B	5102	POV	O21-C21-C22	2.36	116.59	111.50
3	C	5101	POV	O21-C21-C22	2.35	116.56	111.50

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5101	POV	C22-C21-O21-C2
3	A	5101	POV	O22-C21-O21-C2
3	B	5101	POV	C12-C11-O12-P
3	B	5102	POV	C22-C21-O21-C2
3	B	5102	POV	O22-C21-O21-C2
3	C	5101	POV	C22-C21-O21-C2
3	C	5101	POV	O22-C21-O21-C2
3	C	5102	POV	C12-C11-O12-P
3	D	5101	POV	C22-C21-O21-C2
3	D	5101	POV	O22-C21-O21-C2
3	D	5102	POV	C12-C11-O12-P
3	B	5101	POV	C11-O12-P-O11
3	D	5102	POV	C11-O12-P-O11
3	A	5102	POV	C21-C22-C23-C24
3	A	5101	POV	C311-C312-C313-C314
3	C	5101	POV	C311-C312-C313-C314
3	B	5102	POV	C26-C27-C28-C29
3	C	5102	POV	C21-C22-C23-C24
3	D	5101	POV	C311-C310-C39-C38
3	A	5101	POV	C1-C2-C3-O31
3	C	5101	POV	C1-C2-C3-O31
3	D	5101	POV	C1-C2-C3-O31
3	A	5101	POV	C25-C26-C27-C28
3	A	5101	POV	C31-C32-C33-C34
3	A	5102	POV	C29-C210-C211-C212
3	D	5102	POV	C311-C310-C39-C38
3	A	5101	POV	C26-C27-C28-C29
3	B	5102	POV	C25-C26-C27-C28
3	D	5101	POV	C25-C26-C27-C28
3	B	5101	POV	C32-C33-C34-C35
3	B	5102	POV	C2-C1-O11-P
3	B	5102	POV	C1-C2-C3-O31
3	B	5102	POV	O21-C2-C3-O31
3	A	5102	POV	C11-O12-P-O11
3	C	5102	POV	C11-O12-P-O11
3	D	5101	POV	C2-C1-O11-P
3	B	5101	POV	C11-O12-P-O13
3	D	5102	POV	C11-O12-P-O13
3	A	5102	POV	C12-C11-O12-P
3	B	5102	POV	C12-C11-O12-P

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Mol	Chain	Res	Type	Atoms
3	A	5101	POV	O12-C11-C12-N
3	B	5102	POV	O12-C11-C12-N
3	C	5101	POV	O12-C11-C12-N
3	D	5101	POV	O12-C11-C12-N
3	A	5101	POV	O21-C2-C3-O31
3	C	5101	POV	O21-C2-C3-O31
3	D	5101	POV	O21-C2-C3-O31
3	C	5101	POV	C25-C26-C27-C28
3	A	5102	POV	C214-C215-C216-C217
3	A	5101	POV	C2-C1-O11-P
3	B	5102	POV	C311-C310-C39-C38
3	A	5102	POV	C27-C28-C29-C210
3	C	5101	POV	C26-C27-C28-C29
3	B	5101	POV	C22-C23-C24-C25
3	C	5101	POV	C37-C38-C39-C310
3	A	5101	POV	C37-C38-C39-C310
3	A	5101	POV	C11-O12-P-O11
3	B	5102	POV	C11-O12-P-O11
3	C	5101	POV	C11-O12-P-O11
3	D	5101	POV	C11-O12-P-O11
3	A	5102	POV	C211-C212-C213-C214
3	B	5101	POV	C29-C210-C211-C212
3	C	5102	POV	C27-C28-C29-C210
3	A	5101	POV	C29-C210-C211-C212
3	B	5101	POV	C311-C312-C313-C314
3	B	5102	POV	C29-C210-C211-C212
3	A	5102	POV	C24-C25-C26-C27
3	C	5102	POV	C311-C312-C313-C314
3	D	5102	POV	C3-C2-O21-C21
3	D	5101	POV	C26-C27-C28-C29
3	B	5101	POV	C311-C310-C39-C38
3	B	5101	POV	C24-C25-C26-C27
3	D	5101	POV	C37-C38-C39-C310
3	A	5101	POV	C311-C310-C39-C38
3	D	5101	POV	C33-C34-C35-C36
3	D	5101	POV	O31-C31-C32-C33
3	D	5102	POV	C1-C2-O21-C21
3	C	5101	POV	O11-C1-C2-O21
3	C	5101	POV	C2-C1-O11-P
3	D	5102	POV	C22-C23-C24-C25
3	B	5101	POV	C212-C213-C214-C215
3	D	5101	POV	O32-C31-C32-C33

