



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 10:57 PM UTC

PDB ID : 9NMP / pdb_00009nmp
EMDB ID : EMD-49536
Title : Structure of mouse RyR1 with simvastatin (Ca²⁺/CFF/ATP dataset; open pore)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2025-03-04
Resolution : 3.09 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

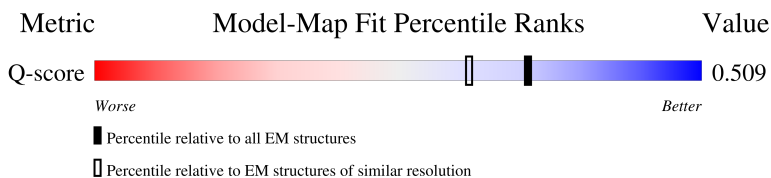
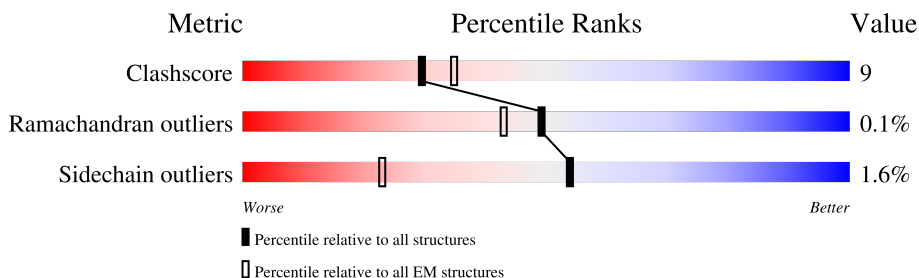
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.09 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	14003 (2.59 - 3.59)

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	E	108	 81% 18% .
1	F	108	 81% 19% .
1	G	108	 81% 19% .
1	H	108	 81% 19% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	A	5035	
2	B	5035	
2	C	5035	
2	D	5035	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	A	8002	-	X	-	-
4	CFF	B	8002	-	X	-	-
4	CFF	C	8002	-	X	-	-
4	CFF	D	8002	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 143492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
1	F	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
1	G	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
1	H	107	Total	C	N	O	S	0	0
			830	526	146	155	3		

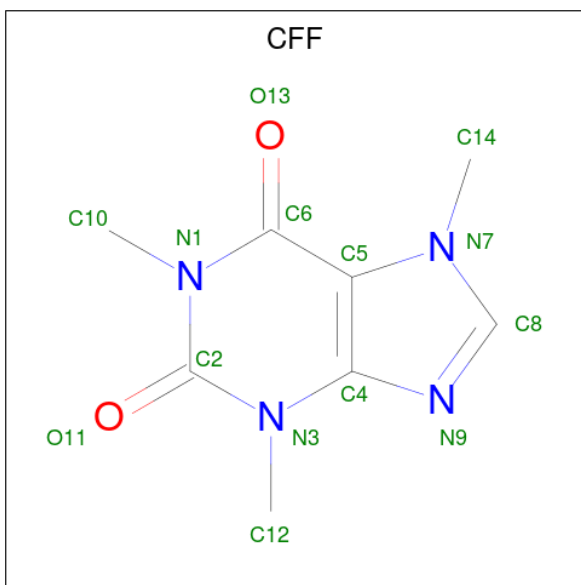
- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
2	A	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
2	B	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
2	C	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

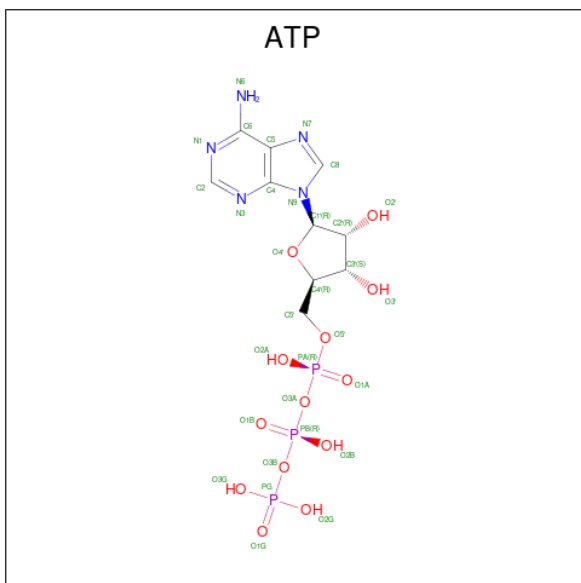
Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Zn	0
			1	1	
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

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



Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	4	2	
4	A	1	Total	C	N	O	0
			14	8	4	2	
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	C	1	Total	C	N	O	0
			14	8	4	2	

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

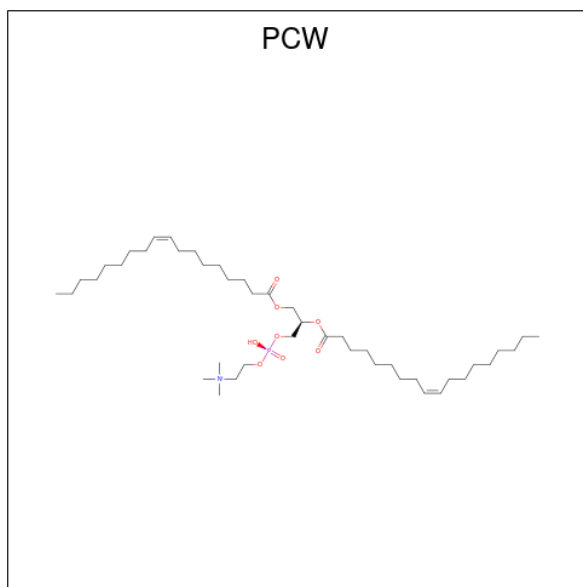


Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

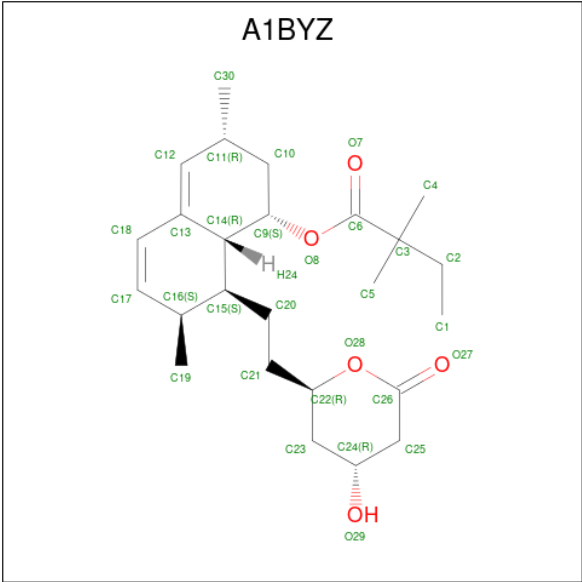
Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Ca	0
			1	1	
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 8 is Simvastatin (CCD ID: A1BYZ) (formula: $C_{25}H_{38}O_5$) (labeled as "Ligand of Interest" by depositor).




Mol	Chain	Residues	Atoms			AltConf
8	D	1	Total	C	O	0
			30	25	5	
8	D	1	Total	C	O	0
			30	25	5	
8	A	1	Total	C	O	0
			30	25	5	
8	A	1	Total	C	O	0
			30	25	5	
8	B	1	Total	C	O	0
			30	25	5	
8	B	1	Total	C	O	0
			30	25	5	
8	C	1	Total	C	O	0
			30	25	5	
8	C	1	Total	C	O	0
			30	25	5	

3 Residue-property plots [i](#)


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

- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E: 




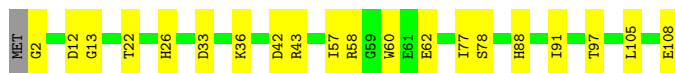
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 




- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 




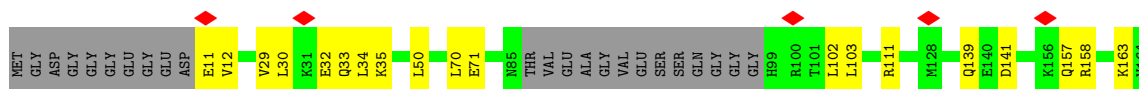
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

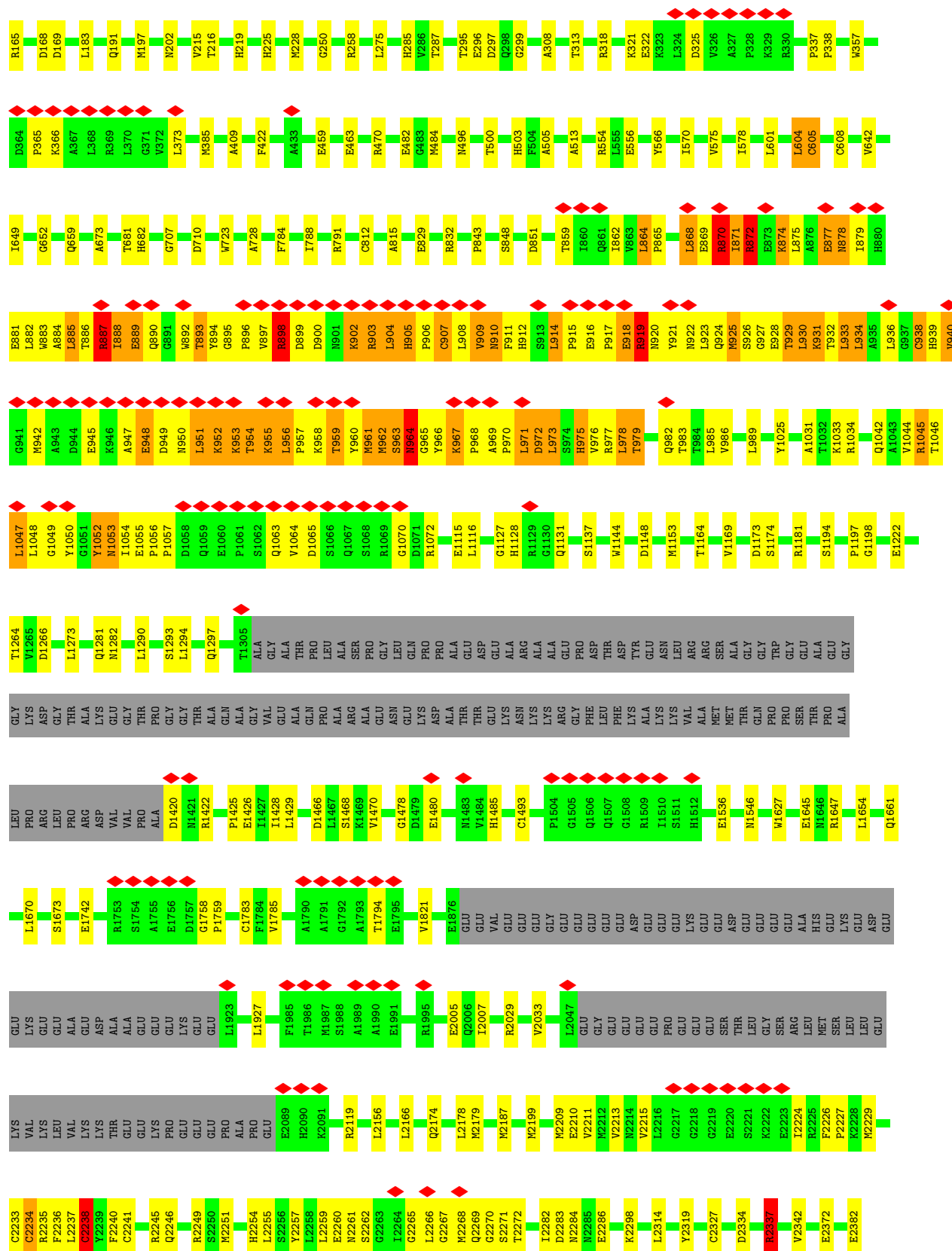
Chain H: 



- Molecule 2: Ryanodine receptor 1

Chain D: 

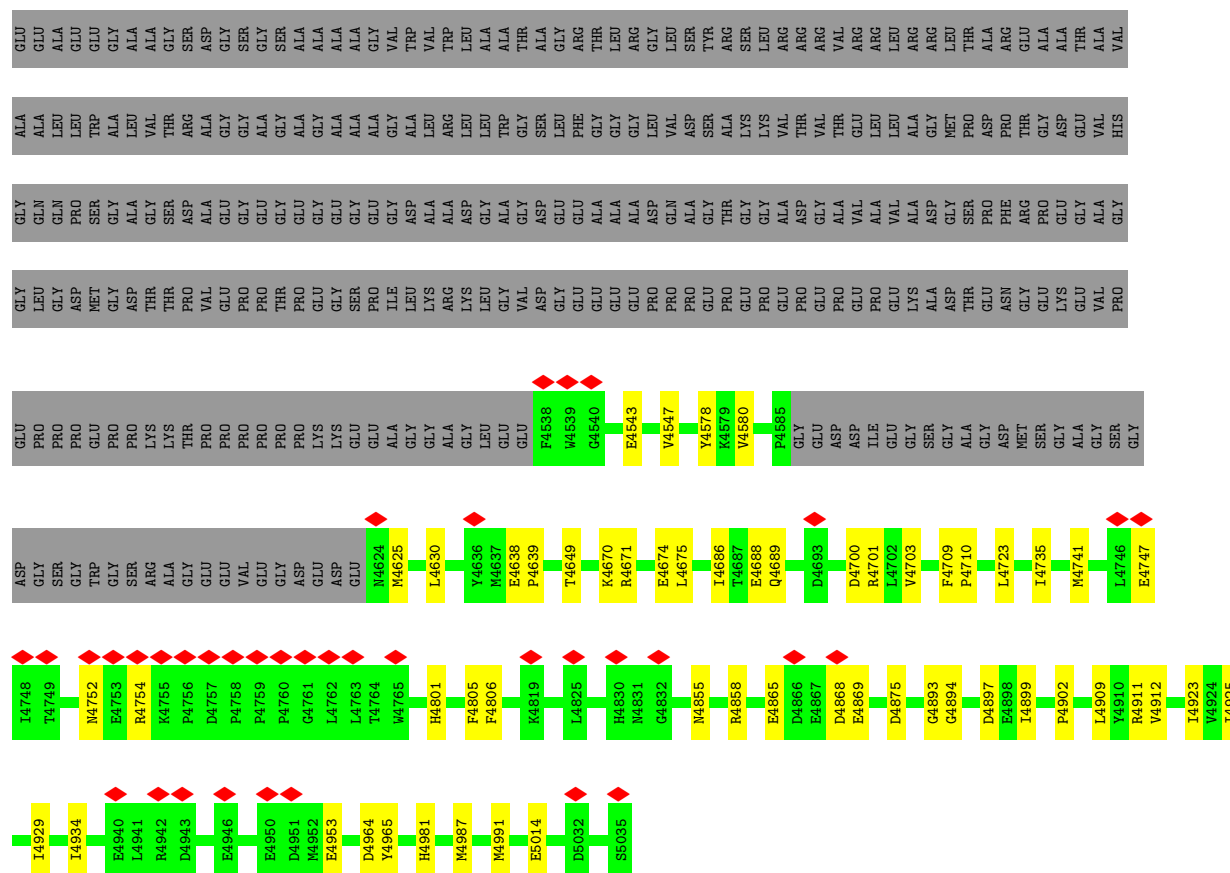




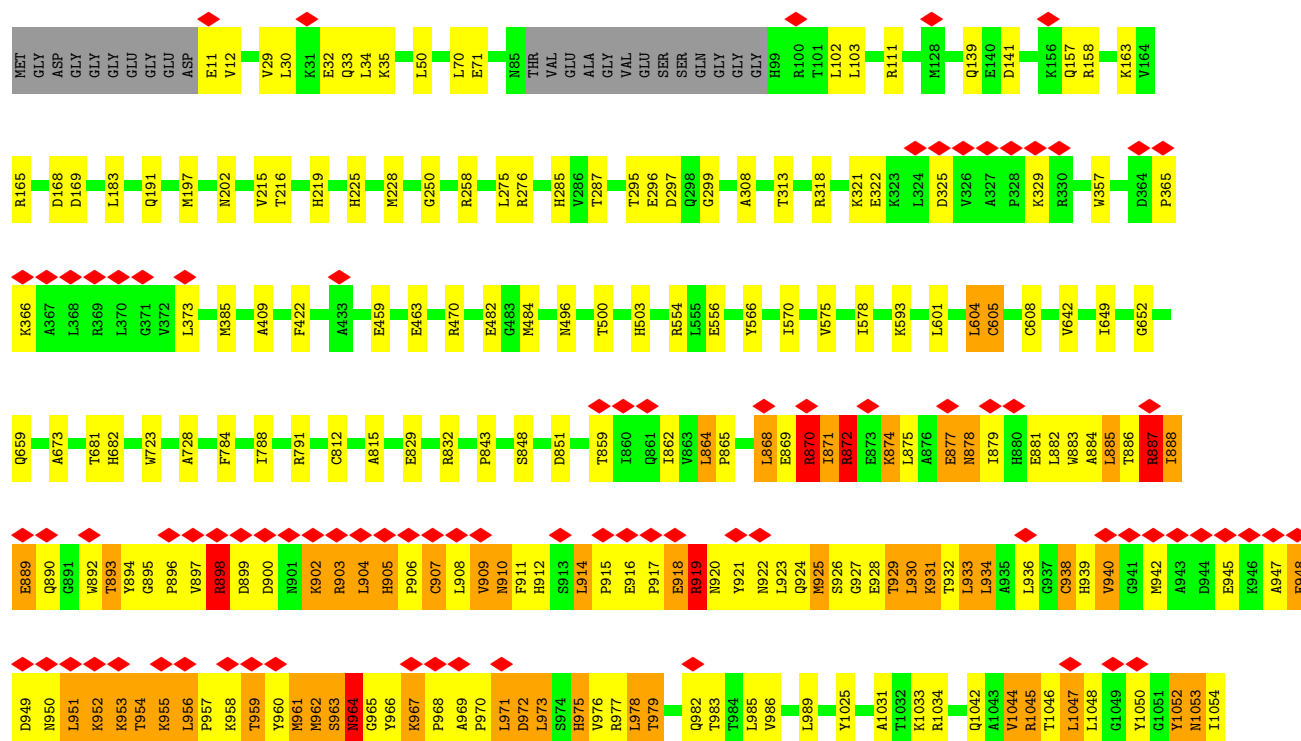
N3653	M3574	ASP	C3403	G3166	V3025	A2924	S2664	E2804	L2744	C3607	E2383
D3672	V3580	GLN	L3406	L3170	L3026	Q2925	V2665	I2805	N2745	L2611	R2386
Q3684	P3581	THR	L3409	L3176	G3027	E2926	T2667	Y2806	V2746	M2619	D2394
E3685	G3582	LYS	Y3410	G3177	K3035	L2927	S2669	W2807	T2747	L2623	V2398
E3686	P3411	LYS	P3411	T3178	I3040	L2928	S2669	W2808	T2748	L2624	ARG
E3687	L3412	LYS	L3412	T3179	T3041	K2929	R2670	P2809	P2749	L2627	ASP
E3688	L3413	ARG	L3413	T3180	V3055	F2930	R2671	I2810	E2750	L2627	ARG
E3689	I3414	ARG	I3414	N3181	S3056	L2931	E2672	E2811	K2751	L2628	ASP
E3687	I3415	GLY	I3415	P3182	L3057	Q2932	Q2673	S2812	L2752	L2634	ARG
E3687	E3434	ASP	E3434	Y3183	D3061	Q2933	A2674	S2813	L2753	N2635	ARG
D3588	L3435	ARG	L3435	V3184	A3062	N2934	A2675	L2814	S2754	L2638	GLU
E3591	M3438	S3505	M3438	I3185	P3063	Q2935	M2675	K2815	P2755	A2638	HIS
E3692	G3439	V3506	G3439	L3195	D3077	G2936	A2676	A2816	T2756	L2645	GLY
E3693	G3440	Q3507	G3440	L3198	R3079	A2937	E2677	M2817	N2757	T2648	GLU
L3711	E3441	T3508	E3441	M3202	T3078	V2938	Q2678	I2818	K2758	T2668	P2411
E3712	I3442	S3509	I3442	P3203	T3080	T2939	A2879	A2819	P2759	L2673	P2412
E3713	F3443	Y3341	F3443	V3204	V3081	R2940	A2880	W2820	H2674	L2675	E2413
D3720	Y3445	Q3344	Y3445	Y3220	M3082	G2941	N2882	W2822	E2761	L2679	E2414
H3735	W3446	V3347	W3446	R3226	K3083	L2942	T2883	T2823	Y2762	L2679	N2415
L3736	S3449	L3354	S3449	R3226	I3088	K2943	H2884	V2824	T2763	L2679	R2416
E3737	K3453	L3355	K3453	R3226	E3105	M2945	T2886	E2825	E2764	L2679	N2417
T3610	E3454	S3357	E3454	R3226	K3106	E2946	W2887	K2826	E2765	L2679	V2417
E3611	E3455	S3357	E3455	R3226	M3107	E2946	Q2888	A2827	E2766	L2679	H2418
H3612	E3456	S3357	E3456	R3226	V3108	D2947	R2889	K2828	W2767	L2679	L2419
P3613	N3463	T3360	N3463	R3226	E3109	D2948	K2890	E2829	A2768	L2679	G2420
TYR	E3464	P3361	E3464	R3226	N3110	T2949	K2891	E2830	P2769	L2679	N2424
LYS	I3465	L3366	I3465	R3226	L3111	K2954	K2892	G2830	D2770	L2679	D2483
SER	V3535	R3367	V3535	R3226	R3112	F2958	Q2893	E2831	K2771	L2679	G2484
LYS	L3536	V3373	L3536	R3226	L3113	F2958	E2894	GLU	I2772	L2679	L2519
ALA	Y3541	L3247	Y3541	R3226	GLY	L2961	L2895	GLU	Q2773	L2679	L2523
ALA	A3542	L3247	A3542	R3226	LYS	L2961	E2896	THR	N2774	L2679	D2524
VAL	L3543	M3267	L3543	R3226	VAL	W2968	A2897	LYS	Q2775	L2679	V2525
TRP	S3469	P3268	S3469	R3226	GLN	S2971	K2898	LYS	W2776	L2679	G2526
HIS	F3470	H3269	F3470	R3226	ALA	Q2972	K2898	THR	E2777	L2679	L2560
LYS	L3471	R3284	L3471	R3226	THR	E2973	G2899	LYS	Y2778	L2679	L2563
LEU	T3472	W3285	T3472	R3226	GLN	F2974	G2900	ARG	Q2779	L2679	T2564
LEU	ALA	A3291	ALA	R3226	VAL	L2975	G2901	LYS	E2780	L2679	T2573
SER	ASP	A3292	ASP	R3226	K3124	A2976	S2902	ILE	W2781	L2679	H2574
LYS	ASN	A3292	ASN	R3226	G3125	H2977	H2903	SER	VAL	L2679	H2575
ARG	LYS	A3292	LYS	R3226	V3126	L2978	P2904	GLN	ASP	L2679	T2578
ARG	LYS	A3292	LYS	R3226	L3130	E2979	L2905	ALA	ALA	L2679	N2579
ALA	MET	A3292	MET	R3226	L3133	K2980	L2906	THR	GLY	L2679	M2583
VAL	ALA	A3292	ALA	R3226	T3133	V2981	V2907	THR	N2735	L2679	L2578
VAL	LYS	A3292	LYS	R3226	D3156	V2982	P2908	ASP	N2736	L2679	H2579
A3635	ALA	A3292	ALA	R3226	D3160	S2983	Y2909	PRO	D2737	L2679	M2583
G3636	GLY	A3292	GLY	R3226	D3160	S2983	D2910	ARG	P2738	L2679	Q2600
F3637	ASP	A3292	ASP	R3226	V3164	S2984	T2911	GLY	P2739	L2679	T2604
R3638	VAL	A3292	VAL	R3226	S3165	G2985	L2912	GLY	P2790	L2679	L2604
L3642	GLN	A3292	GLN	R3226	V2986	G2986	T2913	GLY	M2791	L2679	E2742
L3645	SER	A3292	SER	R3226	V2987	G2986	A2914	GLY	L2792	L2679	T2743
F3650	GLY	A3292	GLY	R3226	E2988	E2988	K2915	GLY	R2793	L2679	
A3656	SER	A3292	SER	R3226	T3306	E2988	E2916	GLY	P2794	L2679	
L3570	SER	A3292	SER	R3226	L3004	E2988	K2917	GLY	Y2795	L2679	
					F3005	E2988	A2918		T2796	L2679	
					N3008	E2988	R2919		T2797	L2679	
						E2988	D2920		F2798	L2679	
						E2988	R2921		S2799	L2679	
						E2988	E2922		E2800	L2679	
						E2988	K2801		D2802	L2679	
						E2988	E2922		K2803	L2679	



