



wwPDB EM Validation Summary Report ⓘ

Apr 10, 2026 – 01:32 PM UTC

PDB ID : 9HEQ / pdb_00009heq
EMDB ID : EMD-52091
Title : Open-state RyR1 in 0.01% POPC micelles, in complex with a nanobody and FKBP12
Authors : Li, C.; Efremov, R.G.
Deposited on : 2024-11-14
Resolution : 3.60 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:

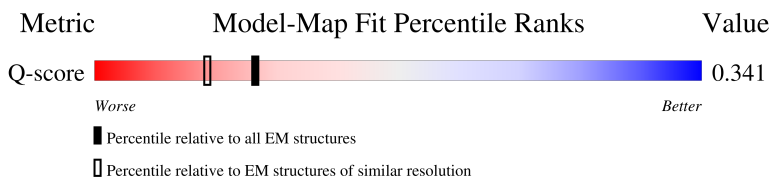
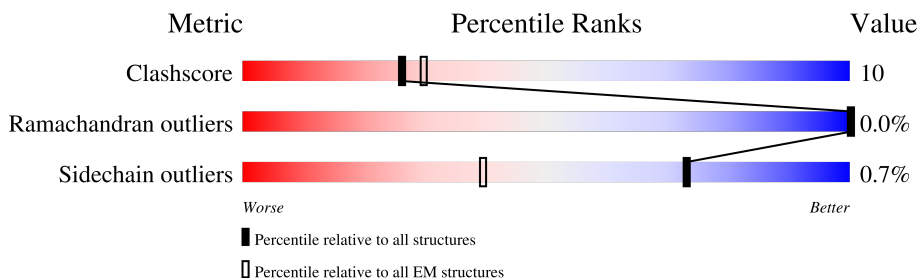
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.60 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	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5027	 5% 66% 20% 14%
1	C	5027	 5% 65% 20% 14%
1	G	5027	 5% 65% 20% 14%
1	J	5027	 5% 66% 20% 14%

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Mol	Chain	Length	Quality of chain
2	B	126	<div> <div>53%</div> <div>73%</div> <div>27%</div> </div>
2	D	126	<div> <div>53%</div> <div>71%</div> <div>29%</div> </div>
2	H	126	<div> <div>53%</div> <div>73%</div> <div>27%</div> </div>
2	K	126	<div> <div>53%</div> <div>73%</div> <div>27%</div> </div>
3	E	107	<div> <div>55%</div> <div>67%</div> <div>31%</div> <div>•</div> </div>
3	F	107	<div> <div>54%</div> <div>72%</div> <div>26%</div> <div>•</div> </div>
3	I	107	<div> <div>53%</div> <div>71%</div> <div>27%</div> <div>•</div> </div>
3	L	107	<div> <div>54%</div> <div>73%</div> <div>25%</div> <div>•</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 145440 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4319	Total	C	N	O	S	0	0
			34138	21741	5891	6279	227		
1	C	4319	Total	C	N	O	S	0	0
			34154	21753	5891	6283	227		
1	G	4319	Total	C	N	O	S	0	0
			34138	21741	5891	6279	227		
1	J	4319	Total	C	N	O	S	0	0
			34138	21741	5891	6279	227		

- Molecule 2 is a protein called Nanobody 9657.

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

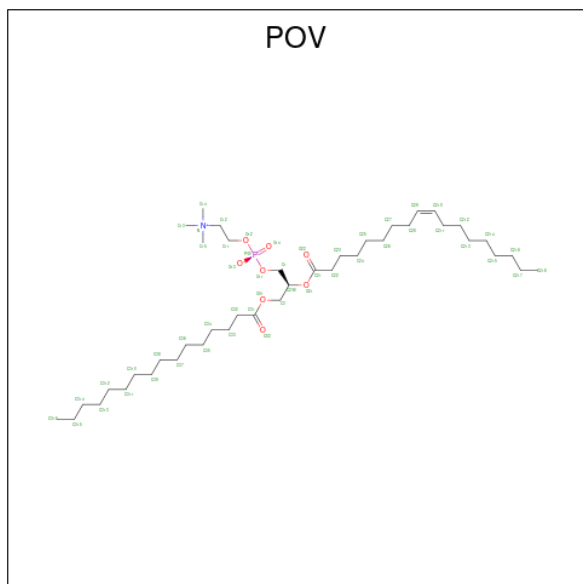
- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
3	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
3	I	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
3	L	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
E	100	ASP	GLY	conflict	UNP Q8HYX6
F	100	ASP	GLY	conflict	UNP Q8HYX6
I	100	ASP	GLY	conflict	UNP Q8HYX6
L	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 4 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
4	A	1	Total 13	C 13				0
4	A	1	Total 47	C 37	N 1	O 8	P 1	0
4	A	1	Total 44	C 34	N 1	O 8	P 1	0
4	A	1	Total 49	C 39	N 1	O 8	P 1	0
4	A	1	Total 13	C 13				0
4	A	1	Total 43	C 33	N 1	O 8	P 1	0
4	A	1	Total 24	C 15	N 1	O 7	P 1	0
4	A	1	Total 39	C 29	N 1	O 8	P 1	0
4	A	1	Total 34	C 24	N 1	O 8	P 1	0

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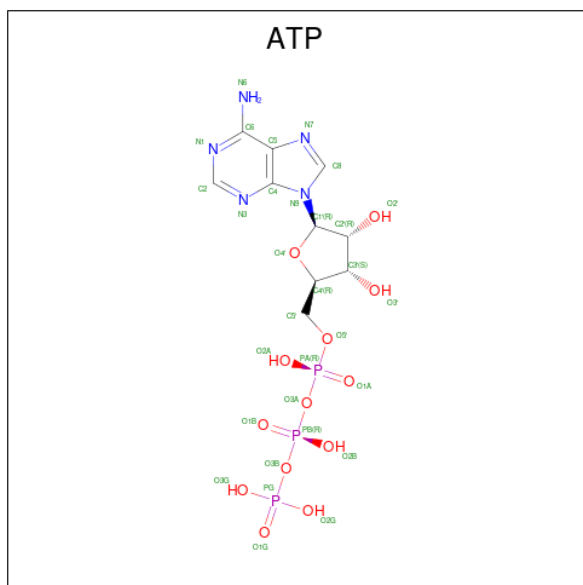
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
4	C	1	Total	C	N	O	P	0
			44	34	1	8	1	
4	C	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	C	1	Total	C	N	O	P	0
			24	15	1	7	1	
4	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	C	1	Total	C	N	O	P	0
			34	24	1	8	1	
4	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	G	1	Total	C	N	O	P	0
			47	37	1	8	1	
4	G	1	Total	C	N	O	P	0
			44	34	1	8	1	
4	G	1	Total	C				0
			13	13				
4	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	G	1	Total	C	N	O	P	0
			24	15	1	7	1	
4	G	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	G	1	Total	C	N	O	P	0
			34	24	1	8	1	
4	G	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	G	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	G	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
4	J	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	J	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	J	1	Total	C	N	O	P	0
			47	37	1	8	1	
4	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
4	J	1	Total	C				0
			13	13				
4	J	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	J	1	Total	C	N	O	P	0
			24	15	1	7	1	
4	J	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	J	1	Total	C	N	O	P	0
			34	24	1	8	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