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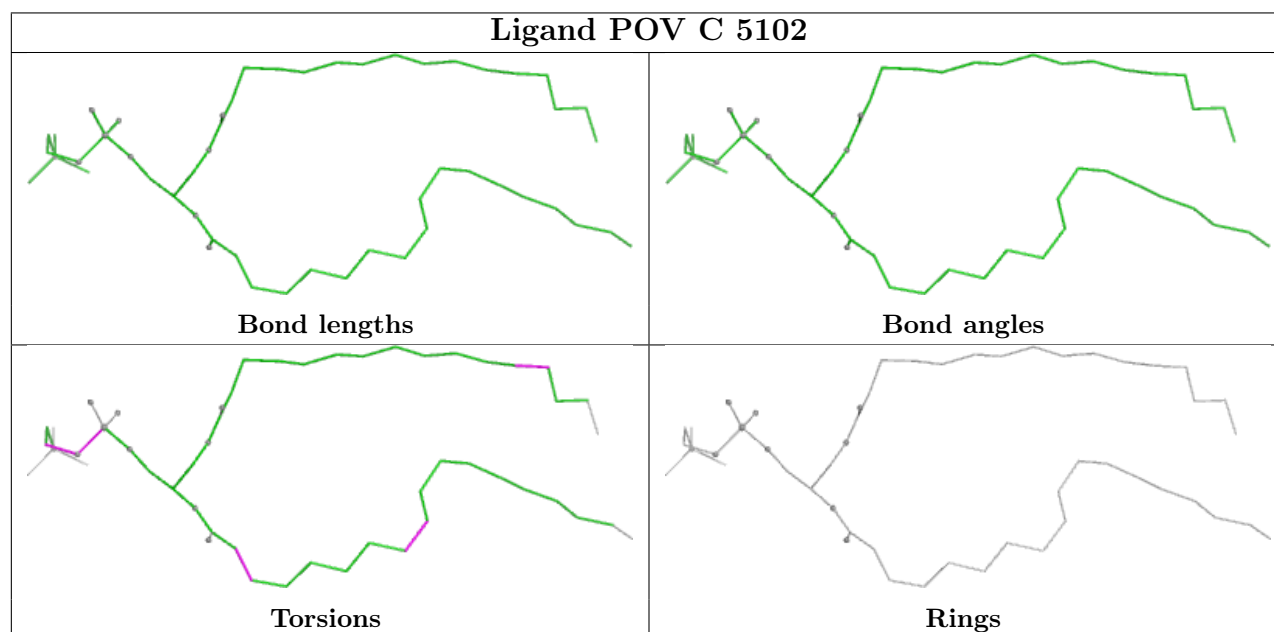
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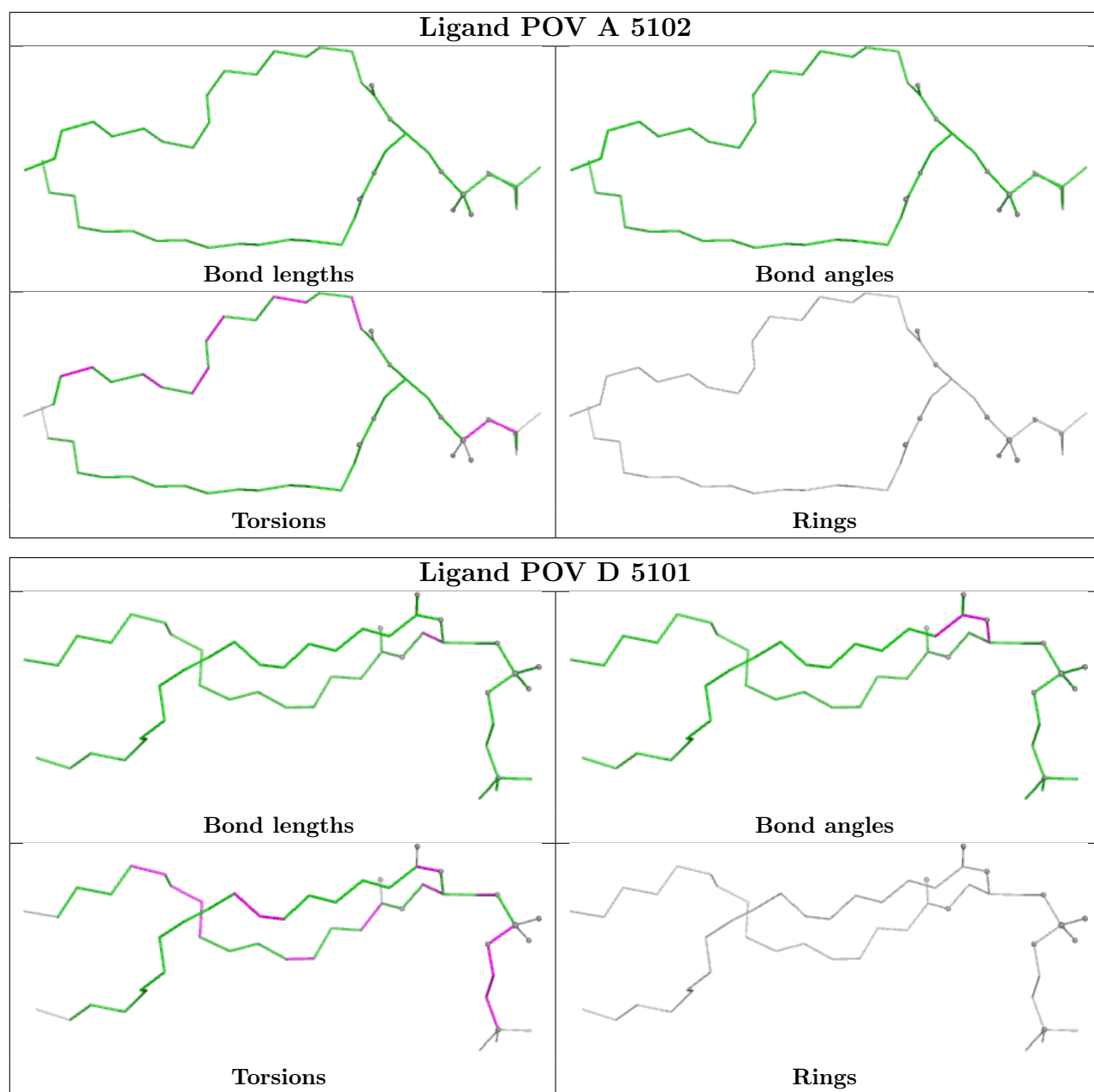
Mol	Chain	Res	Type	Atoms
3	C	5101	POV	C29-C210-C211-C212
3	C	5101	POV	C311-C310-C39-C38
3	D	5101	POV	C11-C12-N-C13
3	D	5101	POV	C310-C311-C312-C313
3	A	5101	POV	C12-C11-O12-P
3	B	5101	POV	C1-C2-O21-C21
3	D	5101	POV	C12-C11-O12-P
3	A	5101	POV	O11-C1-C2-O21
3	A	5101	POV	C11-C12-N-C13