S4055	D4086	F4087	R4088	G4089	L4090	D4095	F4096	M4100	E4122	E4129	M4133	I4142	D4160	I4173	M4187	R4191	K4214	R4218	D4219	F4220	V4224	E4227	G4228	G4229	E4230	S4231	M4248	E4256	F4257	GLY	GLY	PRO	GLY	L4019	D4021	K4024	D4025	V4048	S4054																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
L3859	G3860	M3861	N3862	N3863	E3864	D3865	G3866	T3867	V3868	I3869	N3870	R3871	Q3872	N3873	G3874	D3881	E3882	I3884	G3885	E3886	F3902	Y3940	K3943	D3944	V3945	K3962	E3970	Y3971	I3972	Q3973	G3974	P3975	L3983	F3989	K4005	D4009	S4010	L4019	D4021	K4024	D4025	V4048	S4054																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
D3672	E3683	Q3684	E3685	E3686	E3687	E3688	E3689	E3690	V3691	E3692	E3693	L3711	T3712	E3713	D3720	H3736	L3736	E3737	GLY	GLY	GLY	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
V3580	F3581	G3582	R3583	E3584	E3585	D3586	A3587	D3588	E3591	E3592	I3593	V3594	R3595	R3596	V3597	Q3598	V3603	L3607	T3610	E3611	H3612	P3613	TYR	L3613	L3614	L3615	L3616	L3617	L3618	L3619	L3620	L3621	L3622	L3623	L3624	L3625	L3626	L3627	L3628	L3629	L3630	L3631	L3632	L3633	L3634	L3635	L3636	L3637	L3638	L3639	L3640	L3641	L3642	L3643	L3644	L3645	L3646	L3647	L3648	L3649	L3650	L3651	L3652	L3653	L3654	L3655	L3656	L3657	L3658	L3659	L3660	L3661	L3662	L3663	L3664	L3665	L3666	L3667	L3668	L3669	L3670	L3671	L3672	L3673	L3674	L3675	L3676	L3677	L3678	L3679	L3680	L3681	L3682	L3683	L3684	L3685	L3686	L3687	L3688	L3689	L3690	L3691	L3692	L3693	L3694	L3695	L3696	L3697	L3698	L3699	L3700	L3701	L3702	L3703	L3704	L3705	L3706	L3707	L3708	L3709	L3710	L3711	L3712	L3713	L3714	L3715	L3716	L3717	L3718	L3719	L3720	L3721	L3722	L3723	L3724	L3725	L3726	L3727	L3728	L3729	L3730	L3731	L3732	L3733	L3734	L3735	L3736	L3737	L3738	L3739	L3740	L3741	L3742	L3743	L3744	L3745	L3746	L3747	L3748	L3749	L3750	L3751	L3752	L3753	L3754	L3755	L3756	L3757	L3758	L3759	L3760	L3761	L3762	L3763	L3764	L3765	L3766	L3767	L3768	L3769	L3770	L3771	L3772	L3773	L3774	L3775	L3776	L3777	L3778	L3779	L3780	L3781	L3782	L3783	L3784	L3785	L3786	L3787	L3788	L3789	L3790	L3791	L3792	L3793	L3794	L3795	L3796	L3797	L3798	L3799	L3800	L3801	L3802	L3803	L3804	L3805	L3806	L3807	L3808	L3809	L3810	L3811	L3812	L3813	L3814	L3815	L3816	L3817	L3818	L3819	L3820	L3821	L3822	L3823	L3824	L3825	L3826	L3827	L3828	L3829	L3830	L3831	L3832	L3833	L3834	L3835	L3836	L3837	L3838	L3839	L3840	L3841	L3842	L3843	L3844	L3845	L3846	L3847	L3848	L3849	L3850	L3851	L3852	L3853	L3854	L3855	L3856	L3857	L3858	L3859	L3860	L3861	L3862	L3863	L3864	L3865	L3866	L3867	L3868	L3869	L3870	L3871	L3872	L3873	L3874	L3875	L3876	L3877	L3878	L3879	L3880	L3881	L3882	L3883	L3884	L3885	L3886	L3887	L3888	L3889	L3890	L3891	L3892	L3893	L3894	L3895	L3896	L3897	L3898	L3899	L3900	L3901	L3902	L3903	L3904	L3905	L3906	L3907	L3908	L3909	L3910	L3911	L3912	L3913	L3914	L3915	L3916	L3917	L3918	L3919	L3920	L3921	L3922	L3923	L3924	L3925	L3926	L3927	L3928	L3929	L3930	L3931	L3932	L3933	L3934	L3935	L3936	L3937	L3938	L3939	L3940	L3941	L3942	L3943	L3944	L3945	L3946	L3947	L3948	L3949	L3950	L3951	L3952	L3953	L3954	L3955	L3956	L3957	L3958	L3959	L3960	L3961	L3962	L3963	L3964	L3965	L3966	L3967	L3968	L3969	L3970	L3971	L3972	L3973	L3974	L3975	L3976	L3977	L3978	L3979	L3980	L3981	L3982	L3983	L3984	L3985	L3986	L3987	L3988	L3989	L3990	L3991	L3992	L3993	L3994	L3995	L3996	L3997	L3998	L3999	L4000	L4001	L4002	L4003	L4004	L4005	L4006	L4007	L4008	L4009	L4010	L4011	L4012	L4013	L4014	L4015	L4016	L4017	L4018	L4019	L4020	L4021	L4022	L4023	L4024	L4025	L4026	L4027	L4028	L4029	L4030	L4031	L4032	L4033	L4034	L4035	L4036	L4037	L4038	L4039	L4040	L4041	L4042	L4043	L4044	L4045	L4046	L4047	L4048	L4049	L4050	L4051	L4052	L4053	L4054	L4055	L4056	L4057	L4058	L4059	L4060	L4061	L4062	L4063	L4064	L4065	L4066	L4067	L4068	L4069	L4070	L4071	L4072	L4073	L4074	L4075	L4076	L4077	L4078	L4079	L4080	L4081	L4082	L4083	L4084	L4085	L4086	L4087	L4088	L4089	L4090	L4091	L4092	L4093	L4094	L4095	L4096	L4097	L4098	L4099	L4100	L4101	L4102	L4103	L4104	L4105	L4106	L4107	L4108	L4109	L4110	L4111	L4112	L4113	L4114	L4115	L4116	L4117	L4118	L4119	L4120	L4121	L4122	L4123	L4124	L4125	L4126	L4127	L4128	L4129	L4130	L4131	L4132	L4133	L4134	L4135	L4136	L4137	L4138	L4139	L4140	L4141	L4142	L4143	L4144	L4145	L4146	L4147	L4148	L4149	L4150	L4151	L4152	L4153	L4154	L4155	L4156	L4157	L4158	L4159	L4160	L4161	L4162	L4163	L4164	L4165	L4166	L4167	L4168	L4169	L4170	L4171	L4172	L4173	L4174	L4175	L4176	L4177	L4178	L4179	L4180	L4181	L4182	L4183	L4184	L4185	L4186	L4187	L4188	L4189	L4190	L4191	L4192	L4193	L4194	L4195	L4196	L4197	L4198	L4199	L4200	L4201	L4202	L4203	L4204	L4205	L4206	L4207	L4208	L4209	L4210	L4211	L4212	L4213	L4214	L4215	L4216	L4217	L4218	L4219	L4220	L4221	L4222	L4223	L4224	L4225	L4226	L4227	L4228	L4229	L4230	L4231	L4232	L4233	L4234	L4235	L4236	L4237	L4238	L4239	L4240	L4241	L4242	L4243	L4244	L4245	L4246	L4247	L4248	L4249	L4250	L4251	L4252	L4253	L4254	L4255	L4256	L4257	L4258	L4259	L4260	L4261	L4262	L4263	L4264	L4265	L4266	L4267	L4268	L4269	L4270	L4271	L4272	L4273	L4274	L4275	L4276	L4277	L4278	L4279	L4280	L4281	L4282	L4283	L4284	L4285	L4286	L4287	L4288	L4289	L4290	L4291	L4292	L4293	L4294	L4295	L4296	L4297	L4298	L4299	L4300	L4301	L4302	L4303	L4304	L4305	L4306	L4307	L4308	L4309	L4310	L4311	L4312	L4313	L4314	L4315	L4316	L4317	L4318	L4319	L4320	L4321	L4322	L4323	L4324	L4325	L4326	L4327	L4328	L4329	L4330	L4331	L4332	L4333	L4334	L4335	L4336	L4337	L4338	L4339	L4340	L4341	L4342	L4343	L4344	L4345	L4346	L4347	L4348	L4349	L4350	L4351	L4352	L4353	L4354	L4355	L4356	L4357	L4358	L4359	L4360	L4361	L4362	L4363	L4364	L4365	L4366	L4367	L4368	L4369	L4370	L4371	L4372	L4373	L4374	L4375	L4376	L4377	L4378	L4379	L4380	L4381	L4382	L4383	L4384	L4385	L4386	L4387	L4388	L4389	L4390	L4391	L4392	L4393	L4394	L4395	L4396	L4397	L4398	L4399	L4400	L4401	L4402	L4403	L4404	L4405	L4406	L4407	L4408	L4409	L4410	L4411	L4412	L4413	L4414	L4415	L4416	L4417	L4418	L4419	L4420	L4421	L4422	L4423	L4424	L4425	L4426	L4427	L4428	L4429	L4430	L4431	L4432	L4433	L4434	L4435	L4436	L4437	L4438	L4439	L4440	L4441	L4442	L4443	L4444	L4445	L4446	L4447	L4448	L4449	L4450	L4451	L4452	L4453	L4454	L4455	L4456	L4457	L4458	L4459	L4460	L4461	L4462	L4463	L4464	L4465	L4466	L4467	L4468	L4469	L4470	L4471	L4472	L4473	L4474	L4475	L4476	L4477	L4478	L4479	L4480	L4481	L4482	L4483	L4484	L4485	L4486	L4487	L4488	L4489	L4490	L4491	L4492	L4493	L4494	L4495	L4496	L4497	L4498	L4499	L4500	L4501	L4502	L4503	L4504	L4505	L4506	L4507	L4508	L4509	L4510	L4511	L4512	L4513	L4514	L4515	L4516	L4517	L4518	L4519	L4520	L4521	L4522	L4523	L4524	L4525	L4526	L4527	L4528	L4529	L4530	L4531	L4532	L4533	L4534	L4535	L4536	L4537	L4538	L4539	L4540	L4541	L4542	L4543	L4544	L4545	L4546	L4547	L4548	L4549	L4550	L4551	L4552	L4553	L4554	L4555	L4556	L4557	L4558	L4559	L4560	L4561	L4562	L4563	L4564	L4565	L4566	L4567	L4568	L4569	L4570	L4571	L4572	L4573	L4574	L4575	L4576	L4577	L4578	L4579	L4580	L4581	L4582	L4583	L4584	L4585	L4586	L4587	L4588	L4589	L4590	L4591	L4592	L4593	L4594	L4595	L4596	L4597	L4598	L4599	L4600	L4601	L4602	L4603	L4604	L4605	L4606	L4607	L4608	L4609	L4610	L4611	L4612	L4613	L4614	L4615	L4616	L4617	L4618	L4619	L4620	L4621	L4622	L4623	L4624	L4625	L4626	L4627	L4628	L4629	L4630	L4631	L4632	L4633	L4634	L4635	L4636	L4637	L4638	L4639	L4640	L4641	L4642	L4643	L4644	L4645	L4646	L4647	L4648	L4649	L4650	L4651	L4652	L4653	L4654	L4655	L4656	L4657	L4658	L4659	L4660	L4661	L4662	L4663	L4664	L4665	L4666	L4667	L4668	L4669	L4670	L4671	L4672	L4673	L4674	L4675	L4676	L4677	L4678	L4679	L4680	L4681	L4682	L4683	L4684	L4685	L4686	L4687	L4688	L4689	L4690	L4691	L4692	L4693	L4694	L4695	L4696	L4697	L4698	L4699	L4700	L4701	L4702	L4703	L4704	L4705	L4706	L4707	L4708	L4709	L4710	L4711	L4712	L4713	L4714	L4715	L4716	L4717	L4718	L4719	L4720	L4721	L4722	L4723	L4724	L4725	L4726	L4727	L4728	L4729	L4730	L4731	L4732	L4733	L4734	L4735	L4736	L4737	L4738	L4739	L4740	L4741	L4742	L4743	L4744	L4745	L4746	L4747	L4748	L4749	L4750	L4751	L4752	L4753	L4754	L4755	L4756	L4757	L4758	L4759	L4760	L4761	L4762	L4763	L4764	L4765	L4766	L4767	L4768	L4769	L4770	L4771	L4772	L4773	L4774	L4775	L4776	L4777	L4778	L4779	L4780	L4781	L4782	L4783	L4784	L4785	L4786	L4787	L4788	L4789	L4790	L4791	L4792	L4793	L4794	L4795	L4796	L4797	L4798	L4799	L4800	L4801	L4802	L4803	L4804	L4805	L4806	L4807	L4808	L4809	L4810	L4811	L4812	L4813	L4814	L4815	L4816	L4817	L4818	L4819	L4820	L4821	L4822	L4823	L4824	L

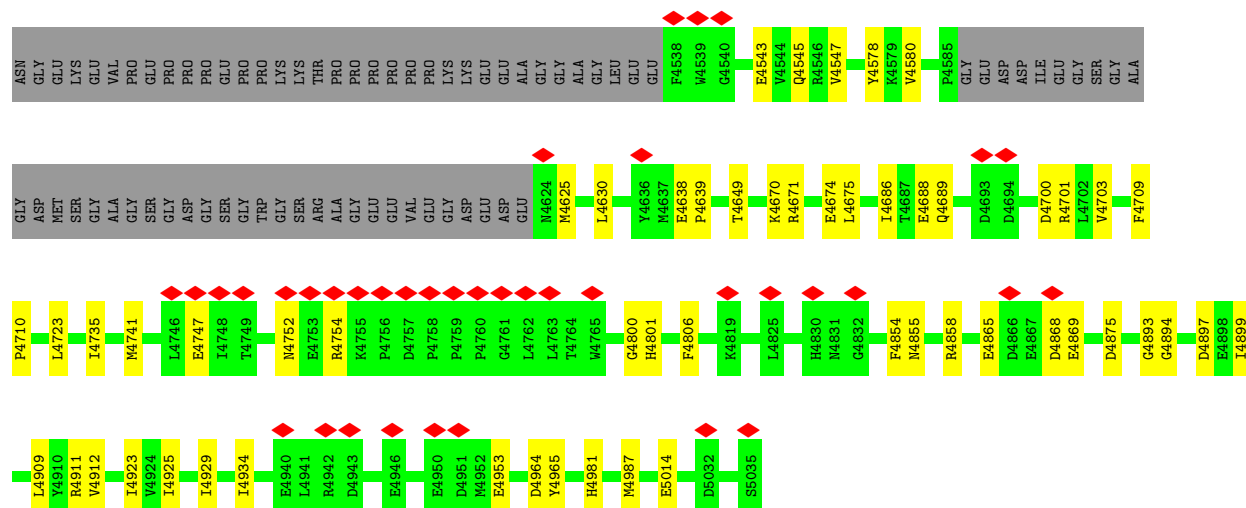


• Molecule 2: Ryanodine receptor 1

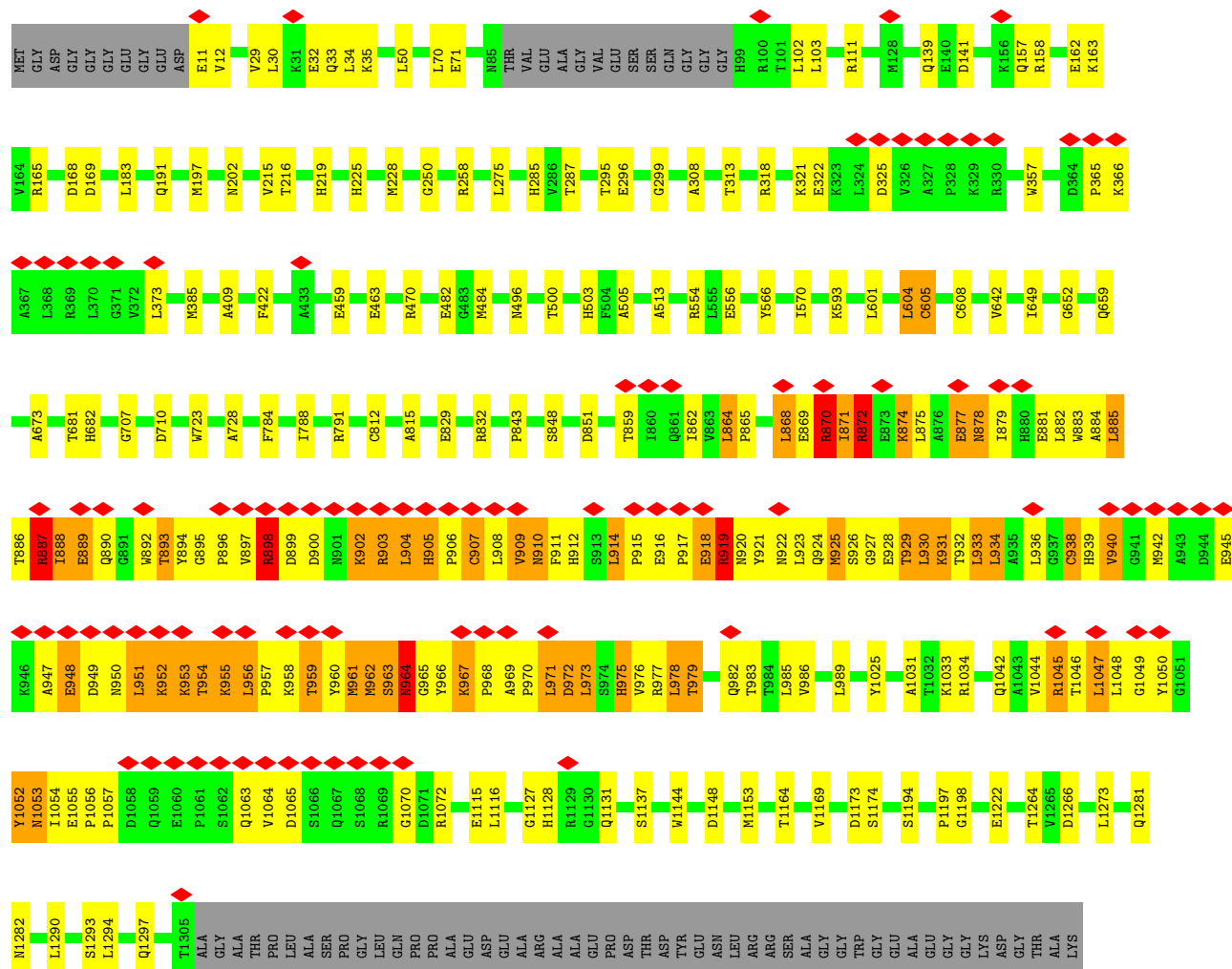
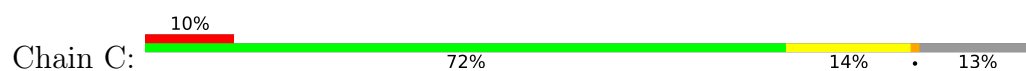






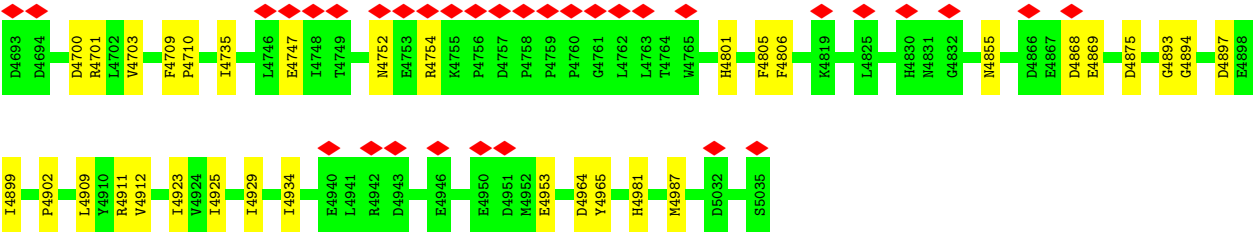


• Molecule 2: Ryanodine receptor 1









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25791	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.628	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	424.448, 424.448, 424.448	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1BYZ, CFF, PCW, ATP, ZN, CA

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	E	0.24	0/848	0.40	0/1143
1	F	0.25	0/848	0.40	0/1143
1	G	0.25	0/848	0.41	0/1143
1	H	0.24	0/848	0.40	0/1143
2	A	0.29	0/35586	0.47	13/48203 (0.0%)
2	B	0.29	0/35586	0.47	14/48203 (0.0%)
2	C	0.29	0/35586	0.47	13/48203 (0.0%)
2	D	0.29	0/35586	0.47	13/48203 (0.0%)
All	All	0.29	0/145736	0.47	53/197384 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	10
2	B	0	10
2	C	0	10
2	D	0	10
All	All	0	40

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2238	CYS	CA-CB-SG	9.57	136.40	114.40
2	B	2238	CYS	CA-CB-SG	9.57	136.40	114.40
2	C	2238	CYS	CA-CB-SG	9.57	136.40	114.40
2	A	2238	CYS	CA-CB-SG	9.55	136.37	114.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3241	CYS	CA-CB-SG	7.71	132.13	114.40

There are no chirality outliers.