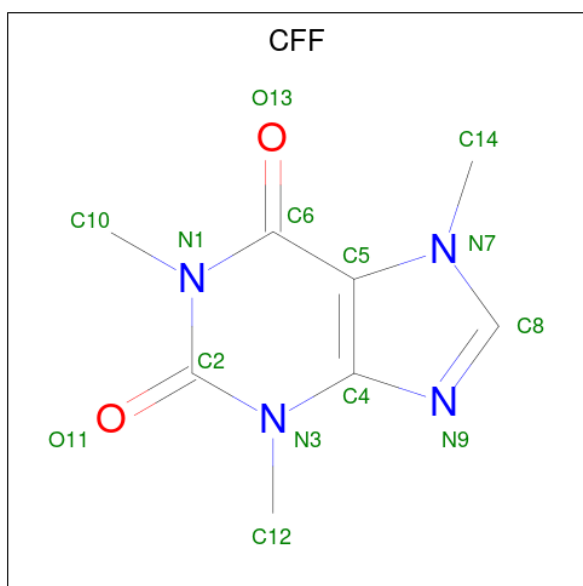
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	J	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	A	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	
6	J	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	A	1	Total	Ca	0
			1	1	

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

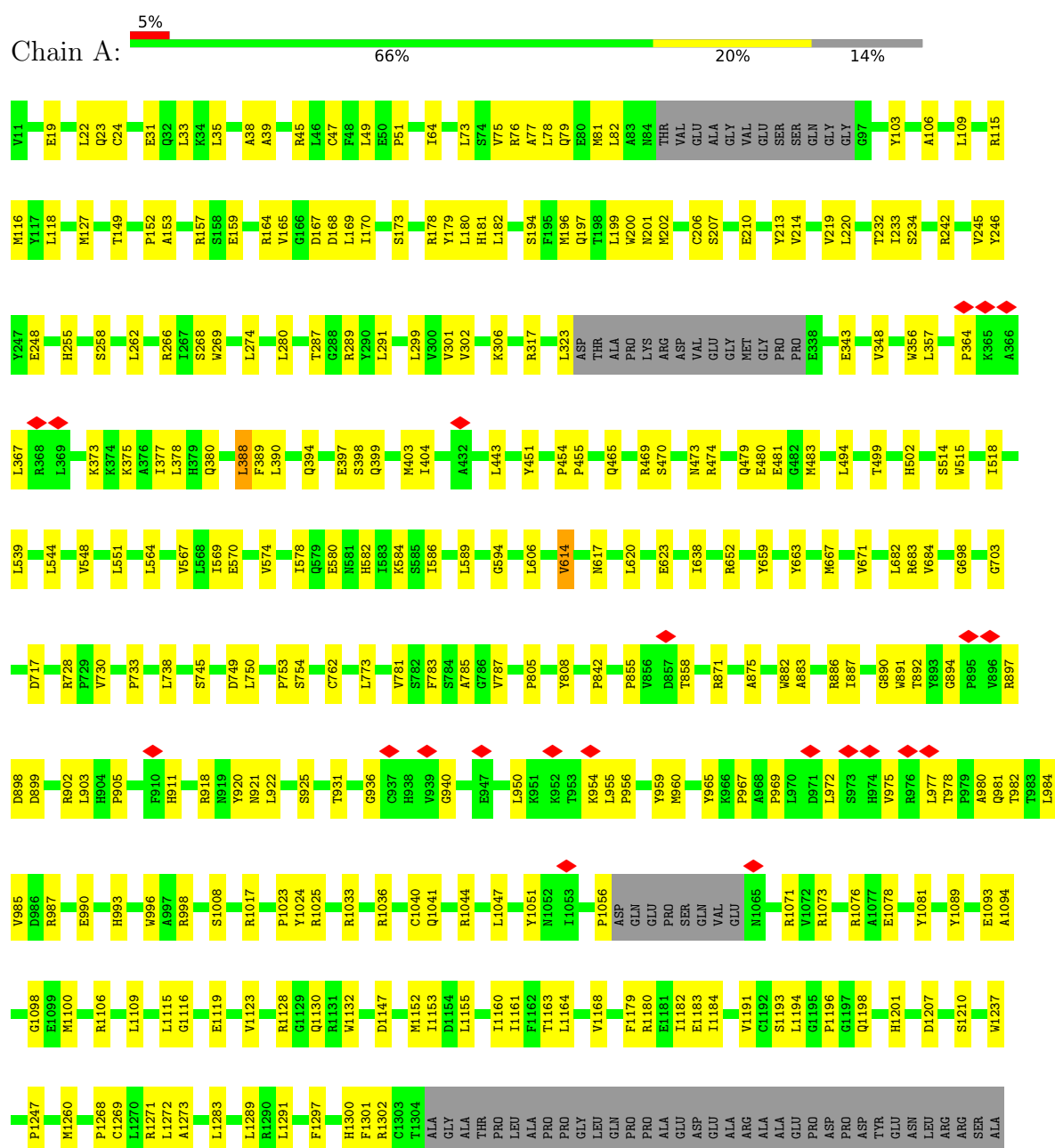
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