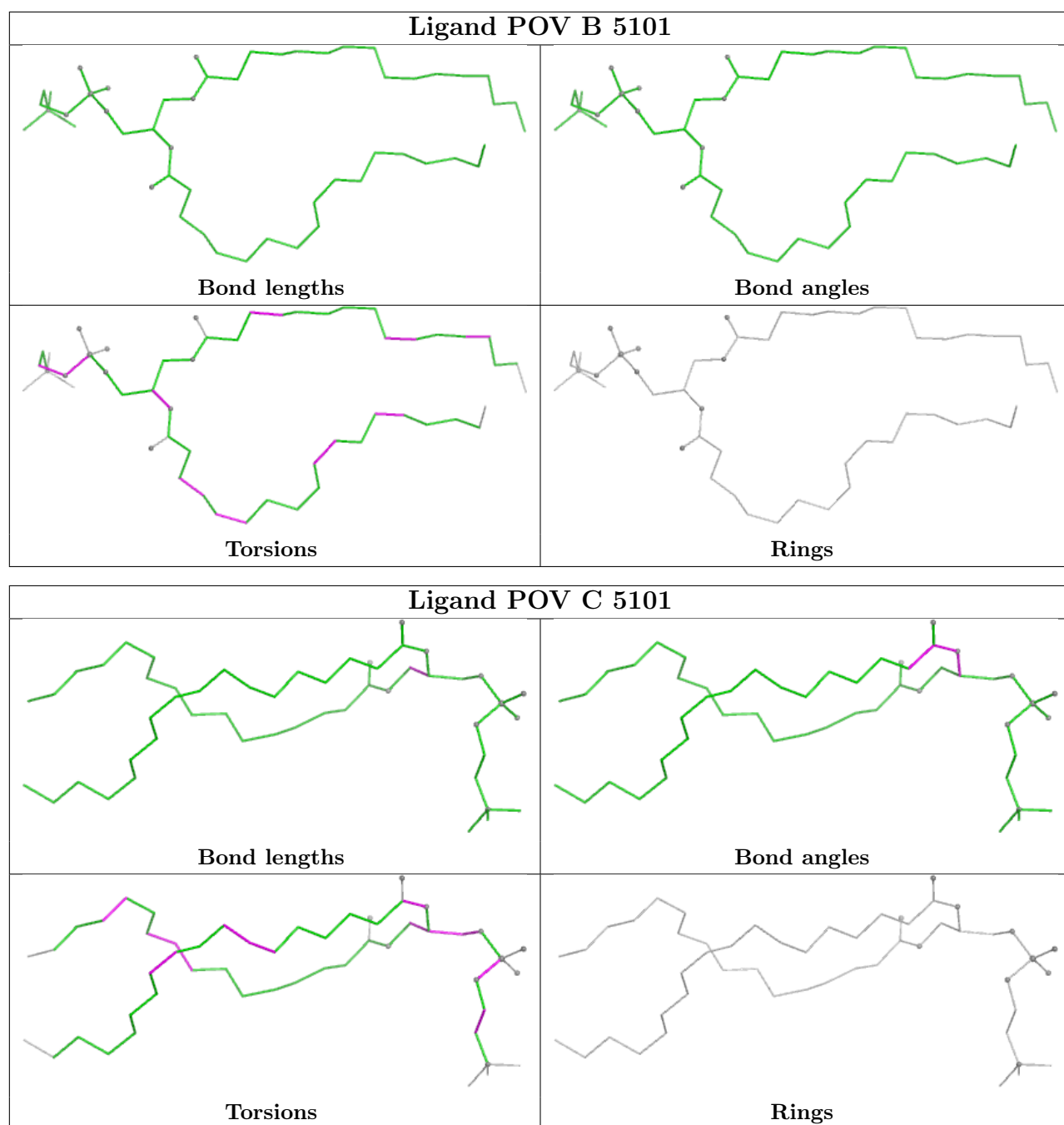
There are no ring outliers.

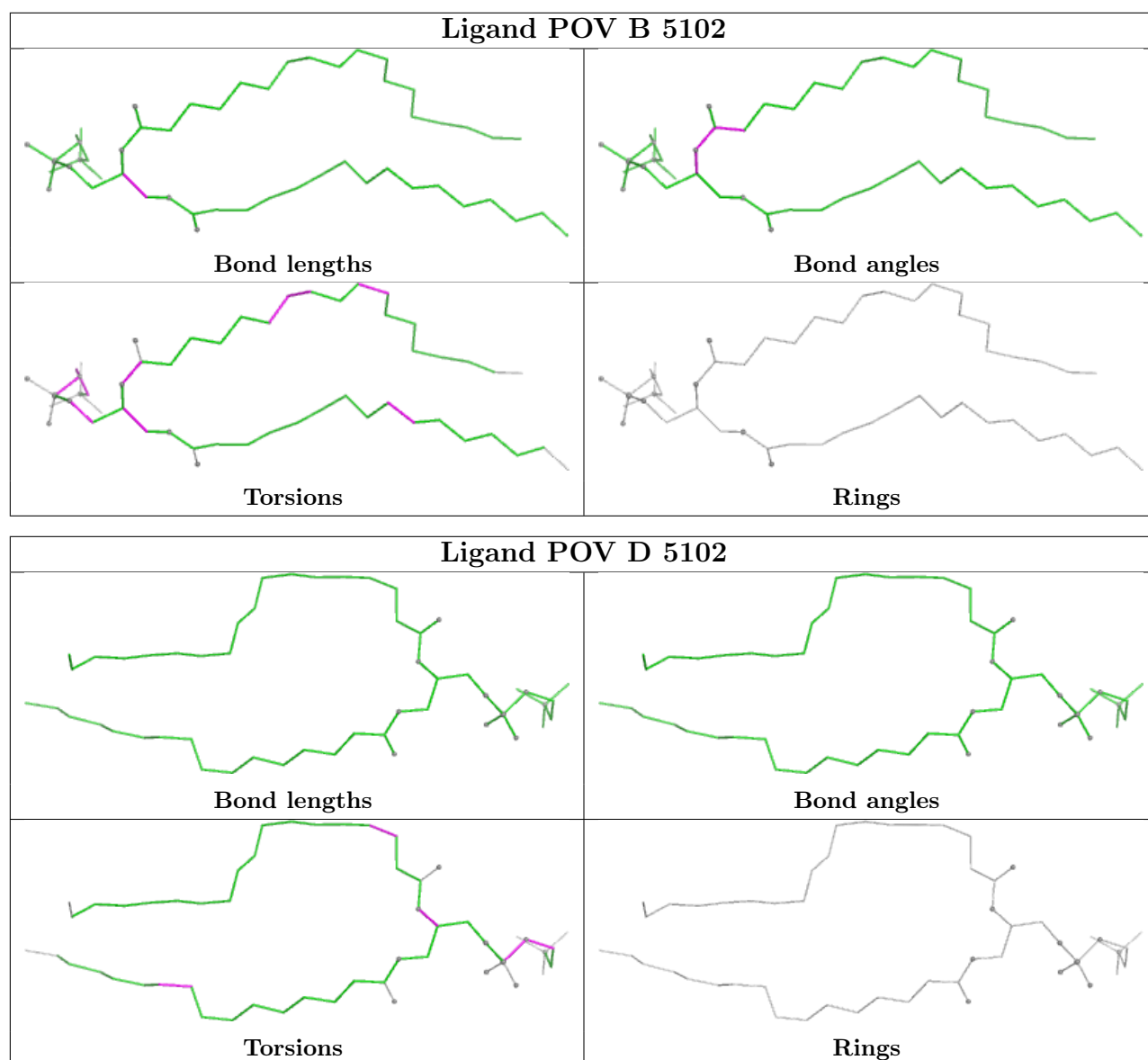
No monomer is involved in short contacts.

