



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 07:14 PM UTC

PDB ID : 9RCW / pdb_00009rcw
EMDB ID : EMD-53924
Title : Primed-state RyR1 in 0.01% POPC micelles, in complex with a nanobody and FKBP12
Authors : Li, C.; Efremov, R.G.
Deposited on : 2025-05-30
Resolution : 3.30 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

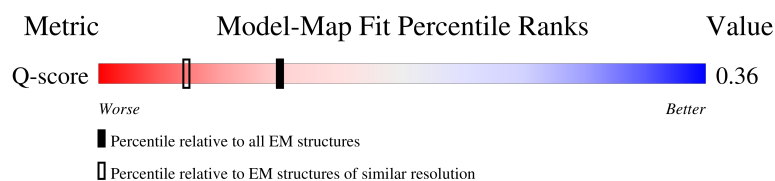
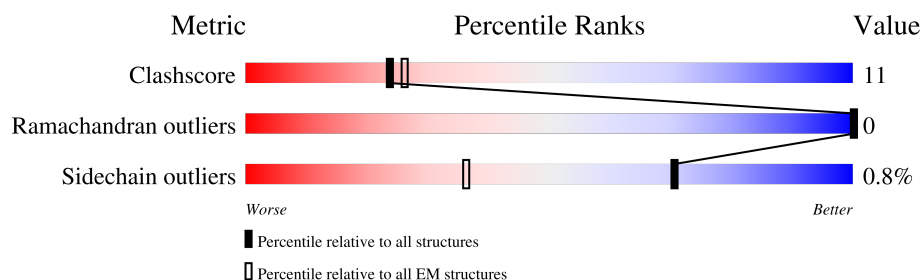
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	B	126	15% 55% 42% ..
1	D	126	13% 56% 41% ..
1	H	126	15% 56% 41% ..
1	K	126	14% 60% 38% ..

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Mol	Chain	Length	Quality of chain
2	E	107	64% 68% 31% .
2	F	107	65% 69% 30% .
2	I	107	64% 65% 34% .
2	L	107	63% 64% 35% .
3	A	5027	. 64% 22% 14%
3	C	5027	. 64% 22% 14%
3	G	5027	. 64% 22% 14%
3	J	5027	. 64% 22% 14%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 144632 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 Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
1	K	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
1	D	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
1	B	126	Total	C	N	O	S	0	0
			967	597	170	195	5		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	L	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	100	ASP	GLY	conflict	UNP Q8HYX6
L	100	ASP	GLY	conflict	UNP Q8HYX6
E	100	ASP	GLY	conflict	UNP Q8HYX6
F	100	ASP	GLY	conflict	UNP Q8HYX6

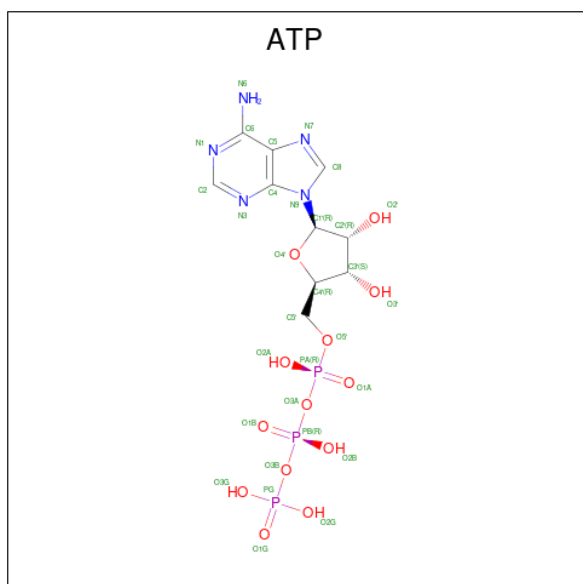
- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	4318	Total	C	N	O	S	0	0
			34131	21738	5887	6282	224		
3	J	4318	Total	C	N	O	S	0	0
			34131	21738	5887	6282	224		
3	C	4318	Total	C	N	O	S	0	0
			34131	21738	5887	6282	224		
3	A	4318	Total	C	N	O	S	0	0
			34131	21738	5887	6282	224		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



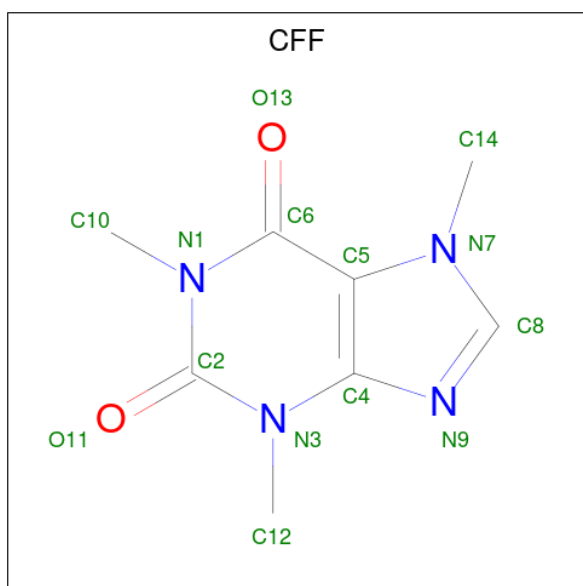
Mol	Chain	Residues	Atoms					AltConf
5	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	G	1	Total	C	N	O	0
			14	8	4	2	
6	J	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	
6	A	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

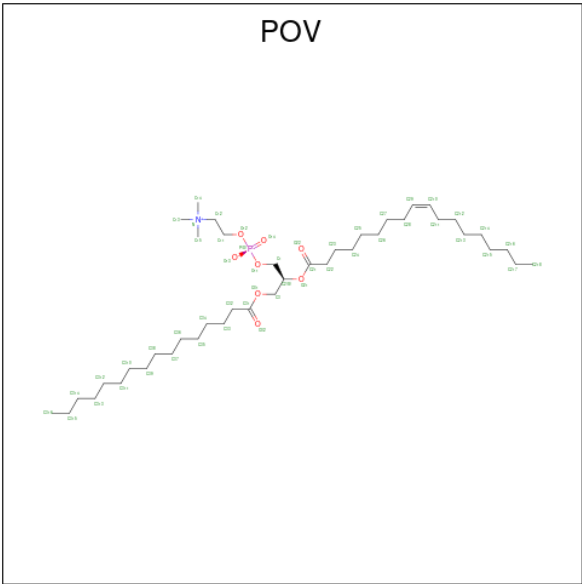
Mol	Chain	Residues	Atoms		AltConf
7	G	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
7	J	1	Total	Ca	0
			1	1	
7	C	1	Total	Ca	0
			1	1	
7	A	1	Total	Ca	0
			1	1	

- Molecule 8 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
8	G	1	Total 34	C 24	N 1	O 8	P 1	0
8	G	1	Total 36	C 26	N 1	O 8	P 1	0
8	G	1	Total 45	C 35	N 1	O 8	P 1	0
8	G	1	Total C 13 13					0
8	G	1	Total 38	C 28	N 1	O 8	P 1	0
8	G	1	Total 29	C 19	N 1	O 8	P 1	0
8	J	1	Total 45	C 35	N 1	O 8	P 1	0

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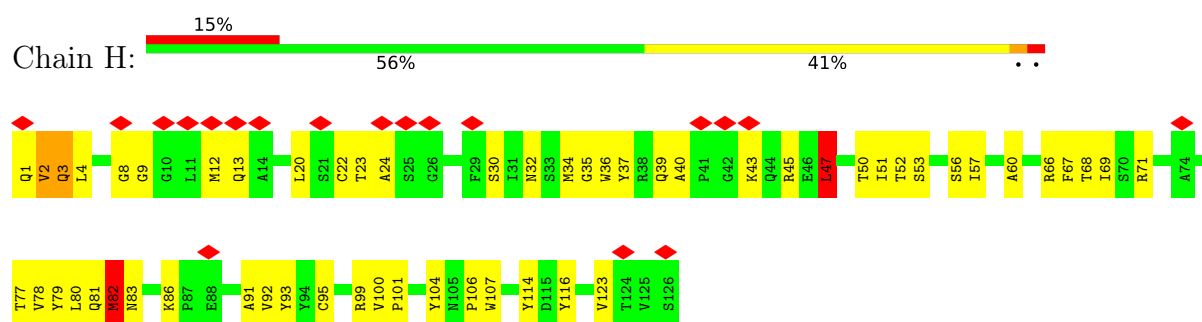
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Mol	Chain	Residues	Atoms					AltConf
8	J	1	Total	C	N	O	P	0
			34	24	1	8	1	
8	J	1	Total	C	N	O	P	0
			36	26	1	8	1	
8	J	1	Total	C	N	O	P	0
			45	35	1	8	1	
8	J	1	Total	C	N	O	P	0
			38	28	1	8	1	
8	J	1	Total	C	N	O	P	0
			29	19	1	8	1	
8	C	1	Total	C	N	O	P	0
			34	24	1	8	1	
8	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
8	C	1	Total	C				0
			13	13				
8	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
8	C	1	Total	C	N	O	P	0
			29	19	1	8	1	
8	C	1	Total	C				0
			13	13				
8	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
8	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
8	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
8	A	1	Total	C				0
			13	13				
8	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
8	A	1	Total	C	N	O	P	0
			29	19	1	8	1	

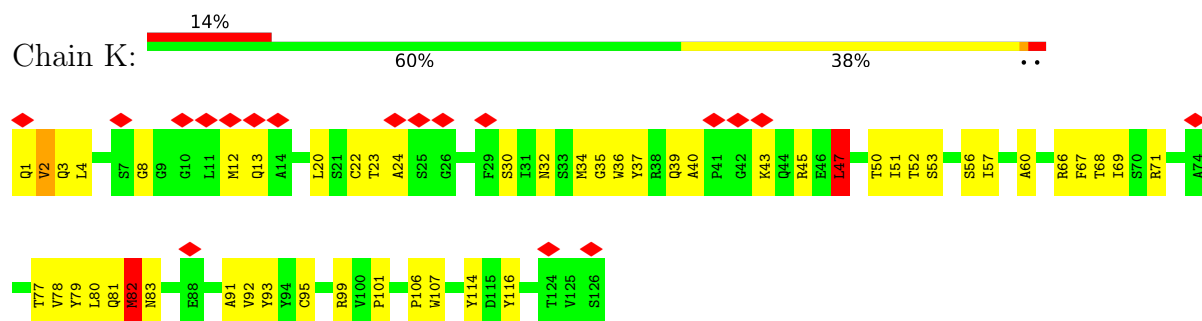
3 Residue-property plots [i](#)

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

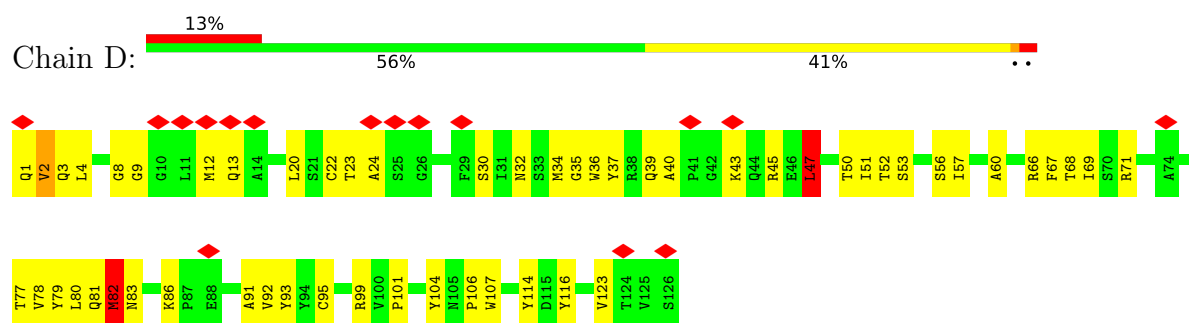
• Molecule 1: Nanobody 9657



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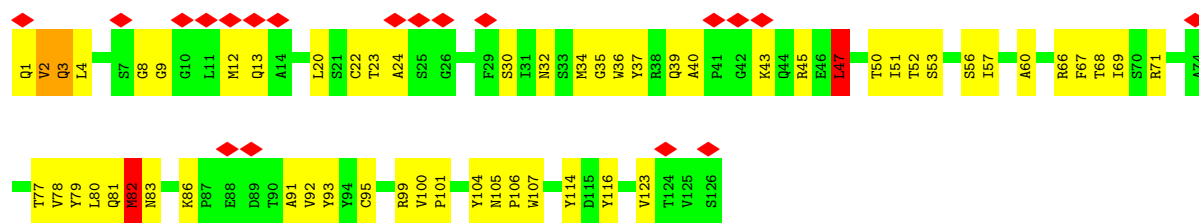


• Molecule 1: Nanobody 9657

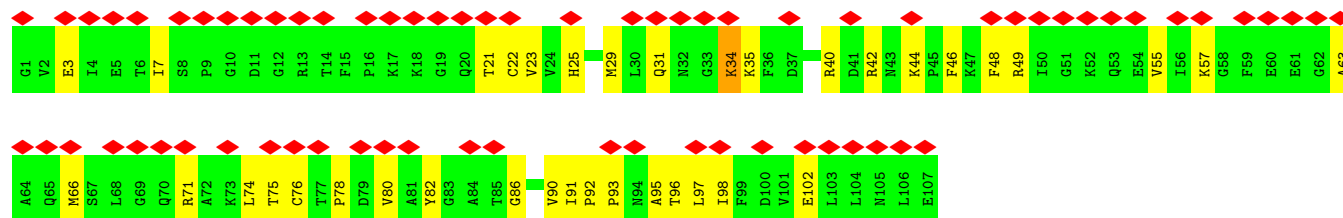


• Molecule 1: Nanobody 9657

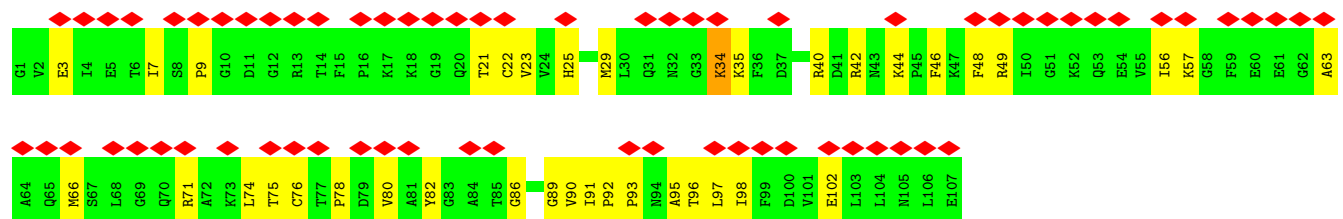




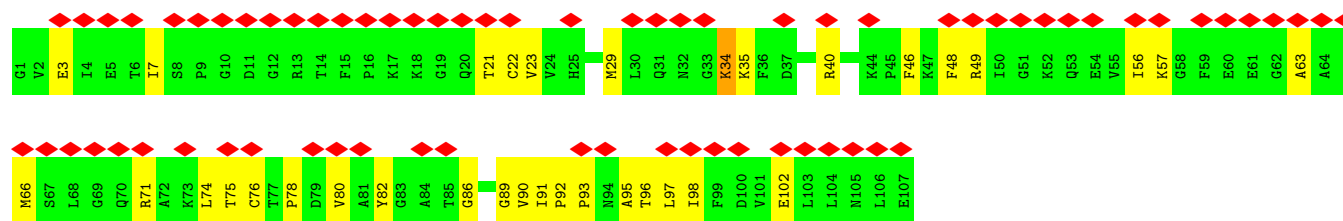
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



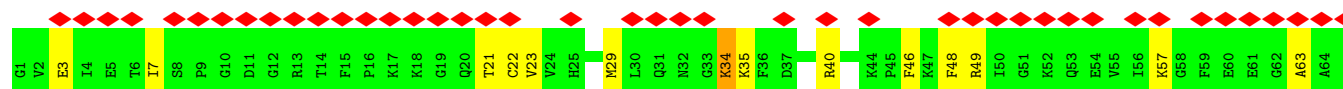
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