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

• Molecule 1: Ryanodine receptor 1







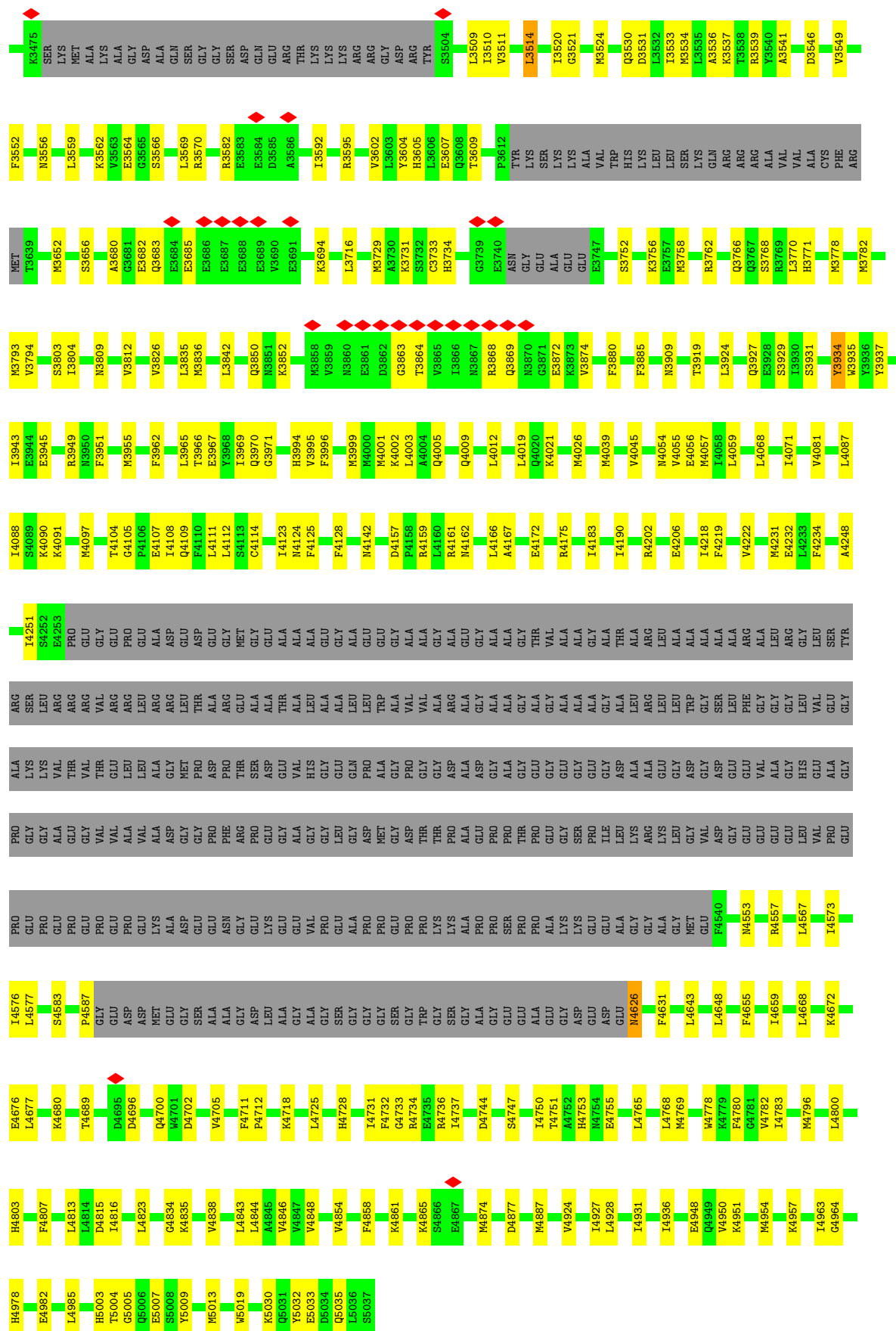


V3812	E3682	G3565	SER	L3322	LYS	S3027	R2939	A2879	W2819	A2759	I2682
V3826	Q3683	S3566	GLY	P3233	GLY	G3028	GLY	E2880	E2820	E2760	F2683
L3835	E3685	L3569	SER	V3236	GLY	G3029	LEU	Y2881	W2821	Y2761	D2692
L3842	E3686	R3570	ASP	V3239	GLY	H3030	ASP	T2882	T2822	T2762	Q2693
Q3850	E3687	R3582	GLN	M3239	L3129	K3036	ASP	H2883	T2823	H2763	E2694
E3688	E3688	E3583	GLU	V3245	T3132	T2885	ASP	H2884	E2824	E2764	L2695
E3689	E3689	E3584	THR	L3246	T3133	E3037	ASP	T2885	K2825	K2765	T2696
V3690	V3690	D3585	LYS	D3247	V3134	Q3038	ASP	C2887	A2826	W2766	R2697
E3691	E3691	A3586	LYS	R3248	A3135	I3039	ASP	K2888	R2827	A2767	A2699
K3694	K3694	L3592	ARG	L3249	L3136	L3049	ASP	K2889	E2828	F2768	W2700
L3716	L3716	R3595	ARG	M3250	L3137	V3051	ASP	K2890	G2829	D2769	P2701
M3729	M3729	R3596	ASP	G3254	L3140	S3055	ASP	K2891	E2830	K2770	I2706
K3730	K3730	V3602	ARG	E3258	F3144	L3056	ASP	Q2892	GLU	I2771	I2706
K3731	K3731	L3603	TYR	E3268	Q3145	E3062	ASP	E2893	ARG	Q2772	L2710
S3732	S3732	H3605	TYR	L3272	H3146	Q3063	ASP	L2894	THR	N2773	P2711
C3733	C3733	L3606	TYR	L3273	H3146	Q3063	ASP	E2895	GLU	N2774	P2712
V3734	V3734	E3607	TYR	L3274	H3150	V3065	ASP	A2896	LYS	W2775	D2713
I3739	I3739	E3608	TYR	P3275	G3153	C3067	ASP	K2897	LYS	W2776	Y2714
E3740	E3740	Q3608	TYR	L3277	V3163	L3068	ASP	G2898	THR	Y2777	K2722
ASN	ASN	T3612	TYR	P3282	R3167	I3070	ASP	G2899	ARG	E2778	A2723
GLY	GLY	L3514	TYR	P3293	S3171	R3073	ASP	G2900	LYS	E2779	E2724
GLU	GLU	L3515	TYR	P3294	I3172	S3074	ASP	G2901	ILE	N2780	K2725
ALA	ALA	G3423	TYR	A3295	L3176	A3077	ASP	H2902	GLN	V2781	LYS
LYS	LYS	E3433	TYR	L3296	G3176	V3080	ASP	H2903	THR	D2782	ALA
VAL	VAL	L3434	TYR	P3297	K3179	E3085	ASP	L2904	ALA	E2783	THR