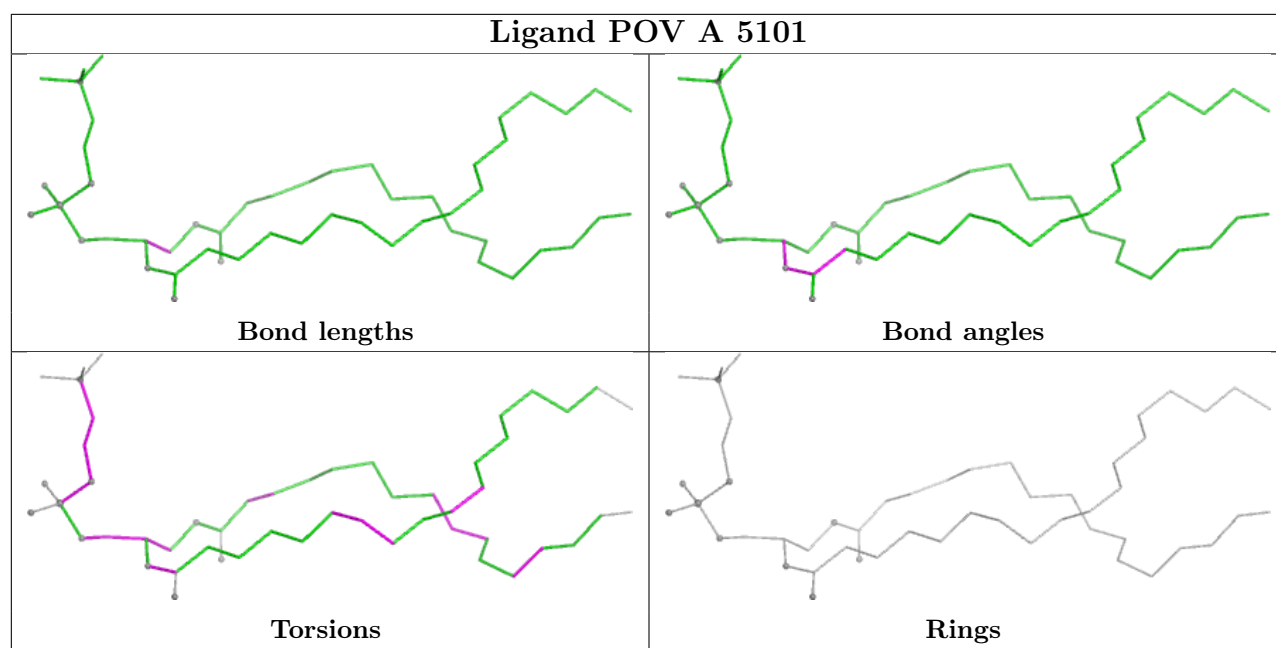
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

There are no chain breaks in this entry.

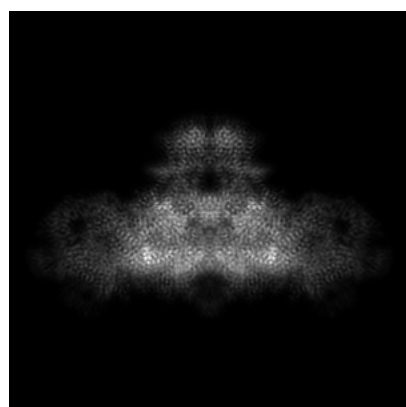
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54590. These allow visual inspection of the internal detail of the map and identification of artifacts.

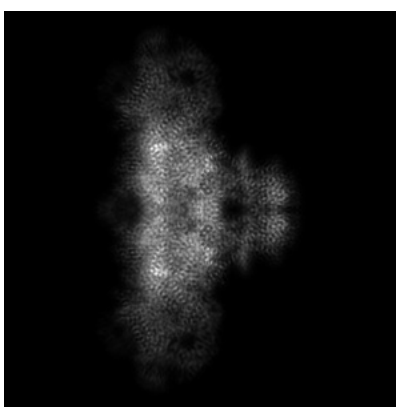
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

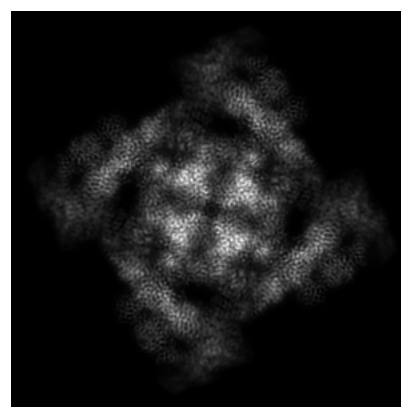
6.1.1 Primary map



X



Y

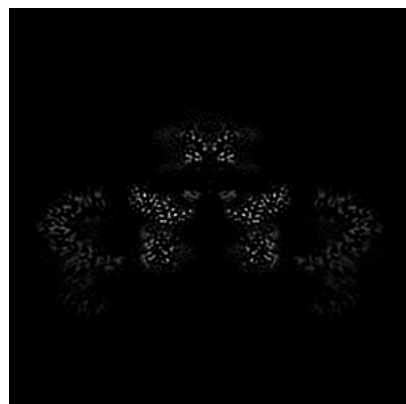


Z

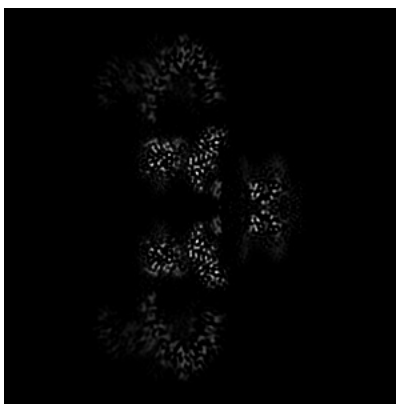
The images above show the map projected in three orthogonal directions.