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	605	CYS	Peptide
2	D	870	ARG	Sidechain
2	D	872	ARG	Sidechain
2	D	887	ARG	Sidechain
2	D	898	ARG	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	E	830	0	828	16	0
1	F	830	0	828	15	0
1	G	830	0	828	16	0
1	H	830	0	828	16	0
2	A	34797	0	34382	638	0
2	B	34797	0	34382	643	0
2	C	34797	0	34382	644	0
2	D	34797	0	34382	642	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	14	0	10	0	0
4	B	14	0	10	0	0
4	C	14	0	10	0	0
4	D	14	0	10	0	0
5	A	62	0	24	1	0
5	B	62	0	24	1	0
5	C	62	0	24	1	0
5	D	62	0	24	1	0
6	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	108	0	168	5	0
7	B	108	0	168	5	0
7	C	108	0	168	5	0
7	D	108	0	168	5	0
8	A	60	0	0	2	0
8	B	60	0	0	3	0
8	C	60	0	0	3	0
8	D	60	0	0	2	0
All	All	143492	0	141648	2626	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 9.

The worst 5 of 2626 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:899:ASP:HB3	2:B:902:LYS:HB2	1.30	1.10
2:A:899:ASP:HB3	2:A:902:LYS:HB2	1.30	1.09
2:D:899:ASP:HB3	2:D:902:LYS:HB2	1.30	1.08
2:C:899:ASP:HB3	2:C:902:LYS:HB2	1.30	1.08
1:H:2:GLY:N	1:H:78:SER:HG	1.55	1.03

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	E	105/108 (97%)	102 (97%)	3 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	A	4345/5035 (86%)	4228 (97%)	114 (3%)	3 (0%)	48	78
2	B	4345/5035 (86%)	4227 (97%)	115 (3%)	3 (0%)	48	78
2	C	4345/5035 (86%)	4227 (97%)	115 (3%)	3 (0%)	48	78
2	D	4345/5035 (86%)	4228 (97%)	114 (3%)	3 (0%)	48	78
All	All	17800/20572 (86%)	17318 (97%)	470 (3%)	12 (0%)	49	78

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2574	GLU
2	D	4055	SER
2	A	2574	GLU
2	A	4055	SER
2	B	2574	GLU

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	E	89/90 (99%)	89 (100%)	0	100	100
1	F	89/90 (99%)	89 (100%)	0	100	100
1	G	89/90 (99%)	89 (100%)	0	100	100
1	H	89/90 (99%)	89 (100%)	0	100	100
2	A	3806/4296 (89%)	3742 (98%)	64 (2%)	53	74
2	B	3806/4296 (89%)	3742 (98%)	64 (2%)	53	74
2	C	3806/4296 (89%)	3742 (98%)	64 (2%)	53	74
2	D	3806/4296 (89%)	3742 (98%)	64 (2%)	53	74
All	All	15580/17544 (89%)	15324 (98%)	256 (2%)	54	75

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	952	LYS
2	C	962	MET
2	A	939	HIS
2	A	933	LEU
2	C	971	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	2037	GLN
2	C	2992	HIS
2	A	1762	HIS
2	A	1641	HIS
2	C	3423	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 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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
8	A1BYZ	A	8008	-	32,32,32	0.67	1 (3%)	40,47,47	0.85	1 (2%)
5	ATP	A	8003	-	32,33,33	0.32	0	48,52,52	0.70	1 (2%)
7	PCW	A	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.12	3 (5%)
5	ATP	B	8007	-	32,33,33	0.27	0	48,52,52	0.66	0
5	ATP	A	8007	-	32,33,33	0.27	0	48,52,52	0.66	0
5	ATP	D	8007	-	32,33,33	0.27	0	48,52,52	0.66	0
8	A1BYZ	D	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
8	A1BYZ	A	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
7	PCW	C	8005	-	53,53,53	1.25	7 (13%)	59,61,61	1.12	3 (5%)
5	ATP	C	8003	-	32,33,33	0.32	0	48,52,52	0.69	1 (2%)
7	PCW	C	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
7	PCW	B	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
8	A1BYZ	C	8008	-	32,32,32	0.68	1 (3%)	40,47,47	0.85	1 (2%)
7	PCW	B	8005	-	53,53,53	1.25	7 (13%)	59,61,61	1.12	3 (5%)
4	CFF	C	8002	-	15,15,15	1.86	6 (40%)	23,23,23	2.94	12 (52%)
7	PCW	D	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.12	3 (5%)
5	ATP	D	8003	-	32,33,33	0.32	0	48,52,52	0.69	1 (2%)
4	CFF	B	8002	-	15,15,15	1.87	6 (40%)	23,23,23	2.94	12 (52%)
7	PCW	A	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
5	ATP	C	8007	-	32,33,33	0.27	0	48,52,52	0.66	0
7	PCW	D	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
5	ATP	B	8003	-	32,33,33	0.32	0	48,52,52	0.69	1 (2%)
8	A1BYZ	D	8008	-	32,32,32	0.68	1 (3%)	40,47,47	0.85	1 (2%)
8	A1BYZ	B	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
4	CFF	A	8002	-	15,15,15	1.87	6 (40%)	23,23,23	2.94	12 (52%)
8	A1BYZ	B	8008	-	32,32,32	0.68	1 (3%)	40,47,47	0.85	1 (2%)
4	CFF	D	8002	-	15,15,15	1.87	6 (40%)	23,23,23	2.94	12 (52%)
8	A1BYZ	C	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)

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
8	A1BYZ	A	8008	-	-	3/18/59/59	0/3/3/3
5	ATP	A	8003	-	-	11/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PCW	A	8005	-	-	25/57/57/57	-
5	ATP	B	8007	-	-	8/22/38/38	0/3/3/3
5	ATP	A	8007	-	-	8/22/38/38	0/3/3/3
5	ATP	D	8007	-	-	8/22/38/38	0/3/3/3
8	A1BYZ	D	8009	-	-	4/18/59/59	0/3/3/3
8	A1BYZ	A	8009	-	-	4/18/59/59	0/3/3/3
7	PCW	C	8005	-	-	25/57/57/57	-
5	ATP	C	8003	-	-	11/22/38/38	0/3/3/3
7	PCW	C	8006	-	-	29/57/57/57	-
7	PCW	B	8006	-	-	29/57/57/57	-
8	A1BYZ	C	8008	-	-	3/18/59/59	0/3/3/3
7	PCW	B	8005	-	-	25/57/57/57	-
4	CFF	C	8002	-	-	-	0/2/2/2
7	PCW	D	8005	-	-	25/57/57/57	-
5	ATP	D	8003	-	-	11/22/38/38	0/3/3/3
4	CFF	B	8002	-	-	-	0/2/2/2
7	PCW	A	8006	-	-	29/57/57/57	-
5	ATP	C	8007	-	-	8/22/38/38	0/3/3/3
7	PCW	D	8006	-	-	29/57/57/57	-
5	ATP	B	8003	-	-	11/22/38/38	0/3/3/3
8	A1BYZ	D	8008	-	-	3/18/59/59	0/3/3/3
8	A1BYZ	B	8009	-	-	4/18/59/59	0/3/3/3
4	CFF	A	8002	-	-	-	0/2/2/2
8	A1BYZ	B	8008	-	-	3/18/59/59	0/3/3/3
8	A1BYZ	C	8009	-	-	4/18/59/59	0/3/3/3
4	CFF	D	8002	-	-	-	0/2/2/2

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8002	CFF	C6-N1	-3.80	1.32	1.40
4	A	8002	CFF	C6-N1	-3.80	1.32	1.40
4	B	8002	CFF	C6-N1	-3.80	1.32	1.40
4	C	8002	CFF	C6-N1	-3.80	1.32	1.40
8	D	8008	A1BYZ	C16-C15	-3.34	1.51	1.54

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8002	CFF	C14-N7-C8	-8.05	111.22	126.28
4	D	8002	CFF	C14-N7-C8	-8.03	111.25	126.28
4	A	8002	CFF	C14-N7-C8	-8.03	111.25	126.28
4	C	8002	CFF	C14-N7-C8	-8.02	111.28	126.28
4	D	8002	CFF	C14-N7-C5	5.48	140.80	127.77

There are no chirality outliers.

5 of 320 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	8003	ATP	C5'-O5'-PA-O1A
5	D	8003	ATP	C5'-O5'-PA-O2A
5	D	8003	ATP	C5'-O5'-PA-O3A
5	D	8007	ATP	PB-O3B-PG-O3G
5	D	8007	ATP	C5'-O5'-PA-O2A

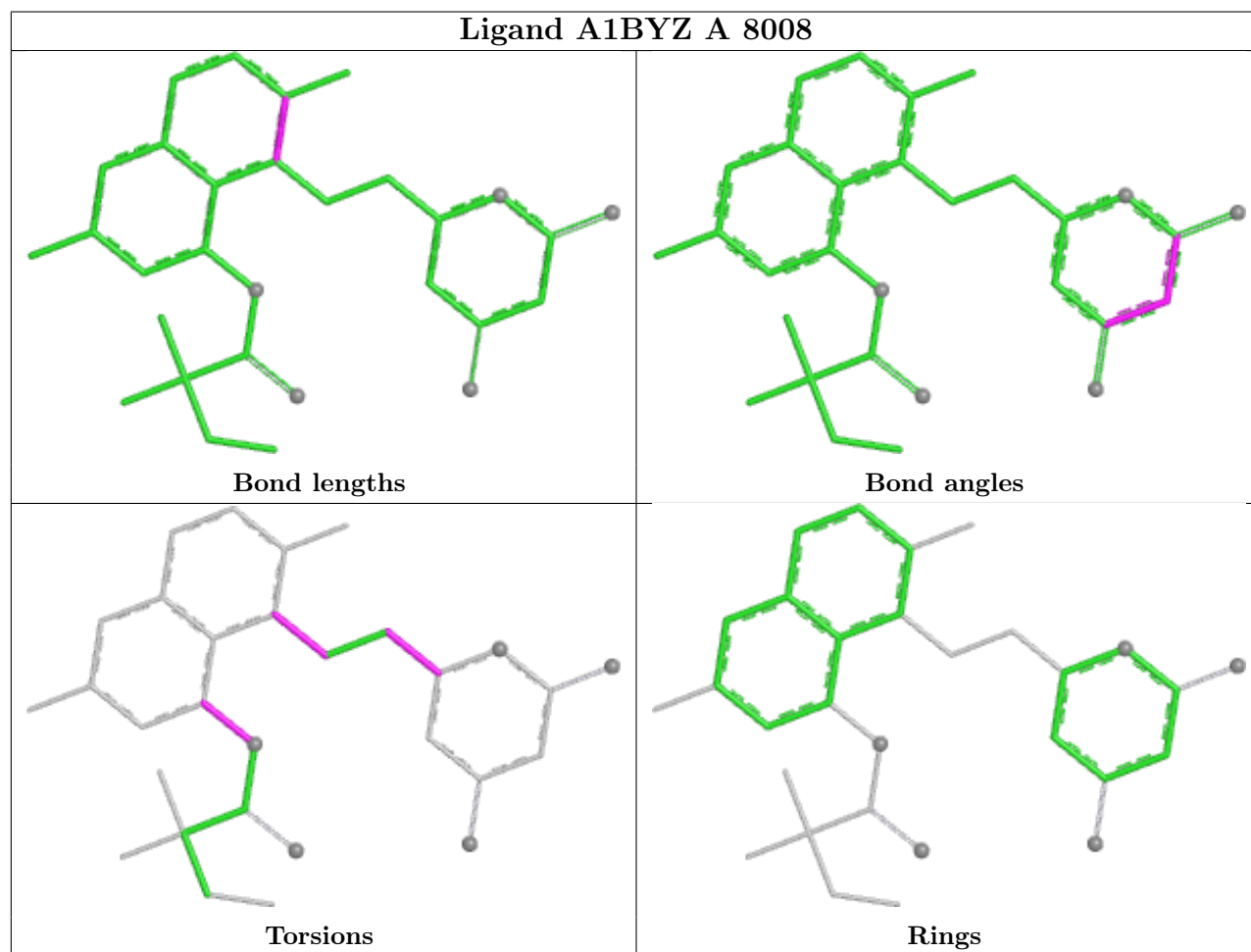
There are no ring outliers.

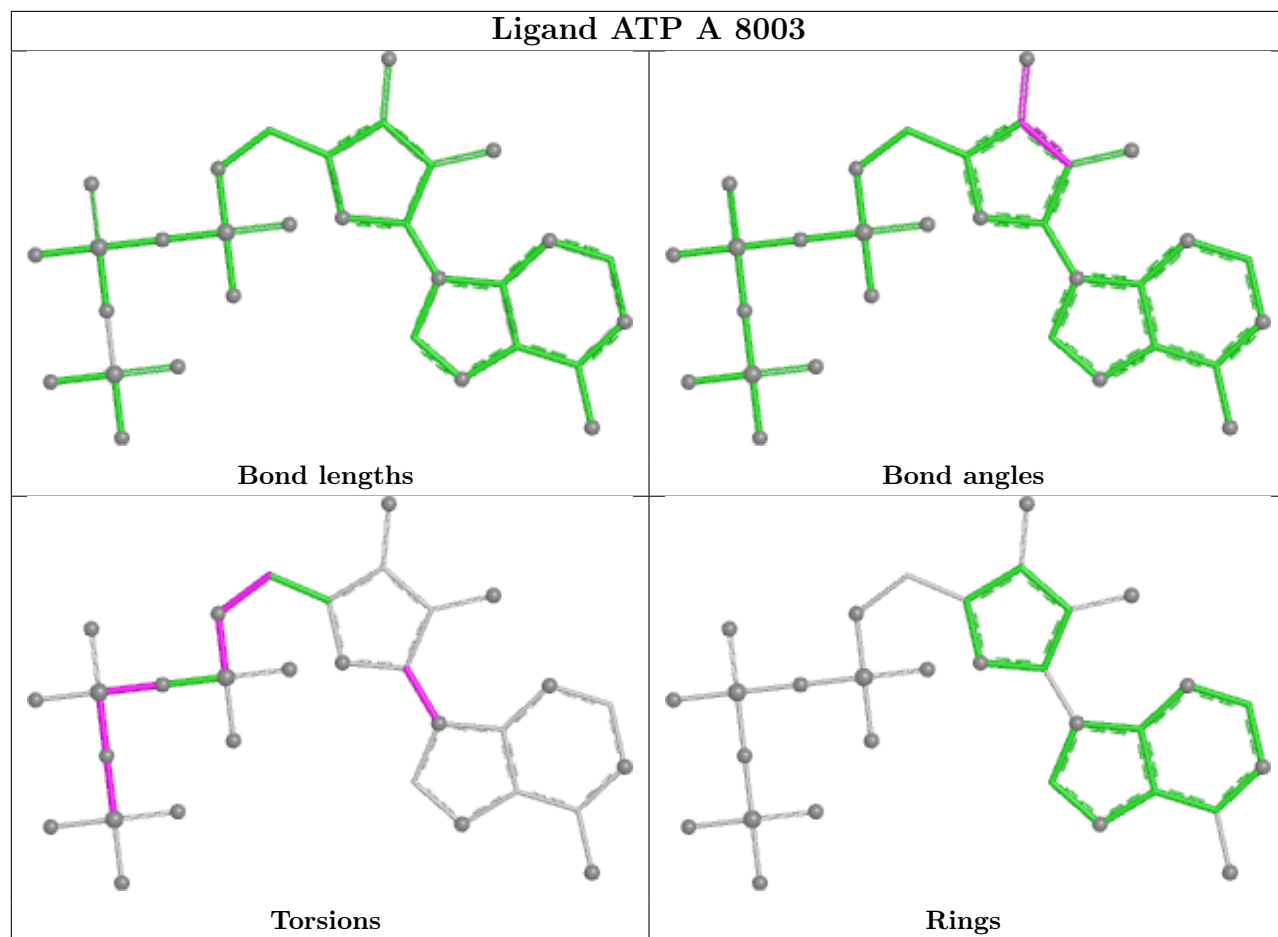
18 monomers are involved in 30 short contacts:

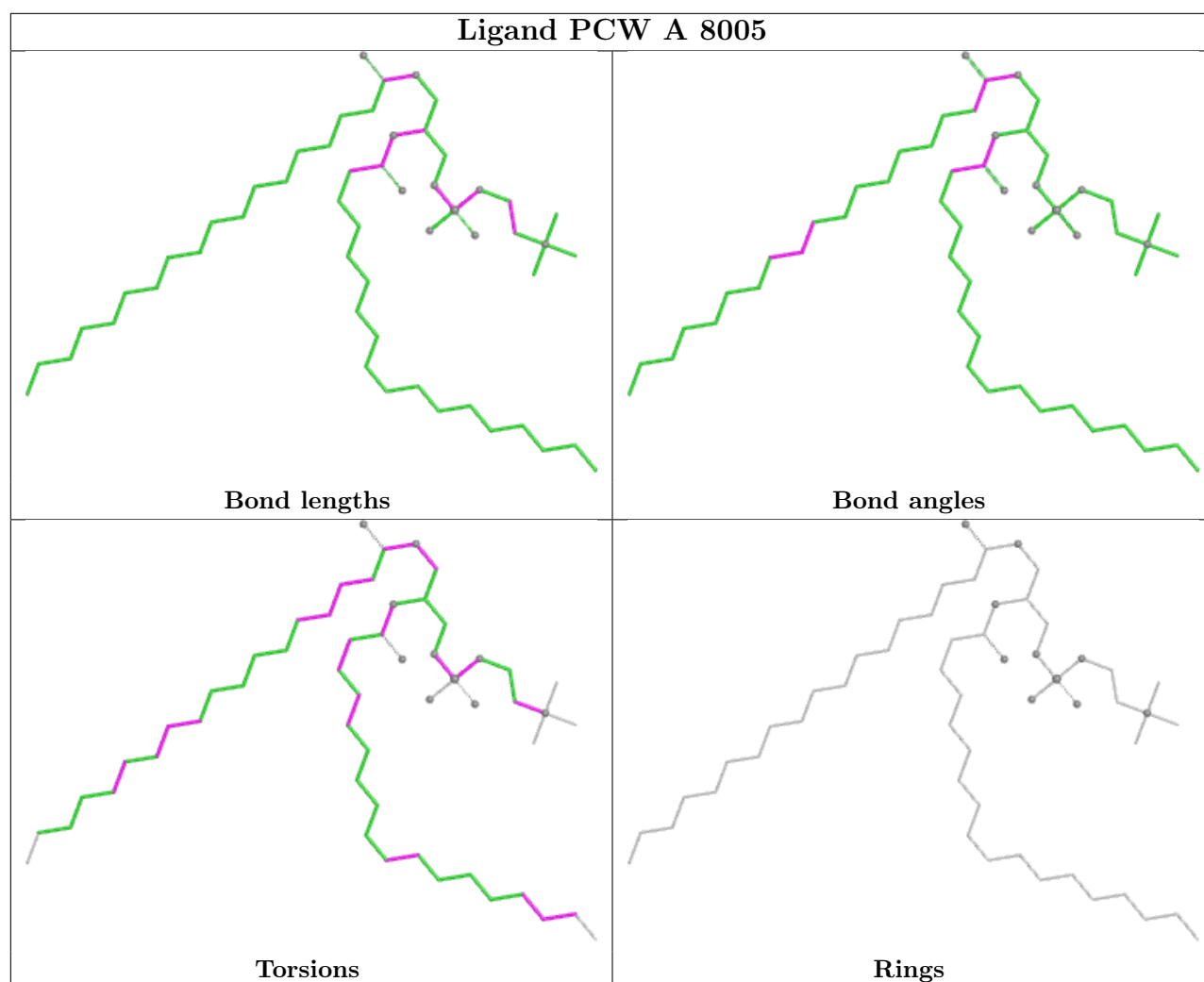
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8003	ATP	1	0
7	A	8005	PCW	2	0
8	D	8009	A1BYZ	2	0
8	A	8009	A1BYZ	2	0
7	C	8005	PCW	2	0
5	C	8003	ATP	1	0
7	C	8006	PCW	3	0
7	B	8006	PCW	3	0
8	C	8008	A1BYZ	1	0
7	B	8005	PCW	2	0
7	D	8005	PCW	2	0
5	D	8003	ATP	1	0
7	A	8006	PCW	3	0
7	D	8006	PCW	3	0
5	B	8003	ATP	1	0
8	B	8009	A1BYZ	2	0
8	B	8008	A1BYZ	1	0
8	C	8009	A1BYZ	2	0

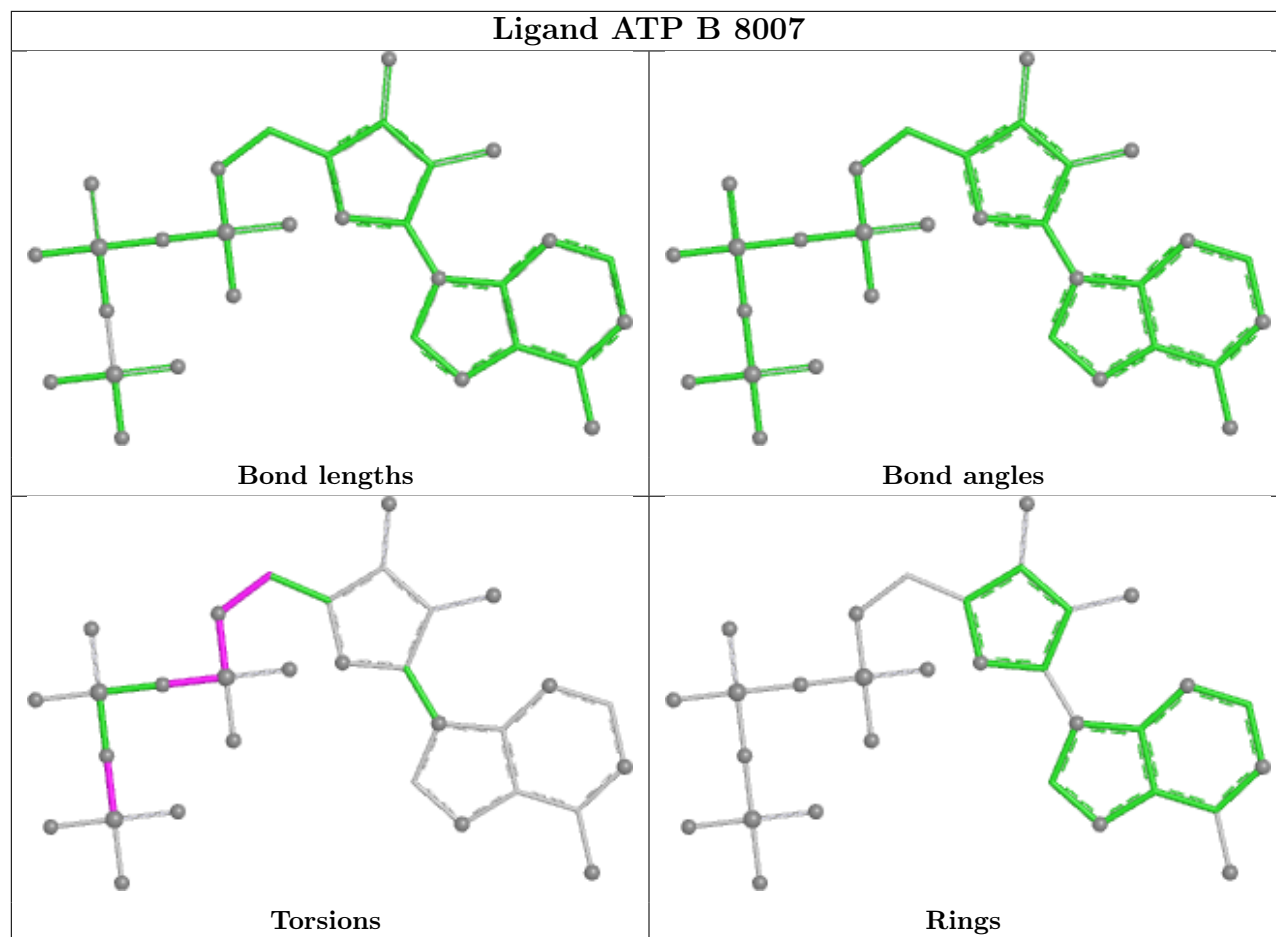
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