TRP	TRP	F3435	TYR	A3298	K3179	E3085	ASP	L2905	GLN	E2784	VAL
HTS	HTS	R3436	TYR	G3299	V3183	E3086	ASP	L2906	THR	E2784	ASP
LYS	LYS	M3437	TYR	A3300	V3183	E3086	ASP	L2907	TVR	L2785	ALA
LEU	LEU	V3438	TYR	E3439	R3187	K3089	ASP	L2908	PRO	K2786	GLU
LEU	LEU	E3440	TYR	T3308	R3188	E3097	ASP	L2909	ARG	T2787	GLY
SER	SER	F3441	TYR	H3311	A3189	E3097	ASP	T2910	GLY	H2788	K2734
LYS	LYS	F3442	TYR	L3315	A3189	E3097	ASP	T2911	GLY	P2789	D2736
GLN	GLN	I3443	TYR	L3316	L3190	E3097	ASP	A2913	GLY	M2790	D2736
ARG	ARG	N3466	TYR	L3319	L3190	E3097	ASP	K2914	GLY	L2791	R2738
ARG	ARG	M3467	TYR	D3330	L3197	E3097	ASP	E2915	GLY	R2792	P2739
ALA	ALA	L3470	TYR	F3341	L3197	E3097	ASP	K2916	GLY	P2793	E2740
VAL	VAL	T3471	TYR	F3341	L3197	E3097	ASP	A2917	GLY	E2741	V2740
VAL	VAL	A3472	TYR	L3345	L3210	E3097	ASP	K2918	GLY	T2742	T2742
CYS	CYS	K3475	TYR	L3346	N3211	E3097	ASP	D2919	GLY	K2796	L2743
PHE	PHE	SER	TYR	V3346	Y3219	E3097	ASP	D2920	GLY	F2797	N2744
MET	MET	LYS	TYR	E3352	R3225	E3097	ASP	E2921	GLY	S2798	V2745
T3639	T3639	ALA	TYR	L3354	E3226	E3097	ASP	K2922	GLY	E2799	I2746
M3652	M3652	ASP	TYR	F3358	R3227	E3097	ASP	A2923	GLY	K2800	I2747
K3656	K3656	ALA	TYR	T3362		E3097	ASP	Q2924	GLY	D2801	P2748
S3656	S3656	LYS	TYR			E3097	ASP	E2925	GLY	K2802	E2749
A3680	A3680	ALA	TYR			E3097	ASP	L2926	GLY	E2803	K2750
G3681	G3681	GLY	TYR			E3097	ASP	L2927	GLY	L2804	L2751
		ASP	TYR			E3097	ASP	K2928	GLY	D2752	D2752
		ALA	TYR			E3097	ASP	F2929	GLY	S2753	F2753
		ALA	TYR			E3097	ASP	L2930	GLY	Q2806	F2754
		GLN	TYR			E3097	ASP	Q2931	GLY	Q2807	K2757
			TYR			E3097	ASP	M2932	GLY	I2809	I2755
			TYR			E3097	ASP	Q2934	GLY	E2810	K2757
			TYR			E3097	ASP	Y2935	GLY	K2810	F2758
			TYR			E3097	ASP	A2936	GLY	S2812	
			TYR			E3097	ASP	V2937	GLY	L2813	
			TYR			E3097	ASP	T2938	GLY	A2815	
			TYR			E3097	ASP		GLY	M2816	
			TYR			E3097	ASP		GLY	L2817	
			TYR			E3097	ASP		GLY	A2818	