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: 182



Y Index: 120

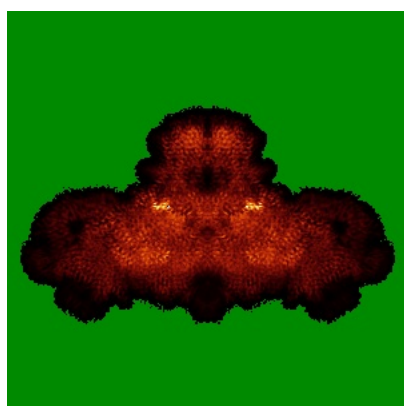


Z Index: 153

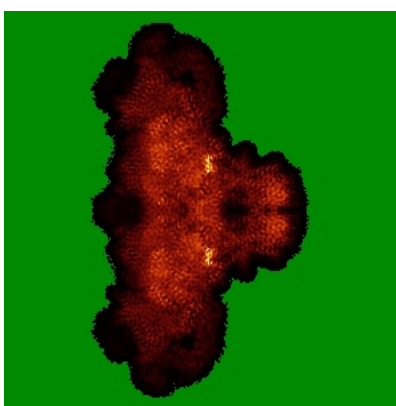
The images above show the largest variance slices of the map in three orthogonal directions.

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

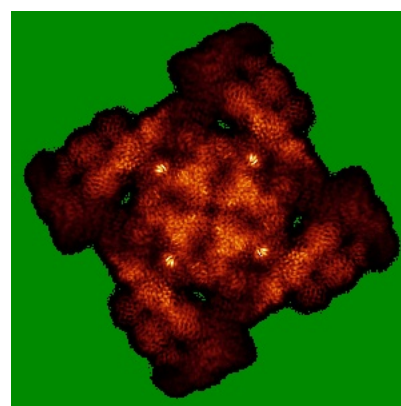
6.4.1 Primary map



X



Y

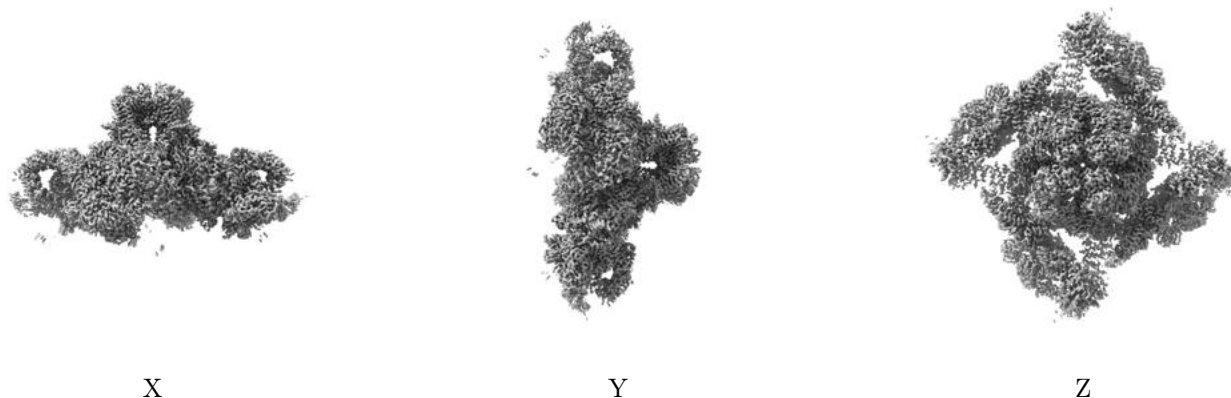


Z

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

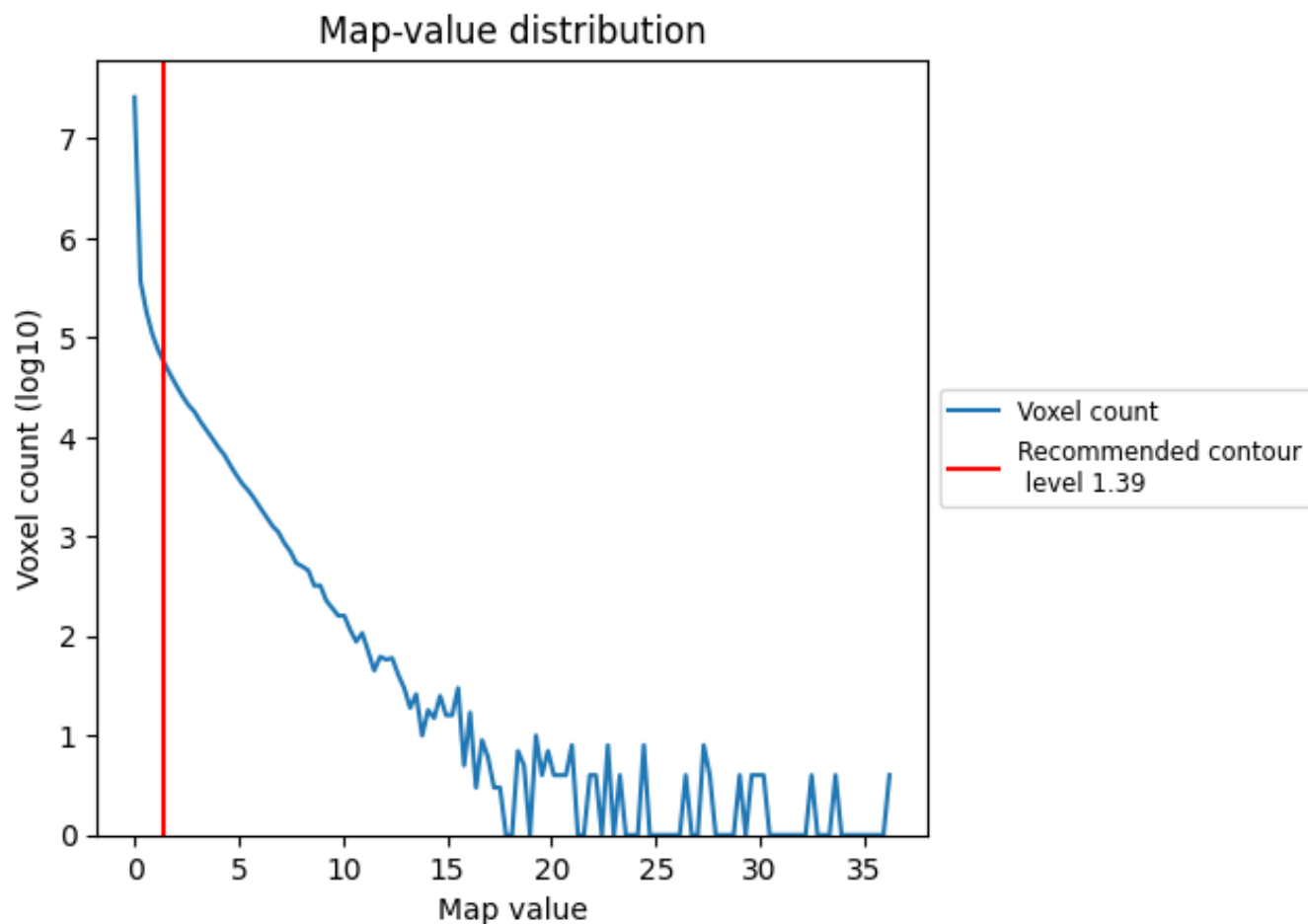
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