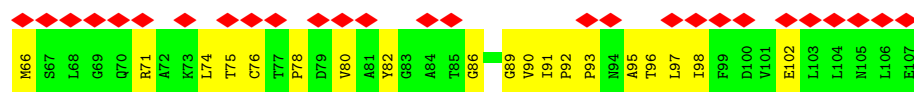


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

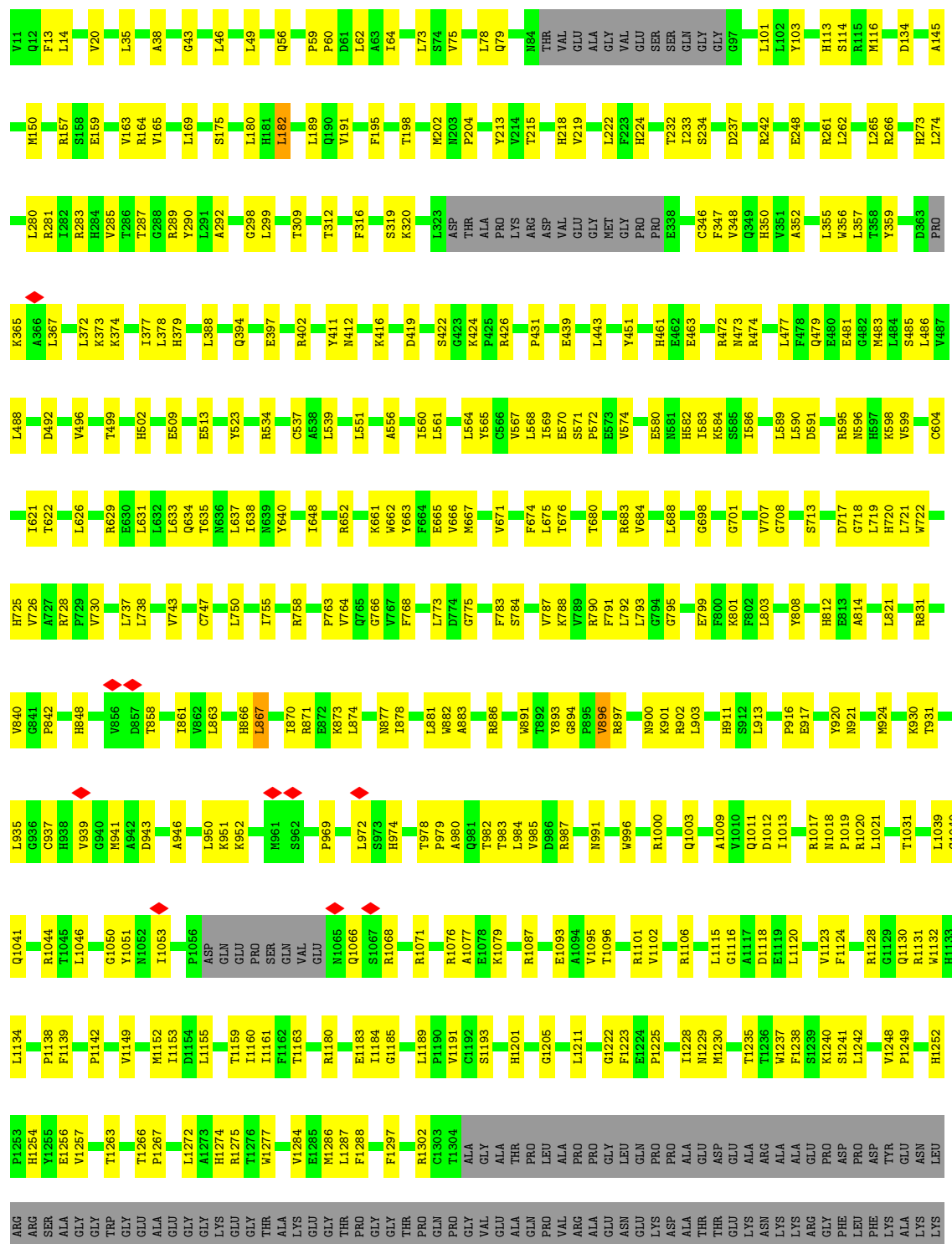


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 3: Ryanodine receptor 1





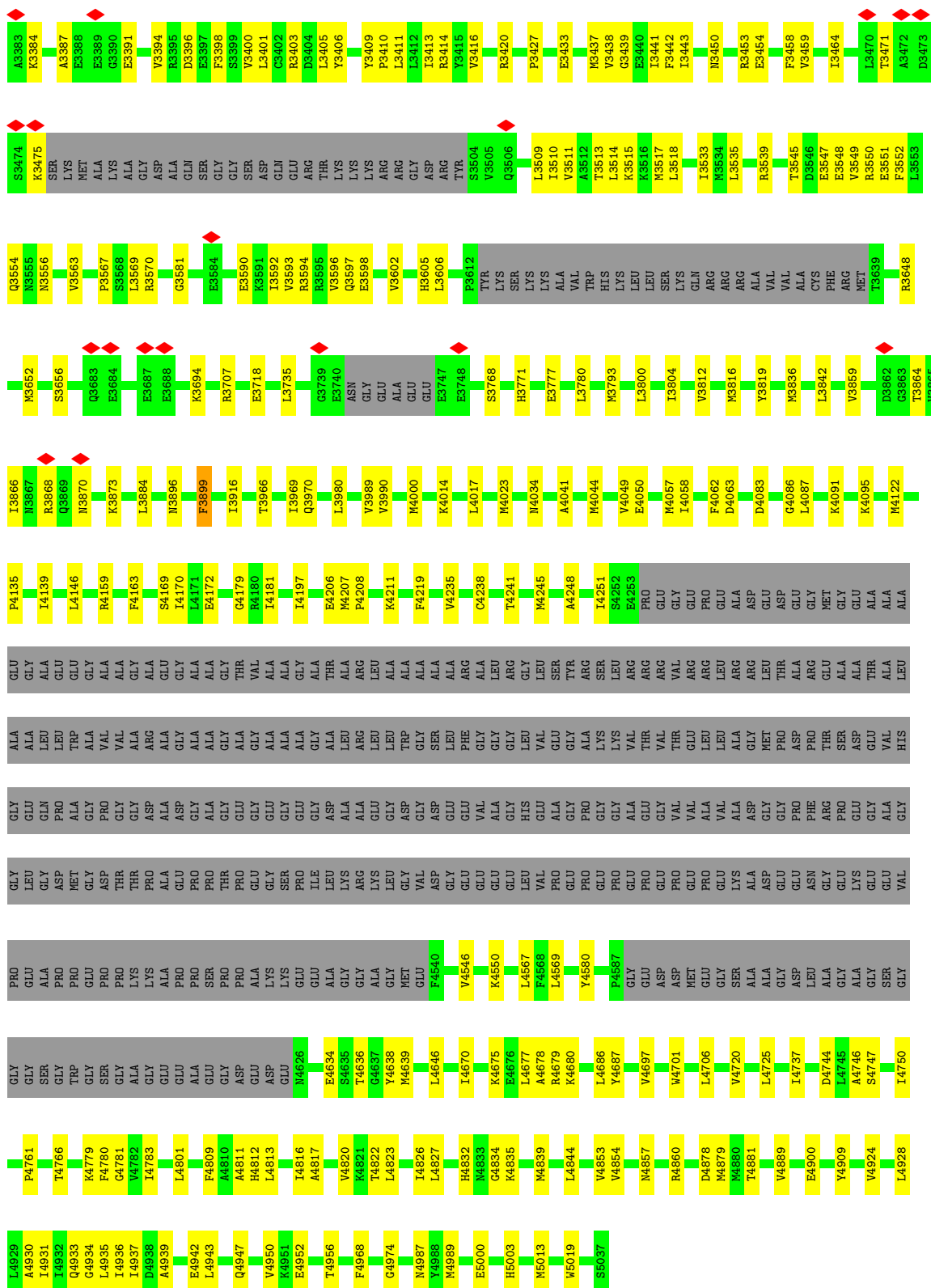
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GLY	THR	ARG	GLY	A4076	L3842	ARG	V3549	L3470	V3346	E3265	GLY	K3036	MEI	Q2877
LEU	ARG	GLY	GLY	D4079	V3859	GLY	E3550	T3471	L3381	M3266	Q3127	E3037	GLU	L2946
ALA	ARG	GLY	GLY	D4083	V3862	GLY	E3551	A3472	E3382	L3270	T3130	I3039	GLY	L2883
GLY	ARG	GLY	GLY	G4086	D3862	GLY	E3552	D3473	A3383	L3274	V3134	S3041	GLY	H2886
PRO	ARG	GLY	GLY	L4087	T3864	GLY	E3553	S3474	E3384	P3275	L3140	L3042	GLY	Q2887
THR	ARG	GLY	GLY	K4091	V3865	GLY	E3554	K3475	E3387	M3276	L3143	V3050	GLY	H2888
ALA	ARG	GLY	GLY	K4095	V3867	GLY	E3555	SER	A3388	C3278	F3144	R3053	GLY	V2955
GLY	ARG	GLY	GLY	M4122	R3868	GLY	E3556	LYS	E3389	G3279	L3157	V3054	GLY	K2890
ALA	ARG	GLY	GLY	P4135	R3869	GLY	E3557	ALA	E3390	Y3280	L3158	R3054	GLY	K2891
GLY	ARG	GLY	GLY	I4139	K3873	GLY	E3558	ASP	E3391	L3281	Q3162	D3060	GLY	Q2892
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GLY	ARG	GLY	GLY	I4181	E3880	GLY	E3565	GLY	E3398	E3290	N3180	I3070	GLY	E2899
GLY	ARG	GLY	GLY	I4197	E3881	GLY	E3566	GLY	E3399	A3291	V3183	Q2971	GLY	E2900
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ALA	ARG	GLY	GLY	M4207	E3883	GLY	E3568	GLY	E3401	L3296	A3195	M3082	GLY	E2902
GLY	ARG	GLY	GLY	P4208	E3884	GLY	E3569	GLY	E3402	P3297	L3196	V3080	GLY	E2903
ASP	ARG	GLY	GLY	K4211	E3885	GLY	E3570	GLY	E3403	A3298	R3197	L2904	GLY	E2904
ALA	ARG	GLY	GLY	F4219	E3886	GLY	E3571	GLY	E3404	G3299	L3198	L2905	GLY	E2905
GLY	ARG	GLY	GLY	D4220	E3887	GLY	E3572	GLY	E3405	A3300	L3199	V2906	GLY	E2906
ASP	ARG	GLY	GLY	E4224	E3888	GLY	E3573	GLY	E3406	T3305	L3206	K3088	GLY	E2907
GLY	ARG	GLY	GLY	V4235	E3889	GLY	E3574	GLY	E3407	T3308	E3207	K3089	GLY	E2908
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ALA	ARG	GLY	GLY	A4248	E3893	GLY	E3578	GLY	E3411	L3316	E3225	Q2993	GLY	E2912
GLY	ARG	GLY	GLY	I4251	E3894	GLY	E3579	GLY	E3412	I3319	E3226	E2994	GLY	E2913
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VAL	ARG	GLY	GLY	E4253	E3896	GLY	E3581	GLY	E3414	A3228	I3229	K2996	GLY	E2915
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ALA	ARG	GLY	GLY			GLY	E3586	GLY	E3419	L3315	E3236	F2929	GLY	E2920
ALA	ARG	GLY	GLY			GLY	E3587	GLY	E3420	L3316	V3236	L2927	GLY	E2921
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ALA	ARG	GLY	GLY			GLY	E3589	GLY	E3422	L3320	ALA	L2930	GLY	E2923
ALA	ARG	GLY	GLY			GLY	E3590	GLY	E3423	R3321	ARG	Q2931	GLY	E2924
ALA	ARG	GLY	GLY			GLY	E3591	GLY	E3424	I3322	THR	M2932	GLY	E2925
ALA	ARG	GLY	GLY			GLY	E3592	GLY	E3425	V3324	GLN	P3021	GLY	E2926
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ALA	ARG	GLY	GLY			GLY	E3594	GLY	E3427	N3326	LYS	H3030	GLY	E2928
ALA	ARG	GLY	GLY			GLY	E3595	GLY	E3428	L3327	LYS	N3033	GLY	E2929
ALA	ARG	GLY	GLY			GLY	E3596	GLY	E3429	G3328	GLY	K3034	GLY	E2930
ALA	ARG	GLY	GLY			GLY	E3597	GLY	E3430	E3331	GLY		GLY	E2931
ALA	ARG	GLY	GLY			GLY	E3598	GLY	E3431	K3336	GLY		GLY	E2932
ALA	ARG	GLY	GLY			GLY	E3599	GLY	E3432	F3341	GLY		GLY	E2933
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ALA	ARG	GLY	GLY			GLY	E3602	GLY	E3435		GLY		GLY	E2936
ALA	ARG	GLY	GLY			GLY	E3603	GLY	E3436		GLY		GLY	E2937
ALA	ARG	GLY	GLY			GLY	E3604	GLY	E3437		GLY		GLY	E2938
ALA	ARG	GLY	GLY			GLY	E3605	GLY	E3438		GLY		GLY	E2939
ALA	ARG	GLY	GLY			GLY	E3606	GLY	E3439		GLY		GLY	E2940
ALA	ARG	GLY	GLY			GLY	E3607	GLY	E3440		GLY		GLY	E2941
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ALA	ARG	GLY	GLY			GLY	E3612	GLY	E3445		GLY		GLY	E2946
ALA	ARG	GLY	GLY			GLY	E3613	GLY	E3446		GLY		GLY	E2947
ALA	ARG	GLY	GLY			GLY	E3614	GLY	E3447		GLY		GLY	E2948
ALA	ARG	GLY	GLY			GLY	E3615	GLY	E3448		GLY		GLY	E2949
ALA	ARG	GLY	GLY			GLY	E3616	GLY	E3449		GLY		GLY	E2950
ALA	ARG	GLY	GLY			GLY	E3617	GLY	E3450		GLY		GLY	E2951
ALA	ARG	GLY	GLY			GLY	E3618	GLY	E3451		GLY		GLY	E2952
ALA	ARG	GLY	GLY			GLY	E3619	GLY	E3452		GLY		GLY	E2953
ALA	ARG	GLY	GLY			GLY	E3620	GLY	E3453		GLY		GLY	E2954
ALA	ARG	GLY	GLY			GLY	E3621	GLY	E3454		GLY		GLY	E2955
ALA	ARG	GLY	GLY			GLY	E3622	GLY	E3455		GLY		GLY	E2956
ALA	ARG	GLY	GLY			GLY	E3623	GLY	E3456		GLY		GLY	E2957
ALA	ARG	GLY	GLY			GLY	E3624	GLY	E3457		GLY		GLY	E2958
ALA	ARG	GLY	GLY			GLY	E3625	GLY	E3458		GLY		GLY	E2959
ALA	ARG	GLY	GLY			GLY	E3626	GLY	E3459		GLY		GLY	E2960
ALA	ARG	GLY	GLY			GLY	E3627	GLY	E3460		GLY		GLY	E2961
ALA	ARG	GLY	GLY			GLY	E3628	GLY	E3461		GLY		GLY	E2962
ALA	ARG	GLY	GLY			GLY	E3629	GLY	E3462		GLY		GLY	E2963
ALA	ARG	GLY	GLY			GLY	E3630	GLY	E3463		GLY		GLY	E2964
ALA	ARG	GLY	GLY			GLY	E3631	GLY	E3464		GLY		GLY	E2965
ALA	ARG	GLY	GLY			GLY	E3632	GLY	E3465		GLY		GLY	E2966
ALA	ARG	GLY	GLY			GLY	E3633	GLY	E3466		GLY		GLY	E2967
ALA	ARG	GLY	GLY			GLY	E3634	GLY	E3467		GLY		GLY	E2968
ALA	ARG	GLY	GLY			GLY	E3635	GLY	E3468		GLY		GLY	E2969
ALA	ARG	GLY	GLY			GLY	E3636	GLY	E3469		GLY		GLY	E2970
ALA	ARG	GLY	GLY			GLY	E3637	GLY	E3470		GLY		GLY	E2971
ALA	ARG	GLY	GLY			GLY	E3638	GLY	E3471		GLY		GLY	E2972
ALA	ARG	GLY	GLY			GLY	E3639	GLY	E3472		GLY		GLY	E2973
ALA	ARG	GLY	GLY			GLY	E3640	GLY	E3473		GLY		GLY	E2974
ALA	ARG	GLY	GLY			GLY	E3641	GLY	E3474		GLY		GLY	E2975
ALA	ARG	GLY	GLY			GLY	E3642	GLY	E3475		GLY		GLY	E2976
ALA	ARG	GLY	GLY			GLY	E3643	GLY	E3476		GLY		GLY	E2977
ALA	ARG	GLY	GLY			GLY	E3644	GLY	E3477		GLY		GLY	E2978
ALA	ARG	GLY	GLY			GLY	E3645	GLY	E3478		GLY		GLY	E2979
ALA	ARG	GLY	GLY			GLY	E3646	GLY	E3479		GLY		GLY	E2980
ALA	ARG	GLY	GLY			GLY	E3647	GLY	E3480		GLY		GLY	E2981
ALA	ARG	GLY	GLY			GLY	E3648	GLY	E3481		GLY		GLY	E2982
ALA	ARG	GLY	GLY			GLY	E3649	GLY	E3482		GLY		GLY	E2983
ALA	ARG	GLY	GLY			GLY	E3650	GLY	E3483		GLY		GLY	E2984
ALA	ARG	GLY	GLY			GLY	E3651	GLY	E3484		GLY		GLY	E2985
ALA	ARG	GLY	GLY			GLY	E3652	GLY	E3485		GLY		GLY	E2986
ALA	ARG	GLY	GLY			GLY	E3653	GLY	E3486		GLY		GLY	E2987
ALA	ARG	GLY	GLY			GLY	E3654	GLY	E3487		GLY		GLY	E2988
ALA	ARG	GLY	GLY			GLY	E3655	GLY	E3488		GLY		GLY	E2989
ALA	ARG	GLY	GLY			GLY	E3656	GLY	E3489		GLY		GLY	E2990
ALA	ARG	GLY	GLY			GLY	E3657</							

R2454	V2354	K2227	W2120	D2037	I1745	Q1614	GLN	PRO	GLY	L1272	M1152	Y1051
L2457	I2358	M2228	L2123	Q2045	T1746	R1619	GLY	ALA	ALA	A1273	I1153	H1052
D2465	C2363	C2233	Q2127	LEU	L1747	A1620	I1509	PRO	PRO	D1274	D1154	I1053
L2466	C2363	F2234	Q2128	GLY	P1779	G1621	C1518	ALA	ALA	R1275	L1155	
V2467	P2366	F2235	Q2128	GLY	F1782	G1622	L1522	LEU	LEU	T1276	T1159	P1056
G2468	A2367	Y2238	P2146	GLY	F1782	W1626	L1522	PRO	ARG	W1277	I1160	ASP
L2469	L2368	S2147	S2147	GLY	L1786	Q1629	T1528	LEU	LEU	V1284	I1161	GLN
I2470	R2369	S2148	Q2149	PRO	P1787	Q1629	F1529	PRO	PRO	E1285	F1162	GLU
S2471	G2370	P2178	V2149	LYS	ALA	D1632	T1539	HIS	HIS	M1286	T1163	SER
L2472	E2371	Q2245	T2152	GLY	ALA	D1632	A1531	VAL	VAL	L1287	R1180	GLN
I2476	L2376	R2248	W2153	GLY	GLY	M1636	S1536	VAL	VAL	F1288		VAL
D2482	L2377	L2258	C2158	THR	GLY	M1636	S1536	PRO	PRO	L1293	E1183	H1065
G2483	L2377	L2258	L2159	SER	VAL	H1640	N1545	PRO	PRO	P1294	I1184	Q1066
	E2381	S2261	L2162	SER	ALA	E1793	N1545	ASP	ASP	F1297	G1185	S1067
V2495	R2385	L2265	W2170	SER	P1800	P1800	L1548	R1421	R1422	R1302	L1189	R1068
P2496	G2266	M2267	W2170	ARG	P1803	P1803	F1549	D1422	D1422	C1303	P1190	P1071
D2497	G2266	M2267	W2170	LEU	P1806	P1806	V1552	Y1433	Y1433	T1304	V1191	R1076
H2498	M2267	M2267	E2175	SER	A1806	A1806	F1553	Y1434	Y1434	GLY	R1076	A1077
K2499	S2270	S2270	W2178	LEU	K1810	K1810	V1554	Y1435	Y1435	ALA	H1201	E1078
S2501	P2395	T2271	T2179	LEU	M1814	M1814	V1561	Y1449	Y1449	ALA		K1079
M2502	GLY	T2271	T2179	GLY	L1815	L1815	I1562	Y1450	Y1450	THR	G1205	R1087
V2503	ARG	D2274	T2182	THR	L1815	L1815	E1565	G1451	G1451	PRO	L1211	E1093
L2504	ARG	D2274	T2182	VAL	L1815	L1815	E1565	W1452	W1452	ALA		A1094
F2505	ASP	V2275	T2185	ARG	H1825	H1825	L1566	W1453	W1453	ARG	G1222	T1095
L2506	ASP	V2275	W2186	VAL	A1826	A1826	G1674	T1454	T1454	PRO	G1222	T1095
D2507	ARG	V2280	W2186	VAL	A1827	A1827	L1676	P1455	P1455	GLY	E1224	T1096
R2508	ARG	E2292	K2189	LYS	D1827	D1827	L1676	P1456	P1456	LEU	P1225	
I2512	ARG	E2292	W2190	LYS	V1845	V1845	H1683	M1462	M1462	GLN	R1101	R1101
E2513	GLY	L2295	V2191	LYS	V1845	V1845	K1570	M1462	M1462	GLN	V1102	V1102
N2514	GLY	L2295	Q2193	GLY	V1845	V1845	N1571	M1462	M1462	PRO	N1229	N1229
F2517	GLY	V2298	H2194	LYS	F1854	F1854	I1572	R1470	R1470	ALA	R1106	R1106
L2518	GLY	L2302	L2201	PRO	G1855	G1855	M1573	M1476	M1476	GLU	L1115	L1115
L2519	PRO	L2302	L2201	GLY	D1856	D1856	P1574	G1477	G1477	GLY	G1116	G1116
L2522	GLY	S2309	Q2202	GLY	E1857	E1857	L1575	M1476	M1476	ALA	F1238	F1238
F2526	GLY	C2310	W2203	LEU	D1858	D1858	A1578	G1477	G1477	ALA	A1117	A1117
L2527	GLY	W2203	W2203	PRO	V1859	V1859	L1581	Q1480	Q1480	ASN	D1118	D1118
M2530	ALA	V2207	V2207	ALA	Q1861	Q1861	L1581	Q1480	Q1480	LYS	E1119	E1119
R2531	L2418	W2207	W2207	ALA	Q1861	Q1861	R1584	Y1483	Y1483	ARG	L1120	L1120
A2532	L2418	W2207	W2207	ALA	Q1861	Q1861	K1585	Y1483	Y1483	GLY	V1123	V1123
L2536	L2418	W2207	W2207	ALA	Q1861	Q1861	K1585	Y1483	Y1483	GLY	F1124	F1124
F2541	L2418	W2207	W2207	ALA	Q1861	Q1861	K1585	Y1483	Y1483	GLY	R1128	R1128
N2551	L2418	W2207	W2207	ALA	Q1861	Q1861	K1585	Y1483	Y1483	GLY	G1129	G1129
R2552	L2418	W2207	W2207	ALA	Q1861	Q1861	K1585	Y1483	Y1483	GLY	Q1130	Q1130
Y2553	L2418	W2207	W2207	ALA	Q1861	Q1861	K1585	Y1483	Y1483	GLY	R1131	R1131
L2554	L2418	W2207	W2207	ALA	Q1861	Q1861	K1585	Y1483	Y1483	GLY	W1132	W1132
C2555	L2418	W2207	W2207	ALA	Q1861	Q1861	K1585	Y1483	Y1483	GLY	F1138	F1138

V2558 L2559																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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P3275	L3143	F2957	K2891	E2824	E2764	E2670	T2563	D2465	L2358	C2233	L2123
R3276	F3144	G2958	Q2892	K2825	K2765	E2671	H2574	L2466	L2357	R2234	Q2127
C3278	C3278	F2959	E2893	A2826	W2766	L2672	R2575	V2467	C2363	F2235	Y2128
S3279	H3150	Q2961	L2894	R2827	A2767	R2676	A2576	G2468	P2366	Y2238	P2146
Y3280	L3157	Q2962	E2895	E2828	F2768	K2677	W2582	I2469	A2367	S2147	S2147
L3281	L3158	L2963	A2896	E2829	K2770	L2678	L2583	I2470	L2368	I2242	S2148
W3284	V3161	W2966	K2897	E2830	L2771	L2679	V2586	S2471	R2369	Q2245	V2149
W3285	Q3162	L2969	G2898	GLU	Q2772	Y2691	I2476	D2472	E2371	R2248	T2152
E3286	L3067	G2899	G2899	ARG	N2773	Y2696	D2482	G2483	L2376	L2258	M2153
R3287	H3069	S2970	G2900	THR	N2774	R2697	V2495	P2496	L2377	L2259	C2158
G3288	I3070	Q2971	L2901	GLU	W2775	M2698	P2496	D2497	I2380	S2261	L2162
P3289	L3071	E2972	H2902	LYS	S2776	A2699	V2495	H2498	E2381	L2265	L2162
E3290	D3076	F2973	P2903	LYS	Q2777	M2700	P2496	K2499	R2386	G2266	W2170
A3291	D3076	L2974	L2904	LYS	Q2778	P2701	I2706	A2500	R2392	M2267	E2175
A3295	V3080	A2975	L2904	THR	E2779	I2706	C2806	S2501	S2270	T2271	W2178
L3296	M3081	H2976	L2905	ARG	E2779	A2709	L2610	M2502	T2272	P2272	L2179
P3297	K3082	L2977	V2906	LYS	Q2778	P2711	C2611	V2503	L2273	L2273	L2182
A3298	V3088	E2978	D2909	THR	W2781	A2709	L2610	L2504	D2274	V2275	L2185
G3299	K3089	V2981	T2912	GLN	D2782	L2710	C2611	F2505	R2281	W2186	L2185
A3300	A3090	R2985	E2915	ALA	E2783	P2711	L2614	L2506	ARG	I2281	W2186
T3306	R3093	P2990	K2915	THR	L2784	A2717	I2618	D2507	ASP	R2281	K2189
T3308	F3096	H2991	A2917	TTR	K2786	K2722	M2618	R2508	ARG	E2292	W2190
H3311	D3102	Q2993	R2918	PRO	T2787	A2723	L2626	L2514	GLU	L2295	F2191
L3312	I3103	E2994	D2919	ARG	H2788	E2724	V2627	M2514	HIS	W2295	Q2193
L3315	E3104	K2996	R2920	GLU	P2789	K2725	W2630	N2514	GLU	V2298	H2194
L3316	K3105	T3001	E2921	GLY	W2790	LYS	V2630	N2514	ARG	L2302	L2201
I3319	M3106	F3010	Q2924	N2855	L2791	ALA	F2636	N2514	GLU	G2202	G2202
R3320	V3107	G3014	E2925	P2857	R2792	THR	M2639	L2518	GLY	M2203	V2207
R3321	R3111	L3014	L2926	Q2858	P2793	VAL	P2640	L2519	GLU	E2209	E2209
I3322	LEU	S3019	L2927	P2859	Y2794	ALA	L2641	L2522	PHO	Y2318	Y2212
V3323	GLY	T3020	K2928	P2860	K2795	GLU	L2643	F2526	GLU	G2322	L2215
V3324	LYS	T3021	L2930	D2861	T2796	GLY	L2644	L2527	GLU	Y2331	G2216
N3325	VAL	P3022	Q2931	L2862	E2799	N2794	T2645	M2530	N2414	F2340	GLY
N3326	GLN	A3022	Q2932	S2863	K2800	F2735	Y2648	R2531	H2420	THR	GLU
N3327	ALA	H3030	M2932	G2864	K2802	D2736	E2649	A2532	L2430	E2348	THR
G3328	THR	N3033	G2934	T2866	E2803	E2741	K2653	L2536	D2431	N2349	GLY
I3329	GLN	K3034	Y2935	L2867	I2804	T2742	Y2654	F2541	M2440	A2350	GLY
D3330	VAL	E3035	A2936	S2868	R2805	L2743	Y2655	N2551	M2440	N2351	T2223
V3245	LYS	V2937	V2937	S2869	W2807	C2856	C2856	R2552	M2440	V2352	K2227
R3248	GLY	E3037	T2938	R2870	P2808	L2857	L2857	Y2553	A2437	V2353	W2228
A3257	VAL	M3038	R2939	E2871	L2809	V2745	G2660	L2558	R2454	V2353	
A3342	GLY	T3040	GLY	L2871	K2810	I2746	I2661	L2559	M2551	V2353	
E3265	T3130	S3041	LYS	M2874	E2811	I2747	I2662	L2559	R2552	V2353	
K3266	V3134	L3042	ASP	Q2877	S2812	I2747	A2662	L2559	Y2553	V2353	
T3270	L3140	F3043	MET	L2878	K2814	K2750	F2664	L2559	C2555	V2353	
L3274	L3140	L3049	GLU	H2883	A2815	K2750	F2664	L2559	V2558	V2353	
		V3050	L2946	H2883	M2816	D2752	T2667	L2559	L2559	V2353	
			D2947	W2886	I2817	S2753					
			T2948	G2887	A2818	F2754					
			I2951	R2888	W2819	I2755					
			E2952		W2821						
			F2955		T2822						
			A2956		I2823						