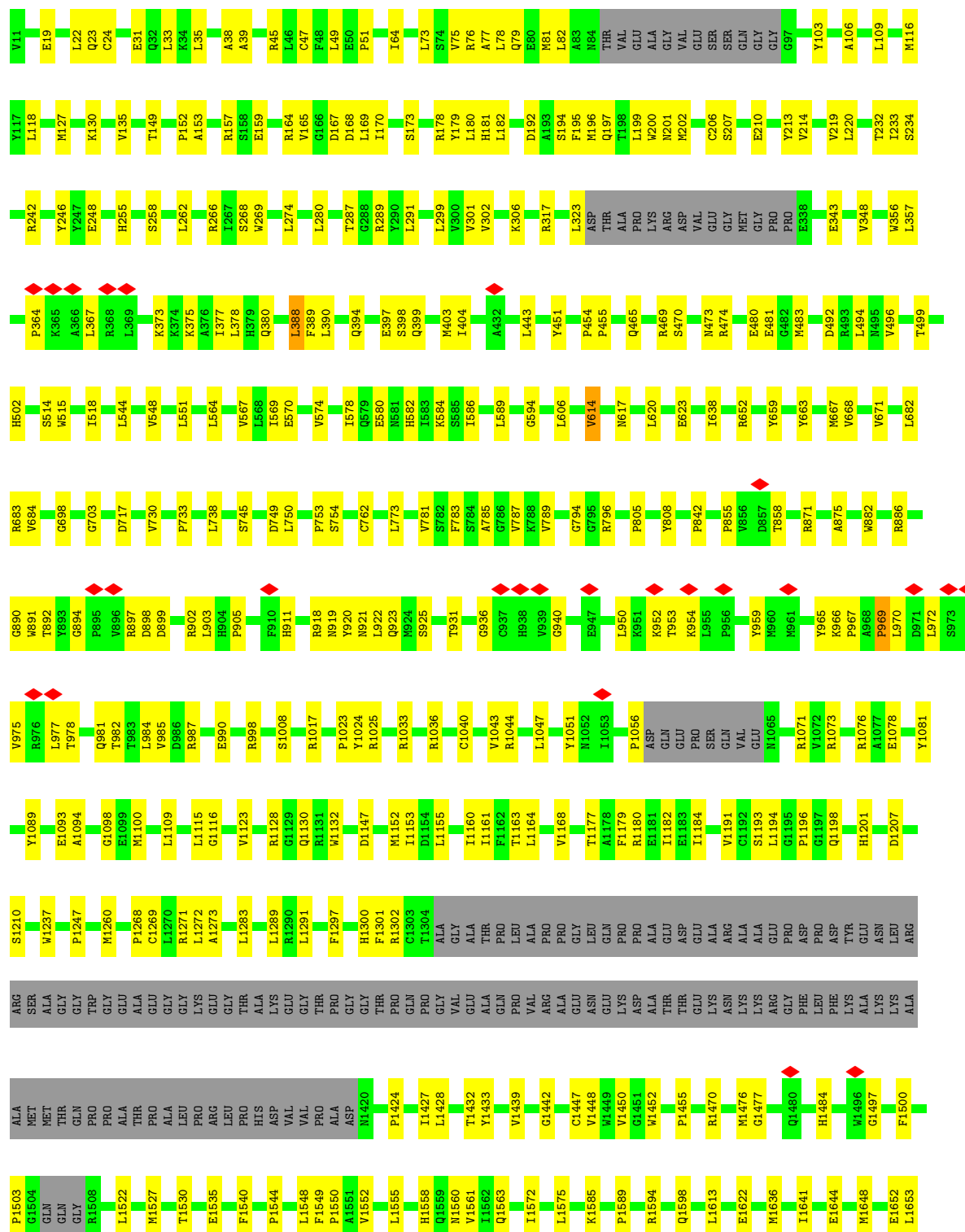


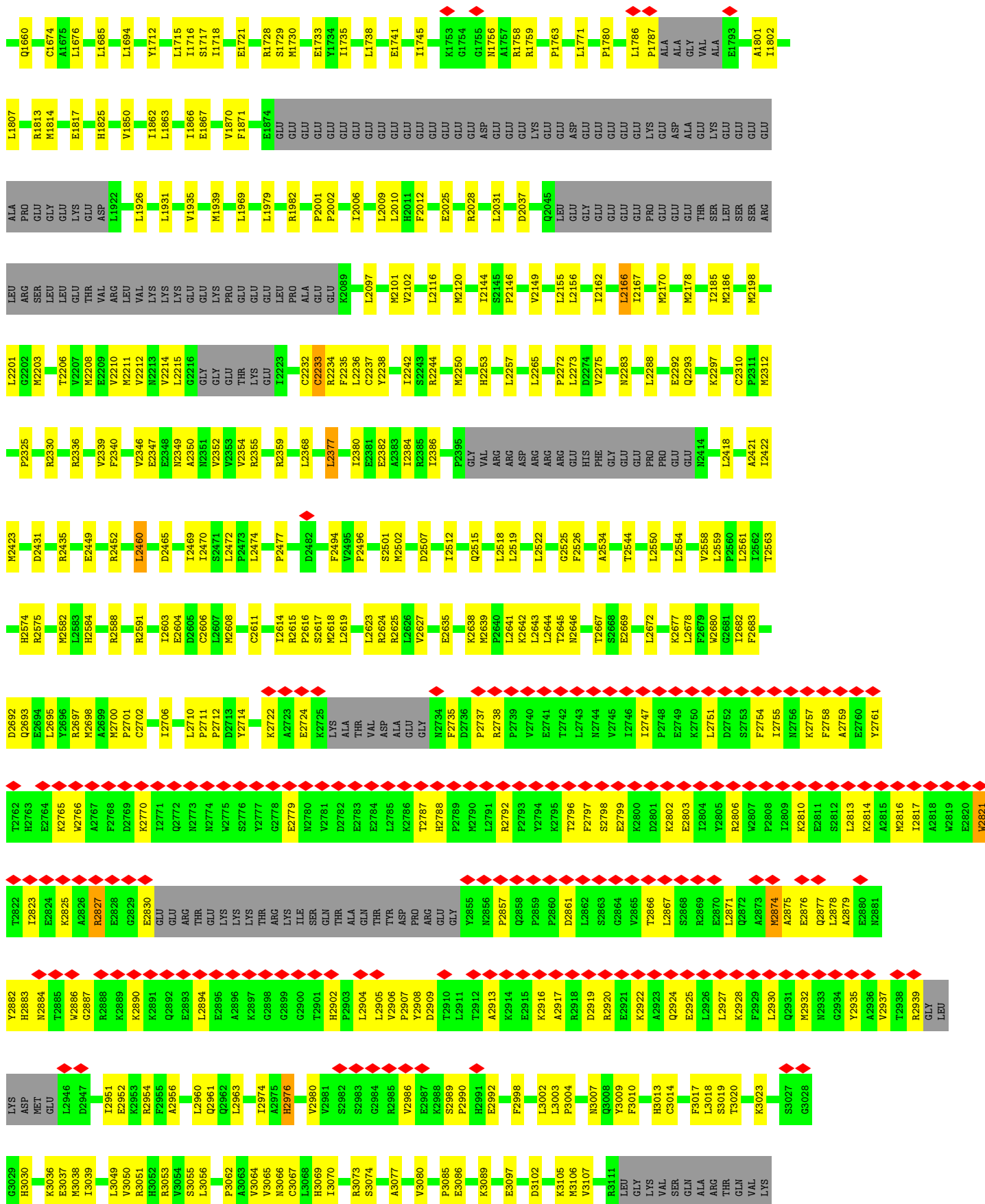






• Molecule 1: Ryanodine receptor 1

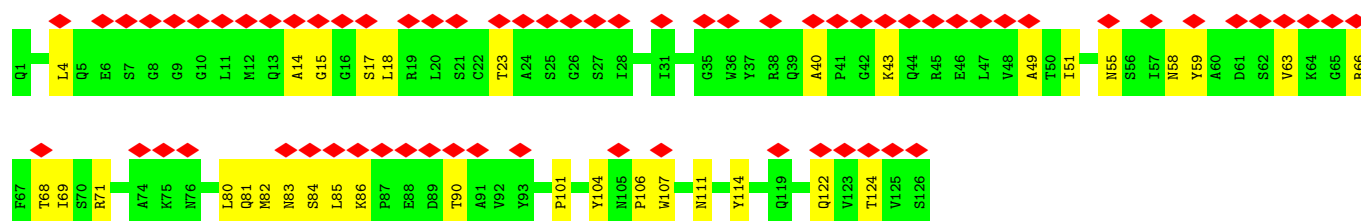




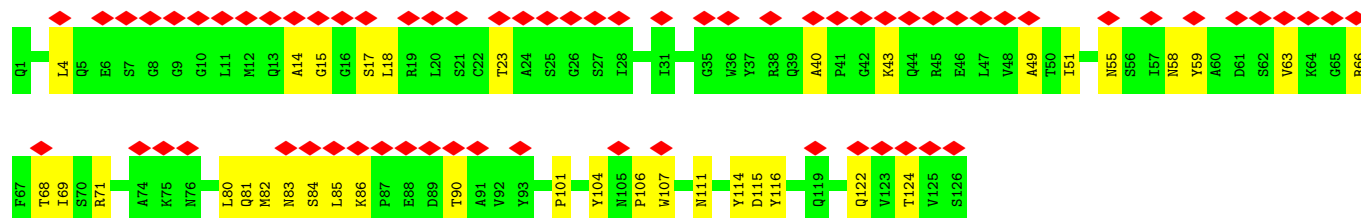




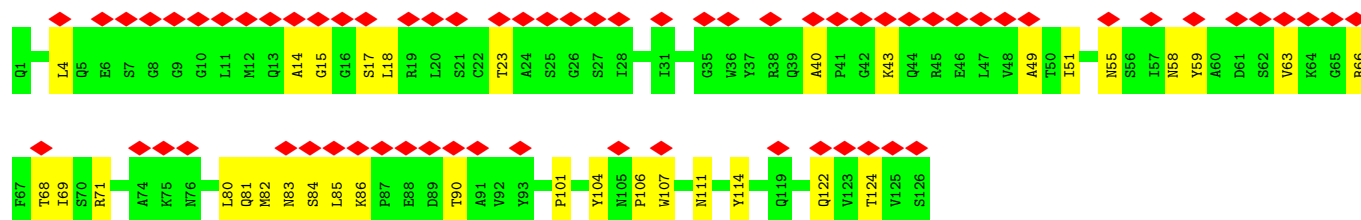
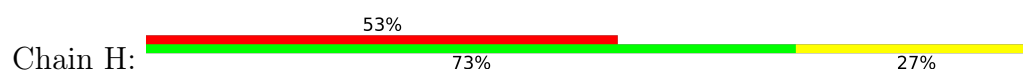
• Molecule 2: Nanobody 9657



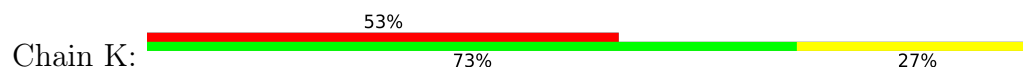
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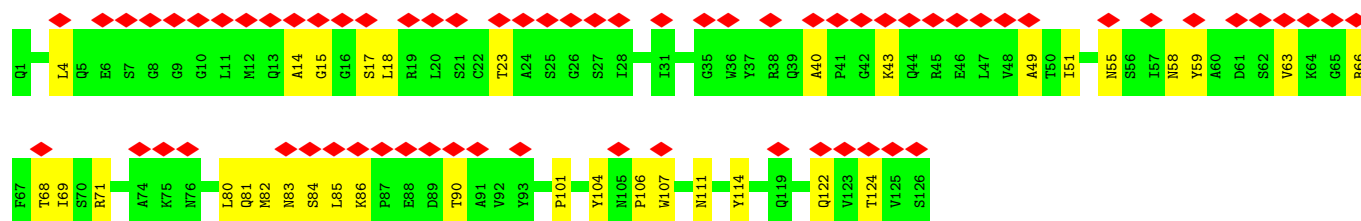


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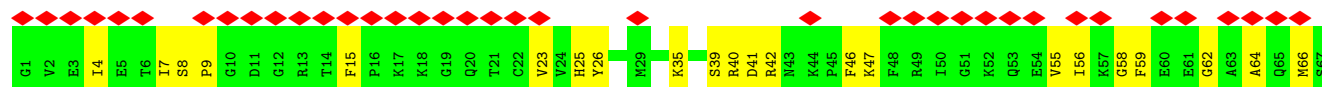


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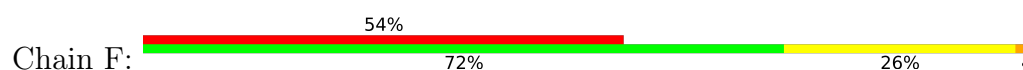




• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B



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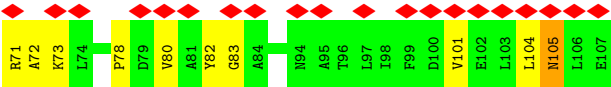


• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80709	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	4.326	Depositor
Minimum map value	-0.162	Depositor
Average map value	0.056	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	488.544, 488.544, 488.544	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ZN, POV, CA, 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	A	0.22	0/34909	0.44	1/47317 (0.0%)
1	C	0.22	0/34926	0.44	1/47340 (0.0%)
1	G	0.22	0/34909	0.43	1/47317 (0.0%)
1	J	0.23	0/34909	0.44	3/47317 (0.0%)