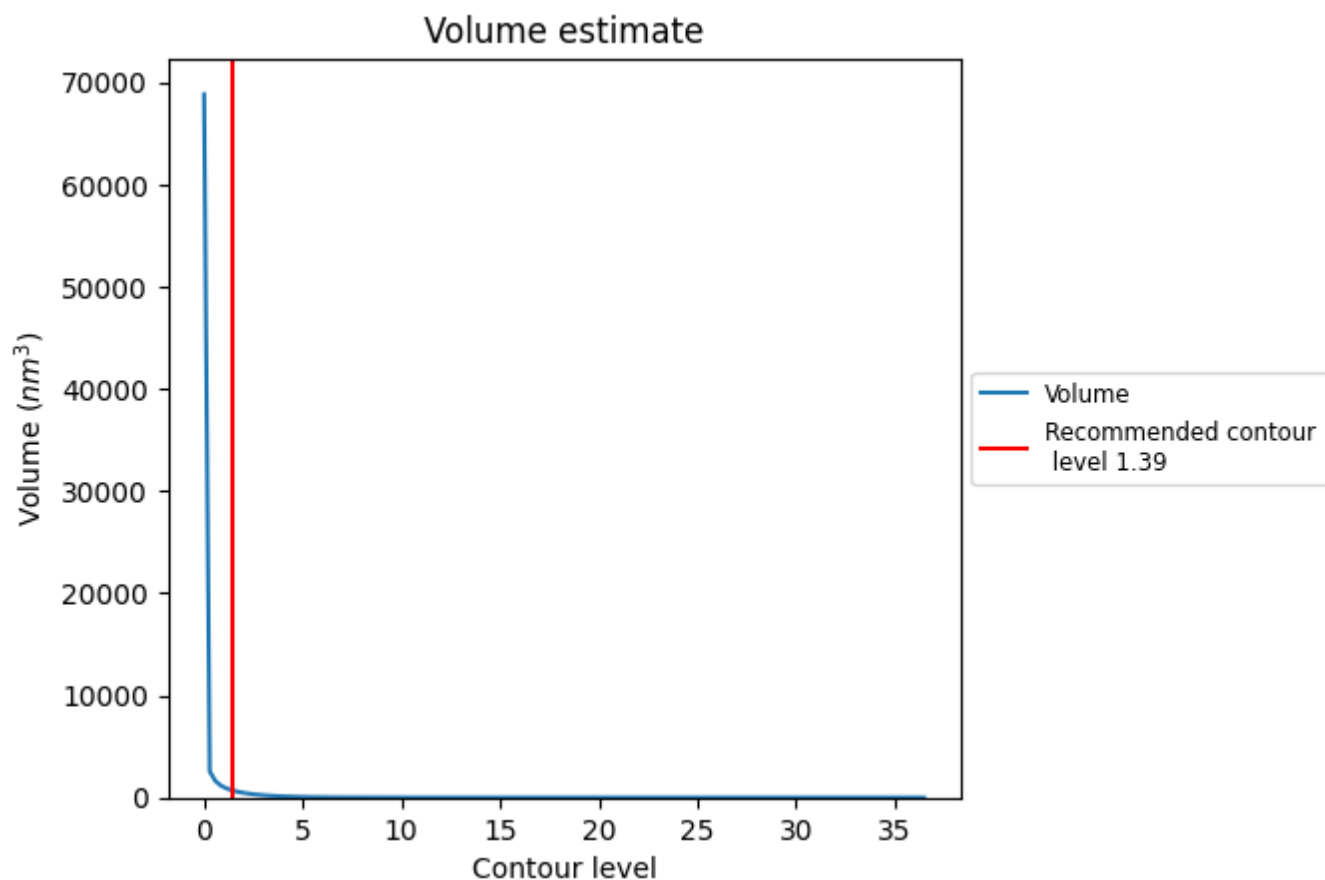
This section contains the results of statistical analysis of the map.

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.