- Molecule 3: Ryanodine receptor 1







L3049 V3050	L3140	L3274 P3276	V3373	I3464	E3547	CYS	L4059	PRO	THR	GLU	P4587
R3053 V3054	L3143 F3144	P3276 L3277	L3379 R3380	L3470 T3471	E3548 V3549	PHE ARG	K4060 F4061	ARG VAL	VAL THR	GLY THR	GLY ASP
D3060	H3150	C3278	E3382 A3383	A3472 D3473	F3552 L3553	T3639	D4063	ARG LEU	LEU ALA	GLY ASP	ASP ALA
V3064 V3065	I3157 L3158	Y3280 L3281	A3383 K3384	D3473 S3474	Q3554 N3556	R3648	D4083	ARG ASP	ALA GLY	ASP GLY	GLY ASP
V3066 C3067	V3161 Q3162	Y3280 L3281	A3387 E3388	K3475 SER	V3563	M3652	G4086 L4087	ARG LEU	ALA THR	ASP GLY	GLY ASP
L3070 L3071	Y3166	Y3288	E3389 G3390	K3475 MET	P3567	S3656	K4090 K4091	ALA GLY	ALA GLY	ASP GLY	GLY ASP
D3076	L3169	P3288	E3391	K3475 ALA	F3568	F3669	K4095	ALA GLY	ALA THR	ASP GLY	GLY ASP
V3080 R3081	L3175	L3295	V3394	SER	P3569	E3682	M4122	ALA GLY	ALA THR	ASP GLY	GLY ASP
K3082	N3180	L3296	R3395	GLY	R3570	Q3683	P4135	ALA GLY	ALA THR	ASP GLY	GLY ASP
V3088 K3089	V3183	P3297	E3396	ASP	G3581	E3684	I4139	ALA GLY	ALA THR	ASP GLY	GLY ASP
A3090	R3187	A3298	D3397	GLN	E3584	E3685	L4146	ALA GLY	ALA THR	ASP GLY	GLY ASP
R3093	A3195	G3299	L3400	SER	E3590	E3686	R4159	ALA GLY	ALA THR	ASP GLY	GLY ASP
F3096	R3196	A3300	L3401	GLY	R3591	E3688	F4163	ALA GLY	ALA THR	ASP GLY	GLY ASP
D3102 I3103	L3206 E3207	T3305	D3402	GLY	I3592	R3707	S4169	ALA GLY	ALA THR	ASP GLY	GLY ASP
E3104 K3105	K3222 S3223	T3308	R3403	ARG	V3593	E3719	I4170	ALA GLY	ALA THR	ASP GLY	GLY ASP
V3107	P3224	L3315	L3405	GLY	R3594	G3739	I4181	ALA GLY	ALA THR	ASP GLY	GLY ASP
R3111	R3225	L3316	Y3406	ARG	V3596	E3740	L3960	ALA GLY	ALA THR	ASP GLY	GLY ASP
LEU	E3226	I3319	Y3409	TYR	Q3597	ASN	I4197	ALA GLY	ALA THR	ASP GLY	GLY ASP
GLY	R3227	L3320	L3410	V3504	E3598	GLU	V3989	ALA GLY	ALA THR	ASP GLY	GLY ASP
LYS	A3228	R3321	L3411	V3505	V3602	ALA	V3990	ALA GLY	ALA THR	ASP GLY	GLY ASP
VAL	LYS	I3322	L3412	Q3506	H3605	LEU	M4000	ALA GLY	ALA THR	ASP GLY	GLY ASP
SER	GLN	V3323	L3413	L3509	L3606	TRP	K4014	ALA GLY	ALA THR	ASP GLY	GLY ASP
ALA	ALA	N3324	R3414	T3510	P3612	VAL	L4017	ALA GLY	ALA THR	ASP GLY	GLY ASP
ARG	THR	N3325	Y3415	A3512	TYR	ARG	M4023	ALA GLY	ALA THR	ASP GLY	GLY ASP
THR	VAL	I3329	V3416	T3513	LYS	ARG	L4031	ALA GLY	ALA THR	ASP GLY	GLY ASP
GLN	LYS	D3330	V3416	K3514	H3605	ARG	L4034	ALA GLY	ALA THR	ASP GLY	GLY ASP
LYS	GLY	F3331	N3440	K3516	L2606	ARG	M4041	ALA GLY	ALA THR	ASP GLY	GLY ASP
GLY	VAL	R3336	Y3444	M3517	L3606	ARG	A4041	ALA GLY	ALA THR	ASP GLY	GLY ASP
GLY	GLY	F3341	Y3444	L3518	P3612	ARG	M4044	ALA GLY	ALA THR	ASP GLY	GLY ASP
R3127	A3257	Q3442	N3450	T3533	TYR	ARG	A4044	ALA GLY	ALA THR	ASP GLY	GLY ASP
T3130	E3265	Q3443	R3453	M3534	LYS	ARG	M4245	ALA GLY	ALA THR	ASP GLY	GLY ASP
V3134	M3266	V3346	E3454	L3535	VAL	ARG	A4248	ALA GLY	ALA THR	ASP GLY	GLY ASP
I3270	I3362	I3362	F3458 V3459	T3545	ALA	ARG	E4253	ALA GLY	ALA THR	ASP GLY	GLY ASP

L4686	Y4687	M4879	M4880	T4881	V4889	E4900	Y4909	V4924	L4928	L4929	A4930	I4931	I4932	Q4933	G4934	L4935	I4936	I4937	D4944	S4747	P4761	T4766	K4779	F4780	Q4781	V4782	L4783	F4809	A4810	H4811	H4812	L4813	T4816	A4817	V4820	K4821	T4822	L4823	I4826	L4827	H4832	K4835	M4839	L4844	V4853	Y4854	M4857	R4860	D4878
L4686	Y4687	M4879	M4880	T4881	V4889	E4900	Y4909	V4924	L4928	L4929	A4930	I4931	I4932	Q4933	G4934	L4935	I4936	I4937	D4944	S4747	P4761	T4766	K4779	F4780	Q4781	V4782	L4783	F4809	A4810	H4811	H4812	L4813	T4816	A4817	V4820	K4821	T4822	L4823	I4826	L4827	H4832	K4835	M4839	L4844	V4853	Y4854	M4857	R4860	D4878

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39983	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.787	Depositor
Minimum map value	-1.672	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	488.544, 488.544, 488.544	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.454, 1.454, 1.454	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.23	0/987	0.64	3/1340 (0.2%)
1	D	0.23	0/987	0.64	3/1340 (0.2%)
1	H	0.23	0/987	0.64	3/1340 (0.2%)
1	K	0.23	0/987	0.64	3/1340 (0.2%)
2	E	0.28	0/834	0.60	1/1123 (0.1%)
2	F	0.28	0/834	0.60	1/1123 (0.1%)
2	I	0.28	0/834	0.60	1/1123 (0.1%)
2	L	0.28	0/834	0.60	1/1123 (0.1%)
3	A	0.21	0/34899	0.42	2/47302 (0.0%)
3	C	0.21	0/34899	0.42	2/47302 (0.0%)
3	G	0.21	0/34899	0.42	2/47302 (0.0%)
3	J	0.21	0/34899	0.42	1/47302 (0.0%)
All	All	0.21	0/146880	0.44	23/199060 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	H	0	1
1	K	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	3	GLN	CA-CB-CG	8.84	131.78	114.10
1	B	3	GLN	CA-CB-CG	8.84	131.78	114.10
1	H	3	GLN	CA-CB-CG	8.84	131.77	114.10
1	D	3	GLN	CA-CB-CG	8.82	131.74	114.10
1	D	82	MET	CB-CG-SD	7.20	134.29	112.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	VAL	Peptide
1	D	2	VAL	Peptide
1	H	2	VAL	Peptide
1	K	2	VAL	Peptide

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	B	967	0	916	43	0
1	D	967	0	916	40	0
1	H	967	0	916	42	0
1	K	967	0	916	37	0
2	E	818	0	824	23	0
2	F	818	0	824	22	0
2	I	818	0	824	31	0
2	L	818	0	824	31	0
3	A	34131	0	33507	732	0
3	C	34131	0	33507	726	0
3	G	34131	0	33507	740	0
3	J	34131	0	33507	732	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	31	0	12	0	0
5	C	31	0	12	0	0
5	G	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	31	0	12	0	0
6	A	14	0	10	0	0
6	C	14	0	10	0	0
6	G	14	0	10	0	0
6	J	14	0	10	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	G	1	0	0	0	0
7	J	1	0	0	0	0
8	A	195	0	256	6	0
8	C	163	0	214	6	0
8	G	195	0	256	6	0
8	J	227	0	298	7	0
All	All	144632	0	142100	3131	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 11.

The worst 5 of 3131 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)
3:J:2806:ARG:HE	3:J:2810:LYS:HE2	1.44	0.83
3:A:2806:ARG:HE	3:A:2810:LYS:HE2	1.44	0.82
3:C:2592:GLY:HA2	3:C:2595:LEU:HD12	1.62	0.82
3:J:2592:GLY:HA2	3:J:2595:LEU:HD12	1.62	0.81
3:A:2592:GLY:HA2	3:A:2595:LEU:HD12	1.62	0.81

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	B	124/126 (98%)	115 (93%)	9 (7%)	0	100	100
1	D	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
1	H	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
1	K	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
2	E	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	F	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	I	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	L	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
3	A	4276/5027 (85%)	4150 (97%)	126 (3%)	0	100	100
3	C	4276/5027 (85%)	4149 (97%)	127 (3%)	0	100	100
3	G	4276/5027 (85%)	4149 (97%)	127 (3%)	0	100	100
3	J	4276/5027 (85%)	4149 (97%)	127 (3%)	0	100	100
All	All	18020/21040 (86%)	17452 (97%)	568 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	104/104 (100%)	100 (96%)	4 (4%)	29	57
1	D	104/104 (100%)	100 (96%)	4 (4%)	29	57
1	H	104/104 (100%)	100 (96%)	4 (4%)	29	57
1	K	104/104 (100%)	100 (96%)	4 (4%)	29	57
2	E	88/88 (100%)	87 (99%)	1 (1%)	65	76
2	F	88/88 (100%)	87 (99%)	1 (1%)	65	76
2	I	88/88 (100%)	87 (99%)	1 (1%)	65	76
2	L	88/88 (100%)	87 (99%)	1 (1%)	65	76
3	A	3670/4270 (86%)	3643 (99%)	27 (1%)	76	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	3670/4270 (86%)	3642 (99%)	28 (1%)	73	79
3	G	3670/4270 (86%)	3642 (99%)	28 (1%)	73	79
3	J	3670/4270 (86%)	3644 (99%)	26 (1%)	76	80
All	All	15448/17848 (87%)	15319 (99%)	129 (1%)	70	79

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	2267	MET
3	A	2906	VAL
3	J	2128	TYR
3	J	1736	VAL
3	A	3157	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	122	GLN
3	A	2772	GLN
3	A	226	HIS
3	A	1066	GLN
3	A	4216	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 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	POV	C	5106	-	35,35,51	0.61	0	41,43,59	0.58	0
8	POV	C	5107	-	12,12,51	0.20	0	11,11,59	0.28	0
5	ATP	A	5102	-	32,33,33	0.53	0	48,52,52	0.39	0
8	POV	G	5108	-	12,12,51	0.20	0	11,11,59	0.28	0
8	POV	J	5107	-	35,35,51	0.61	0	41,43,59	0.58	0
8	POV	C	5110	-	12,12,51	0.20	0	11,11,59	0.28	0
6	CFF	G	5103	-	15,15,15	0.72	0	23,23,23	0.78	1 (4%)
6	CFF	J	5104	-	15,15,15	0.72	0	23,23,23	0.78	1 (4%)
8	POV	A	5106	-	35,35,51	0.61	0	41,43,59	0.58	0
8	POV	G	5107	-	44,44,51	0.53	0	50,52,59	0.51	1 (2%)
5	ATP	G	5102	-	32,33,33	0.53	0	48,52,52	0.39	0
6	CFF	C	5103	-	15,15,15	0.72	0	23,23,23	0.78	1 (4%)
8	POV	J	5109	-	37,37,51	0.59	0	43,45,59	0.52	0
5	ATP	C	5102	-	32,33,33	0.53	0	48,52,52	0.39	0
6	CFF	A	5103	-	15,15,15	0.72	0	23,23,23	0.78	1 (4%)
5	ATP	J	5103	-	32,33,33	0.53	0	48,52,52	0.39	0
8	POV	J	5108	-	44,44,51	0.53	0	50,52,59	0.51	1 (2%)
8	POV	C	5109	-	28,28,51	0.65	0	34,36,59	0.64	0
8	POV	J	5110	-	28,28,51	0.65	0	34,36,59	0.64	0
8	POV	A	5109	-	37,37,51	0.59	0	43,45,59	0.52	0
8	POV	G	5109	-	37,37,51	0.59	0	43,45,59	0.52	0
8	POV	A	5105	-	33,33,51	0.60	0	39,41,59	0.50	0
8	POV	G	5105	-	33,33,51	0.60	0	39,41,59	0.50	0
8	POV	J	5101	-	44,44,51	0.53	0	50,52,59	0.51	1 (2%)
8	POV	A	5108	-	12,12,51	0.20	0	11,11,59	0.28	0
8	POV	C	5105	-	33,33,51	0.60	0	39,41,59	0.50	0
8	POV	J	5106	-	33,33,51	0.60	0	39,41,59	0.50	0
8	POV	C	5108	-	37,37,51	0.59	0	43,45,59	0.52	0
8	POV	A	5110	-	28,28,51	0.65	0	34,36,59	0.64	0
8	POV	G	5110	-	28,28,51	0.65	0	34,36,59	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	POV	A	5107	-	44,44,51	0.53	0	50,52,59	0.51	1 (2%)
8	POV	G	5106	-	35,35,51	0.61	0	41,43,59	0.58	0

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	POV	C	5106	-	-	10/39/39/55	-
8	POV	C	5107	-	-	2/10/10/55	-
5	ATP	A	5102	-	-	2/22/38/38	0/3/3/3
8	POV	G	5108	-	-	2/10/10/55	-
8	POV	J	5107	-	-	10/39/39/55	-
8	POV	C	5110	-	-	2/10/10/55	-
6	CFF	G	5103	-	-	-	0/2/2/2
6	CFF	J	5104	-	-	-	0/2/2/2
8	POV	A	5106	-	-	10/39/39/55	-
8	POV	G	5107	-	-	12/48/48/55	-
5	ATP	G	5102	-	-	2/22/38/38	0/3/3/3
8	POV	J	5109	-	-	16/41/41/55	-
6	CFF	C	5103	-	-	-	0/2/2/2
5	ATP	C	5102	-	-	2/22/38/38	0/3/3/3
6	CFF	A	5103	-	-	-	0/2/2/2
5	ATP	J	5103	-	-	2/22/38/38	0/3/3/3
8	POV	J	5108	-	-	12/48/48/55	-
8	POV	C	5109	-	-	9/32/32/55	-
8	POV	J	5110	-	-	9/32/32/55	-
8	POV	A	5109	-	-	16/41/41/55	-
8	POV	G	5109	-	-	16/41/41/55	-
8	POV	A	5105	-	-	9/37/37/55	-
8	POV	G	5105	-	-	9/37/37/55	-
8	POV	J	5101	-	-	12/48/48/55	-
8	POV	A	5108	-	-	2/10/10/55	-
8	POV	C	5105	-	-	9/37/37/55	-
8	POV	J	5106	-	-	9/37/37/55	-
8	POV	C	5108	-	-	16/41/41/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	POV	A	5110	-	-	9/32/32/55	-
8	POV	G	5110	-	-	9/32/32/55	-
8	POV	A	5107	-	-	12/48/48/55	-
8	POV	G	5106	-	-	10/39/39/55	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	5103	CFF	C12-N3-C2	2.65	121.95	117.33
6	J	5104	CFF	C12-N3-C2	2.65	121.95	117.33
6	A	5103	CFF	C12-N3-C2	2.65	121.95	117.33
6	C	5103	CFF	C12-N3-C2	2.65	121.94	117.33
8	G	5107	POV	O13-P-O14	2.02	121.82	112.44

There are no chirality outliers.

5 of 240 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	G	5105	POV	C11-O12-P-O11
8	G	5105	POV	O22-C21-O21-C2
8	G	5106	POV	C1-O11-P-O12
8	G	5106	POV	C1-O11-P-O13
8	G	5106	POV	C1-O11-P-O14

There are no ring outliers.

16 monomers are involved in 25 short contacts:

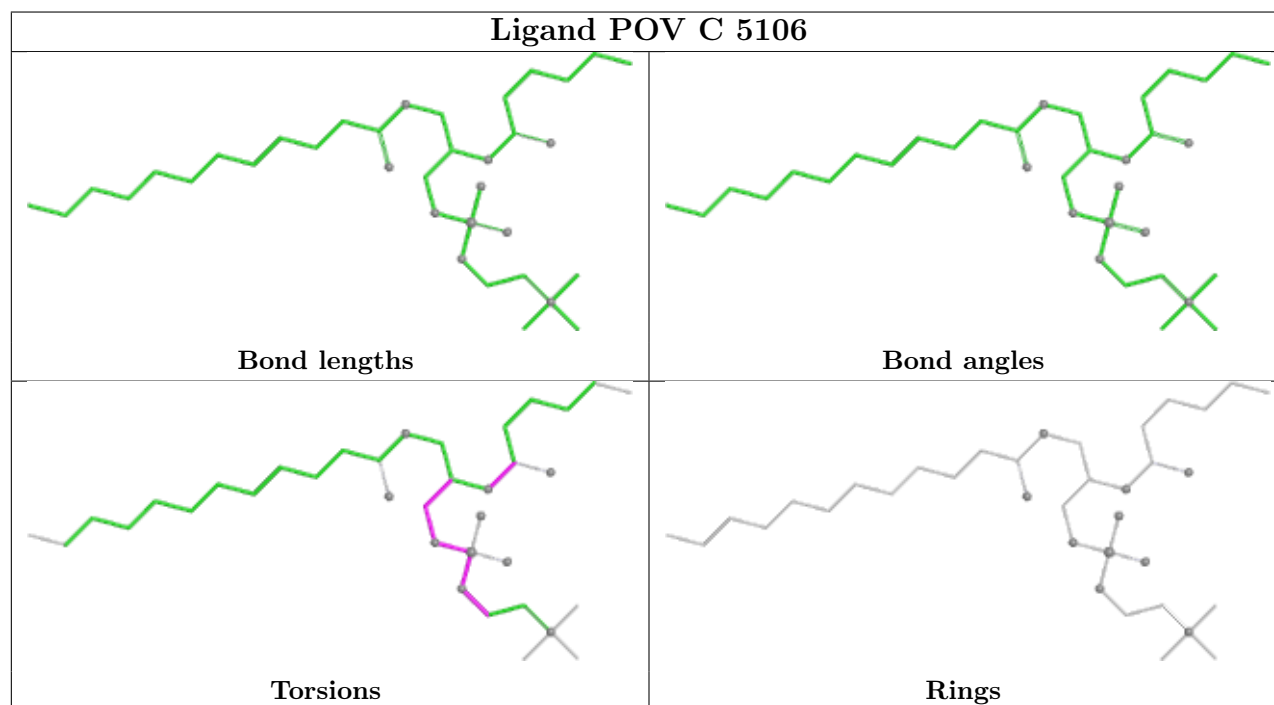
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	5106	POV	2	0
8	C	5107	POV	1	0
8	G	5108	POV	1	0
8	J	5107	POV	2	0
8	C	5110	POV	1	0
8	A	5106	POV	2	0
8	G	5107	POV	2	0
8	J	5108	POV	2	0
8	C	5109	POV	1	0
8	J	5101	POV	3	0
8	A	5108	POV	1	0