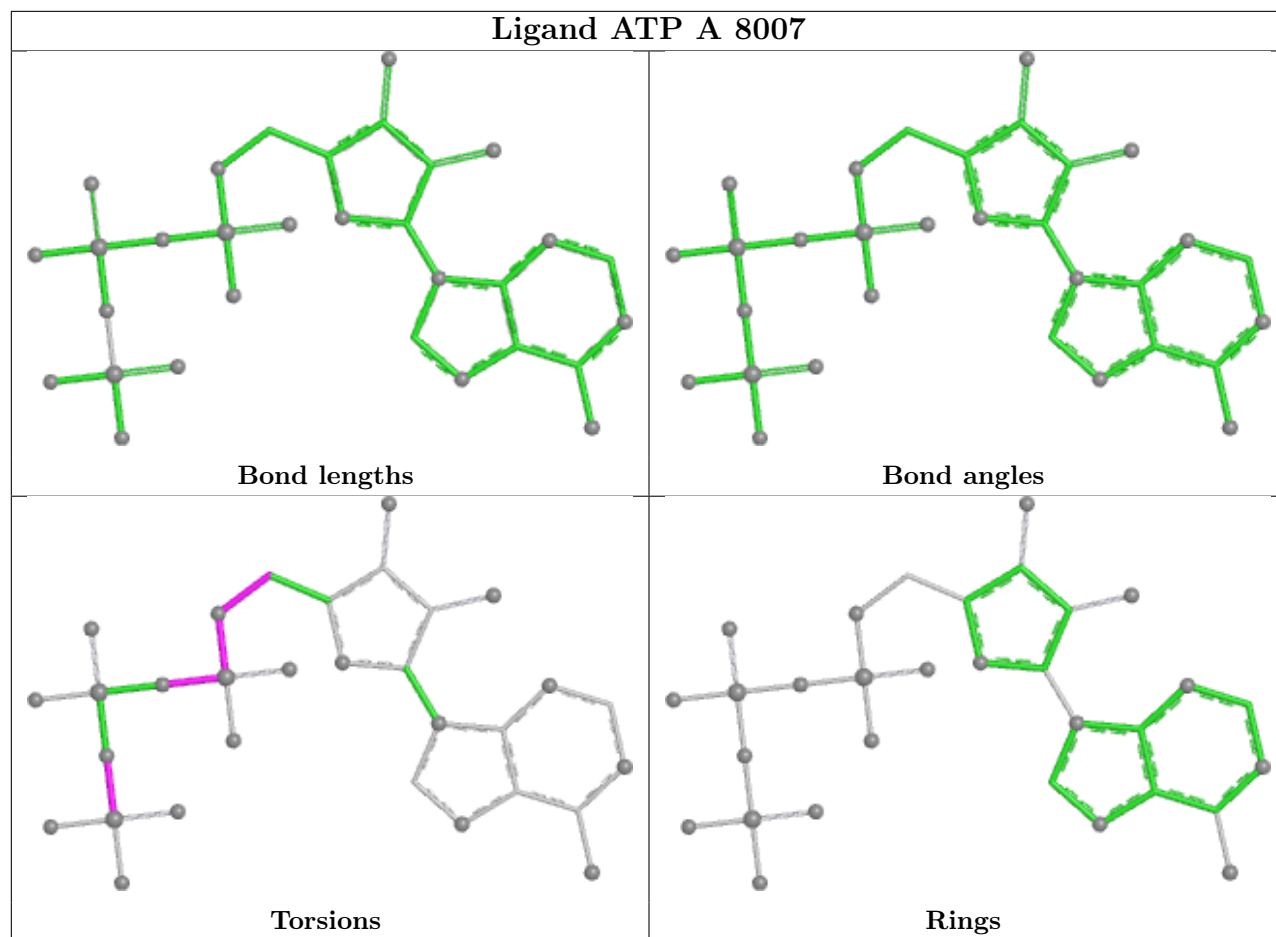
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