2	B	0.18	0/987	0.49	0/1340
2	D	0.27	0/987	0.54	0/1340
2	H	0.18	0/987	0.49	0/1340
2	K	0.18	0/987	0.49	0/1340
3	E	0.33	0/834	0.73	0/1123
3	F	0.38	0/834	0.74	0/1123
3	I	0.39	0/834	0.72	0/1123
3	L	0.40	0/834	0.73	0/1123
All	All	0.23	0/146937	0.45	6/199143 (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	C	0	1
1	J	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1503	PRO	N-CA-CB	6.00	110.16	103.44
1	G	1503	PRO	N-CA-CB	6.00	110.16	103.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1503	PRO	N-CA-CB	5.98	110.14	103.44
1	J	1503	PRO	N-CA-CB	5.97	110.13	103.44
1	J	794	GLY	CA-C-O	-5.69	118.22	122.37

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1020	ARG	Sidechain
1	J	987	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	A	34138	0	33528	683	0
1	C	34154	0	33553	690	0
1	G	34138	0	33528	682	0
1	J	34138	0	33528	683	0
2	B	967	0	916	28	0
2	D	967	0	916	28	0
2	H	967	0	916	27	0
2	K	967	0	916	27	0
3	E	818	0	824	25	0
3	F	818	0	824	24	0
3	I	818	0	824	24	0
3	L	818	0	824	23	0
4	A	448	0	640	12	0
4	C	324	0	448	10	0
4	G	386	0	544	9	0
4	J	386	0	544	13	0
5	A	31	0	12	0	0
5	C	31	0	12	0	0
5	G	31	0	12	0	0
5	J	31	0	12	0	0
6	A	14	0	10	0	0
6	C	14	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0	0	0	0
8	C	1	0	0	0	0
8	G	1	0	0	0	0
8	J	1	0	0	0	0
All	All	145440	0	143361	2925	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 10.