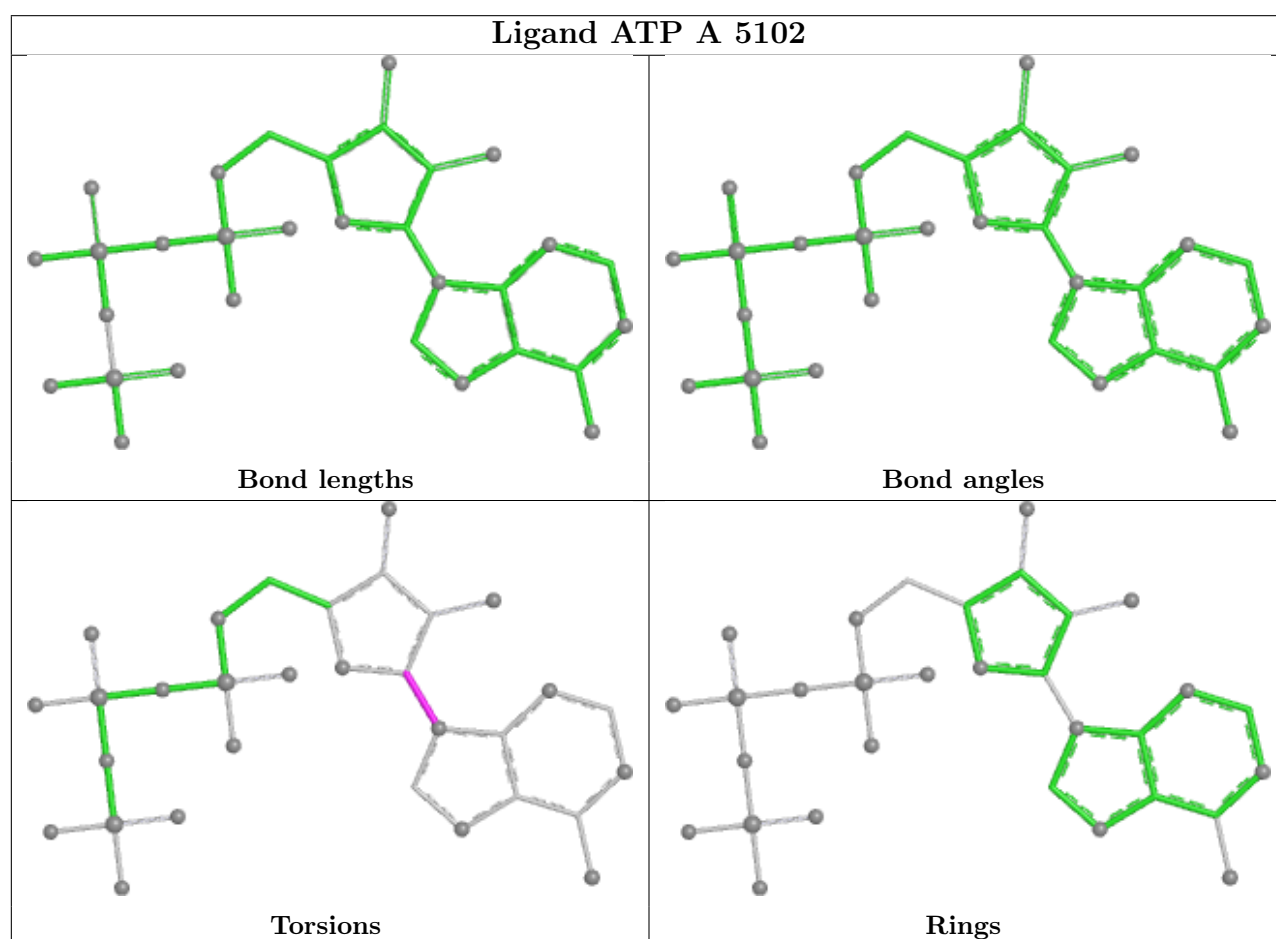
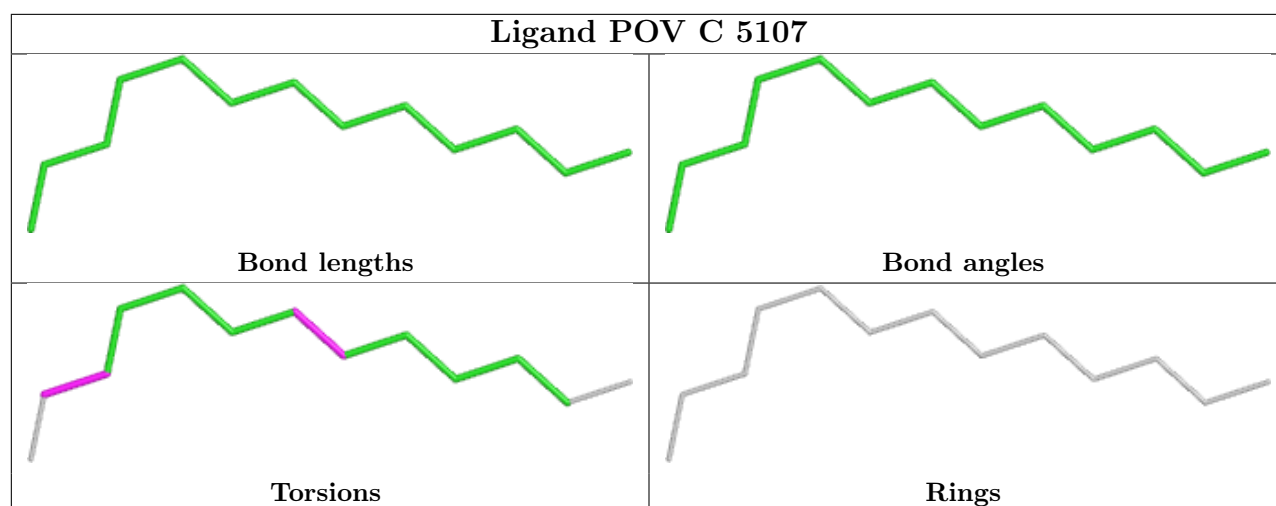
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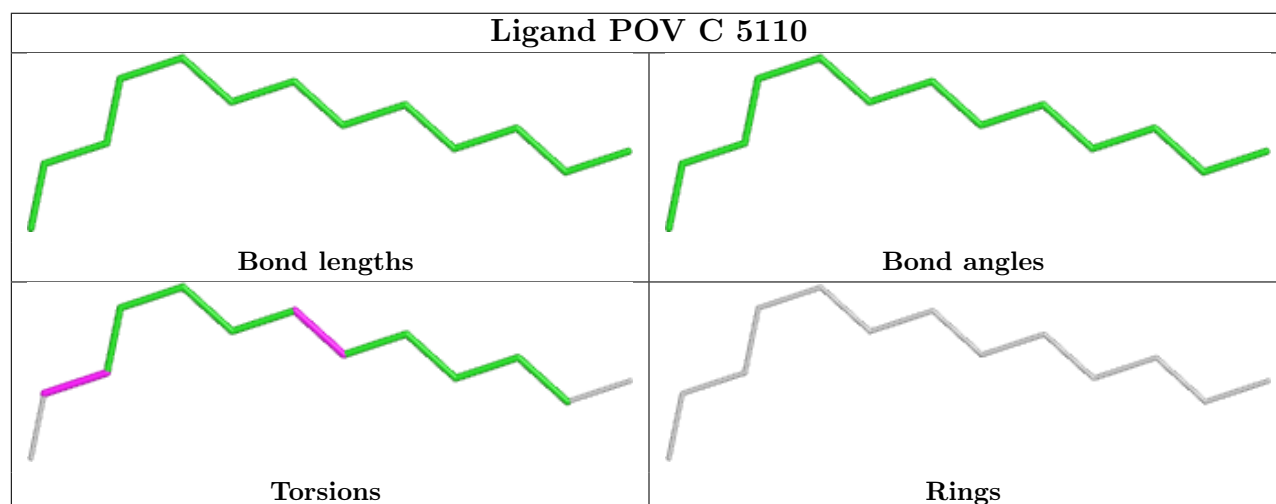
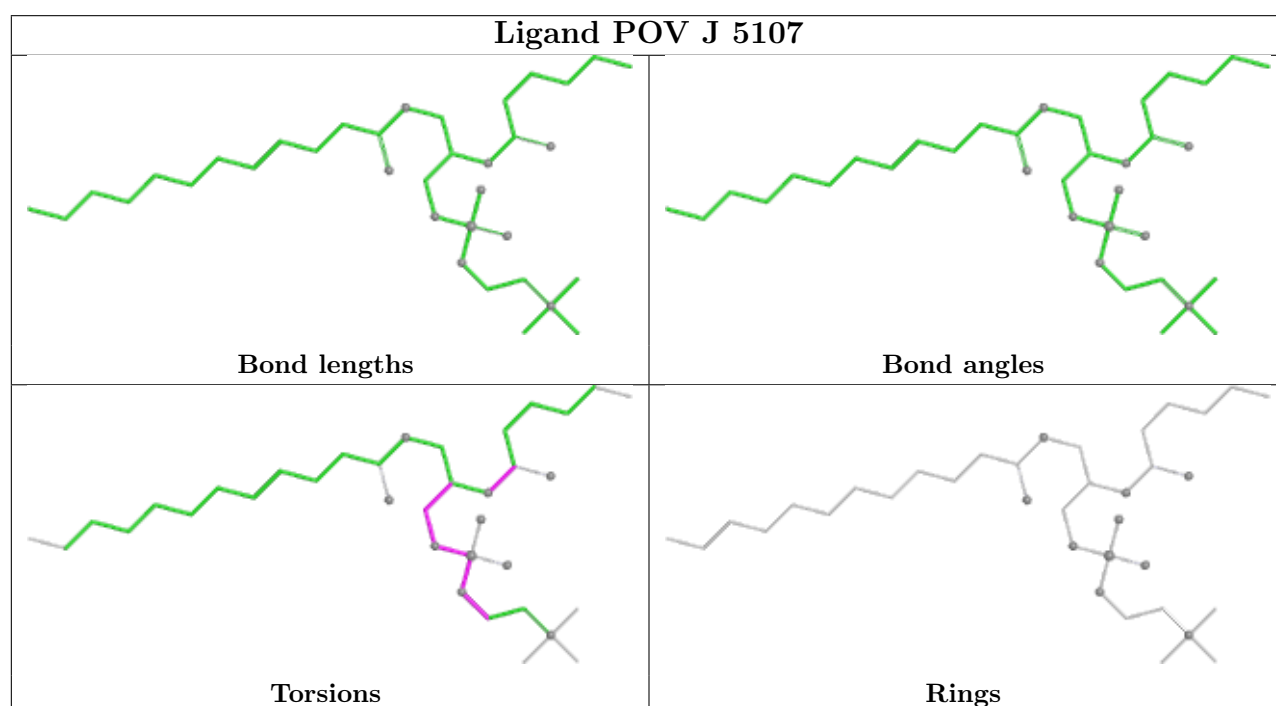
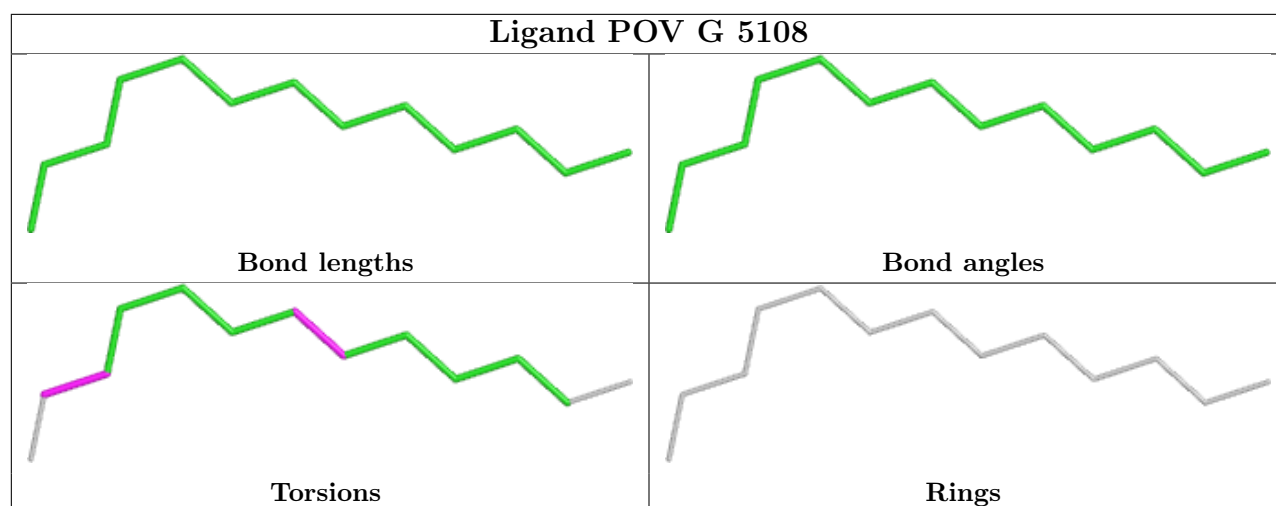
Continued from previous page...

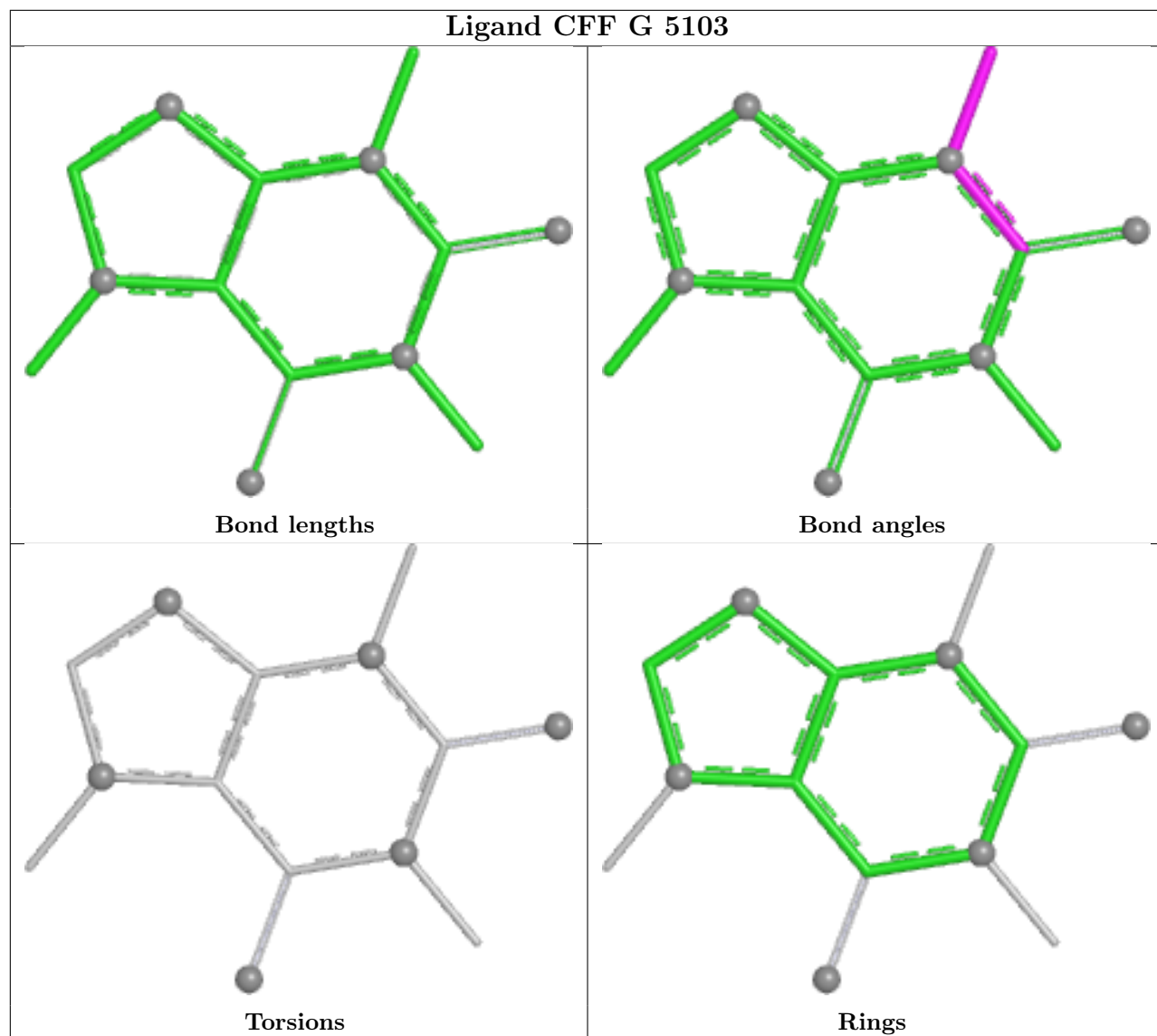
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	5108	POV	1	0
8	A	5110	POV	1	0
8	G	5110	POV	1	0
8	A	5107	POV	2	0
8	G	5106	POV	2	0

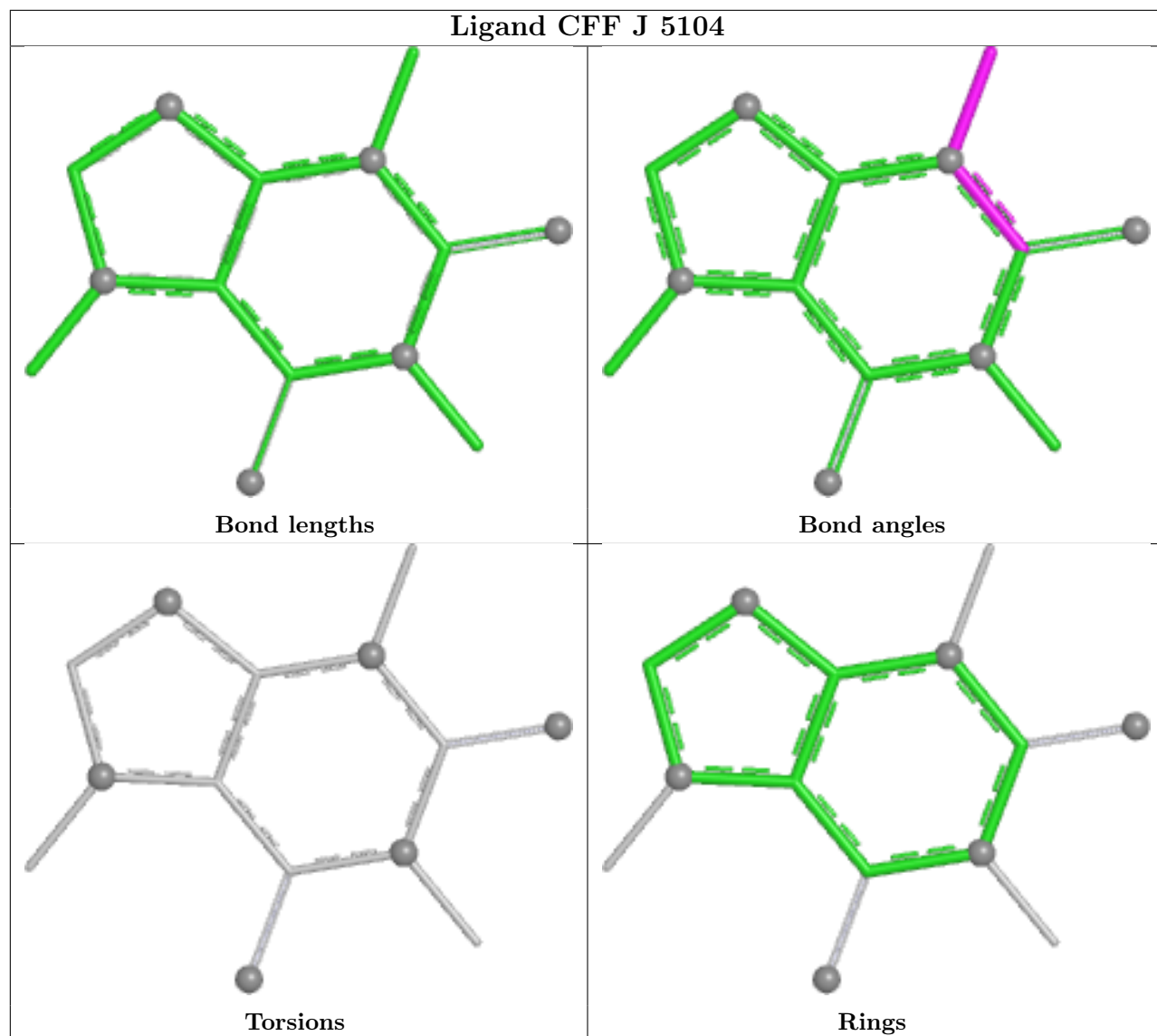
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