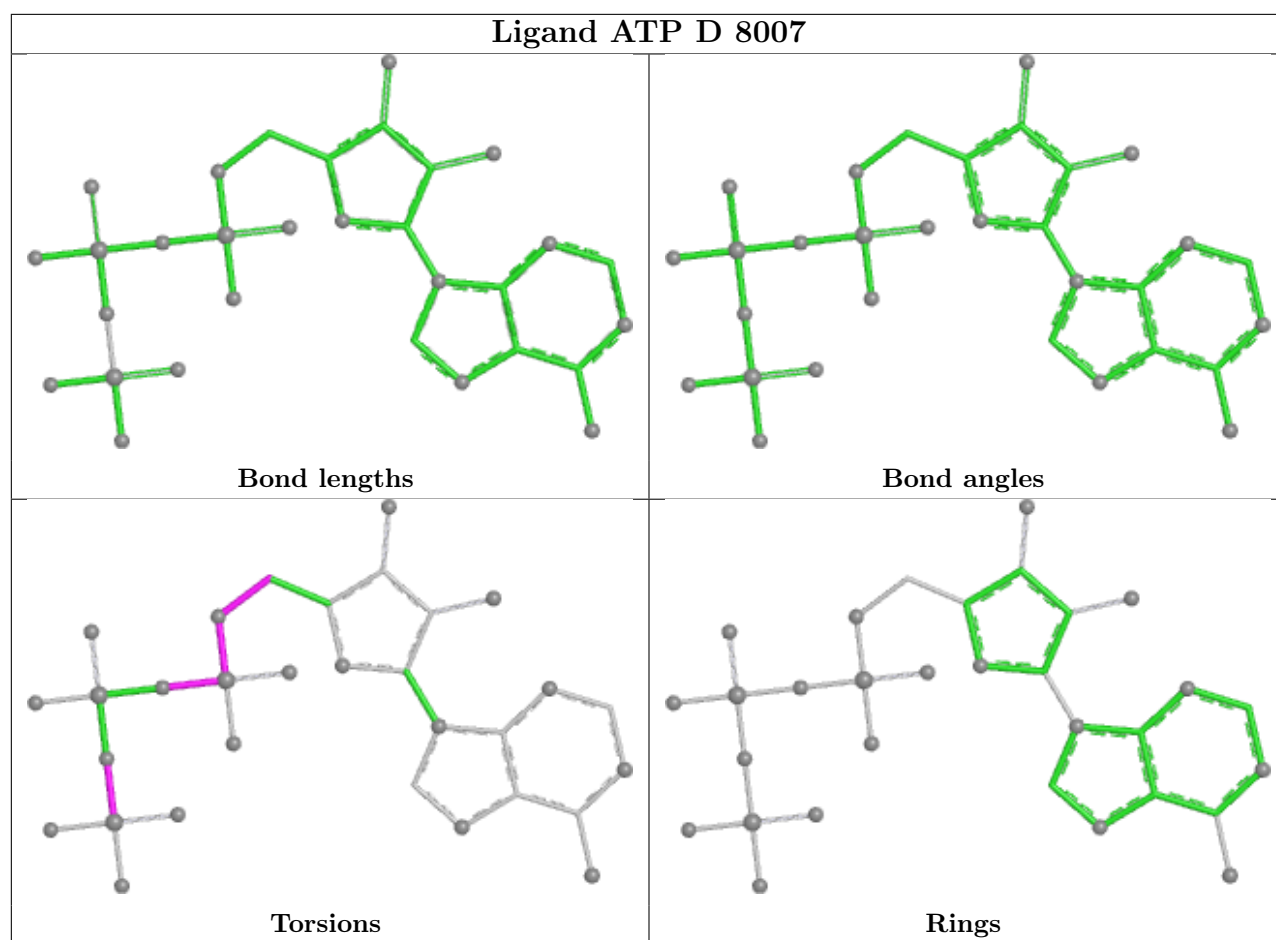




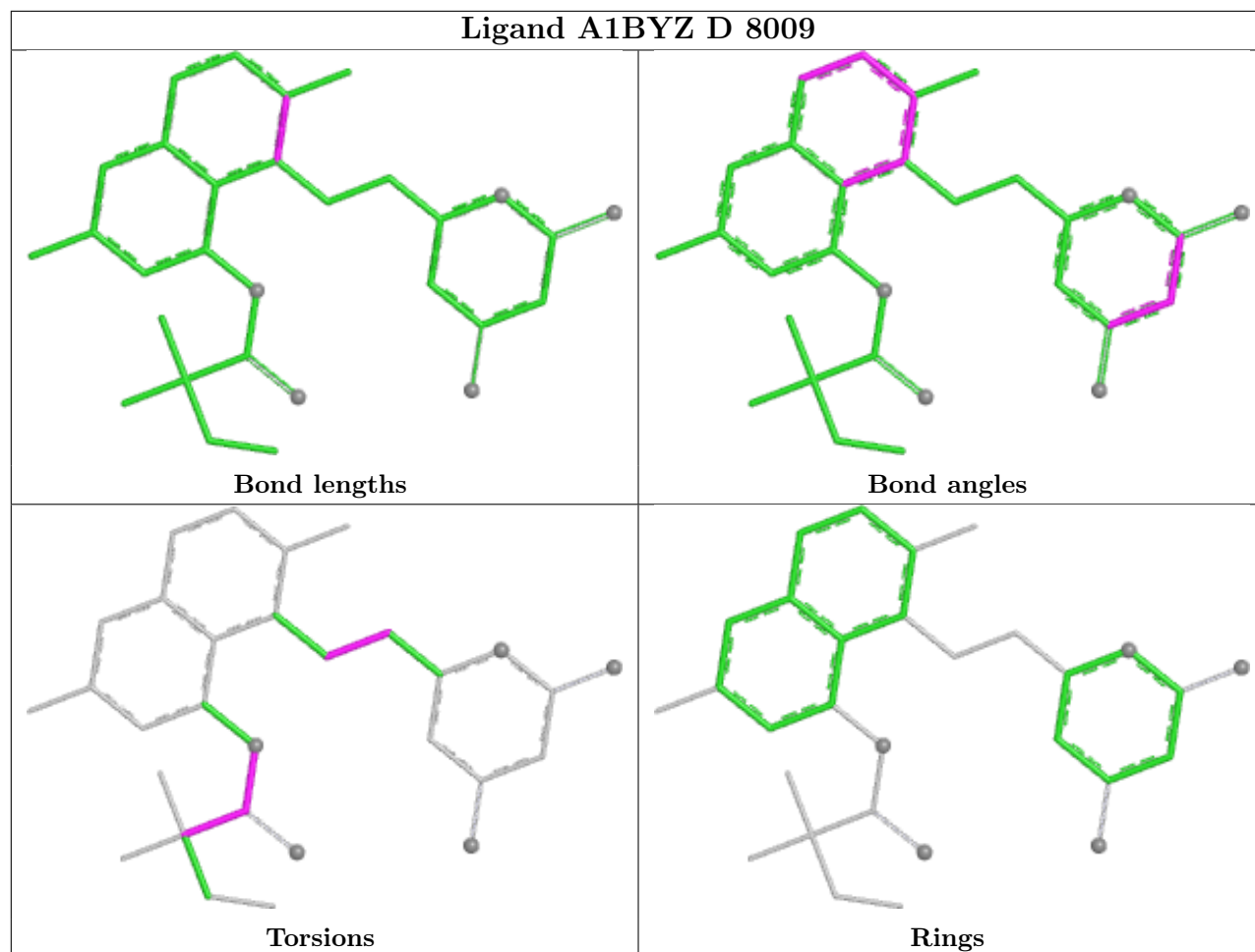




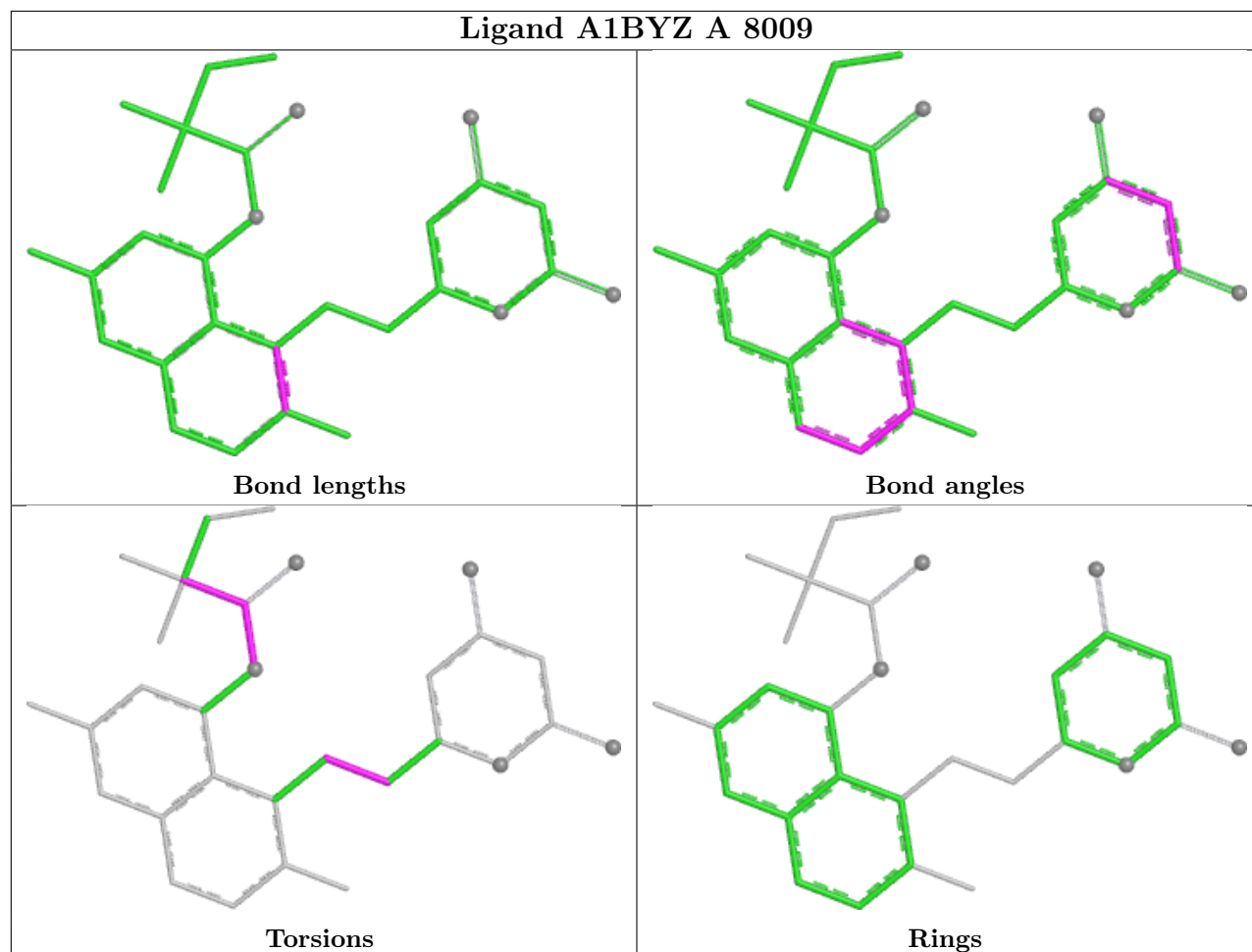


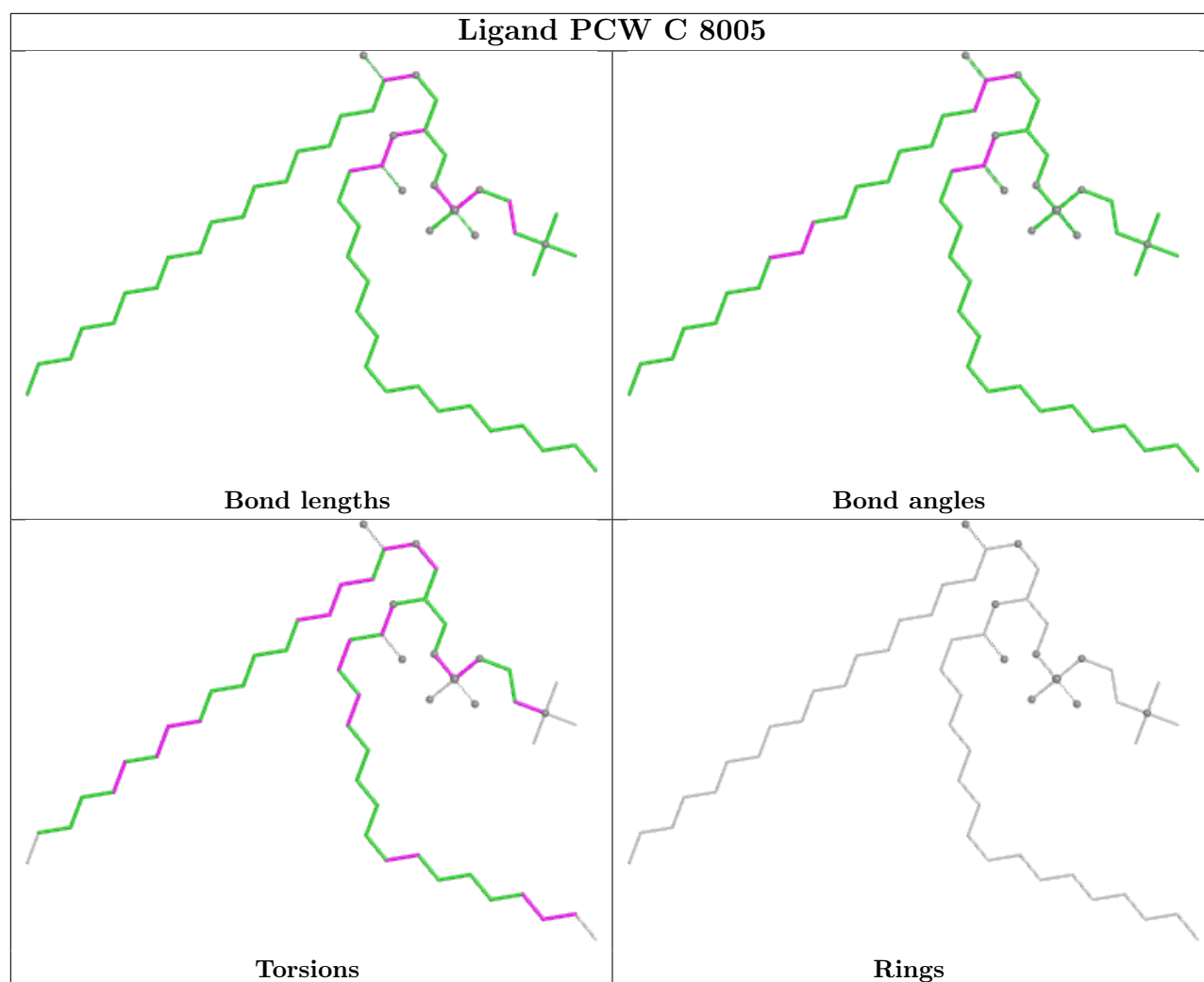


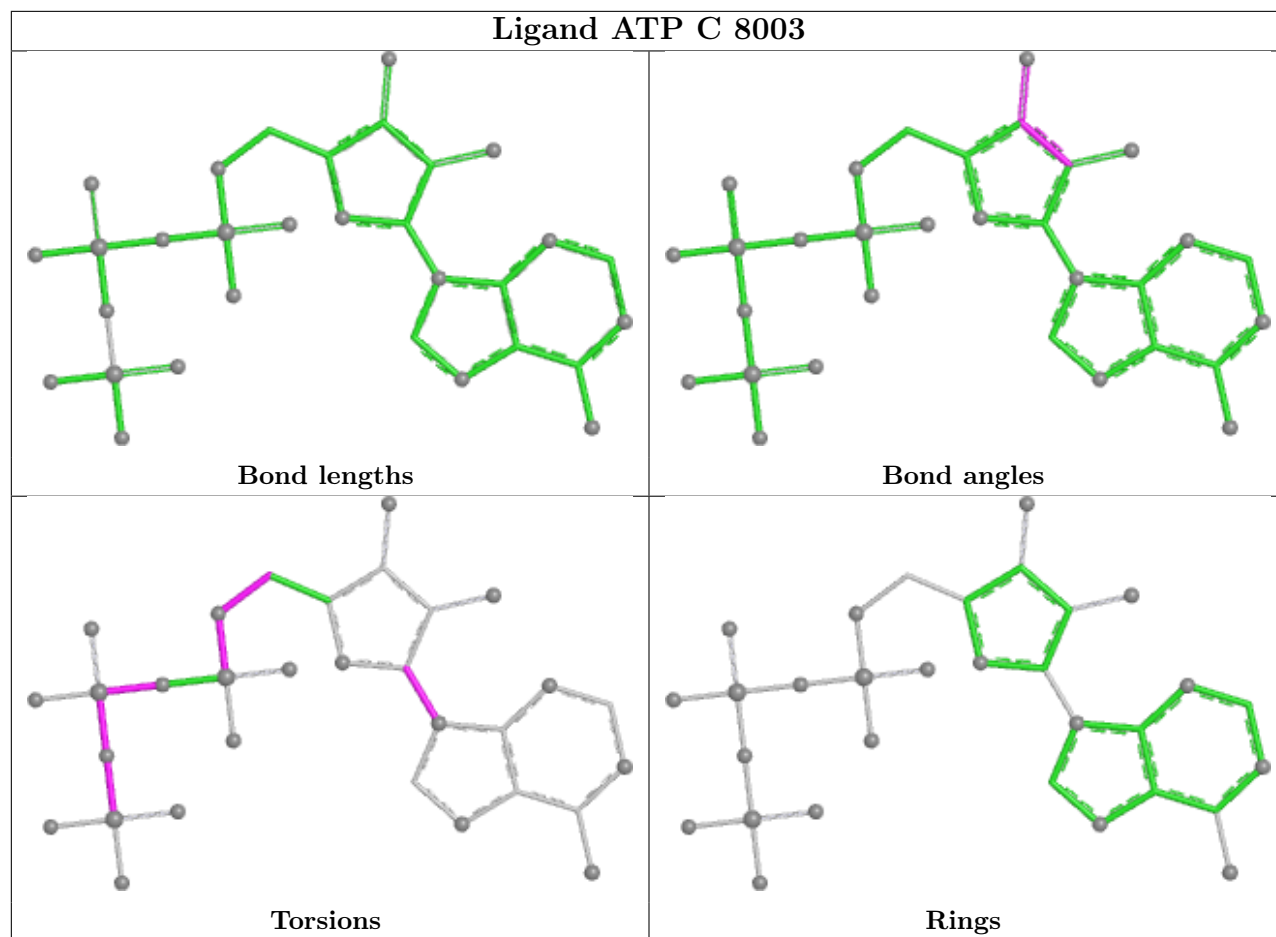
Ligand A1BYZ D 8009

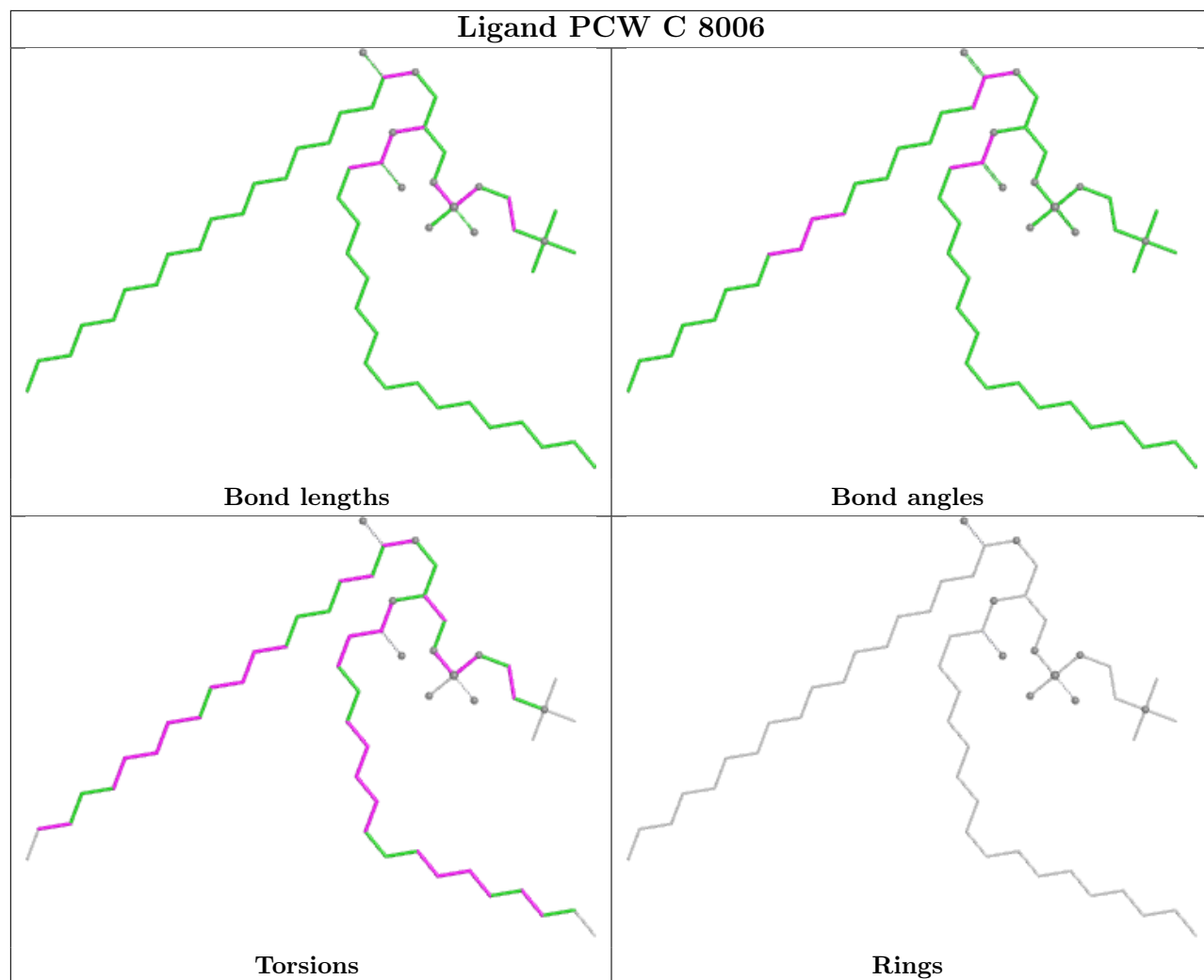


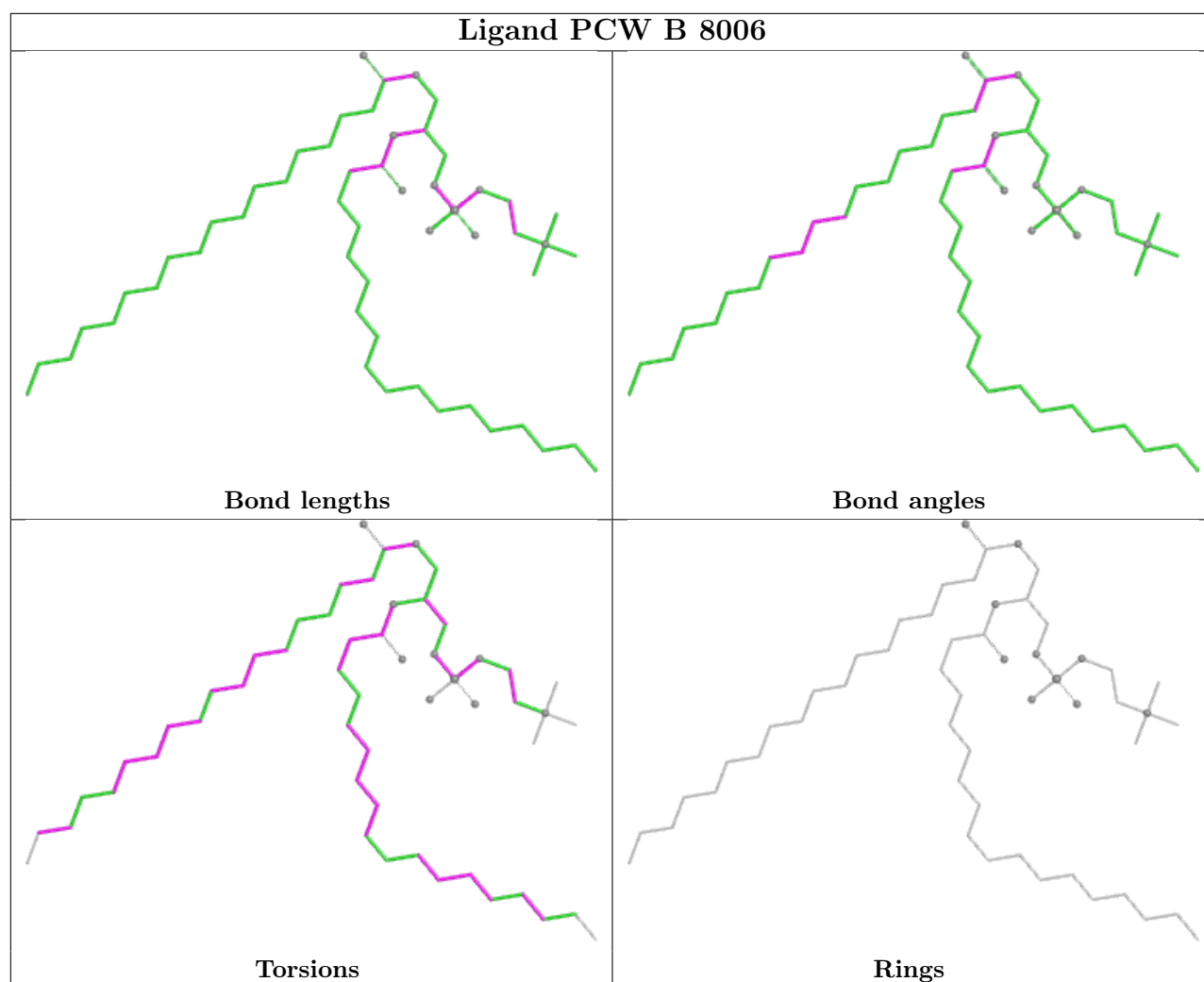
Ligand A1BYZ A 8009

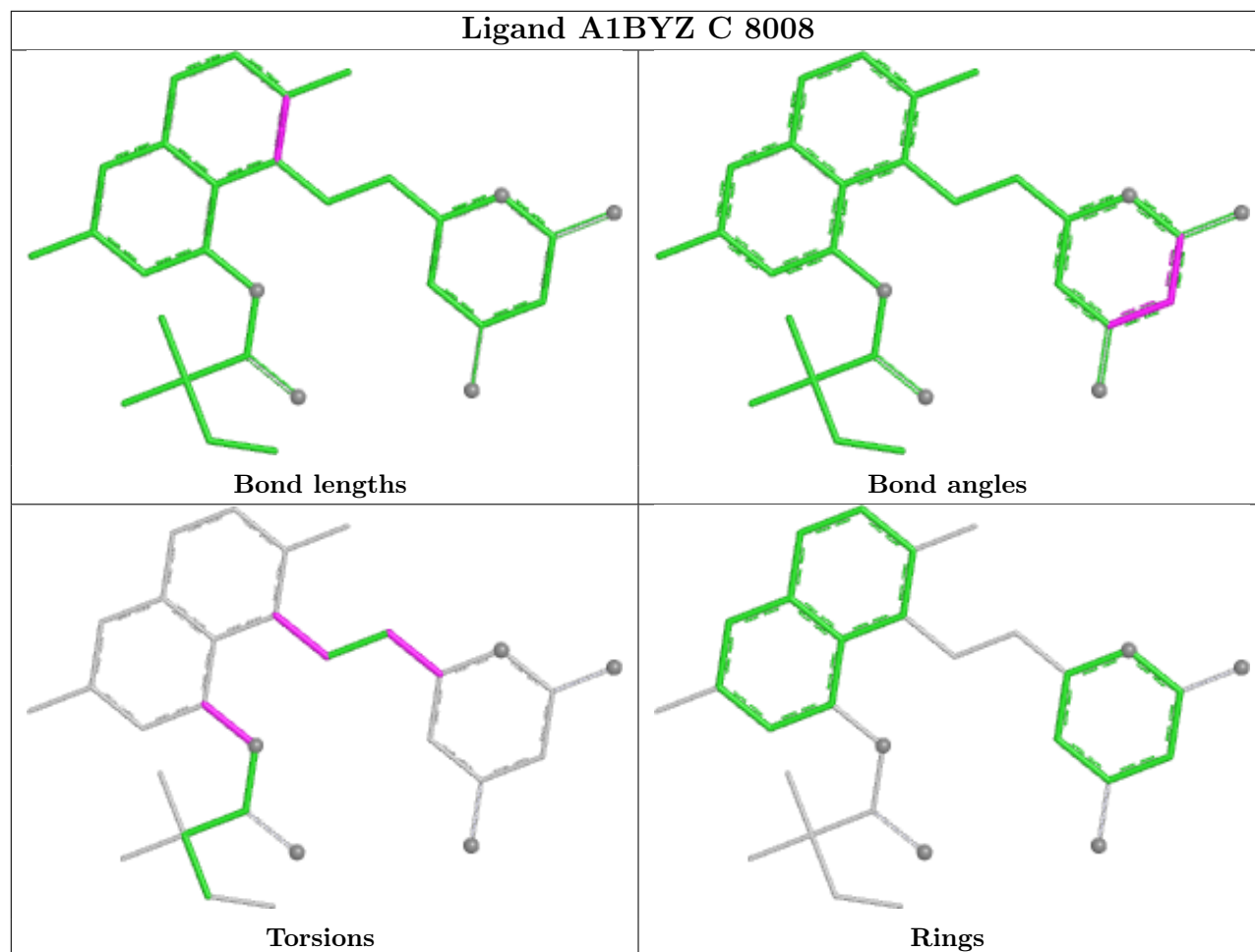


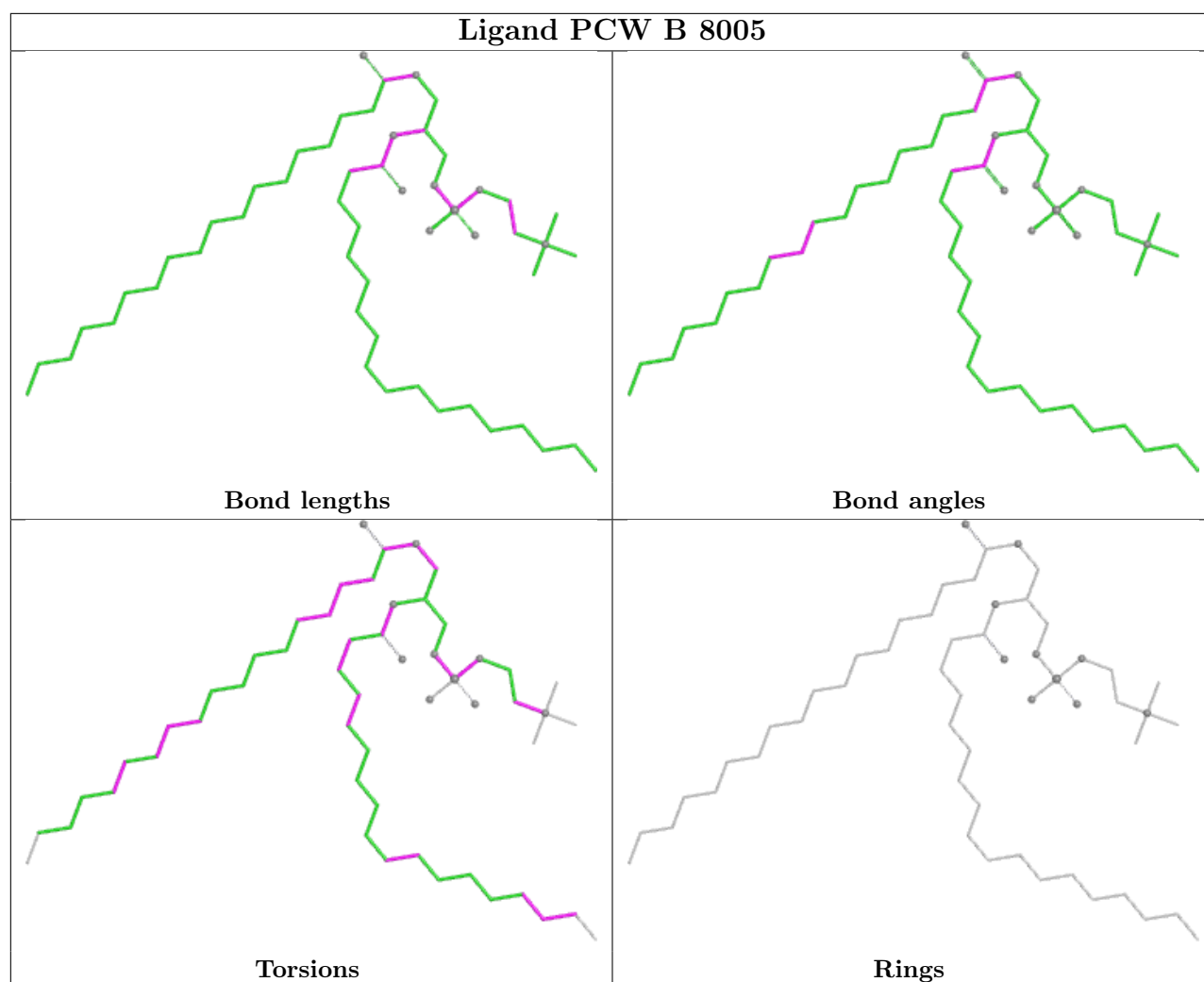


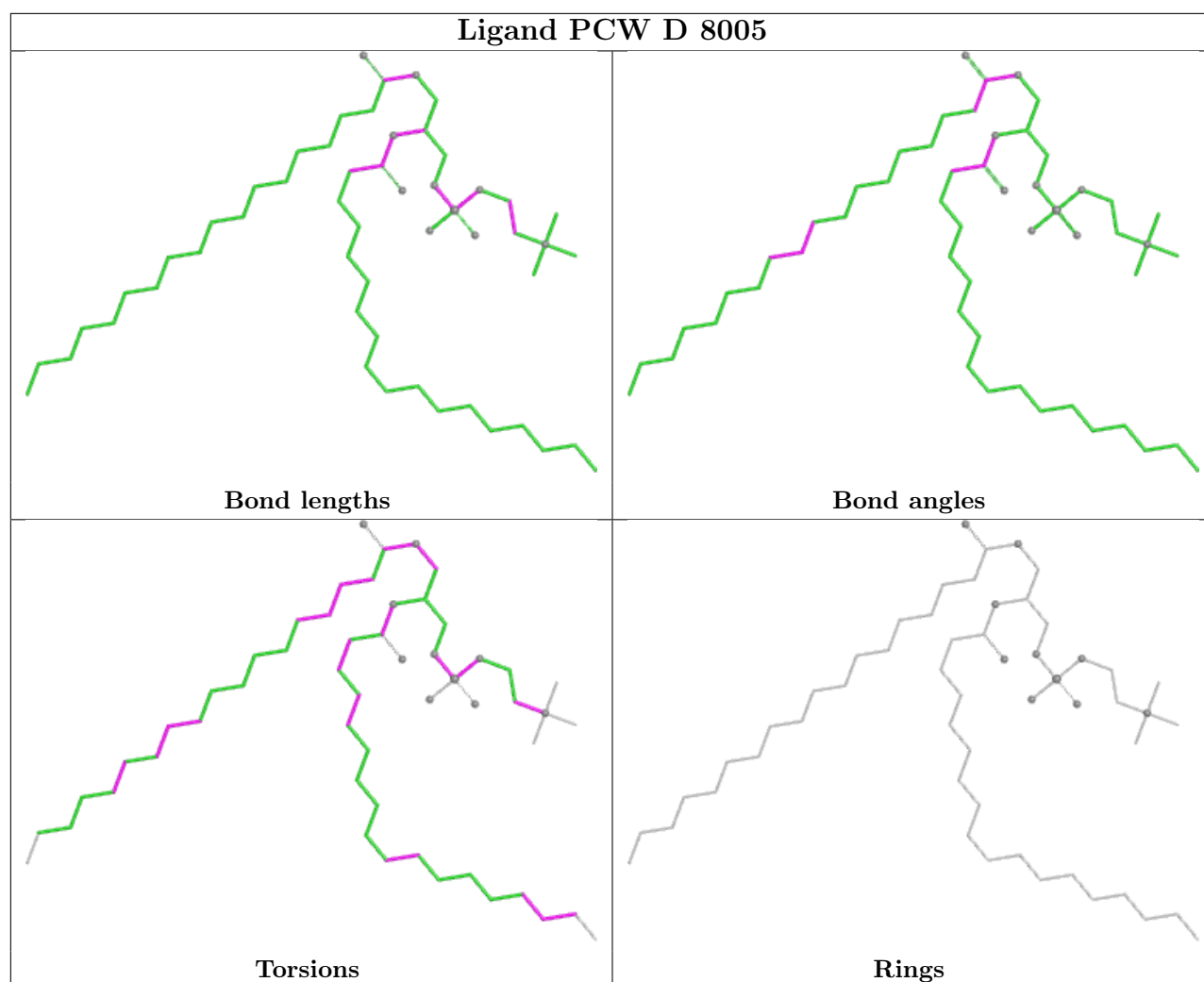


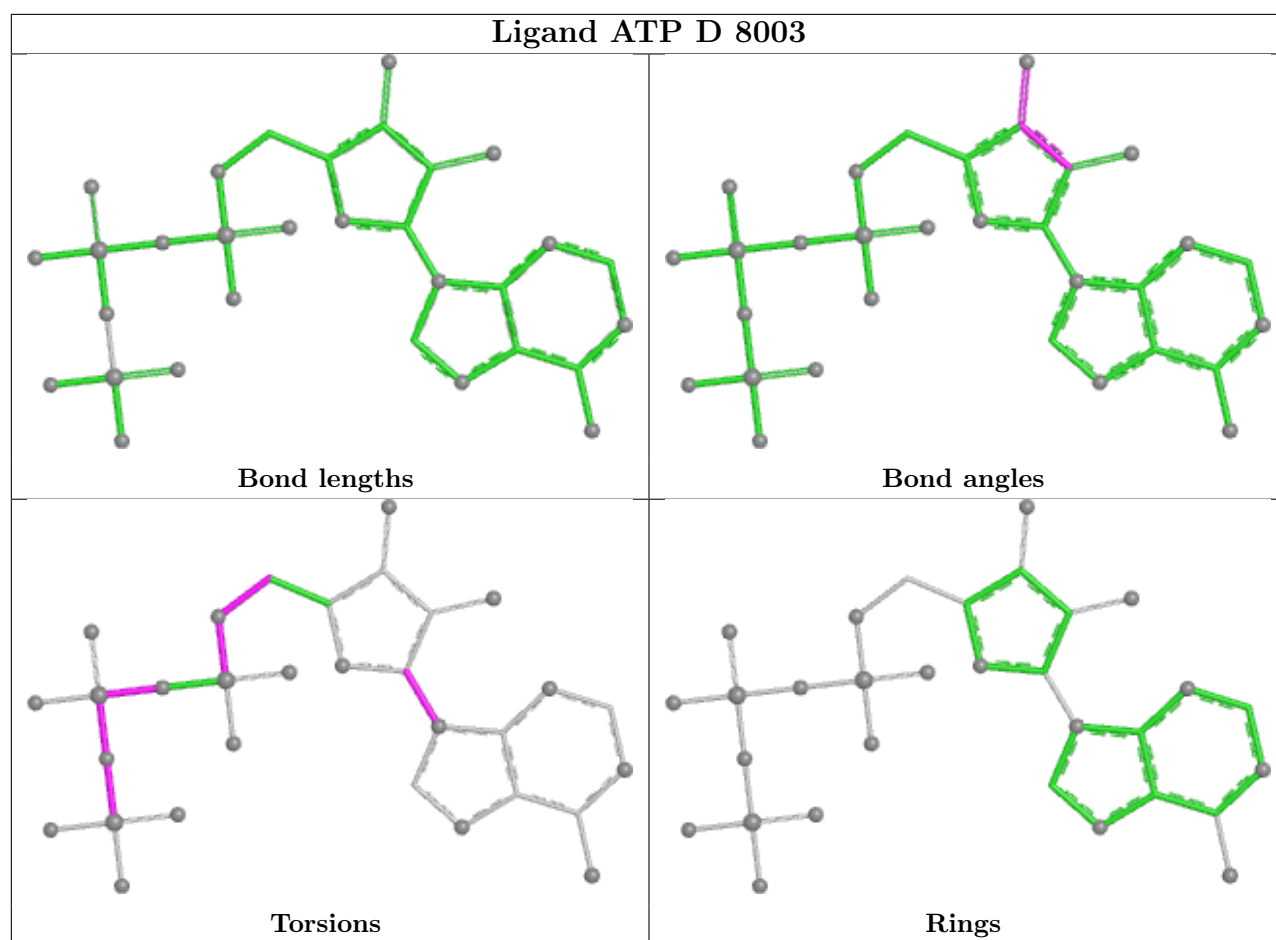


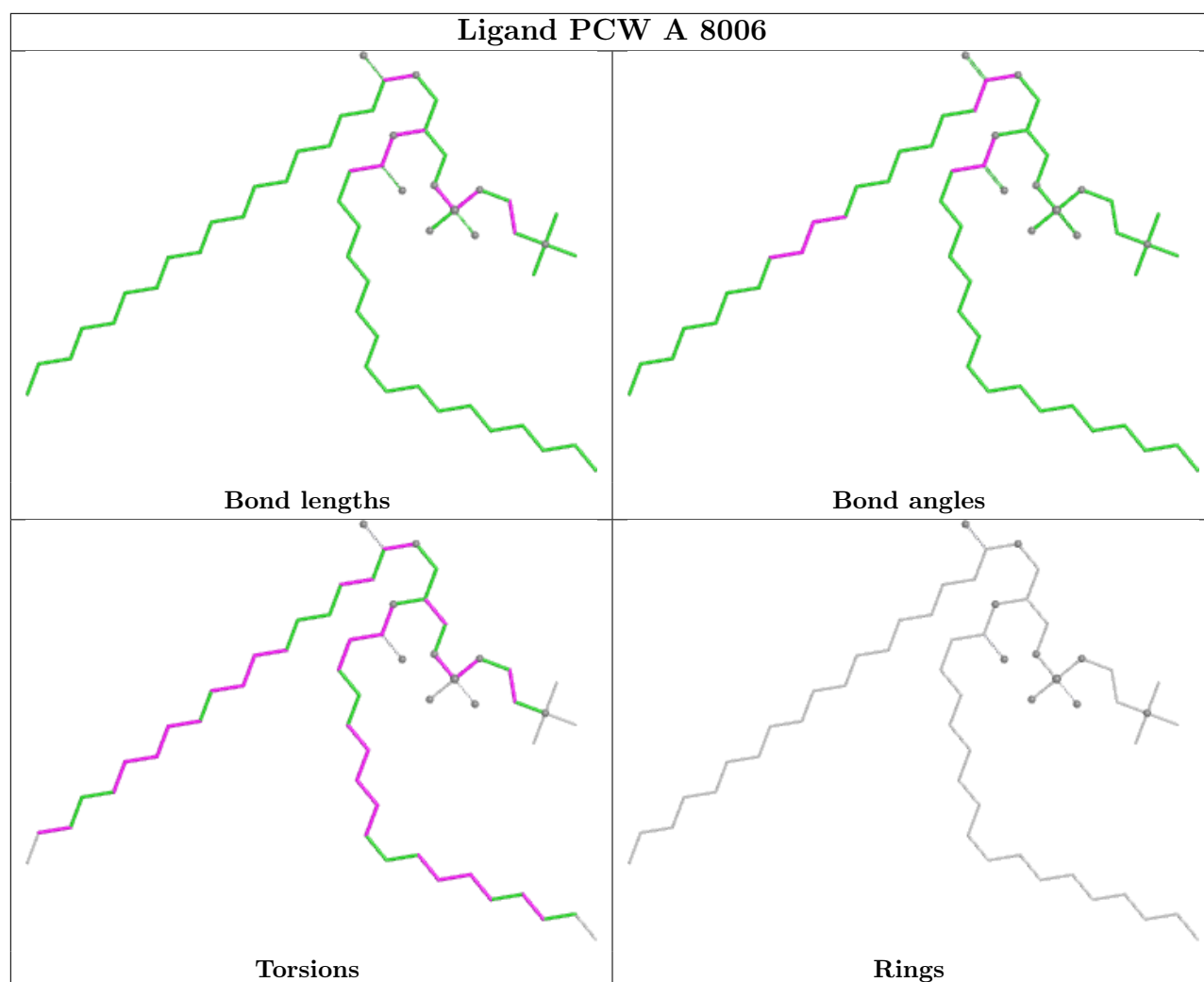


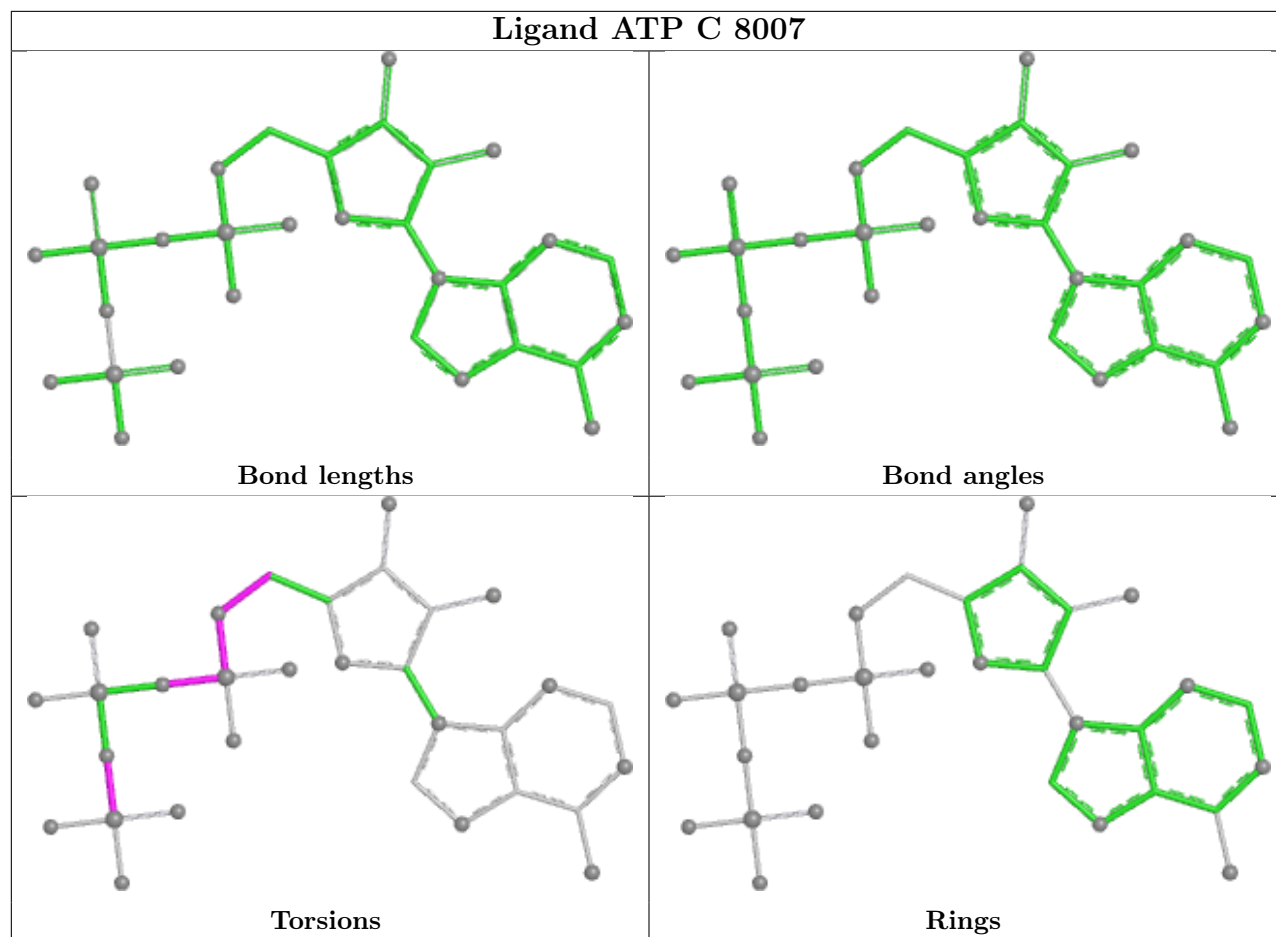


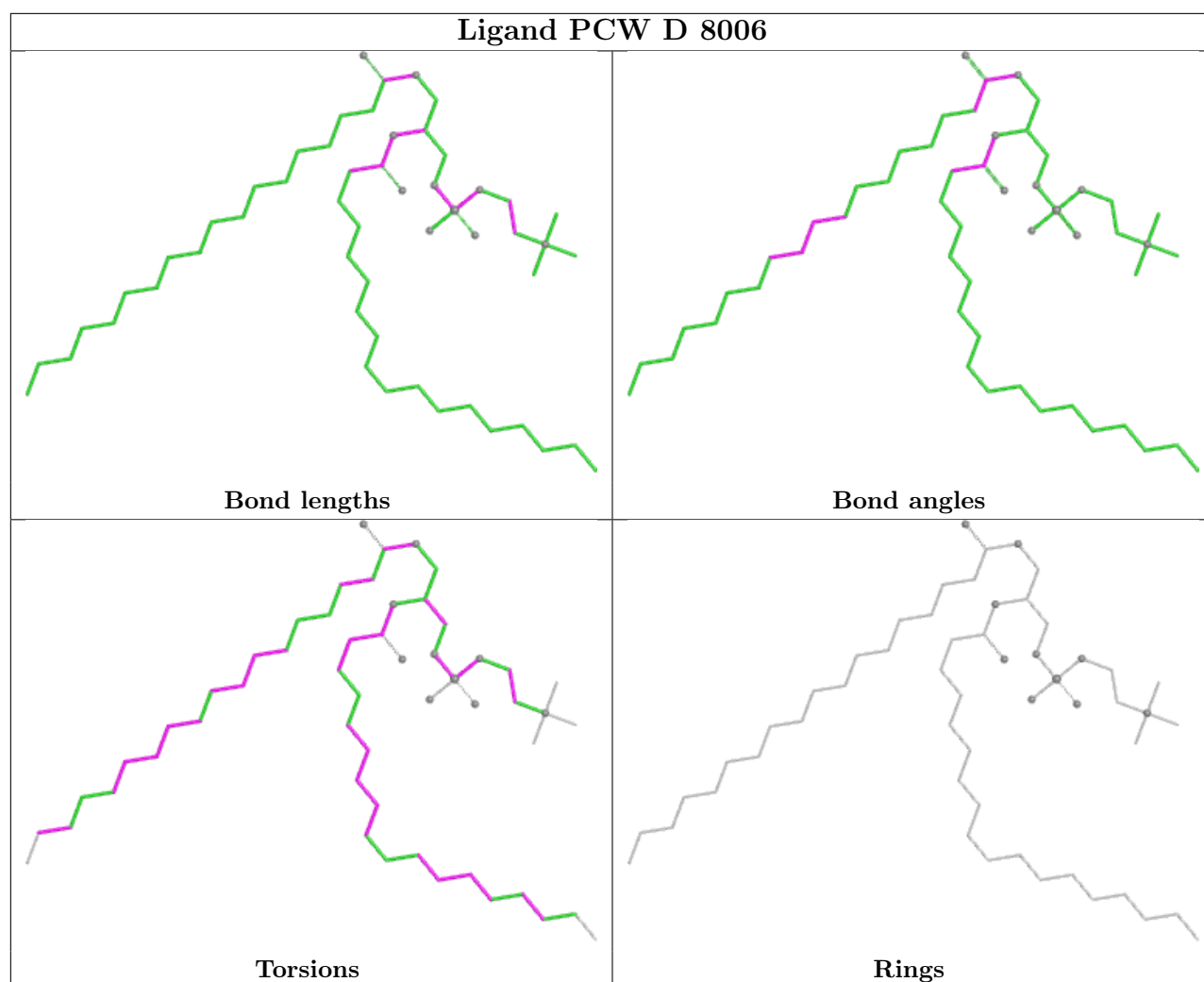


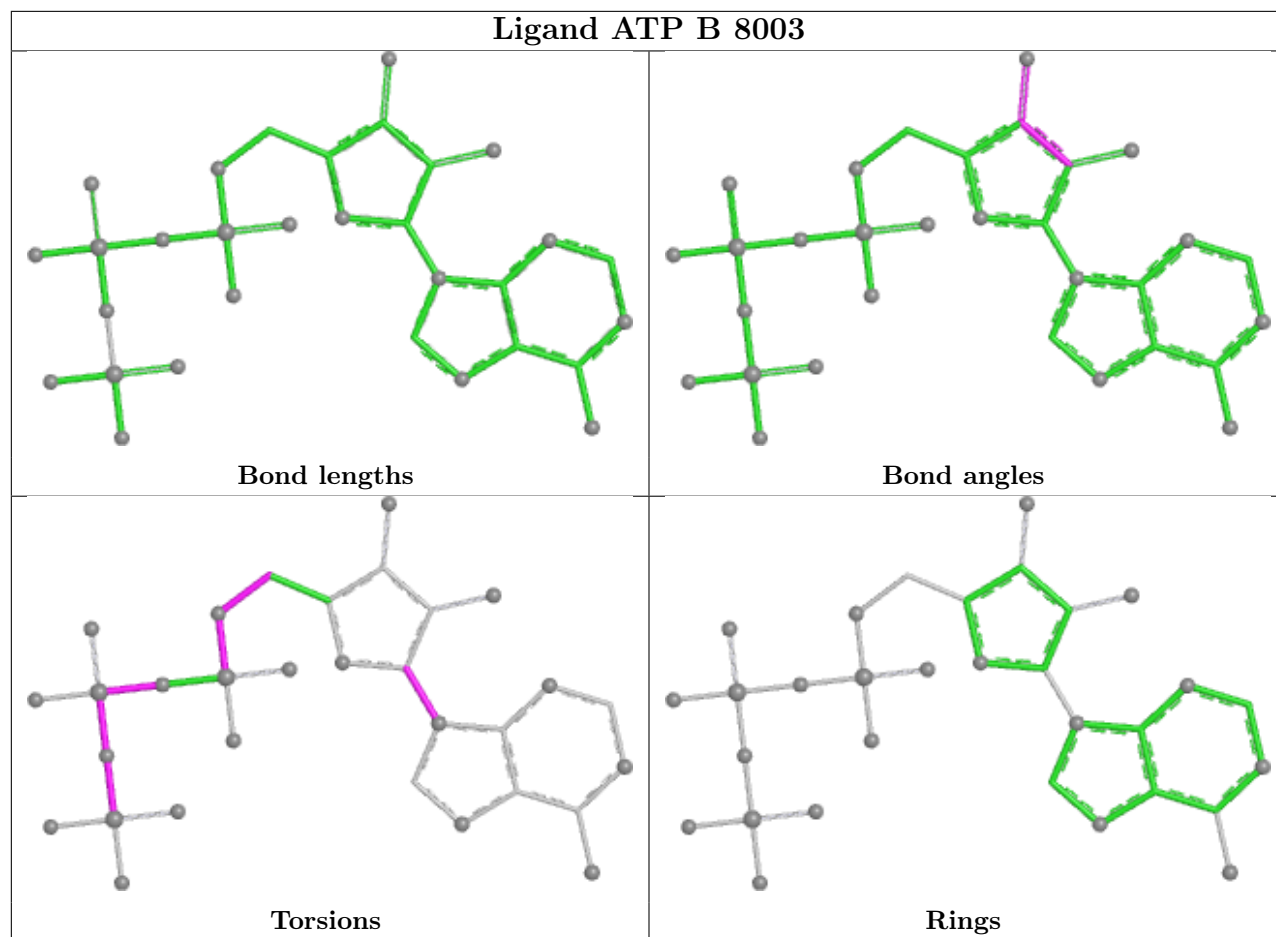




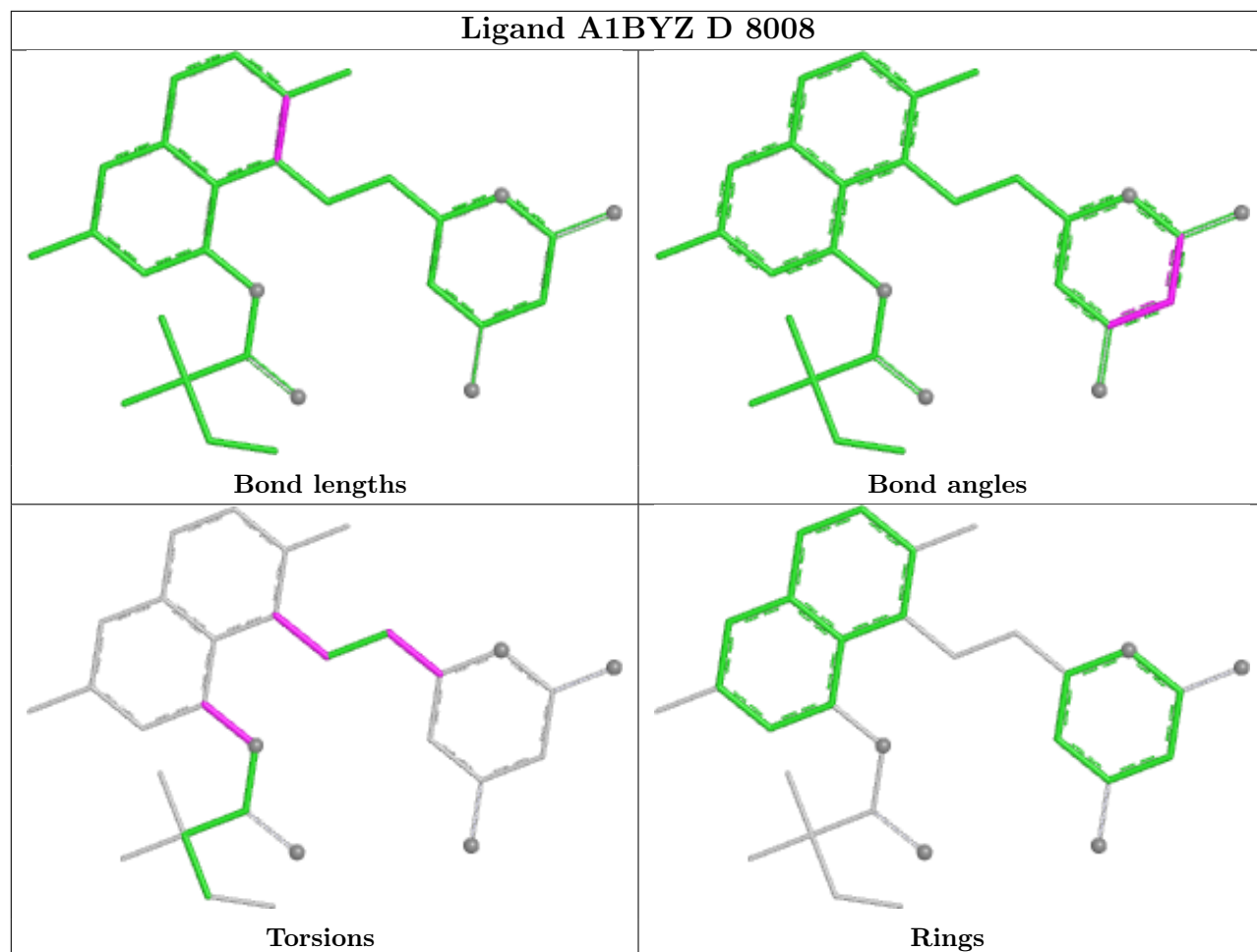




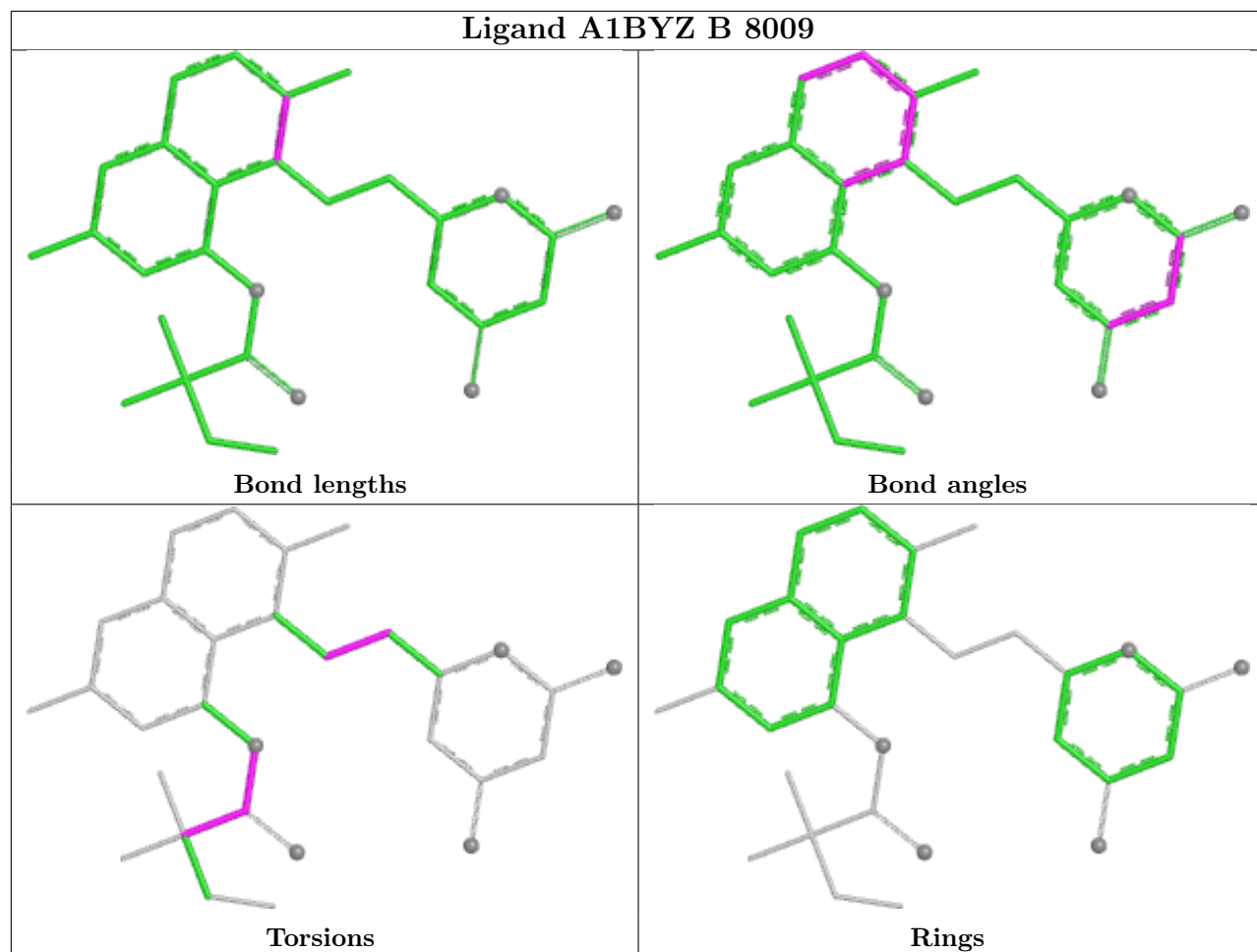




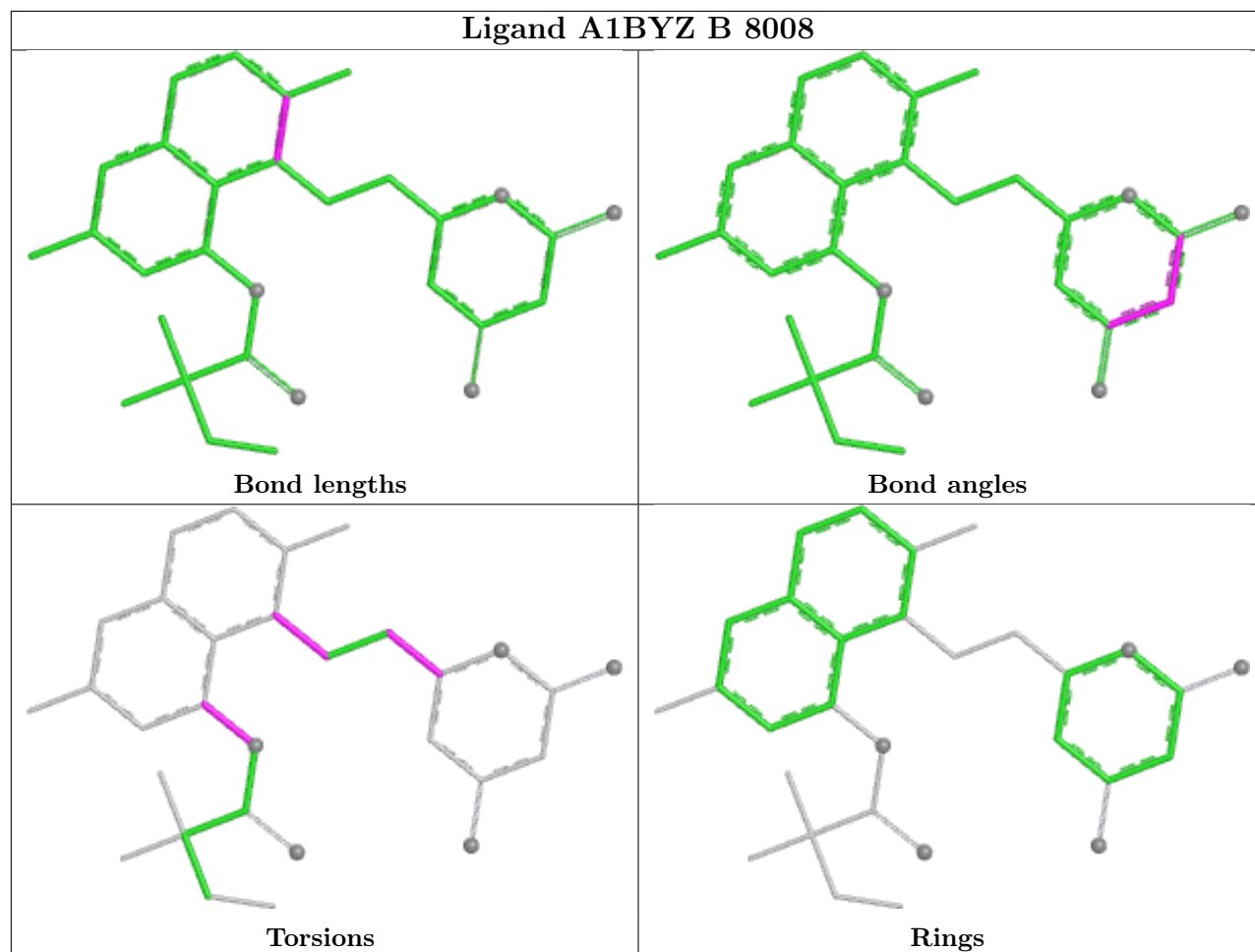
Ligand A1BYZ D 8008

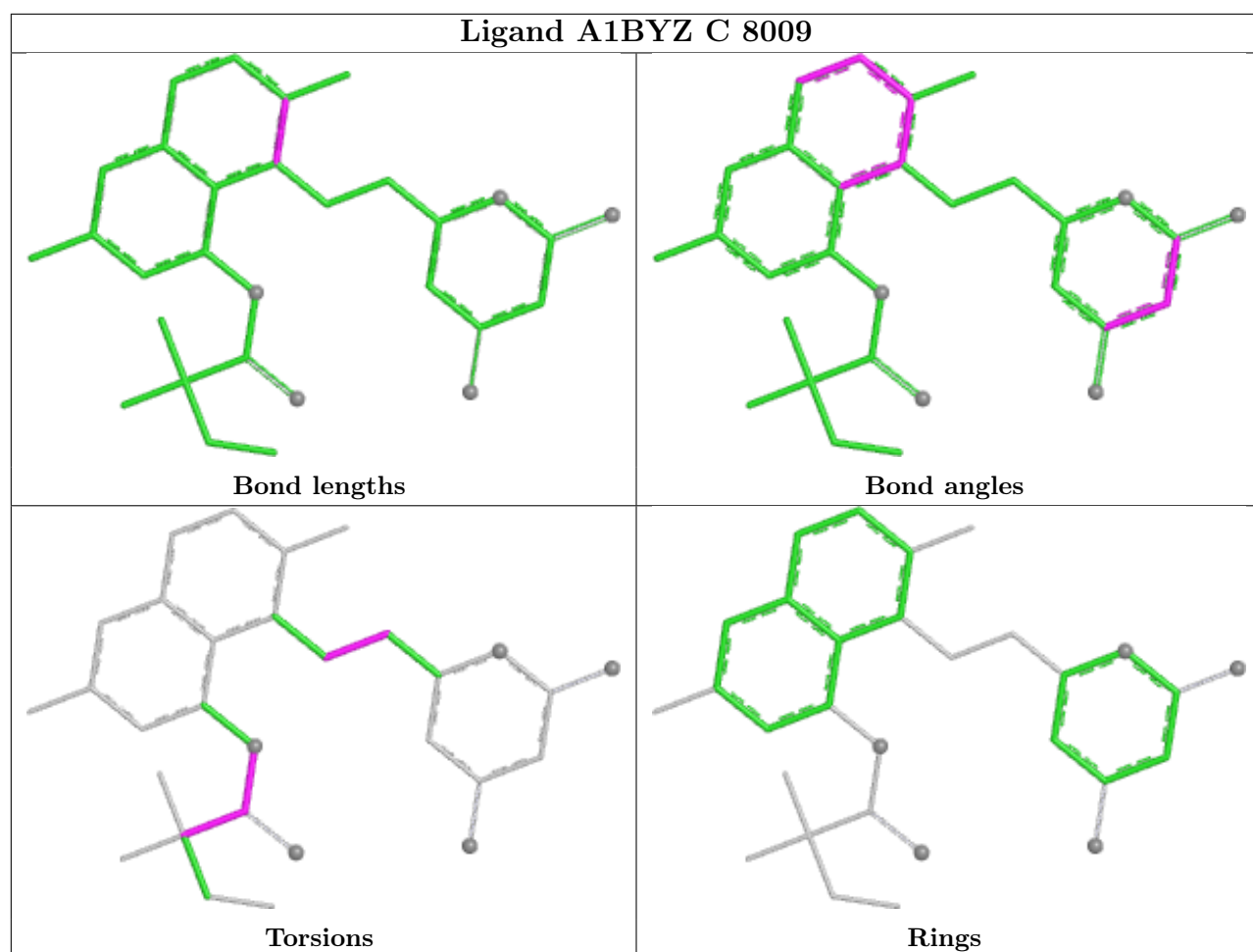


Ligand A1BYZ B 8009



Ligand A1BYZ B 8008