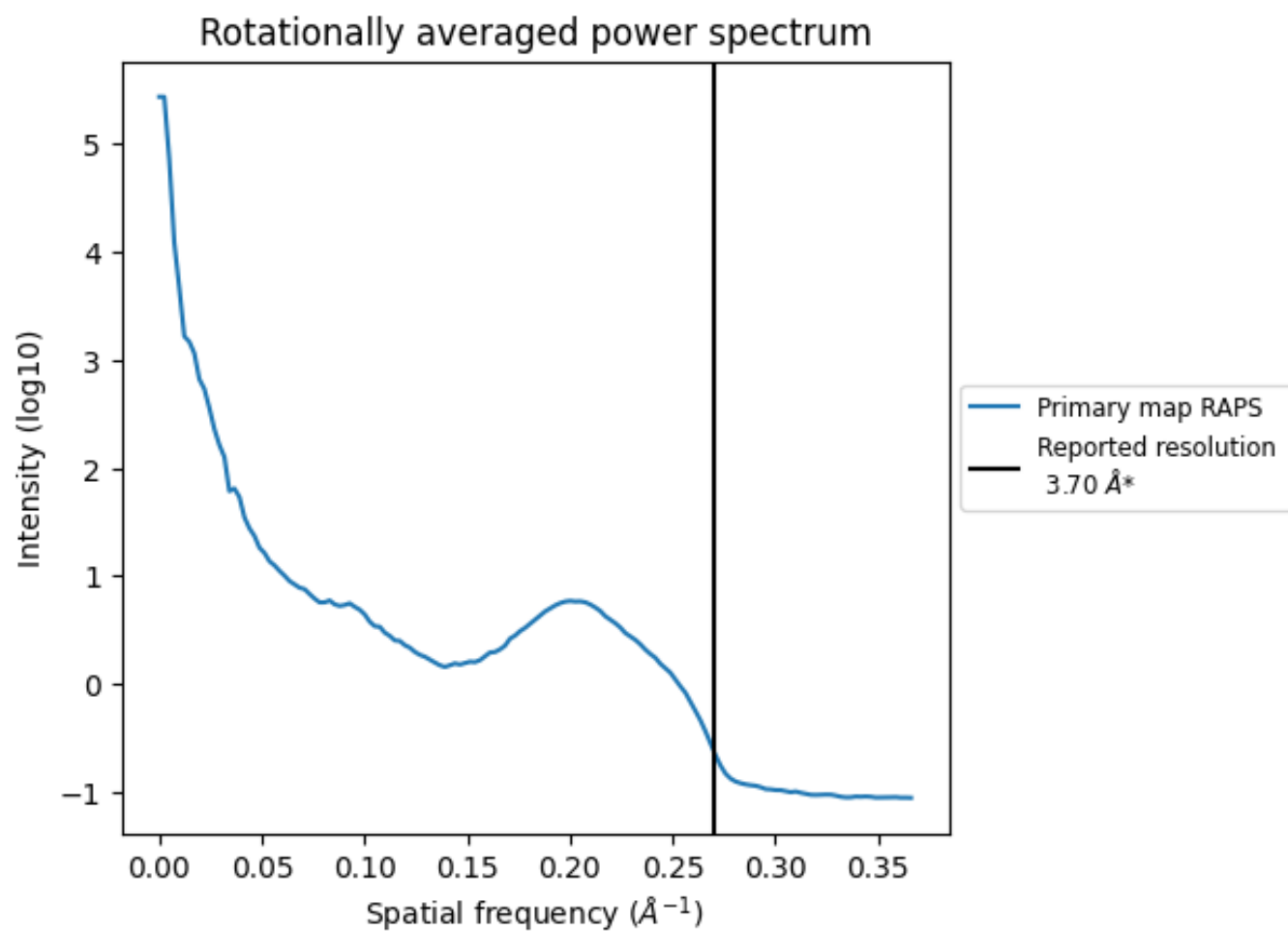
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 729 nm³; this corresponds to an approximate mass of 658 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 0.270 Å⁻¹

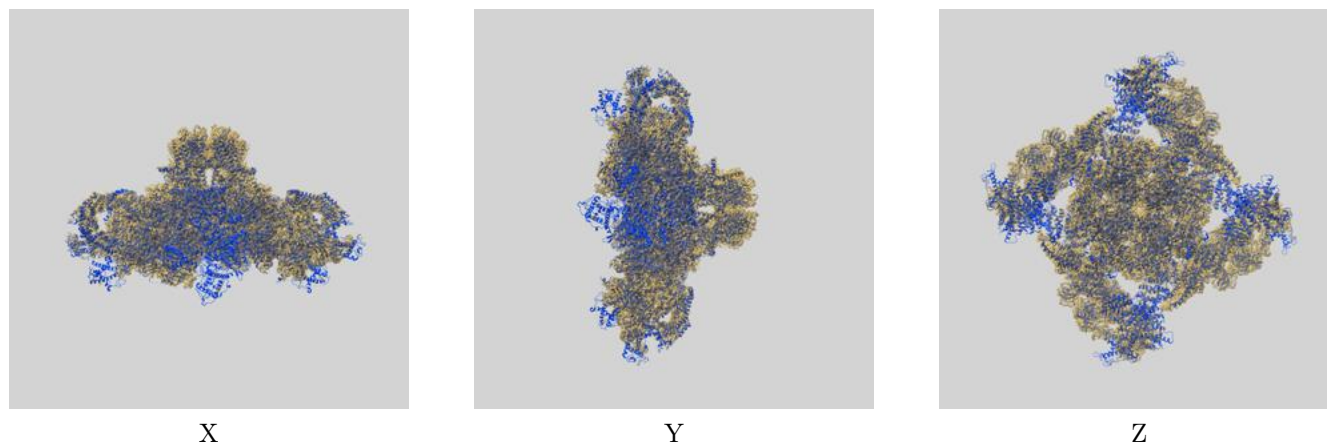
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

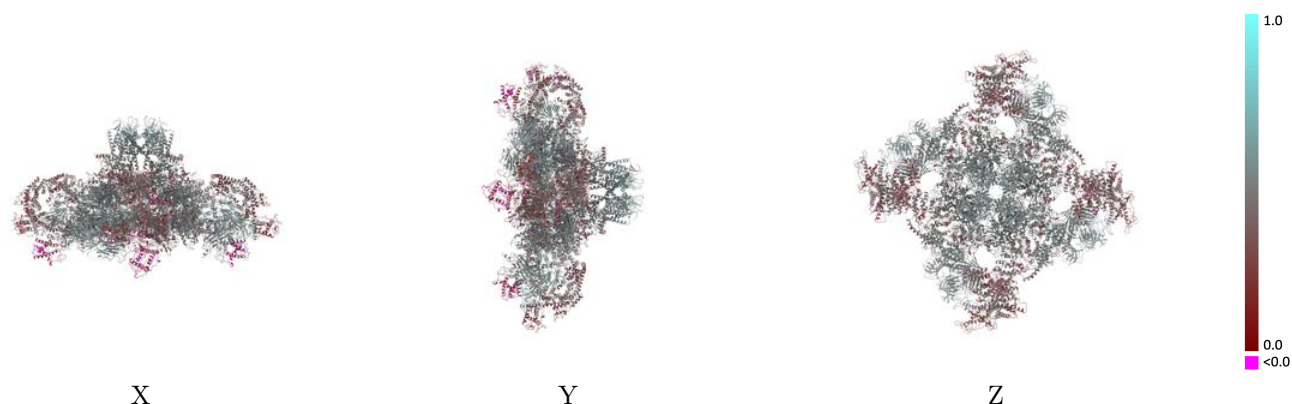
This section contains information regarding the fit between EMDB map EMD-54590 and PDB model 9S55. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