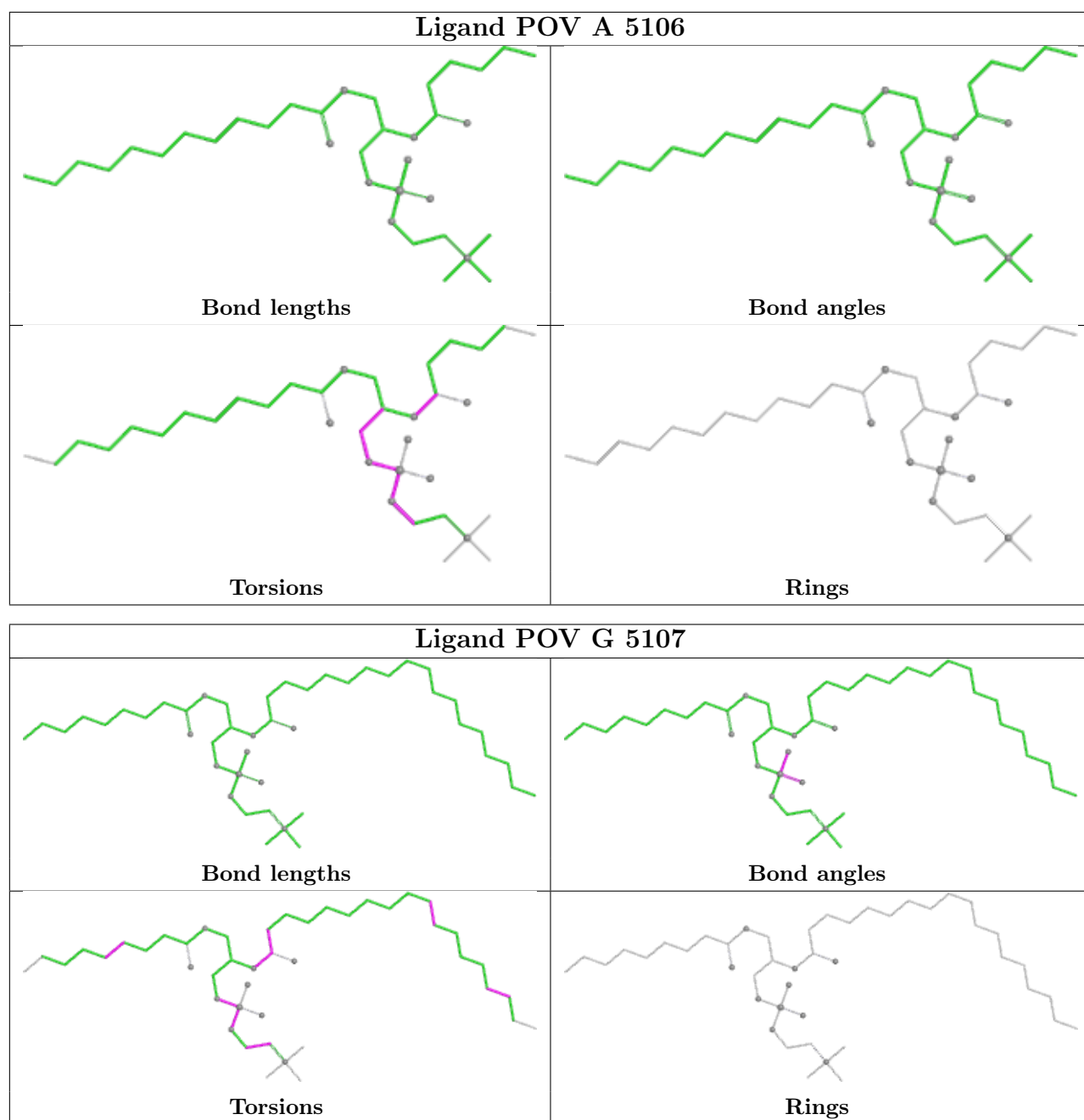


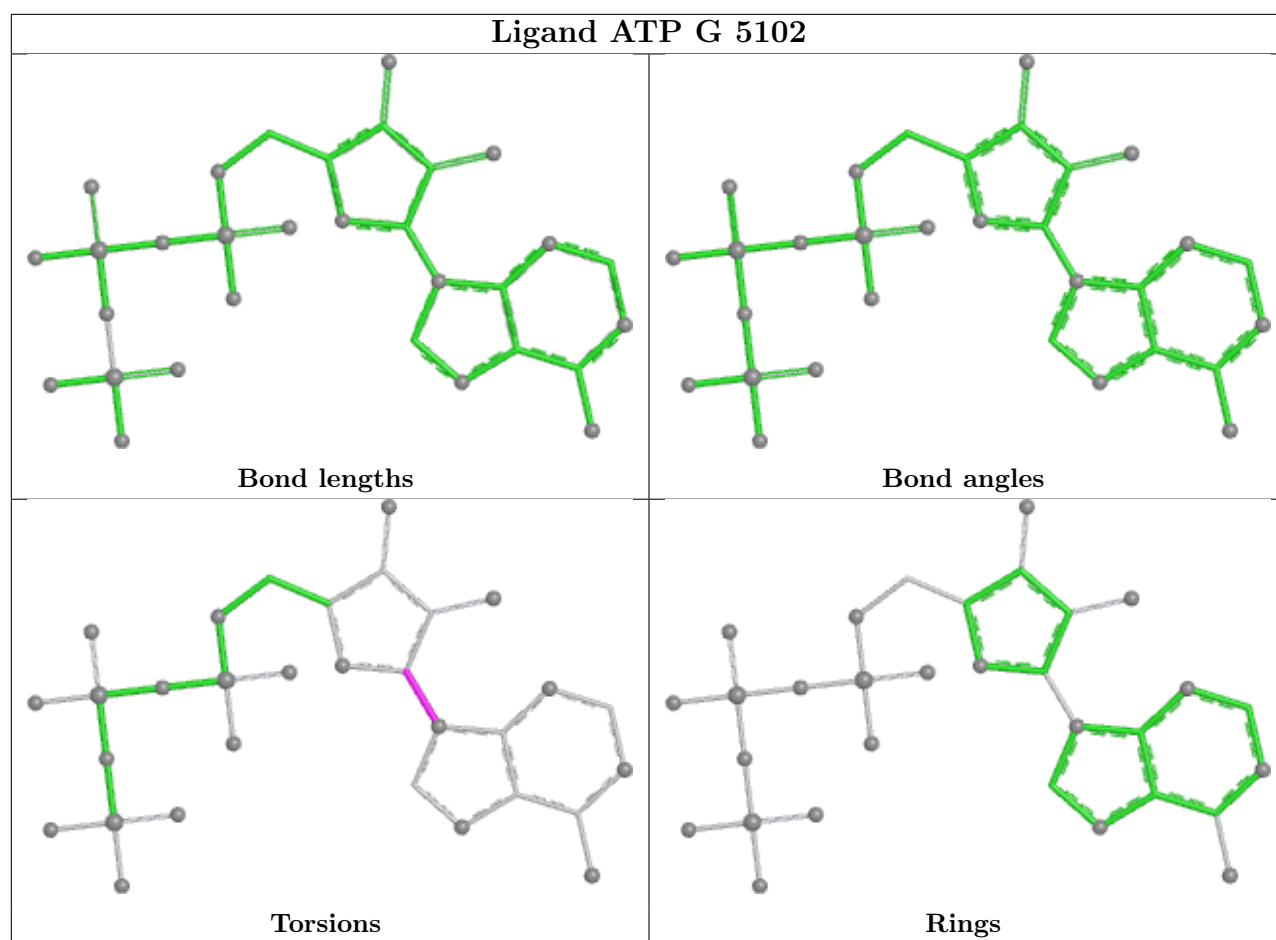


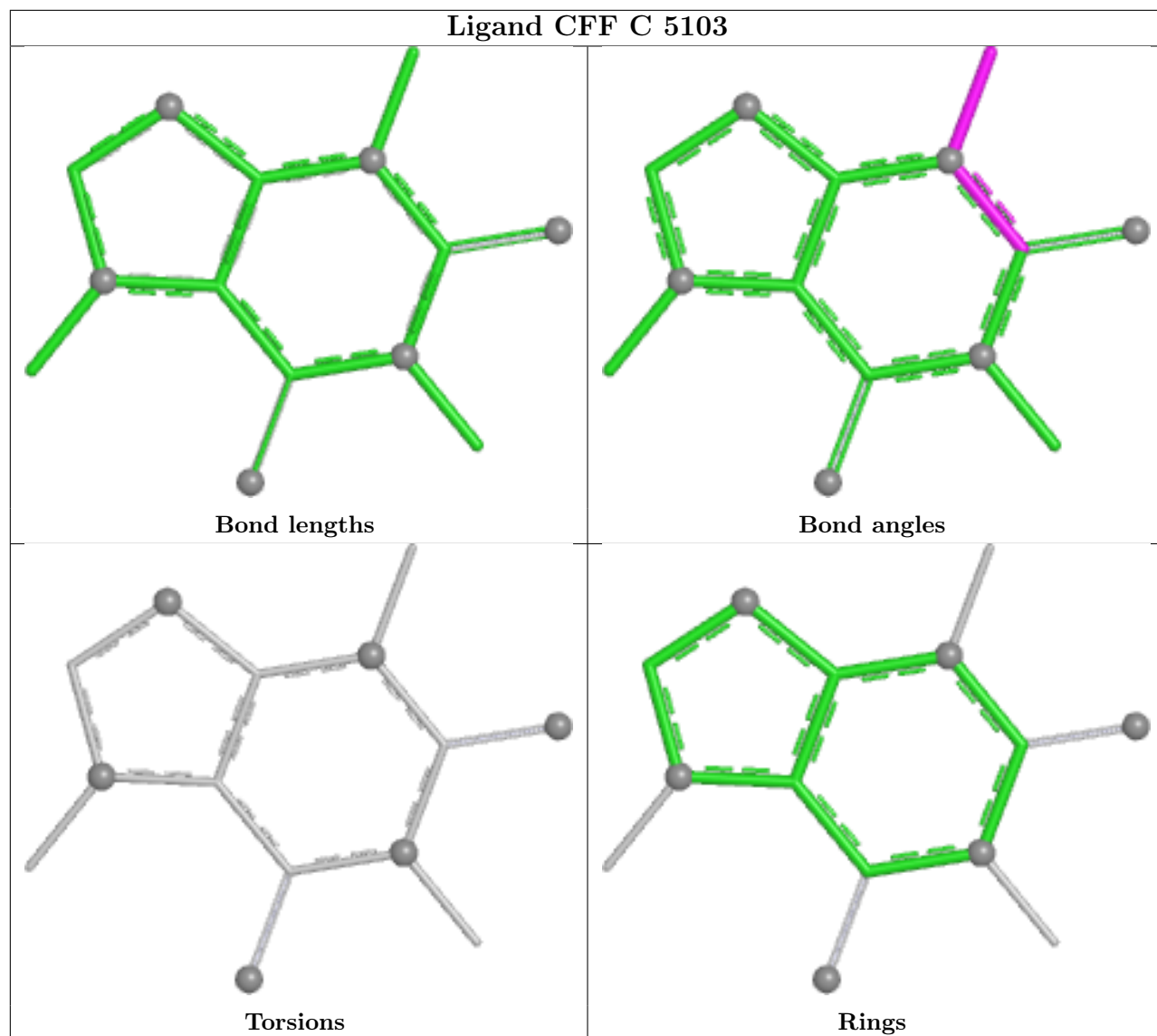


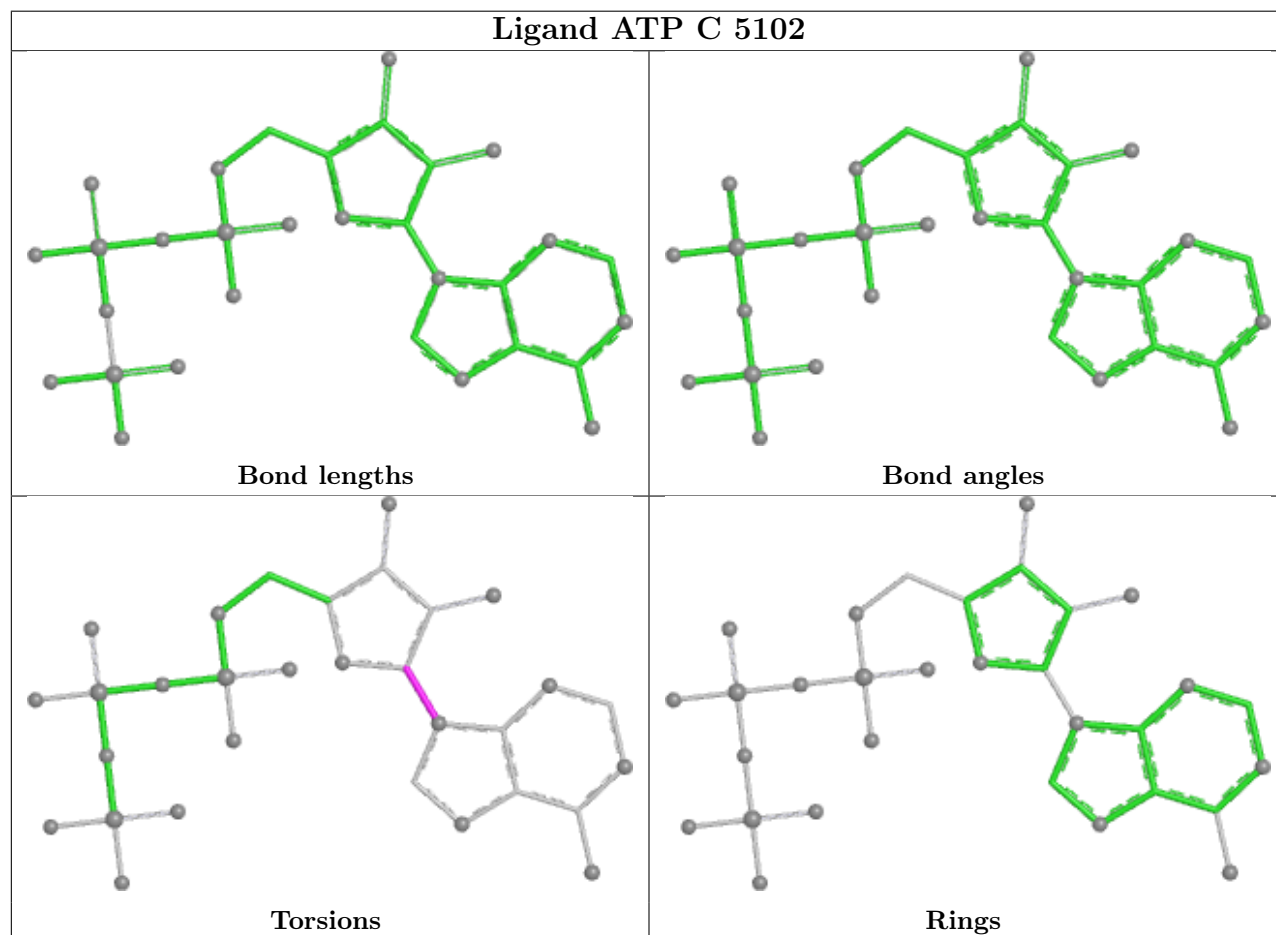
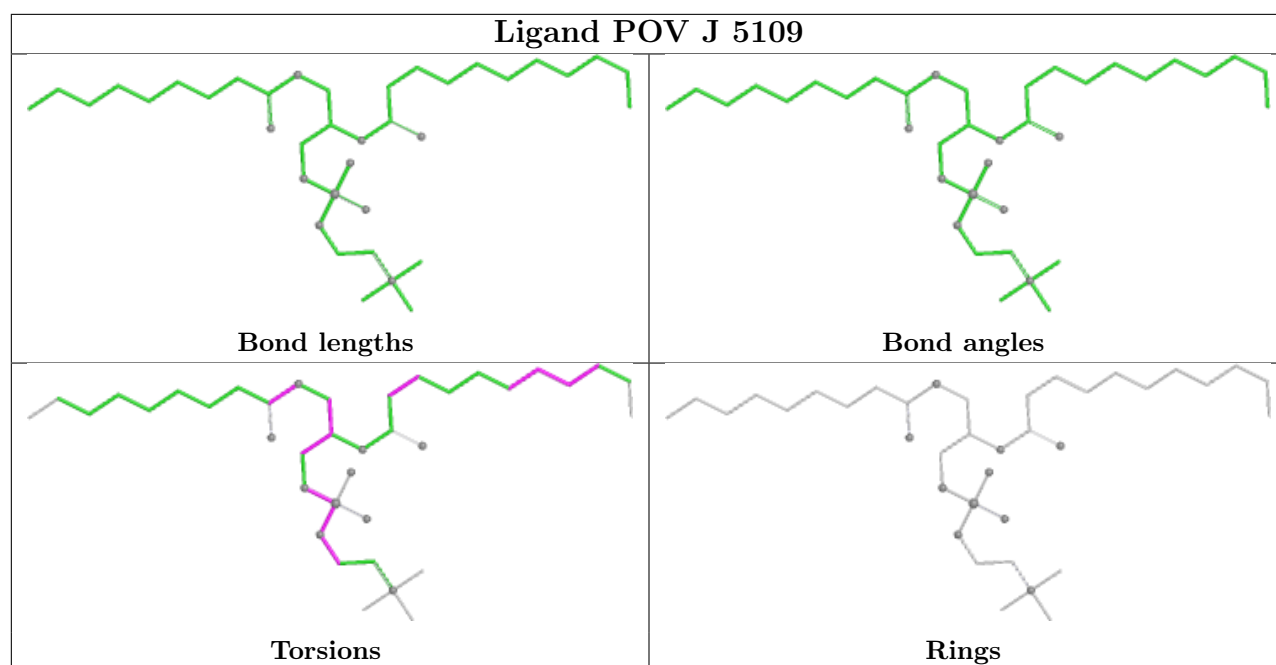