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.

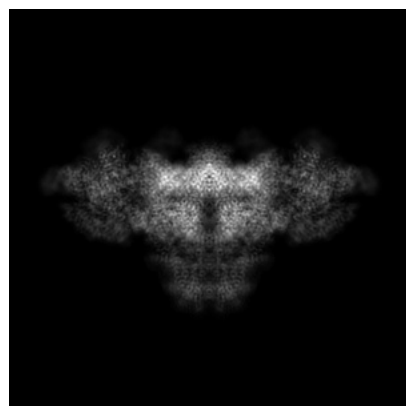
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49536. These allow visual inspection of the internal detail of the map and identification of artifacts.

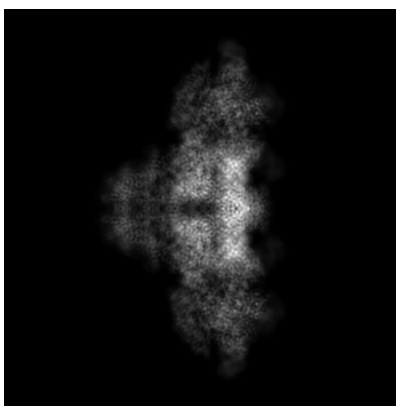
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

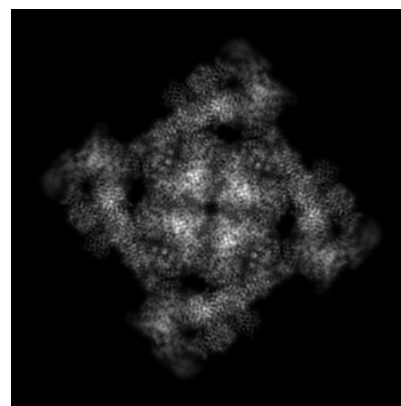
6.1.1 Primary map



X

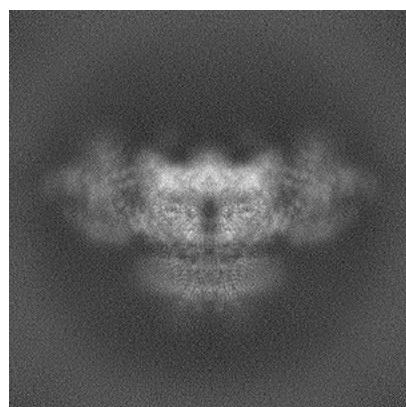


Y

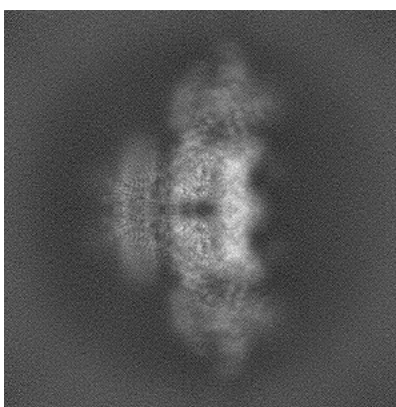


Z

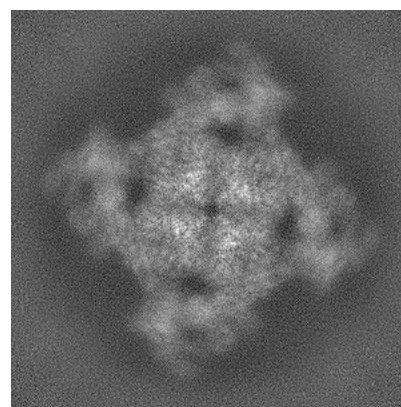
6.1.2 Raw map



X



Y



Z

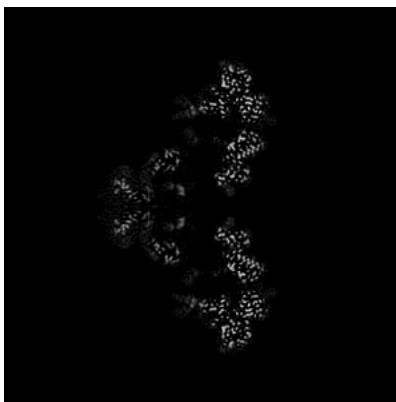
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

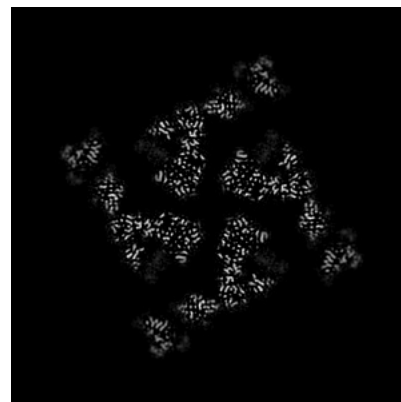
6.2.1 Primary map



X Index: 256



Y Index: 256

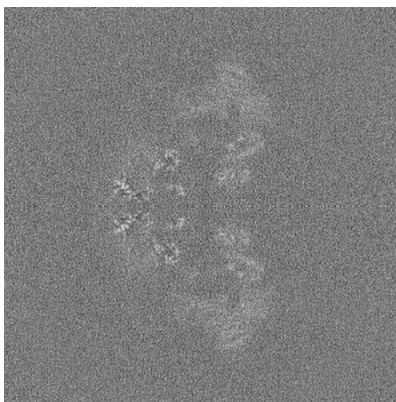


Z Index: 256

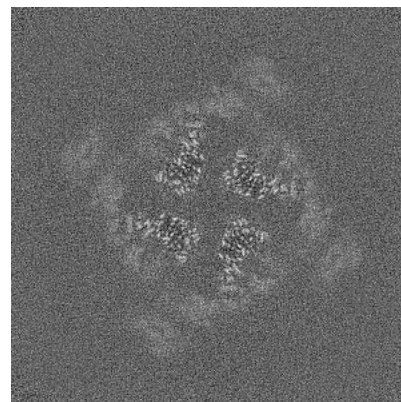
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