The worst 5 of 2925 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:959:TYR:HA	1:J:965:TYR:HA	1.31	1.06
1:A:959:TYR:HA	1:A:965:TYR:HA	1.38	1.05
1:C:181:HIS:HD2	1:C:194:SER:HB2	1.42	0.84
1:A:181:HIS:HD2	1:A:194:SER:HB2	1.41	0.84
1:G:181:HIS:HD2	1:G:194:SER:HB2	1.41	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4279/5027 (85%)	4176 (98%)	101 (2%)	2 (0%)	100	100
1	C	4279/5027 (85%)	4174 (98%)	104 (2%)	1 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	4279/5027 (85%)	4180 (98%)	98 (2%)	1 (0%)	100	100
1	J	4279/5027 (85%)	4179 (98%)	99 (2%)	1 (0%)	100	100
2	B	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
2	D	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
2	H	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
2	K	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
3	E	105/107 (98%)	98 (93%)	5 (5%)	2 (2%)	6	33
3	F	105/107 (98%)	100 (95%)	4 (4%)	1 (1%)	12	45
3	I	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
3	L	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
All	All	18032/21040 (86%)	17587 (98%)	437 (2%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	LYS
1	C	375	LYS
3	E	85	THR
1	G	375	LYS
1	J	375	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3672/4270 (86%)	3648 (99%)	24 (1%)	76	78
1	C	3676/4270 (86%)	3650 (99%)	26 (1%)	76	78
1	G	3672/4270 (86%)	3645 (99%)	27 (1%)	76	78
1	J	3672/4270 (86%)	3648 (99%)	24 (1%)	76	78
2	B	104/104 (100%)	104 (100%)	0	100	100
2	D	104/104 (100%)	103 (99%)	1 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	104/104 (100%)	104 (100%)	0	100	100
2	K	104/104 (100%)	104 (100%)	0	100	100
3	E	88/88 (100%)	85 (97%)	3 (3%)	32	57
3	F	88/88 (100%)	86 (98%)	2 (2%)	44	64
3	I	88/88 (100%)	85 (97%)	3 (3%)	32	57
3	L	88/88 (100%)	86 (98%)	2 (2%)	44	64
All	All	15460/17848 (87%)	15348 (99%)	112 (1%)	73	78

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	377	ILE
3	L	35	LYS
1	G	2460	LEU
1	J	4858	PHE
1	J	2460	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 160 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	4803	HIS
1	J	2991	HIS
3	I	31	GLN
1	J	1429	ASN
1	J	3851	ASN

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 56 ligands modelled in this entry, 8 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	POV	J	5102	-	40,40,51	0.55	0	46,48,59	0.52	0
4	POV	C	5111	-	40,40,51	0.55	0	46,48,59	0.51	0
4	POV	G	5113	-	40,40,51	0.55	0	46,48,59	0.51	0
4	POV	J	5112	-	38,38,51	0.56	0	44,46,59	0.52	0
4	POV	G	5114	-	51,51,51	0.50	0	57,59,59	0.45	0
4	POV	G	5112	-	48,48,51	0.52	0	54,56,59	0.48	0
4	POV	A	5109	-	42,42,51	0.54	0	48,50,59	0.48	0
4	POV	J	5101	-	48,48,51	0.51	0	54,56,59	0.48	0
4	POV	A	5101	-	12,12,51	0.22	0	11,11,59	0.25	0
4	POV	J	5108	-	43,43,51	0.54	0	49,51,59	0.50	0
4	POV	A	5111	-	38,38,51	0.56	0	44,46,59	0.52	0
4	POV	A	5108	-	12,12,51	0.22	0	11,11,59	0.25	0
4	POV	C	5105	-	43,43,51	0.54	0	49,51,59	0.50	0
4	POV	G	5104	-	46,46,51	0.52	0	52,54,59	0.48	0
5	ATP	A	5102	-	32,33,33	0.28	0	48,52,52	0.33	0
5	ATP	J	5104	-	32,33,33	0.28	0	48,52,52	0.33	0
4	POV	A	5105	-	46,46,51	0.52	0	52,54,59	0.48	0
4	POV	J	5103	-	51,51,51	0.50	0	57,59,59	0.45	0
4	POV	J	5110	-	42,42,51	0.54	0	48,50,59	0.48	0
4	POV	A	5107	-	48,48,51	0.52	0	54,56,59	0.48	0
4	POV	G	5109	-	38,38,51	0.56	0	44,46,59	0.52	0
4	POV	J	5107	-	46,46,51	0.52	0	52,54,59	0.48	0
4	POV	J	5109	-	12,12,51	0.22	0	11,11,59	0.25	0
4	POV	A	5112	-	33,33,51	0.60	0	39,41,59	0.54	0
5	ATP	C	5101	-	32,33,33	0.28	0	48,52,52	0.33	0
4	POV	C	5106	-	42,42,51	0.55	0	48,50,59	0.49	0
6	CFF	C	5102	-	15,15,15	0.52	0	23,23,23	0.74	1 (4%)
4	POV	G	5108	-	23,23,51	0.67	0	28,30,59	0.61	0
6	CFF	J	5105	-	15,15,15	0.54	0	23,23,23	0.74	1 (4%)
4	POV	C	5108	-	38,38,51	0.57	0	44,46,59	0.52	0
4	POV	C	5109	-	33,33,51	0.60	0	39,41,59	0.54	0
4	POV	A	5114	-	48,48,51	0.52	0	54,56,59	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	C	5104	-	46,46,51	0.52	0	52,54,59	0.48	0
4	POV	G	5110	-	33,33,51	0.60	0	39,41,59	0.54	0
4	POV	J	5111	-	23,23,51	0.67	0	28,30,59	0.61	0
4	POV	G	5105	-	43,43,51	0.54	0	49,51,59	0.50	0
6	CFF	G	5102	-	15,15,15	0.54	0	23,23,23	0.74	1 (4%)
4	POV	C	5112	-	51,51,51	0.50	0	57,59,59	0.45	0
4	POV	J	5113	-	33,33,51	0.60	0	39,41,59	0.54	0
4	POV	G	5107	-	42,42,51	0.54	0	48,50,59	0.48	0
4	POV	A	5106	-	43,43,51	0.54	0	49,51,59	0.50	0
4	POV	C	5107	-	23,23,51	0.66	0	28,30,59	0.61	0
4	POV	A	5116	-	51,51,51	0.50	0	57,59,59	0.45	0
5	ATP	G	5101	-	32,33,33	0.28	0	48,52,52	0.33	0
6	CFF	A	5103	-	15,15,15	0.54	0	23,23,23	0.74	1 (4%)
4	POV	G	5106	-	12,12,51	0.22	0	11,11,59	0.25	0
4	POV	A	5115	-	40,40,51	0.55	0	46,48,59	0.51	0
4	POV	A	5110	-	23,23,51	0.67	0	28,30,59	0.61	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
4	POV	J	5102	-	-	6/44/44/55	-
4	POV	C	5111	-	-	6/44/44/55	-
4	POV	G	5113	-	-	6/44/44/55	-
4	POV	J	5112	-	-	12/42/42/55	-
4	POV	G	5114	-	-	21/55/55/55	-
4	POV	G	5112	-	-	18/52/52/55	-
4	POV	A	5109	-	-	12/46/46/55	-
4	POV	J	5101	-	-	18/52/52/55	-
4	POV	A	5101	-	-	2/10/10/55	-
4	POV	J	5108	-	-	9/47/47/55	-
4	POV	A	5111	-	-	12/42/42/55	-
4	POV	A	5108	-	-	2/10/10/55	-
4	POV	C	5105	-	-	9/47/47/55	-
4	POV	G	5104	-	-	16/50/50/55	-
5	ATP	A	5102	-	-	3/22/38/38	0/3/3/3
5	ATP	J	5104	-	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POV	A	5105	-	-	16/50/50/55	-
4	POV	J	5103	-	-	21/55/55/55	-
4	POV	J	5110	-	-	12/46/46/55	-
4	POV	A	5107	-	-	18/52/52/55	-
4	POV	G	5109	-	-	12/42/42/55	-
4	POV	J	5107	-	-	16/50/50/55	-
4	POV	J	5109	-	-	2/10/10/55	-
4	POV	A	5112	-	-	10/37/37/55	-
5	ATP	C	5101	-	-	3/22/38/38	0/3/3/3
4	POV	C	5106	-	-	12/46/46/55	-
6	CFF	C	5102	-	-	-	0/2/2/2
4	POV	G	5108	-	-	10/26/26/55	-
6	CFF	J	5105	-	-	-	0/2/2/2
4	POV	C	5108	-	-	12/42/42/55	-
4	POV	C	5109	-	-	10/37/37/55	-
4	POV	A	5114	-	-	18/52/52/55	-
4	POV	C	5104	-	-	16/50/50/55	-
4	POV	G	5110	-	-	10/37/37/55	-
4	POV	J	5111	-	-	10/26/26/55	-
4	POV	G	5105	-	-	9/47/47/55	-
6	CFF	G	5102	-	-	-	0/2/2/2
4	POV	C	5112	-	-	21/55/55/55	-
4	POV	J	5113	-	-	10/37/37/55	-
4	POV	G	5107	-	-	12/46/46/55	-
4	POV	A	5106	-	-	9/47/47/55	-
4	POV	C	5107	-	-	10/26/26/55	-
4	POV	A	5116	-	-	21/55/55/55	-
5	ATP	G	5101	-	-	3/22/38/38	0/3/3/3
6	CFF	A	5103	-	-	-	0/2/2/2
4	POV	G	5106	-	-	2/10/10/55	-
4	POV	A	5115	-	-	6/44/44/55	-
4	POV	A	5110	-	-	10/26/26/55	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	5102	CFF	C12-N3-C2	2.28	121.30	117.33
6	A	5103	CFF	C12-N3-C2	2.26	121.27	117.33
6	G	5102	CFF	C12-N3-C2	2.26	121.27	117.33
6	J	5105	CFF	C12-N3-C2	2.26	121.27	117.33