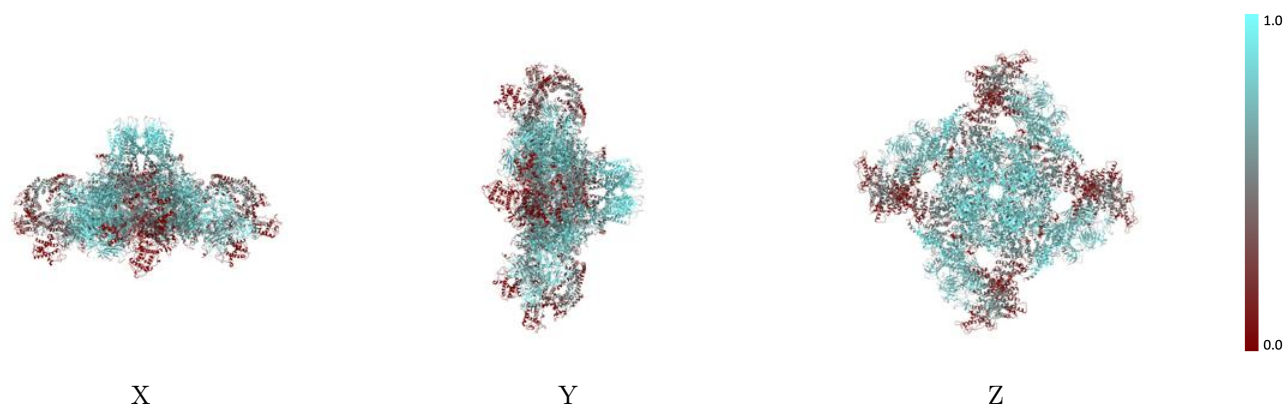
The images above show the 3D surface view of the map at the recommended contour level 1.39 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



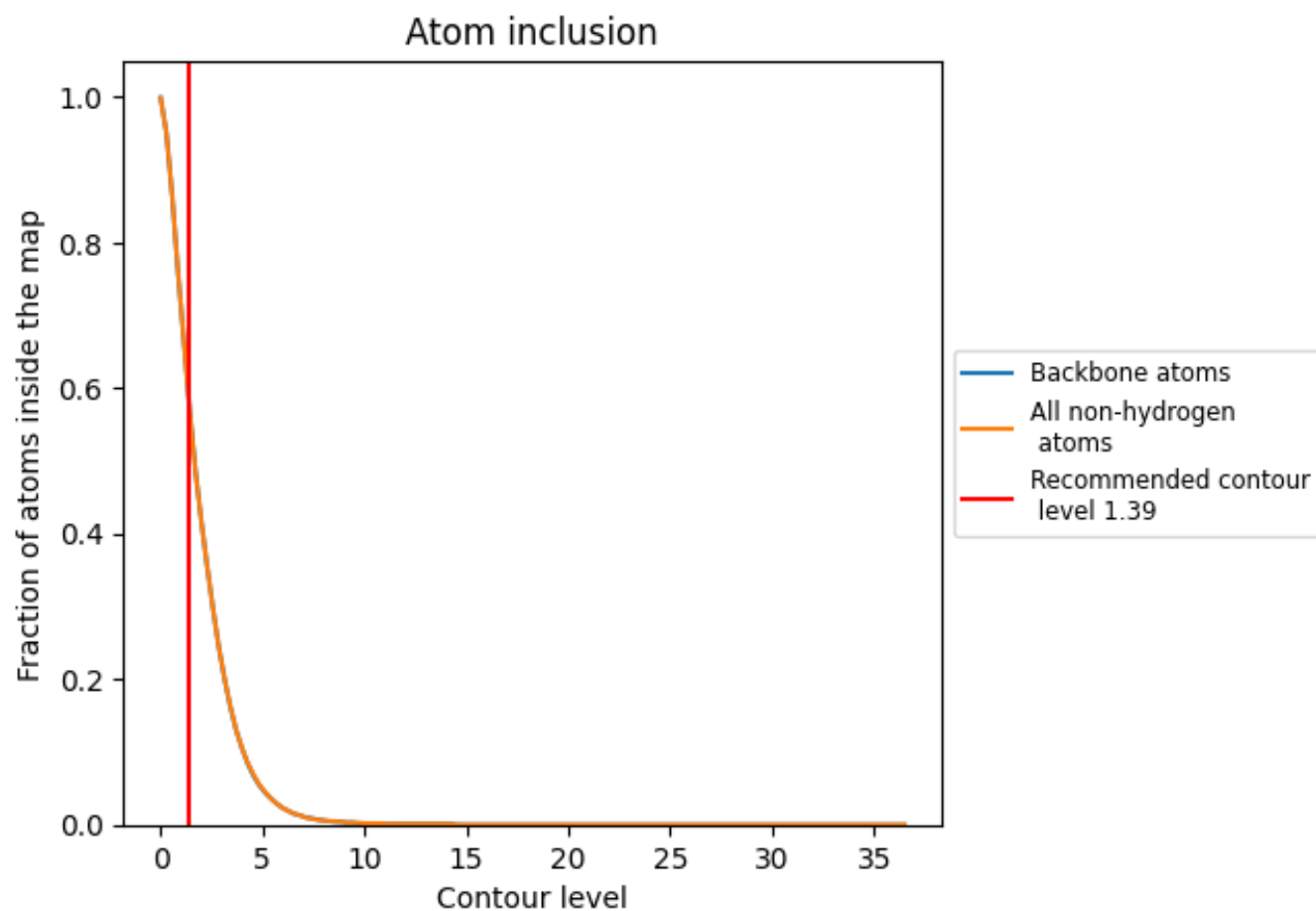
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.39).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 58% 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 (1.39) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5810	0.4370
A	0.5760	0.4340
B	0.5770	0.4340
C	0.5770	0.4340
D	0.6110	0.4370
E	0.7100	0.5240
F	0.7020	0.5260
G	0.7030	0.5270
H	0.7280	0.5290

1.0

0.0

<0.0