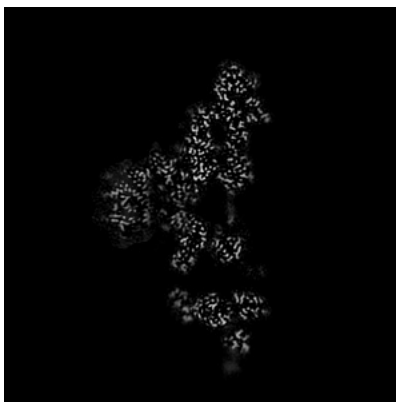
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

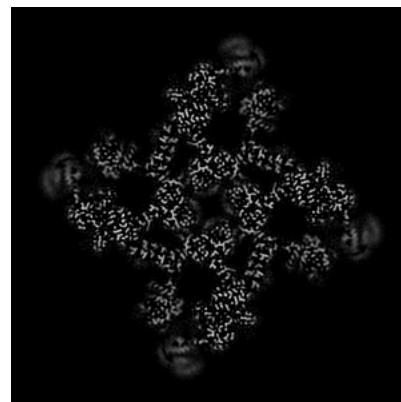
6.3.1 Primary map



X Index: 238

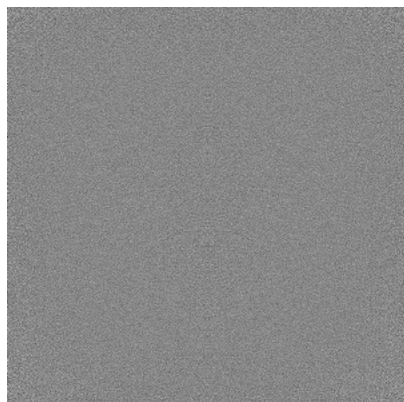


Y Index: 274

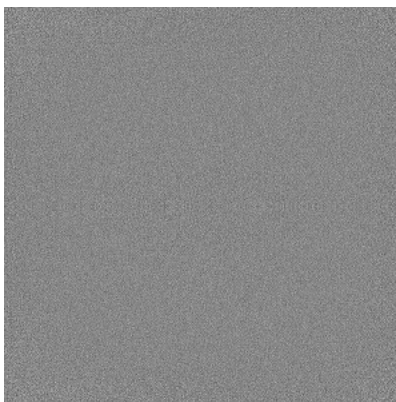


Z Index: 287

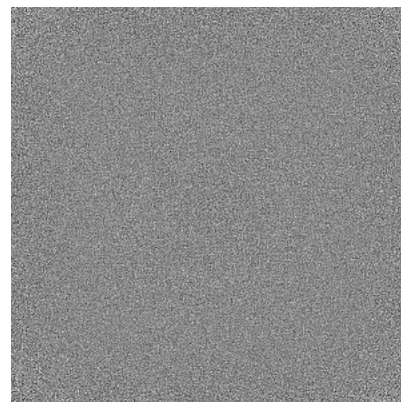
6.3.2 Raw map



X Index: 0



Y Index: 0

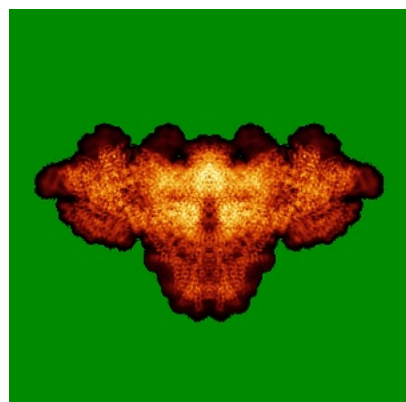


Z Index: 0

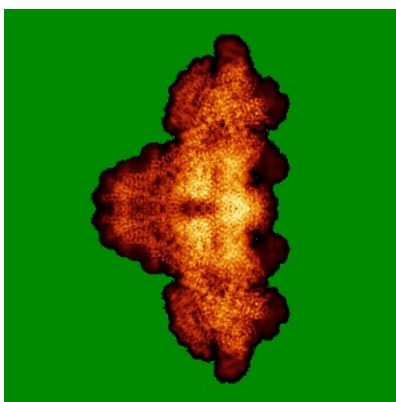
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

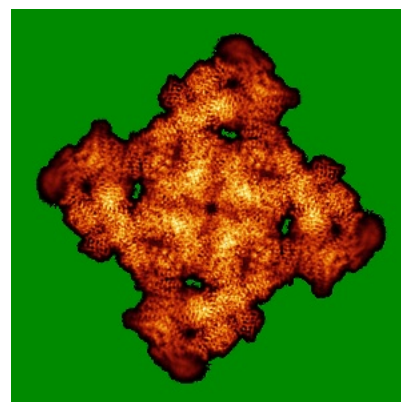
6.4.1 Primary map



X

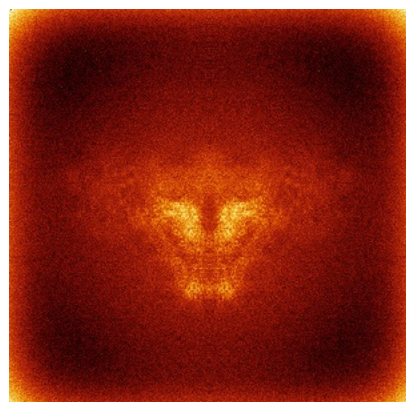


Y

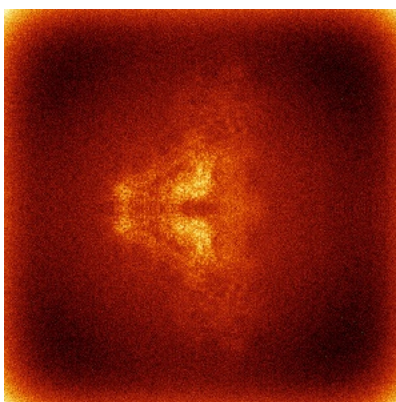


Z

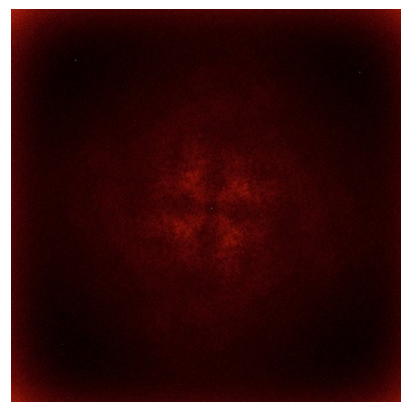
6.4.2 Raw map



X



Y

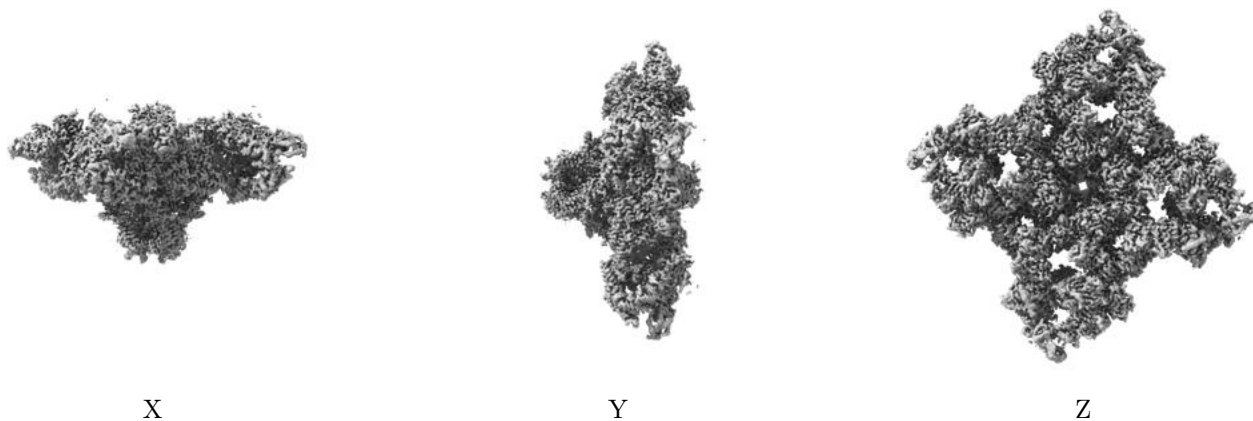


Z

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

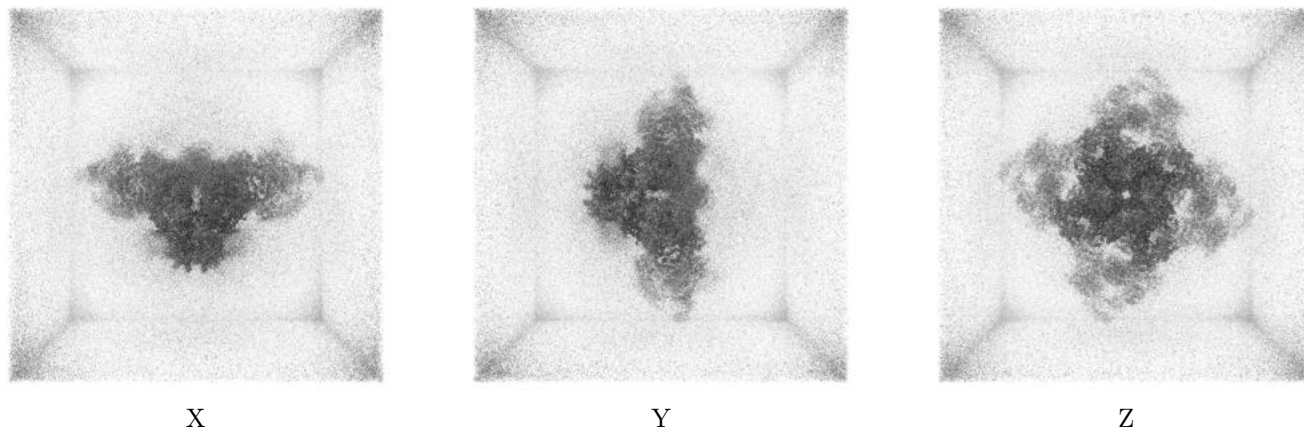
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