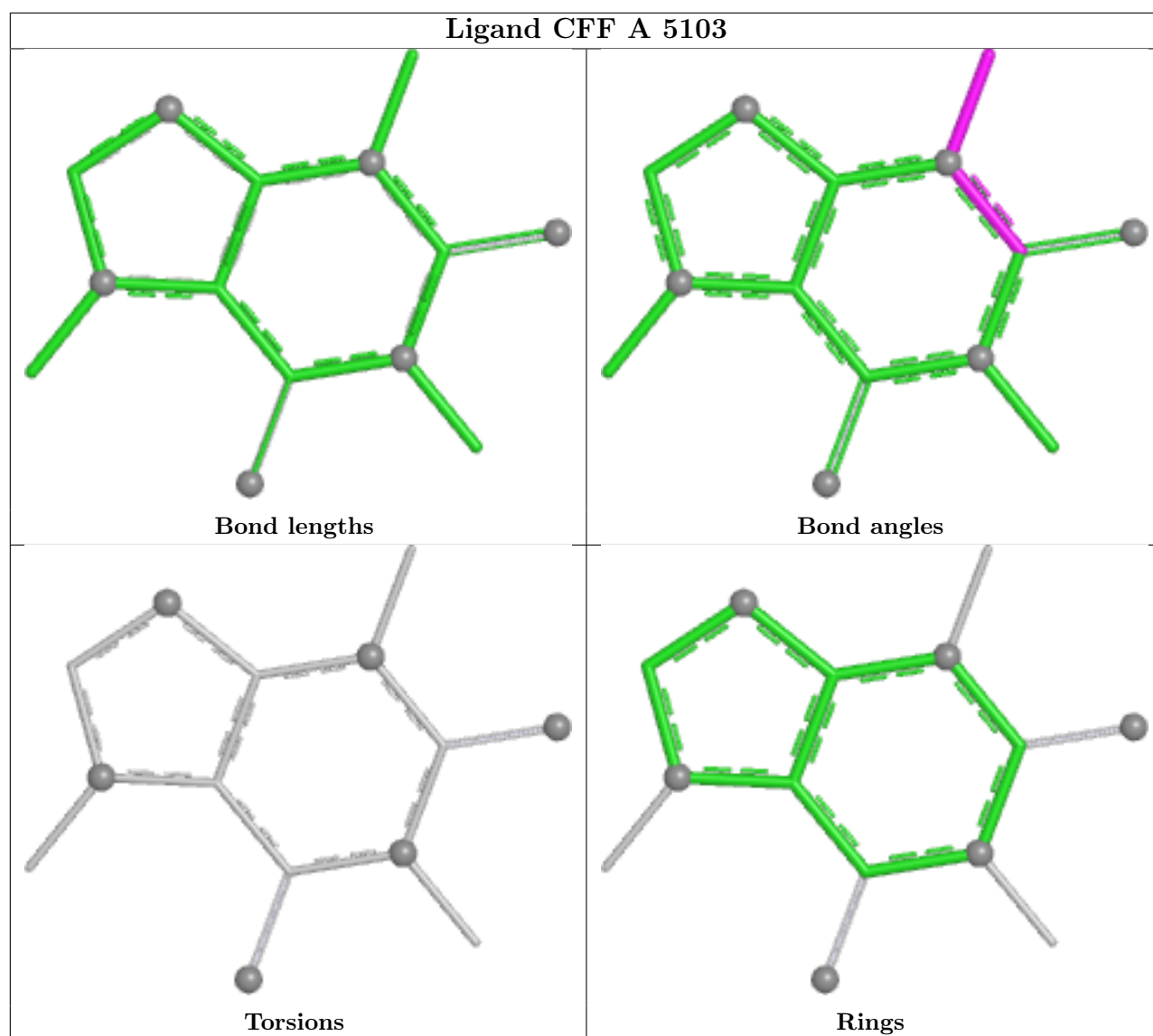


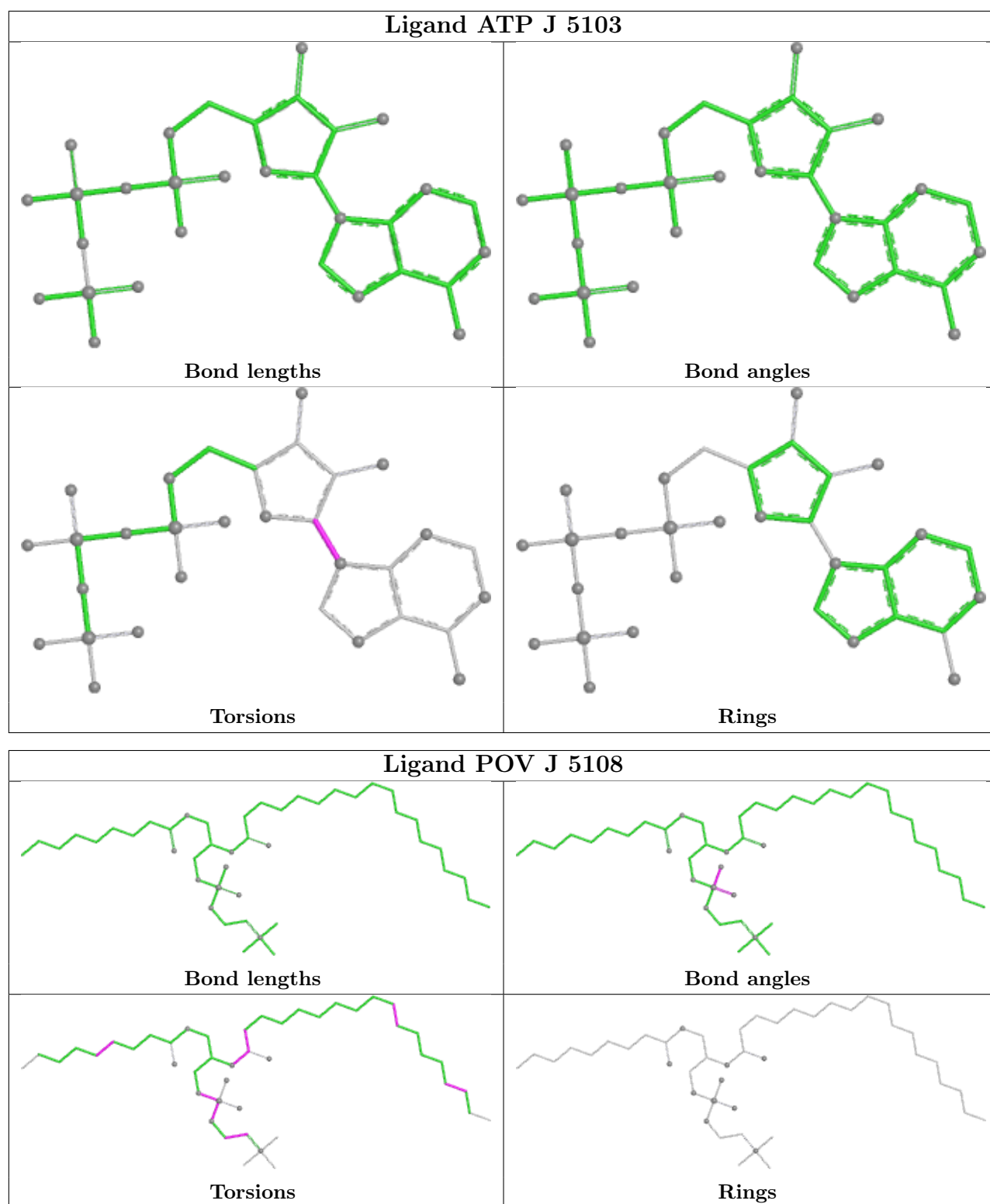


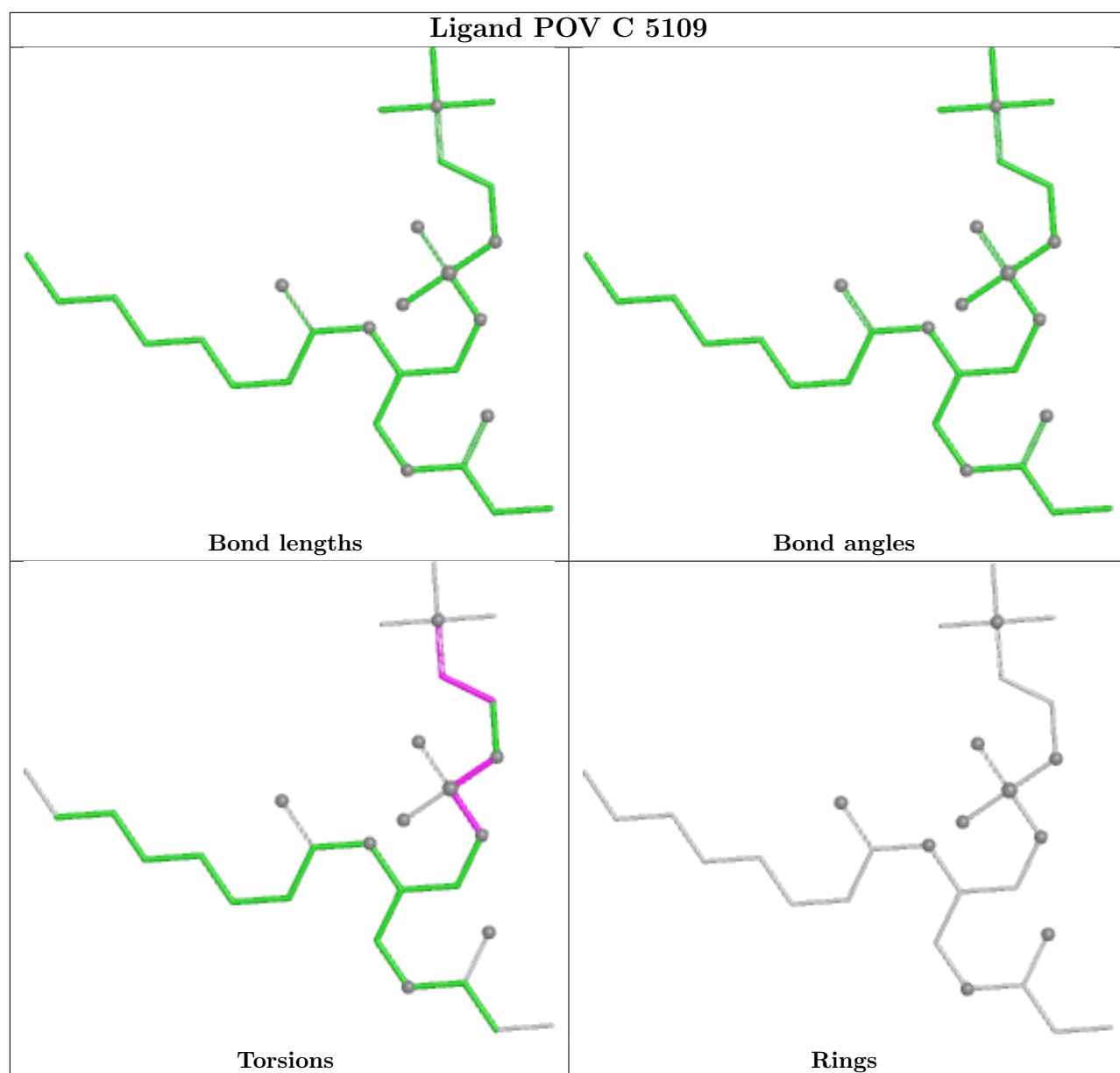


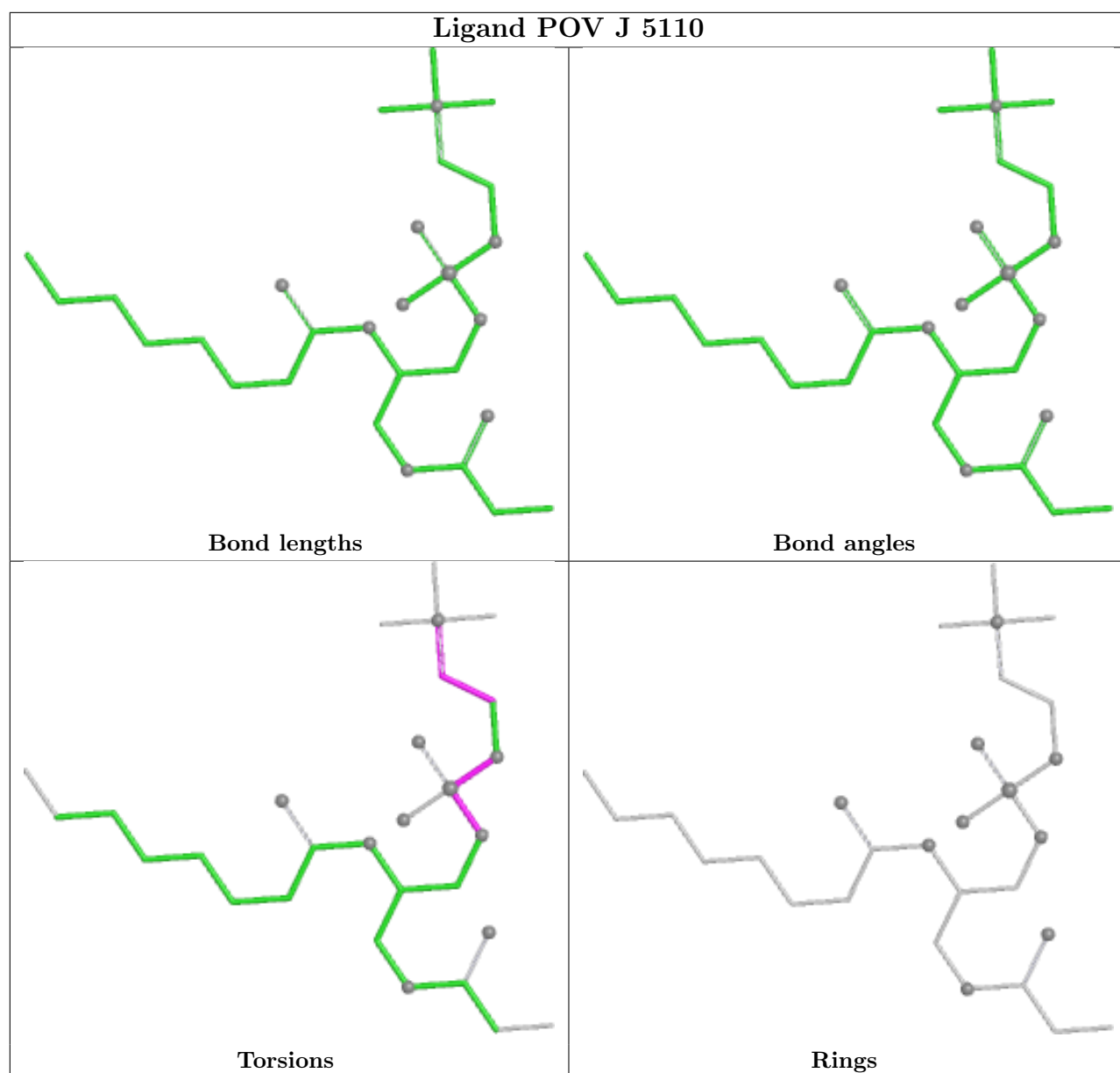


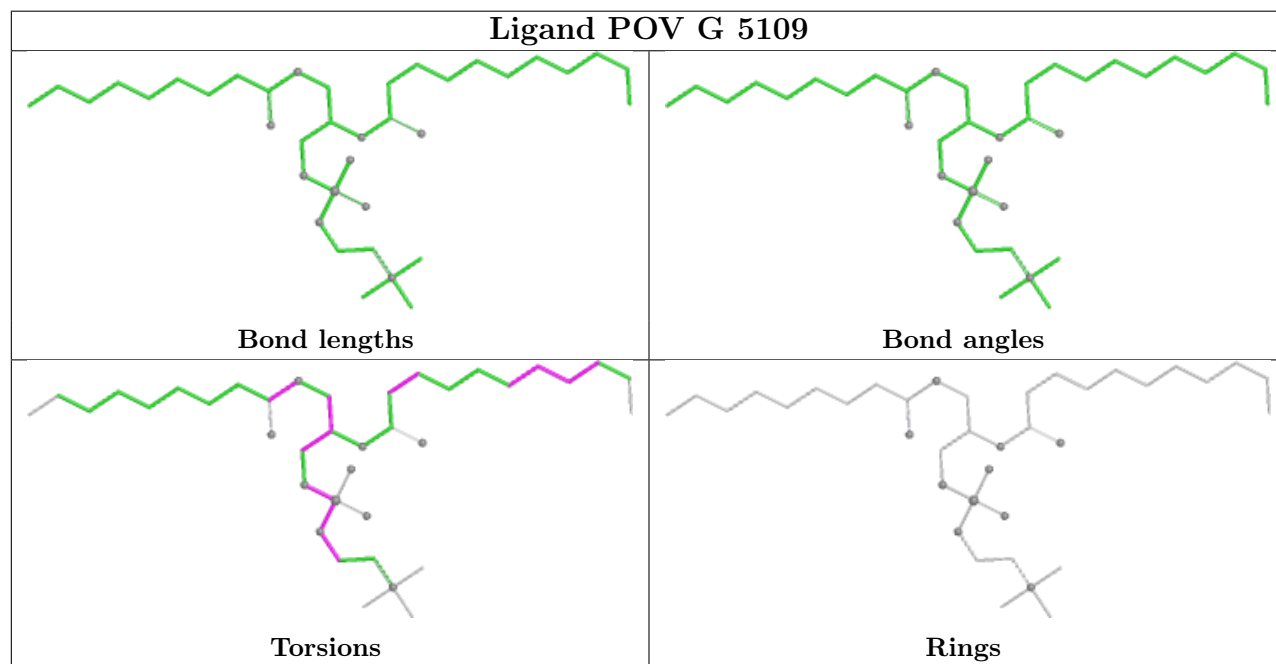
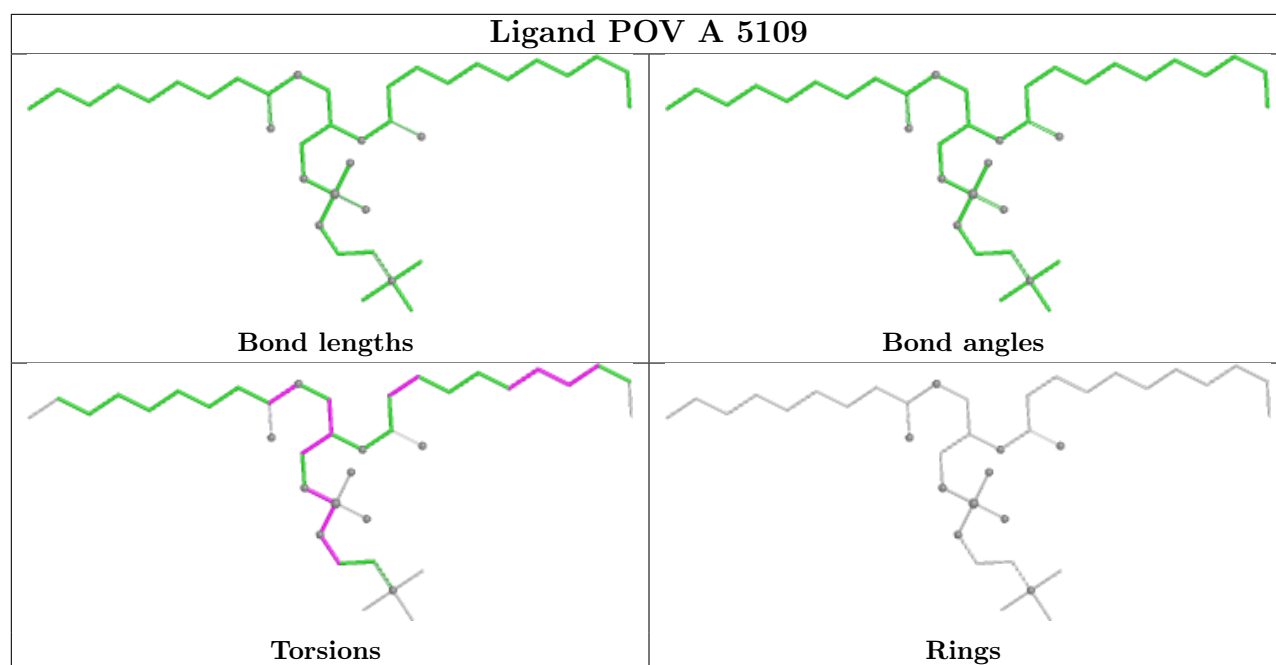


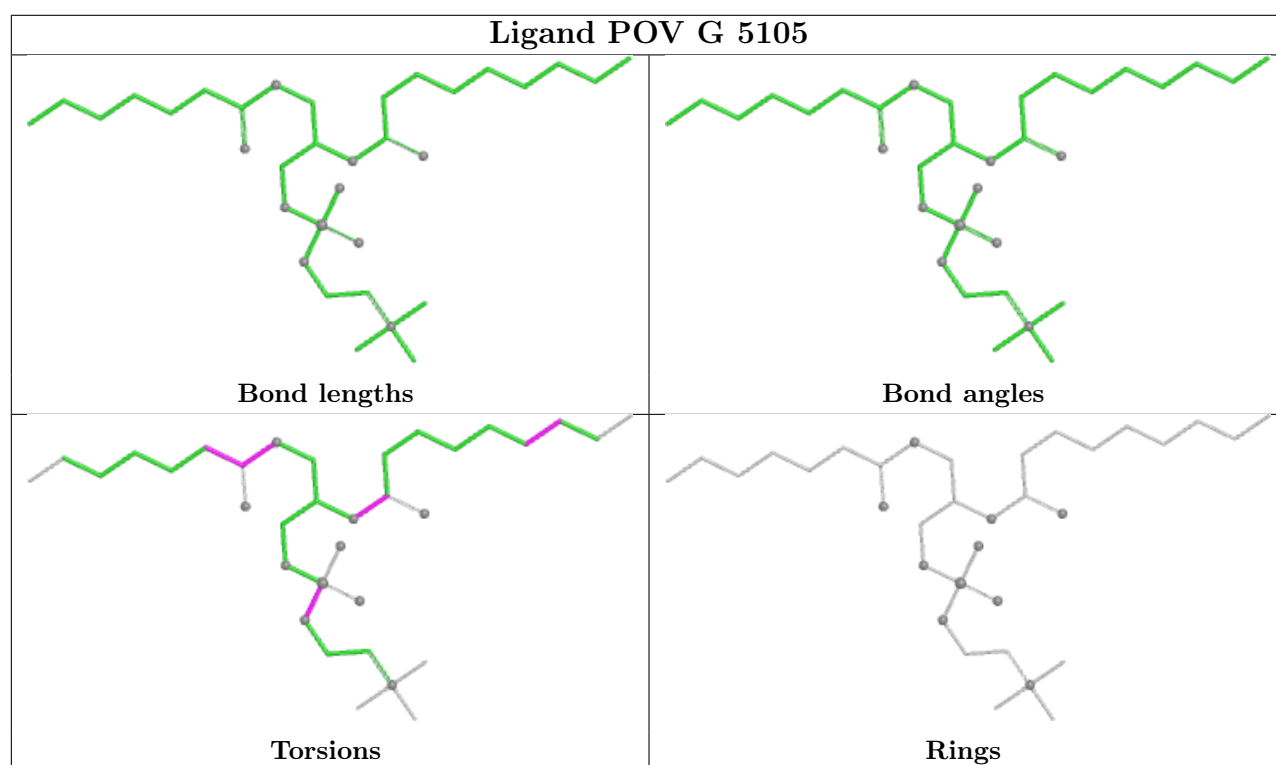
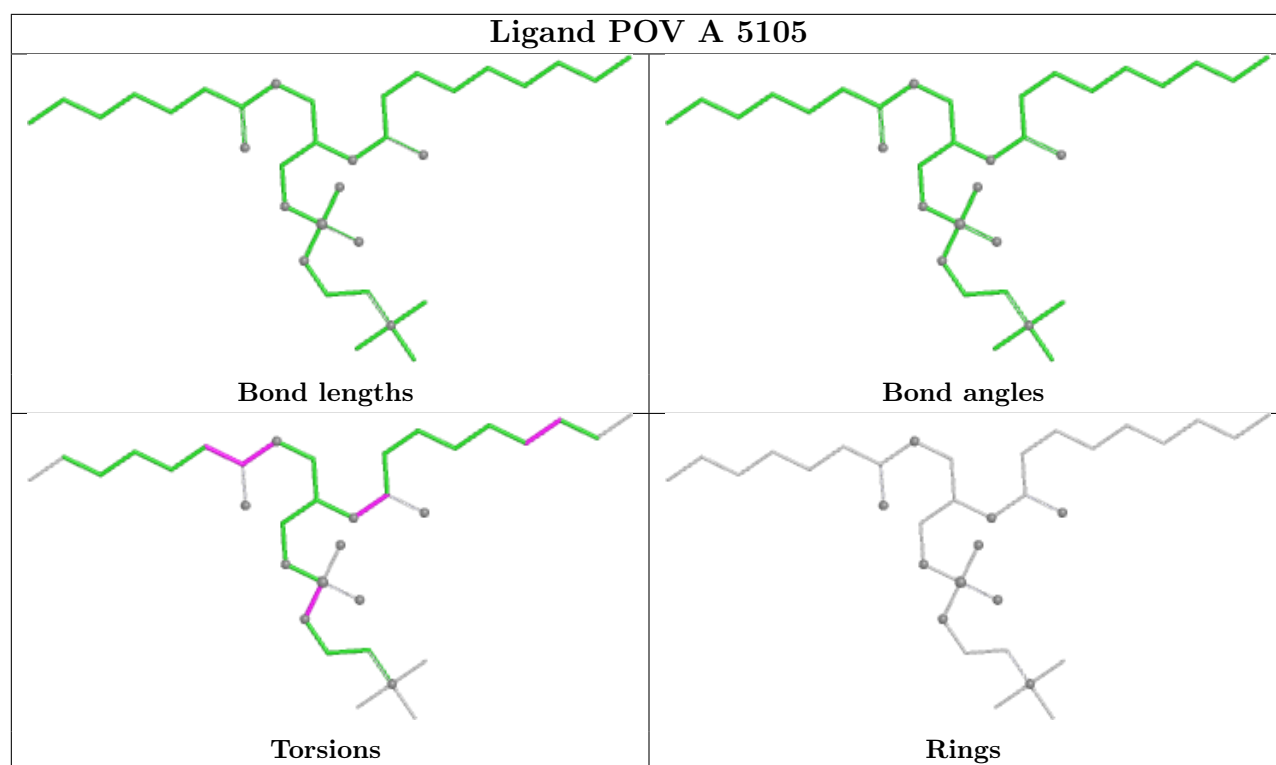


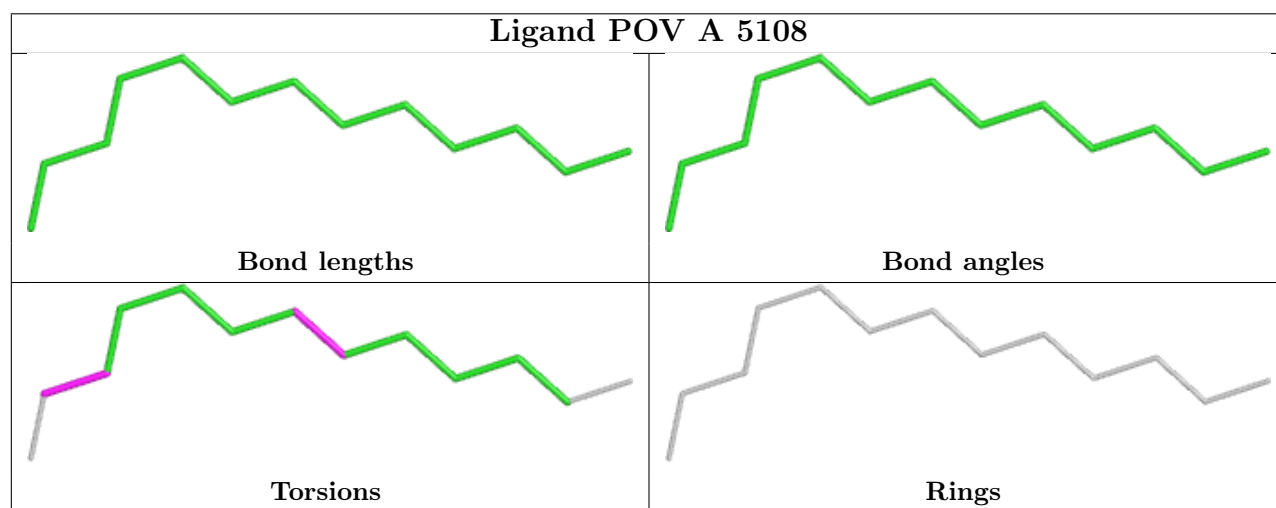
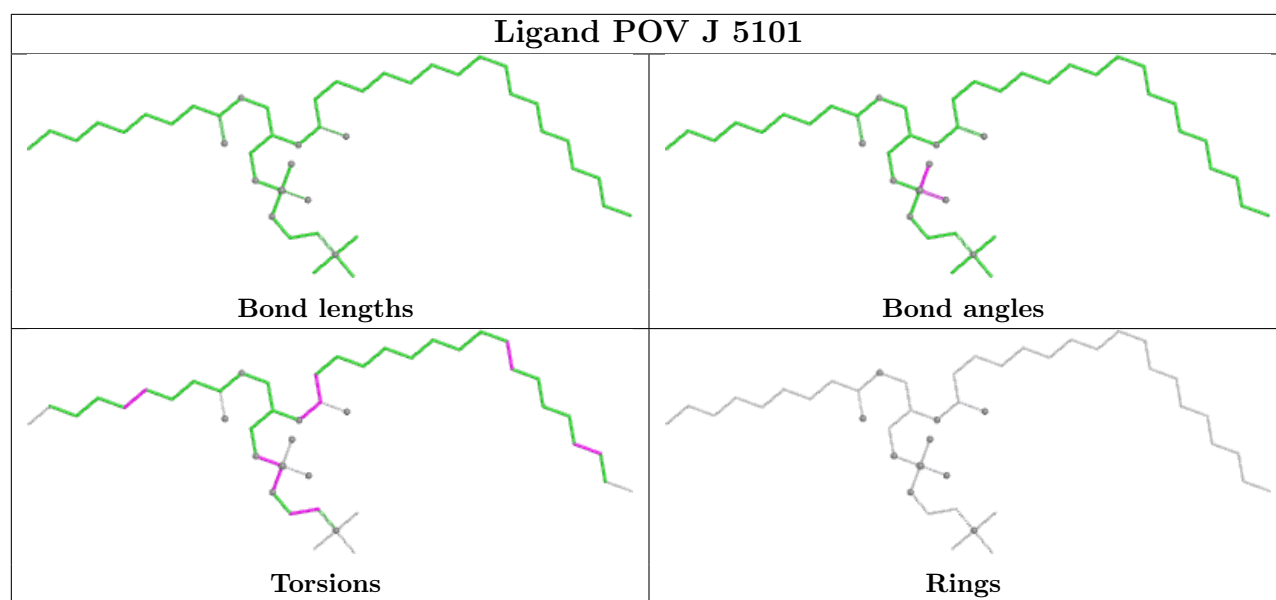


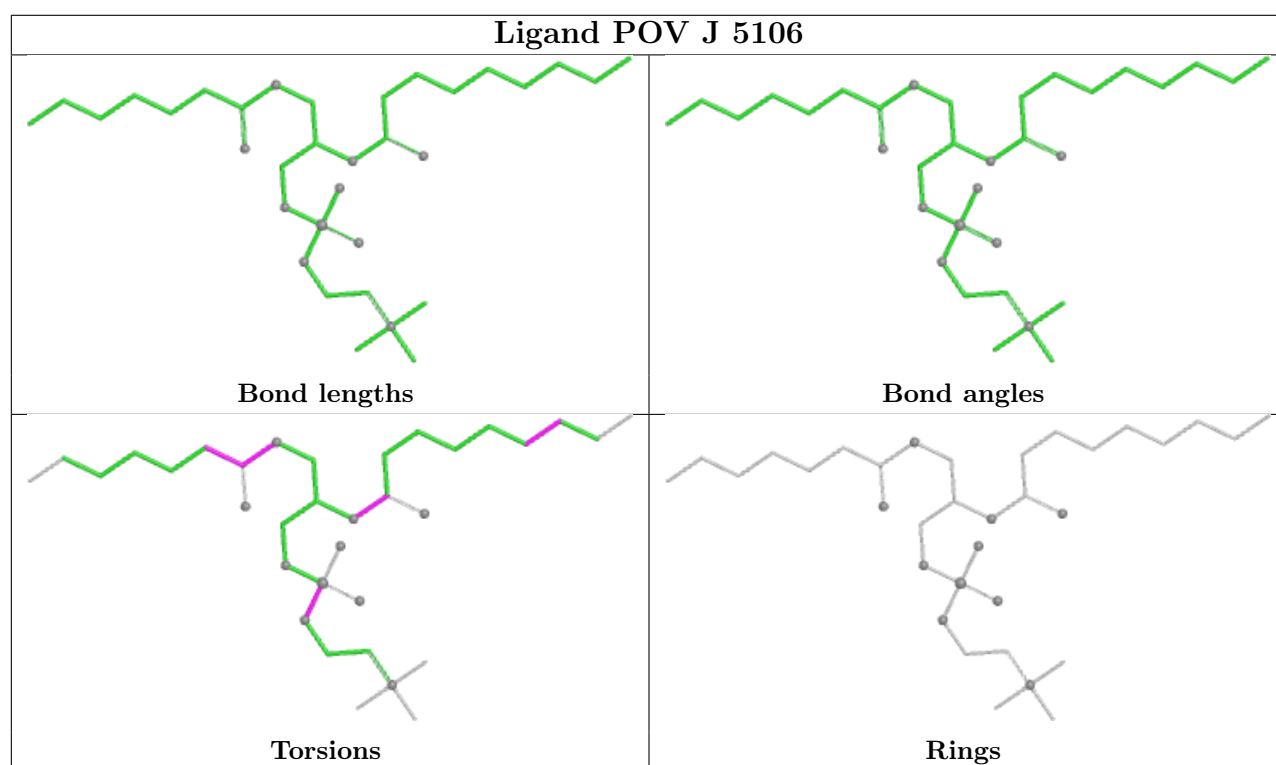
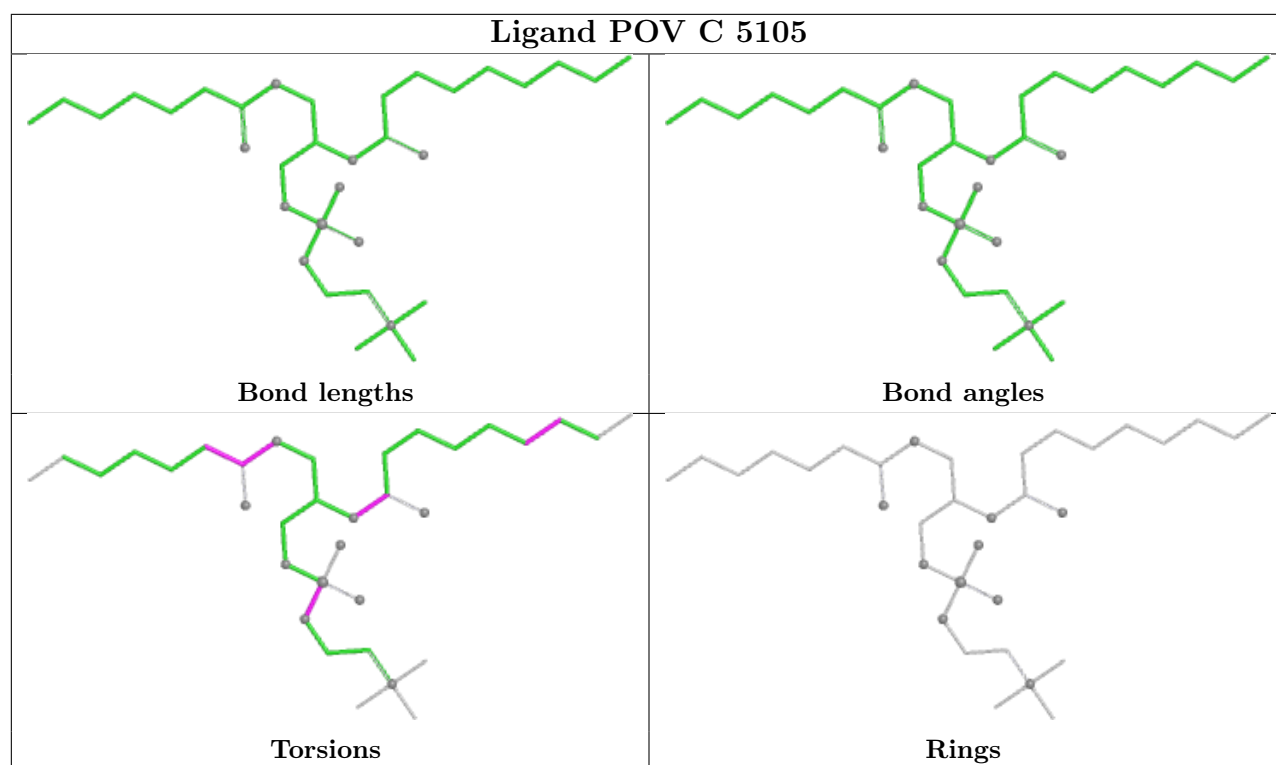


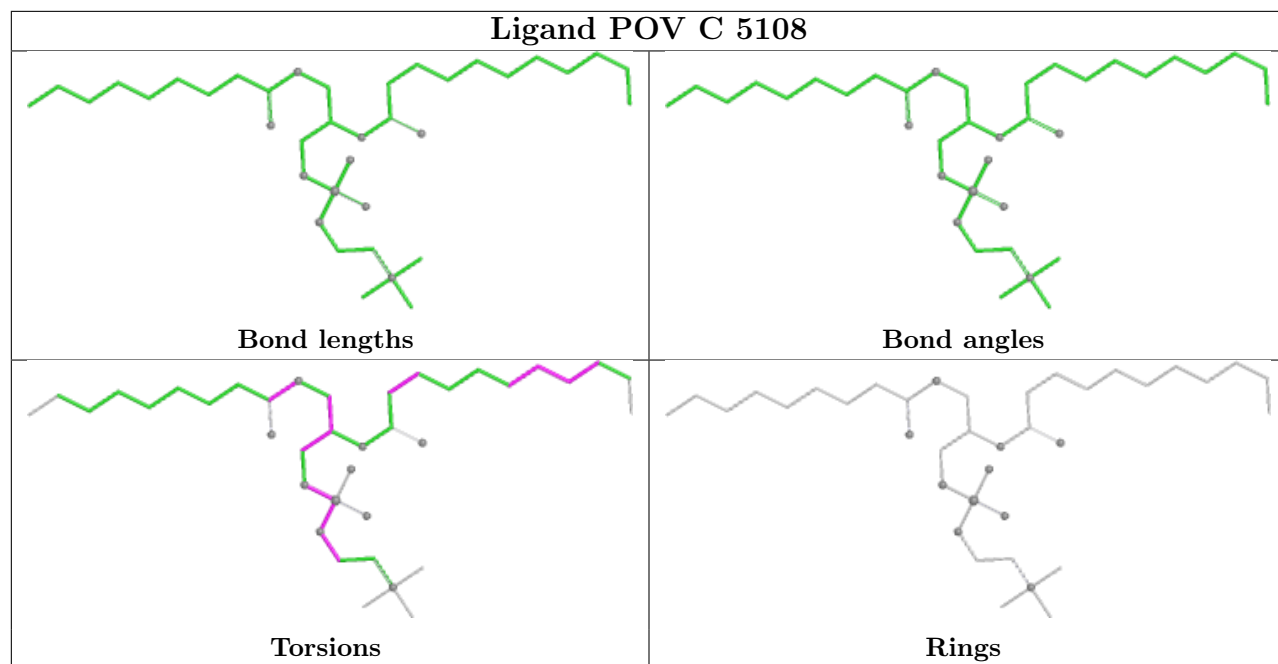


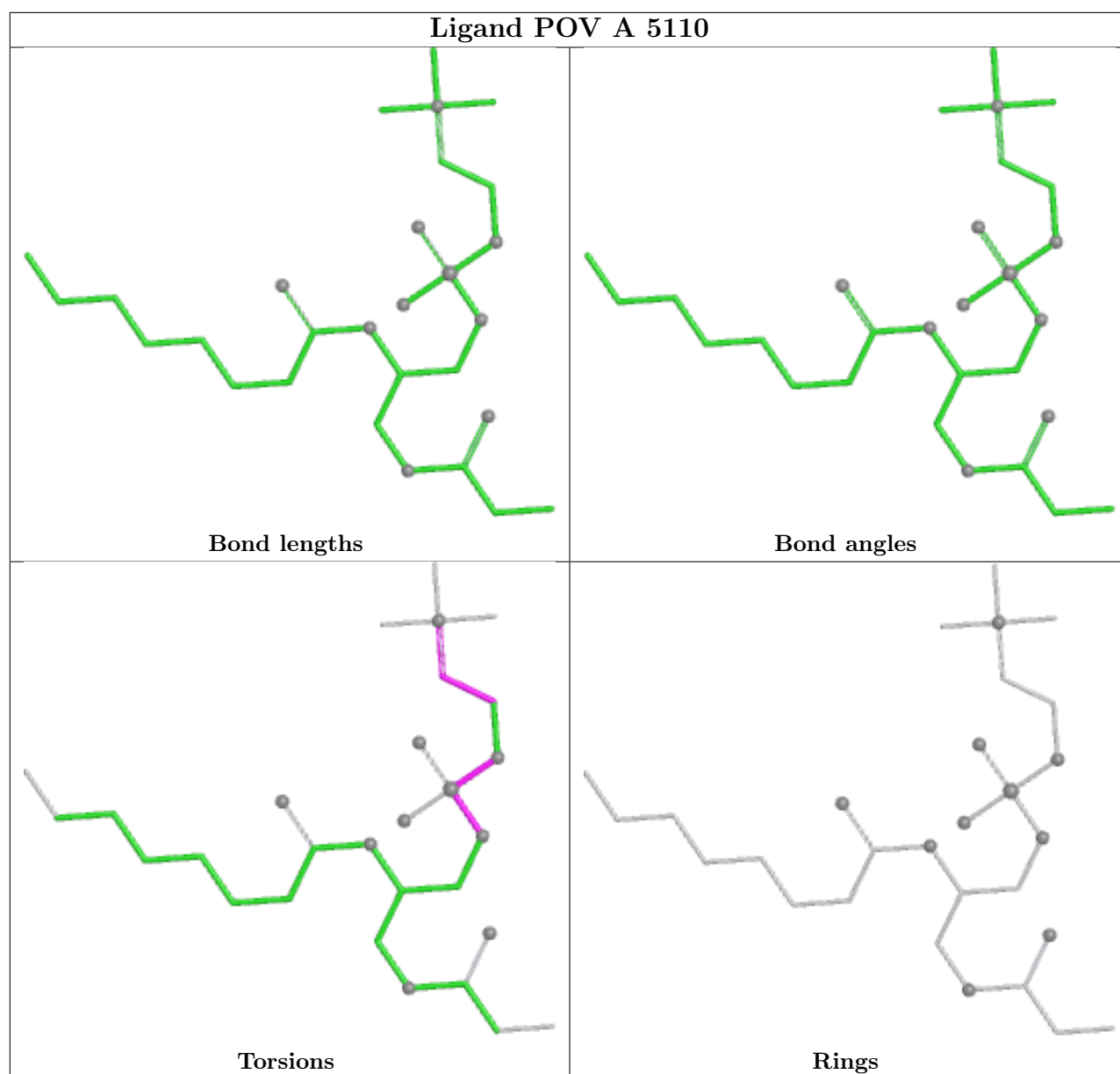


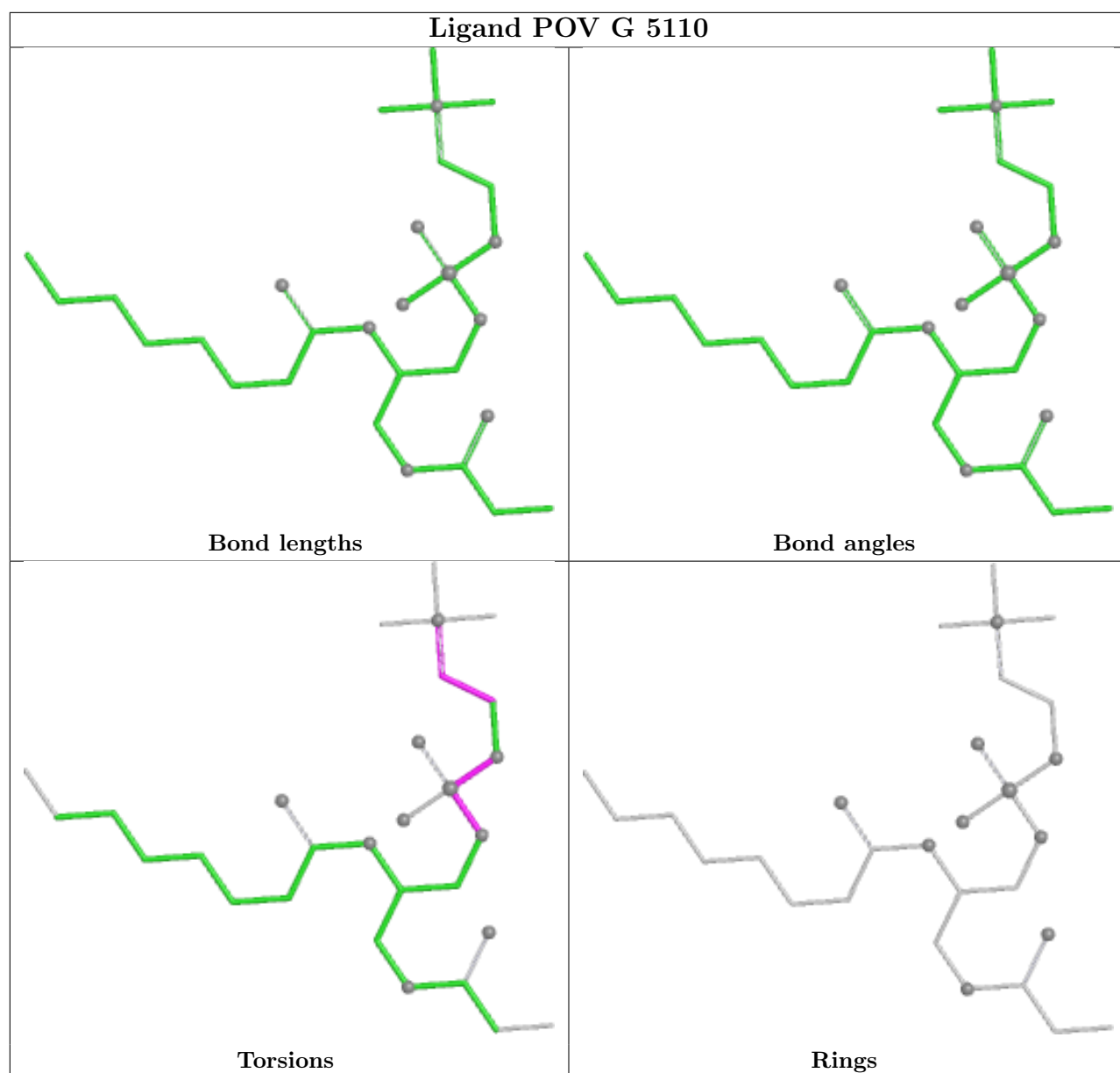


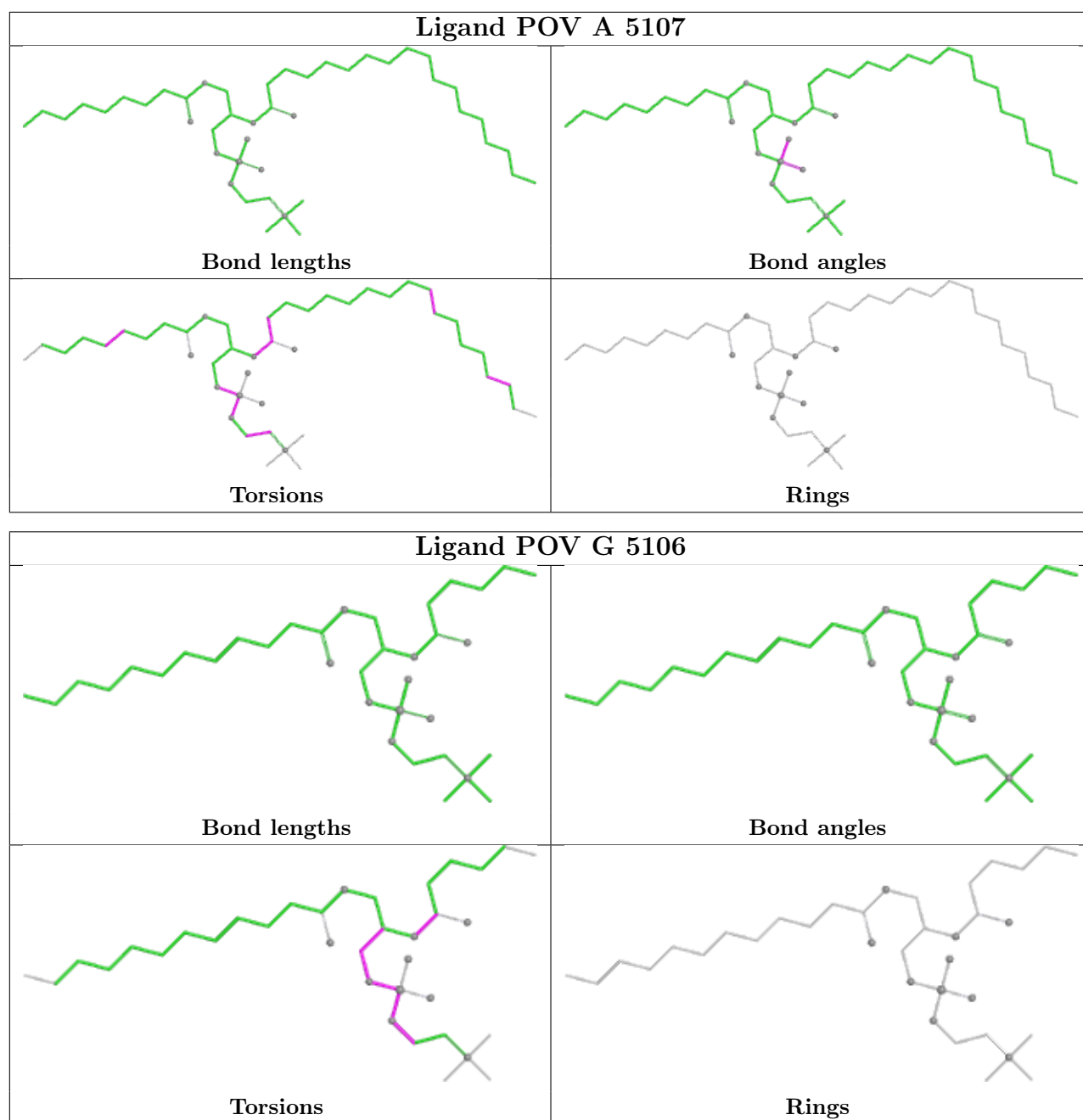












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

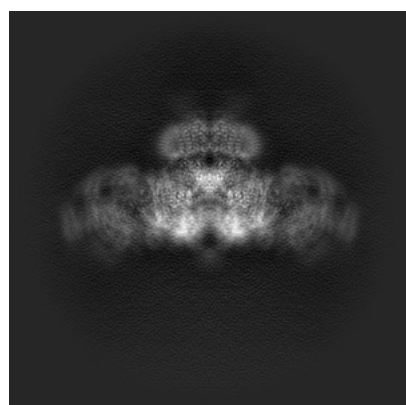
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53924. These allow visual inspection of the internal detail of the map and identification of artifacts.

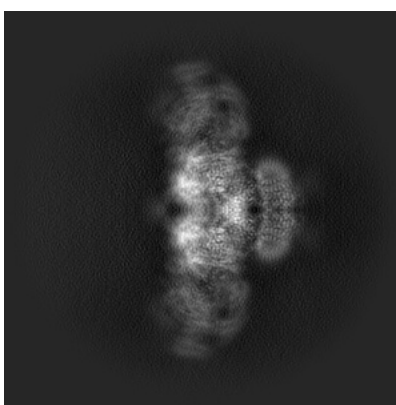
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

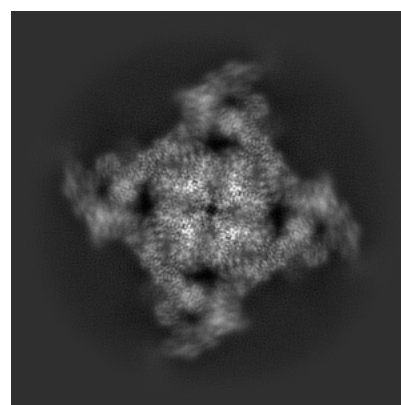
6.1.1 Primary map



X



Y

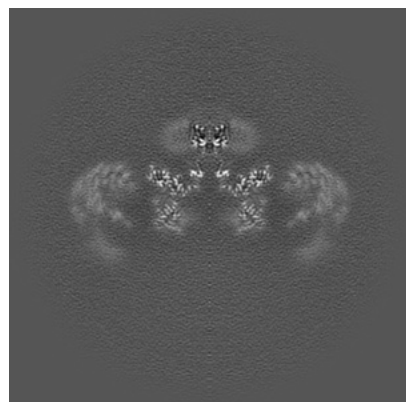


Z

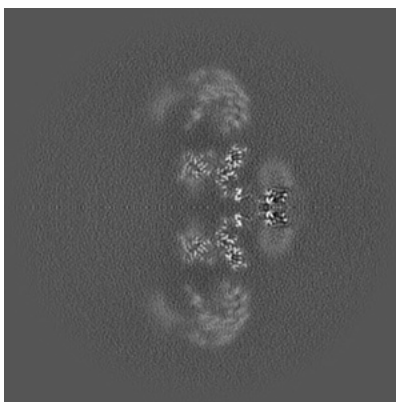
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

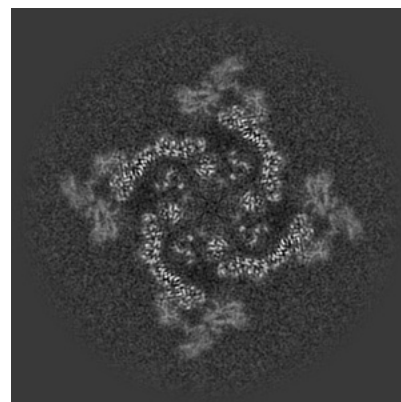
6.2.1 Primary map



X Index: 168



Y Index: 168

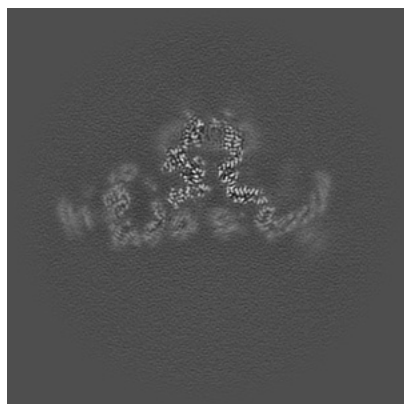


Z Index: 168

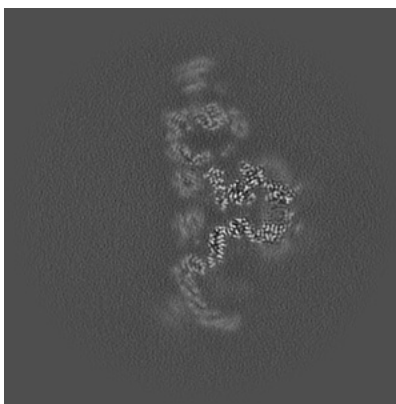
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

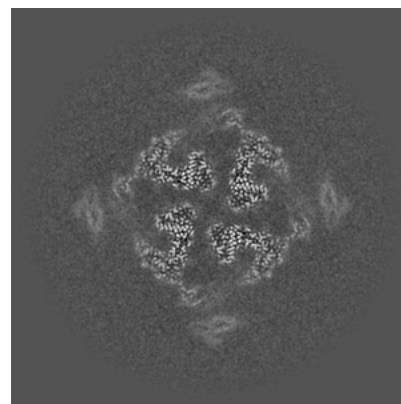
6.3.1 Primary map



X Index: 151



Y Index: 151

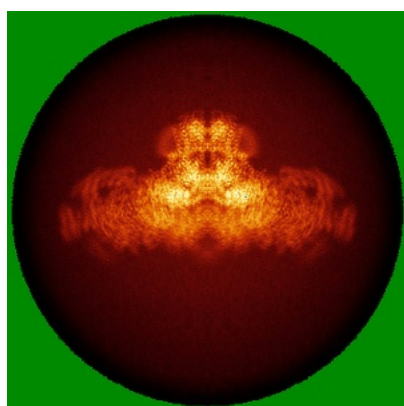


Z Index: 182

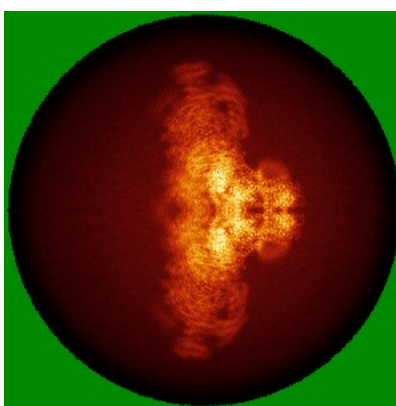
The images above show the largest variance slices of the map in three orthogonal directions.