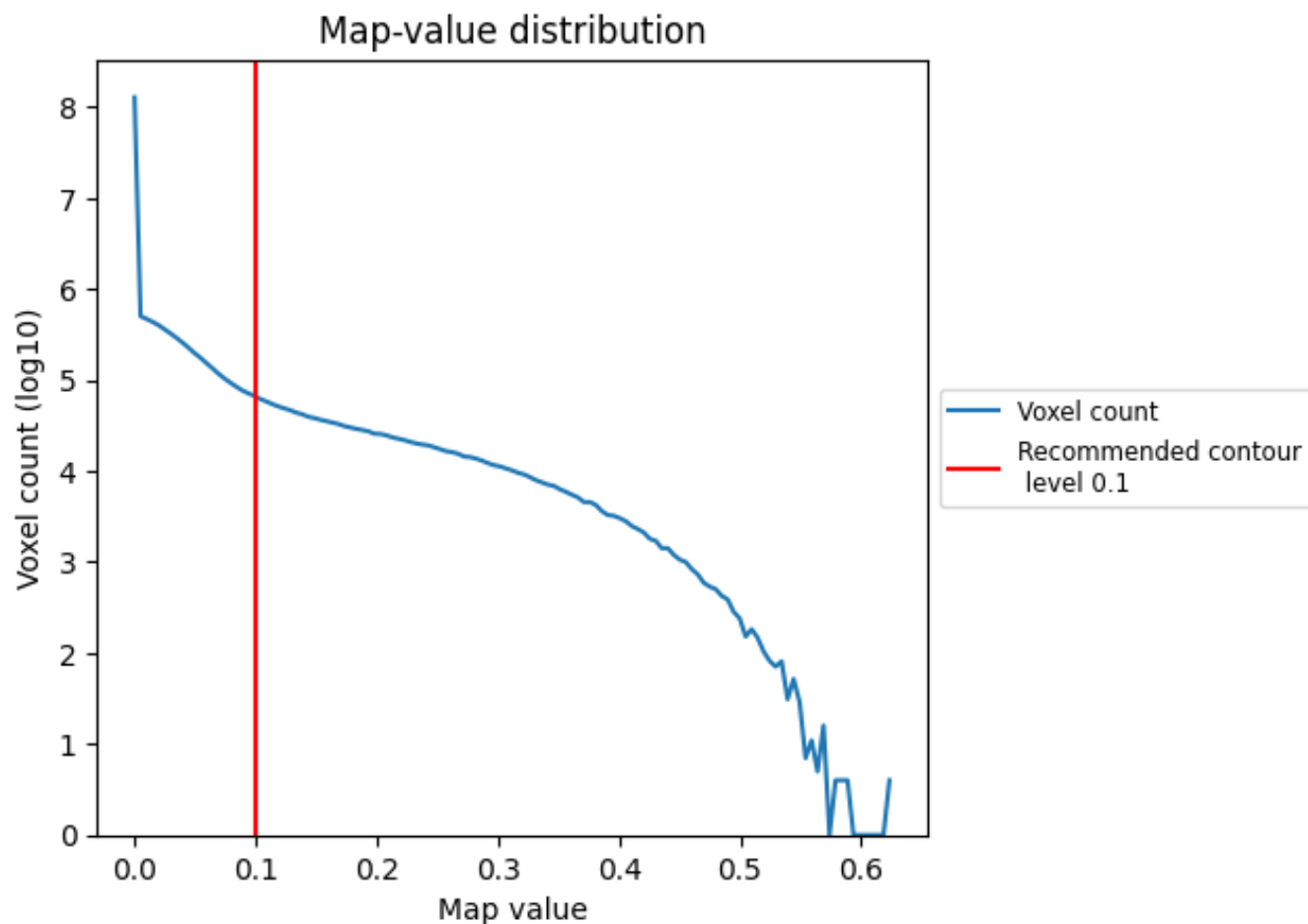
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

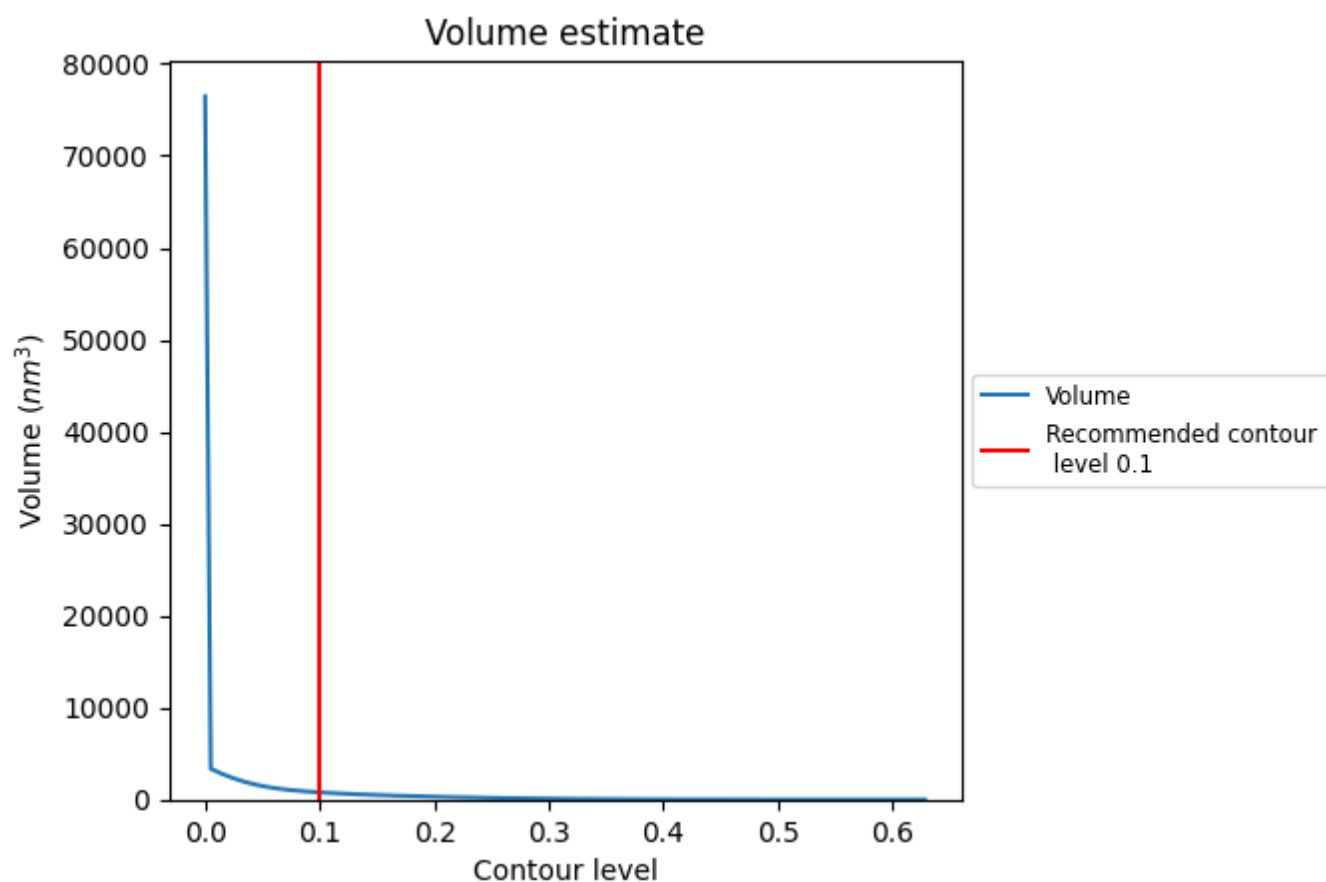
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

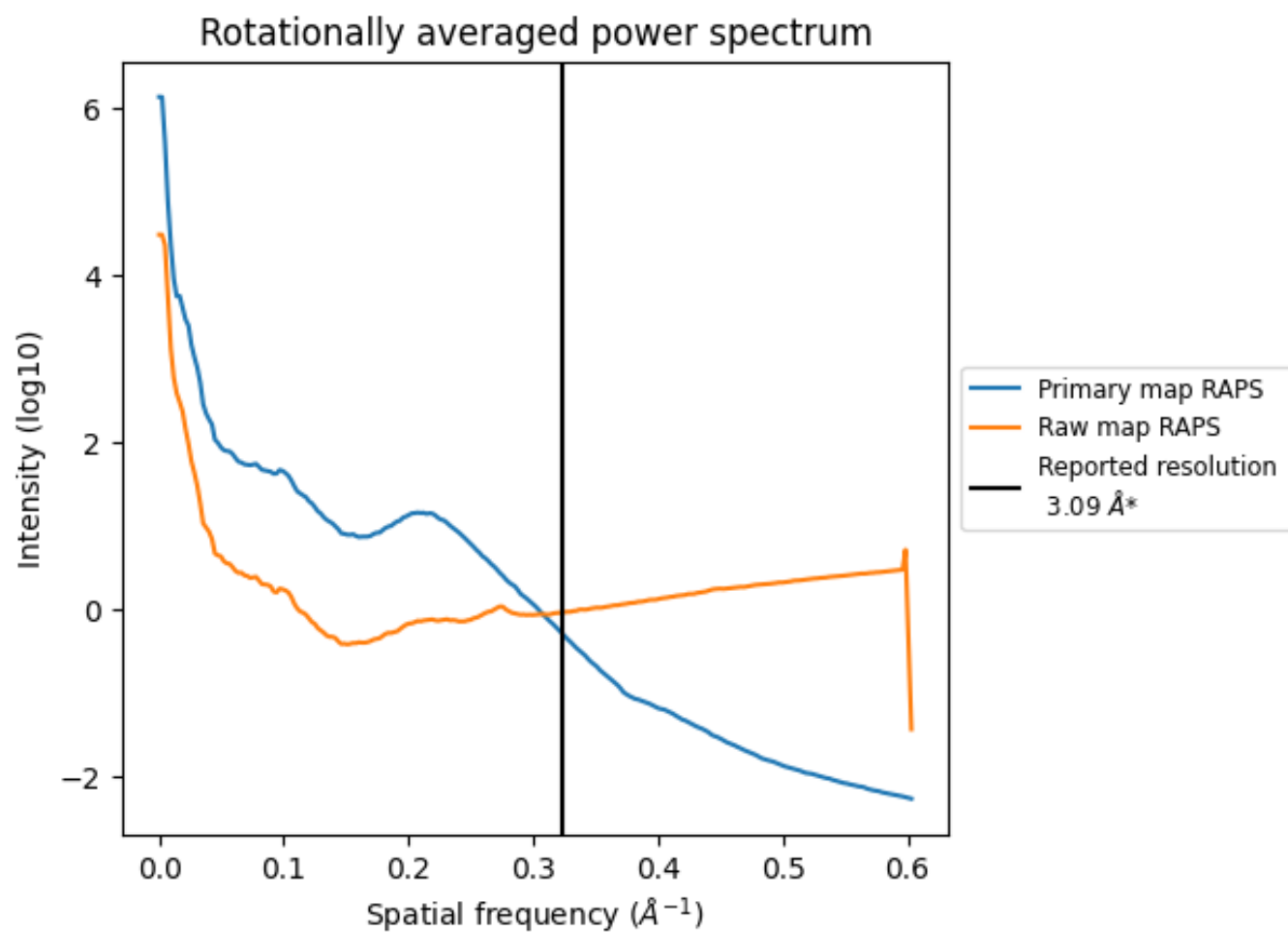
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 783 nm^3 ; this corresponds to an approximate mass of 707 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 ⓘ

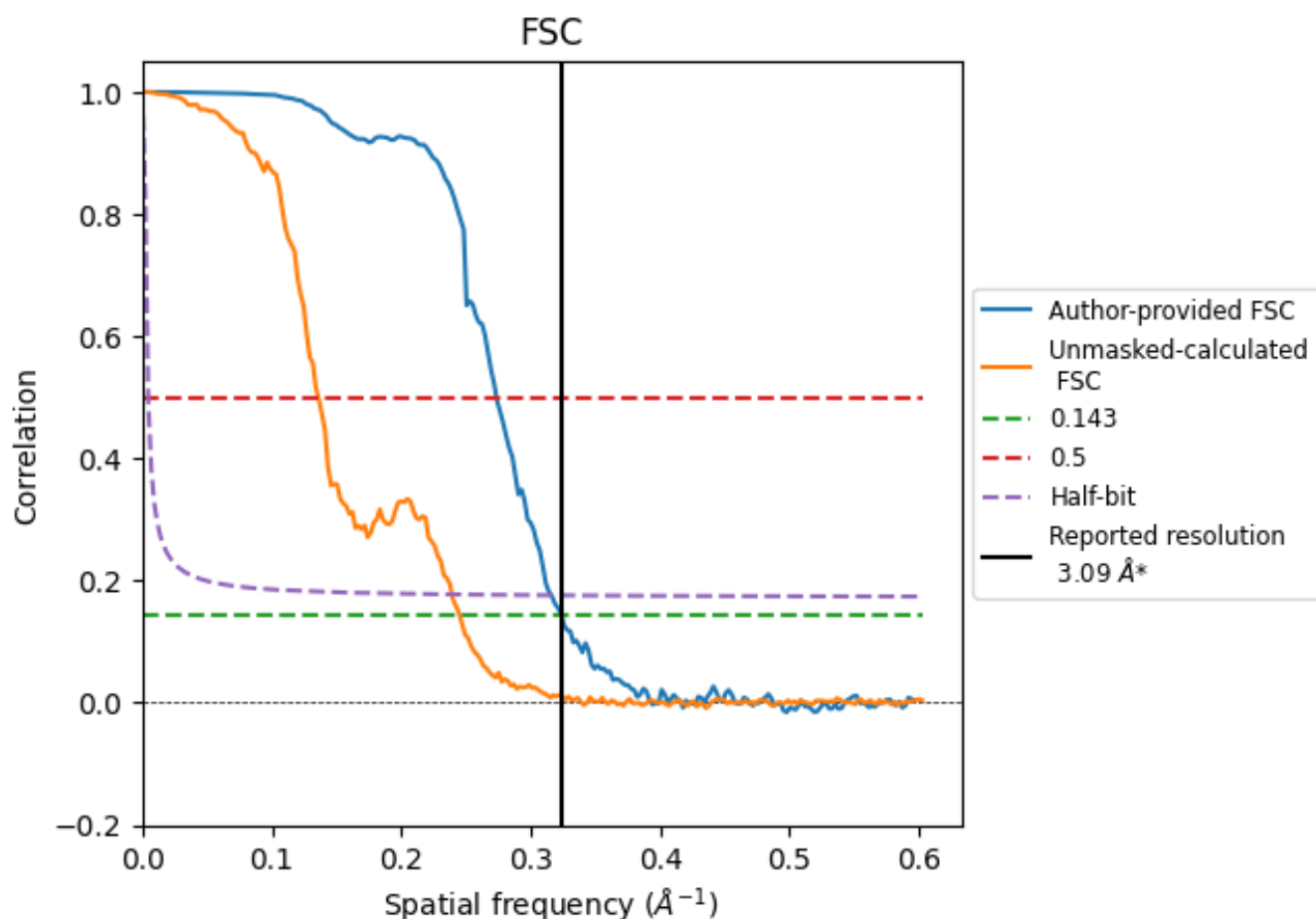


*Reported resolution corresponds to spatial frequency of 0.324 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.324 \AA^{-1}

8.2 Resolution estimates [i](#)

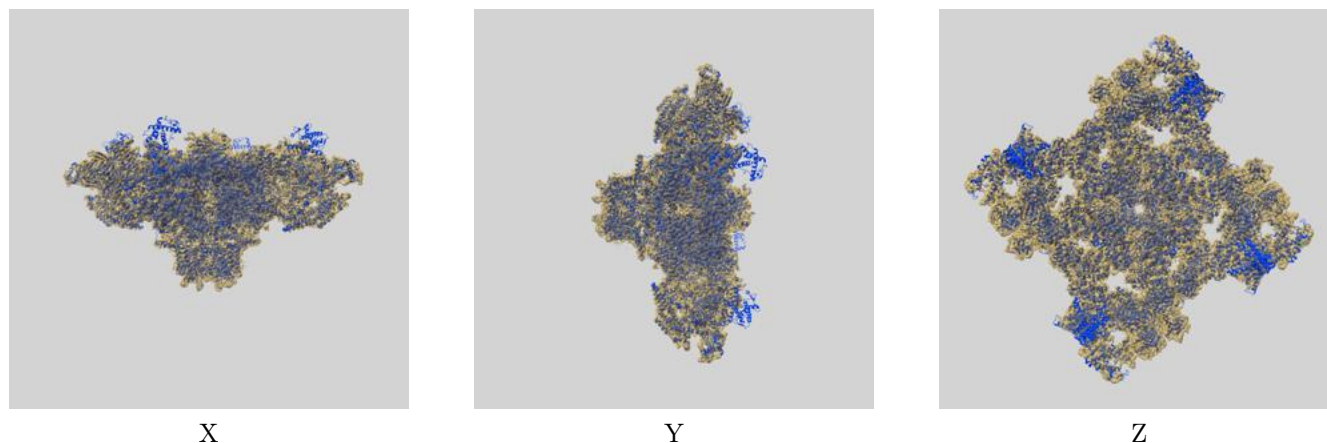
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.65	3.16
Unmasked-calculated*	4.08	7.35	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 3.09 by more than 10 %

9 Map-model fit [i](#)

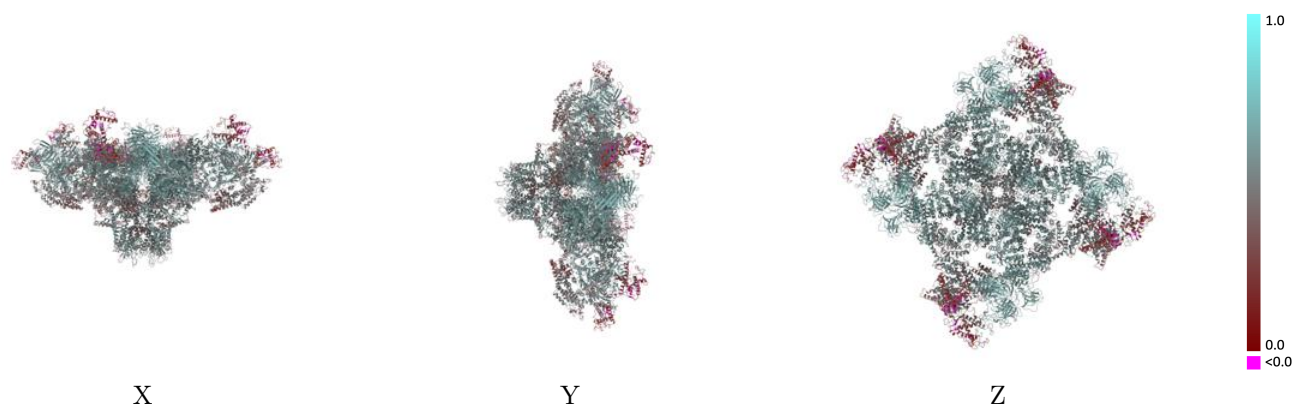
This section contains information regarding the fit between EMDB map EMD-49536 and PDB model 9NMP. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



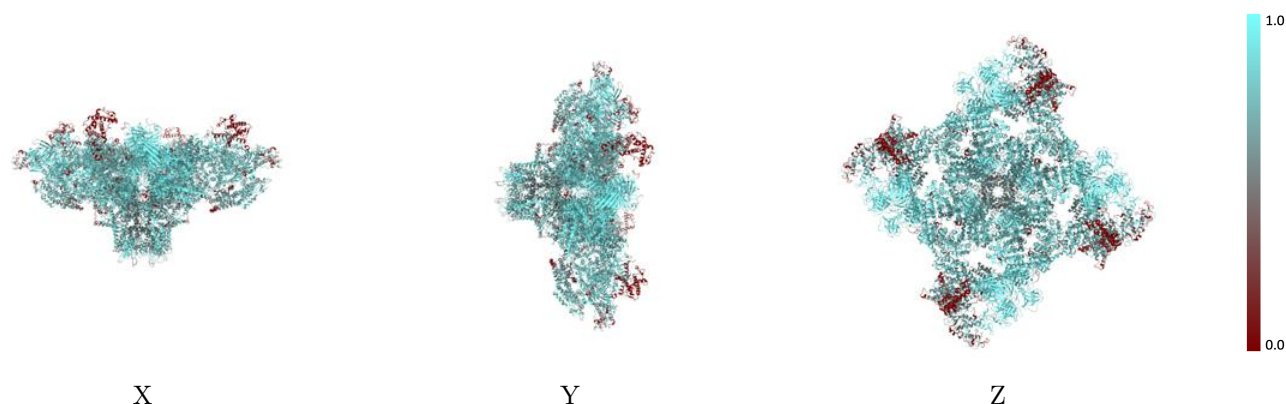
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



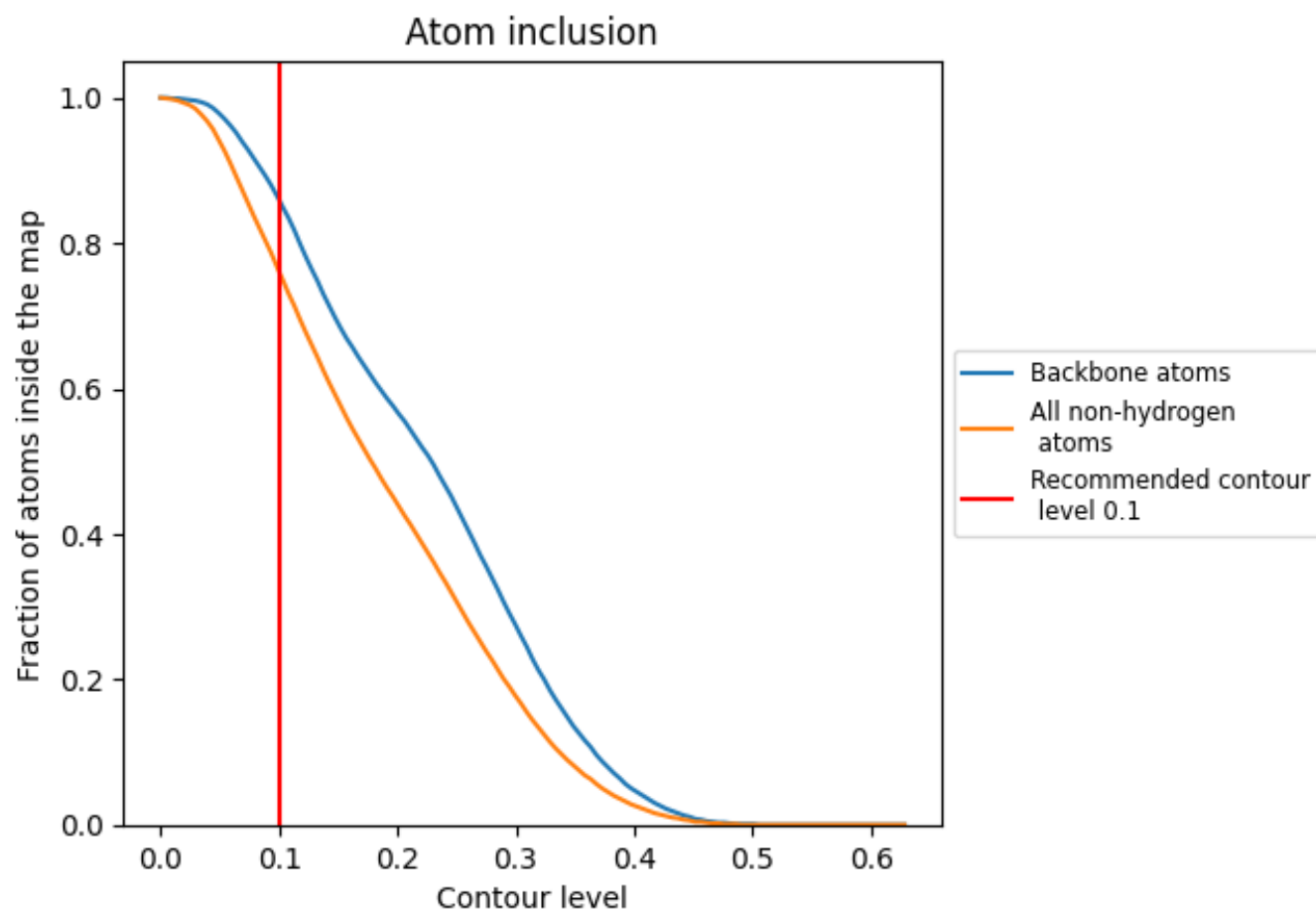
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7610	<div></div> 0.5090
A	<div></div> 0.7600	<div></div> 0.5080
B	<div></div> 0.7580	<div></div> 0.5070
C	<div></div> 0.7580	<div></div> 0.5070
D	<div></div> 0.7580	<div></div> 0.5070
E	<div></div> 0.8810	<div></div> 0.5870
F	<div></div> 0.8840	<div></div> 0.5890
G	<div></div> 0.8770	<div></div> 0.5850
H	<div></div> 0.8840	<div></div> 0.5910