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

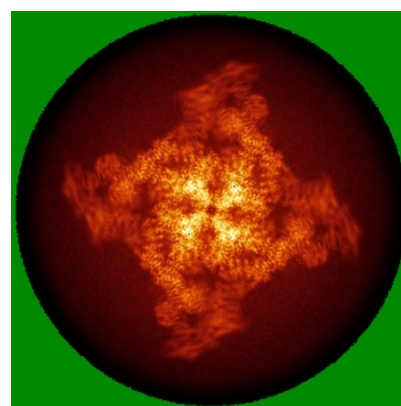
6.4.1 Primary map



X



Y

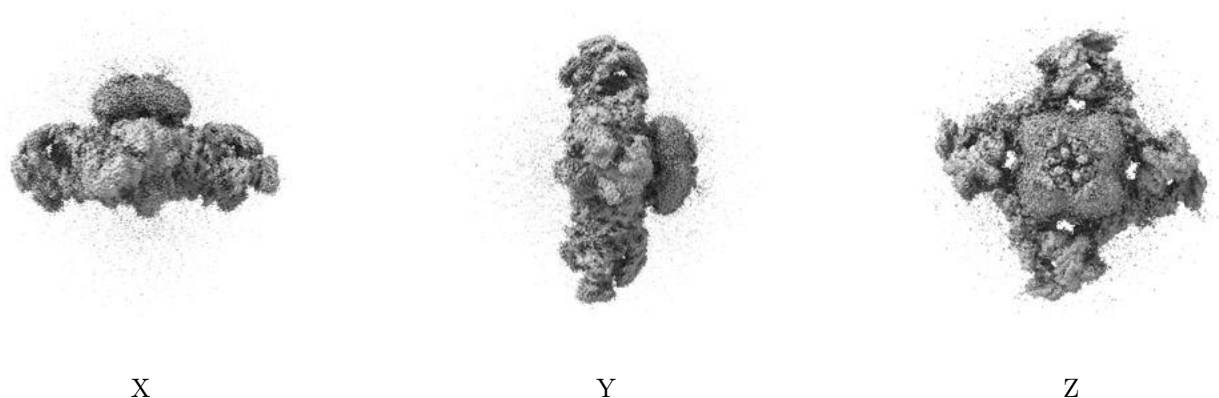


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

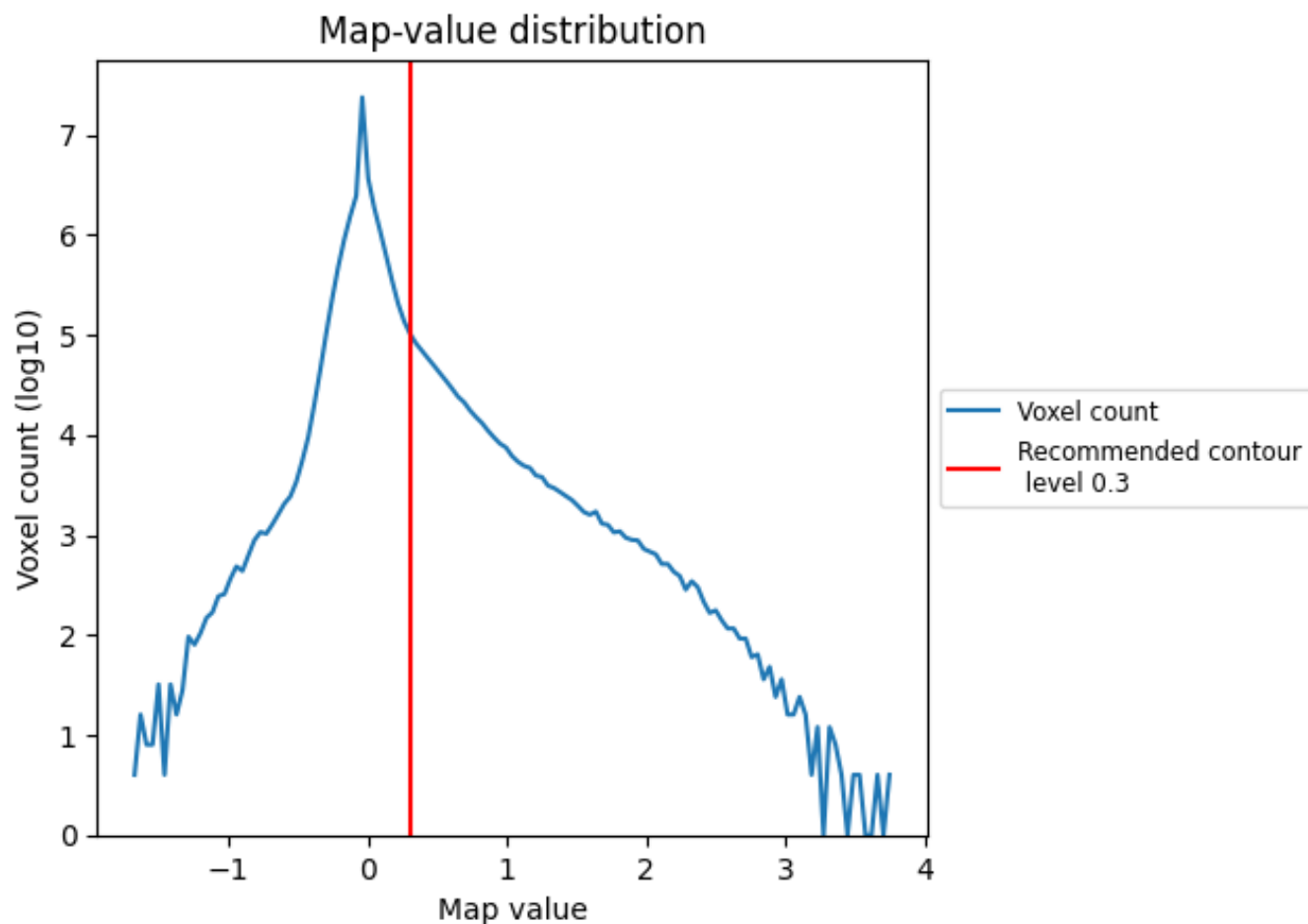
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

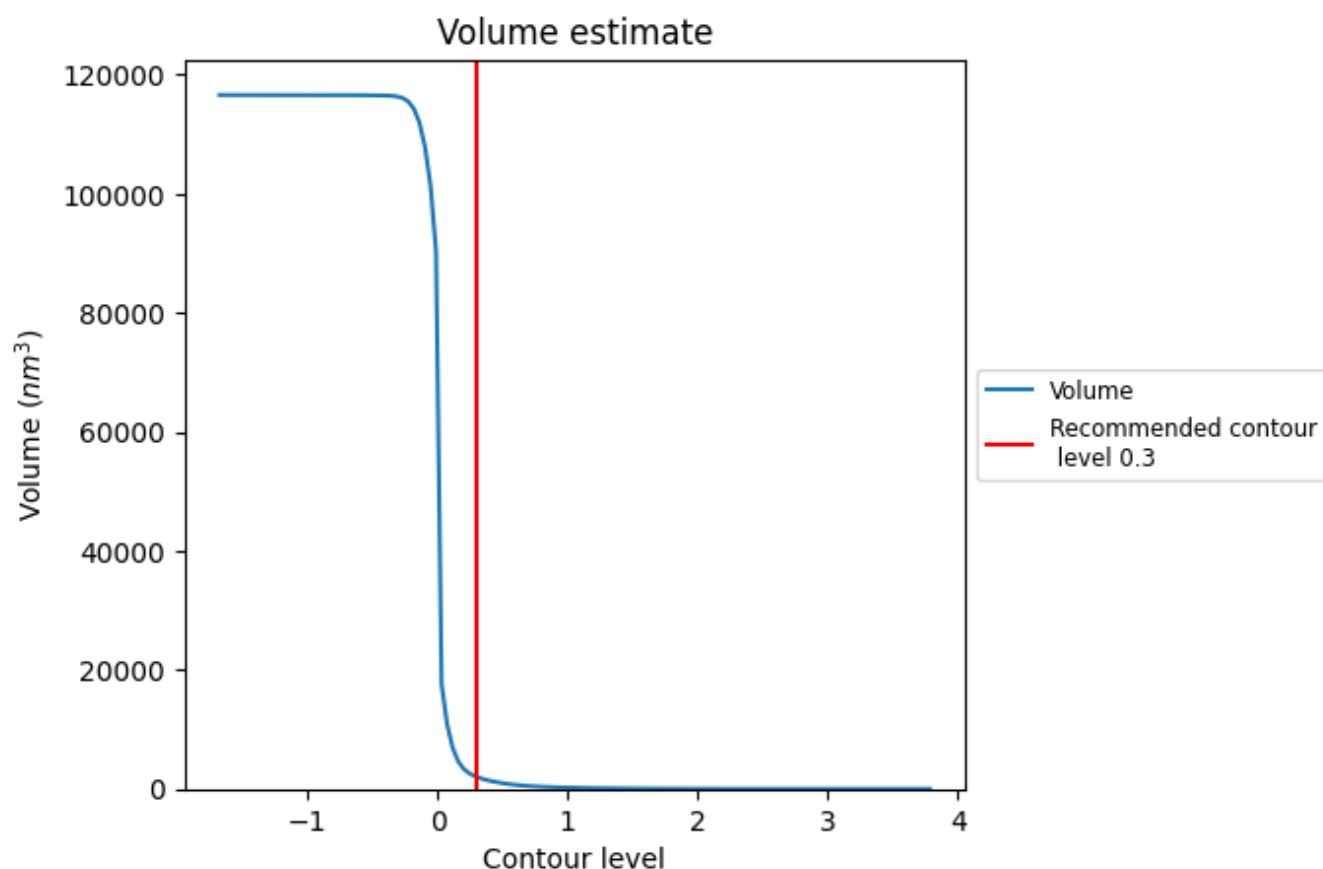
This section contains the results of statistical analysis of the map.

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.

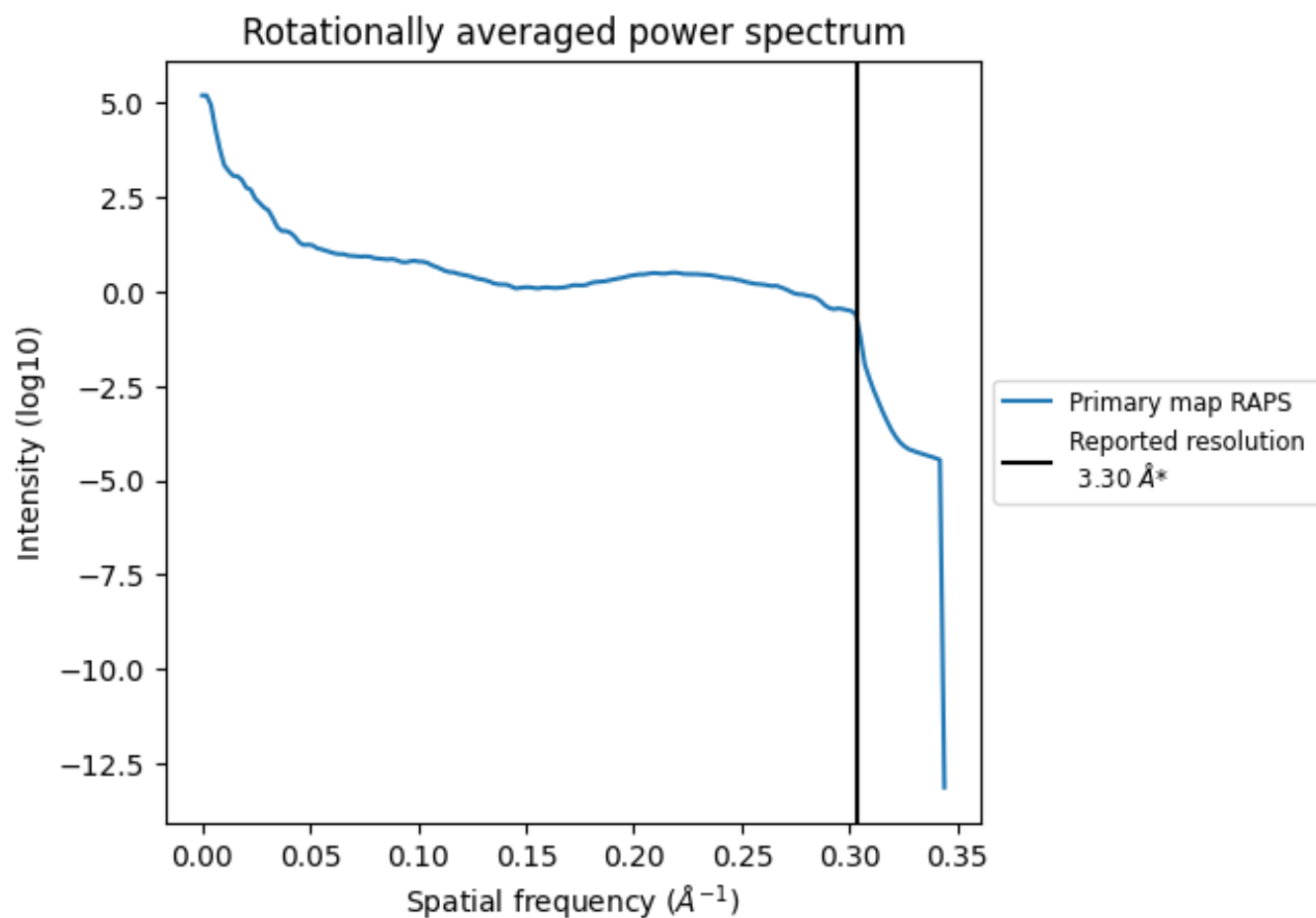
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2061 nm³; this corresponds to an approximate mass of 1861 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 0.303 Å⁻¹

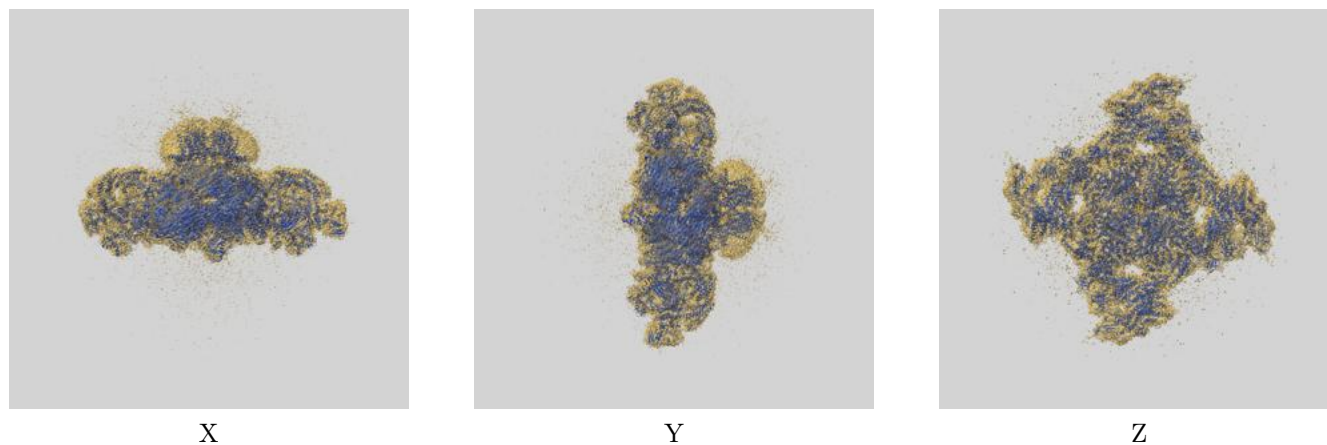
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

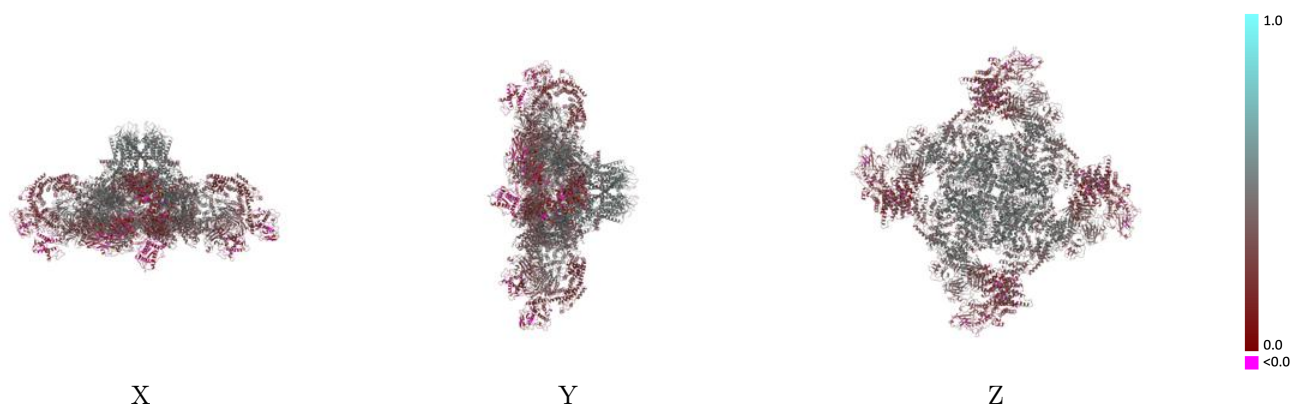
This section contains information regarding the fit between EMDB map EMD-53924 and PDB model 9RCW. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



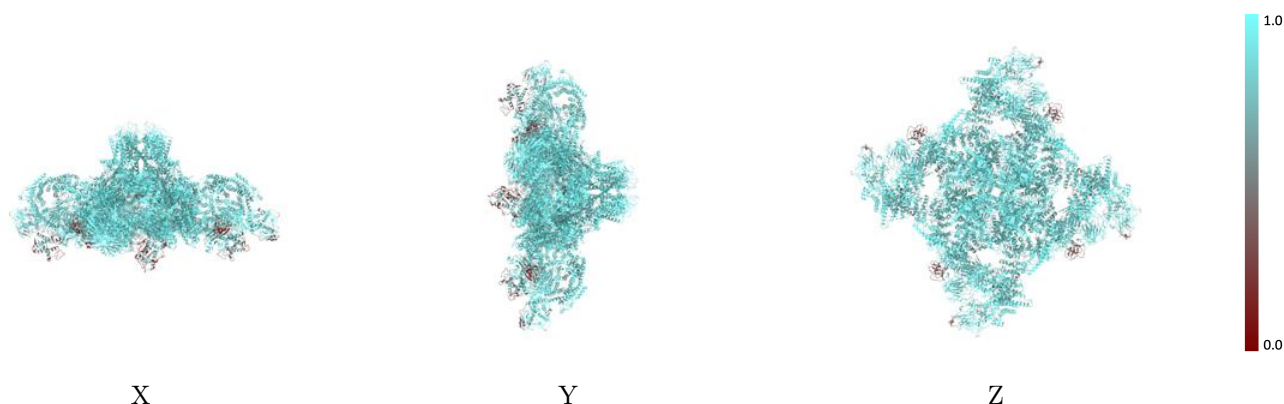
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



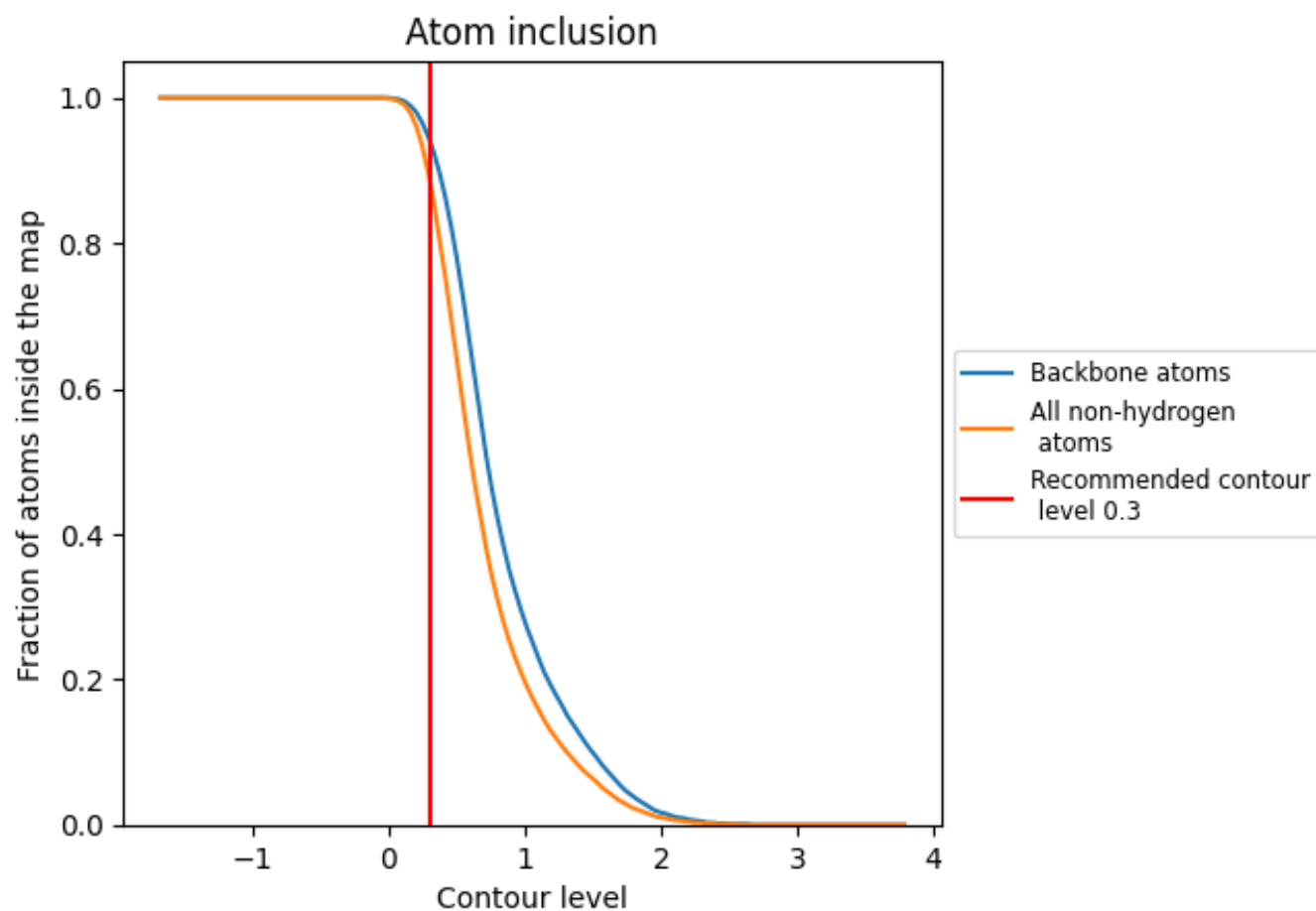
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8900	0.3600
A	0.9070	0.3660
B	0.7750	0.1840
C	0.9060	0.3660
D	0.7670	0.1810
E	0.3450	0.2990
F	0.3450	0.2960
G	0.9070	0.3670
H	0.7810	0.1790
I	0.3450	0.3020
J	0.9070	0.3670
K	0.7730	0.1820
L	0.3470	0.3010

1.0

0.0

<0.0