There are no chirality outliers.

5 of 476 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5105	POV	C22-C21-O21-C2
4	A	5105	POV	O22-C21-O21-C2
4	A	5106	POV	C1-O11-P-O14
4	A	5106	POV	C11-O12-P-O13
4	A	5106	POV	O12-C11-C12-N

There are no ring outliers.

27 monomers are involved in 42 short contacts:

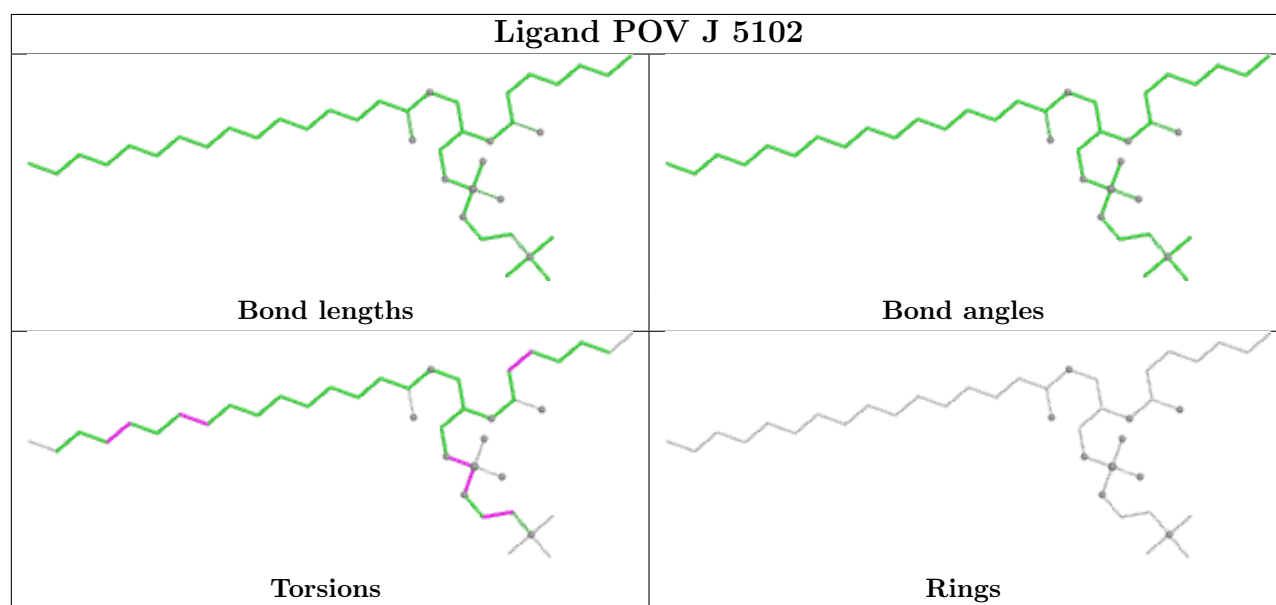
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	5102	POV	3	0
4	C	5111	POV	2	0
4	G	5113	POV	3	0
4	J	5112	POV	1	0
4	G	5114	POV	1	0
4	G	5112	POV	3	0
4	A	5109	POV	1	0
4	J	5101	POV	4	0
4	A	5111	POV	1	0
4	C	5105	POV	2	0
4	G	5104	POV	2	0
4	A	5105	POV	1	0
4	J	5103	POV	4	0
4	J	5110	POV	1	0
4	A	5107	POV	3	0
4	J	5107	POV	1	0
4	A	5112	POV	1	0
4	C	5106	POV	1	0
4	C	5109	POV	2	0
4	A	5114	POV	3	0
4	C	5104	POV	2	0
4	G	5110	POV	1	0
4	C	5112	POV	1	0

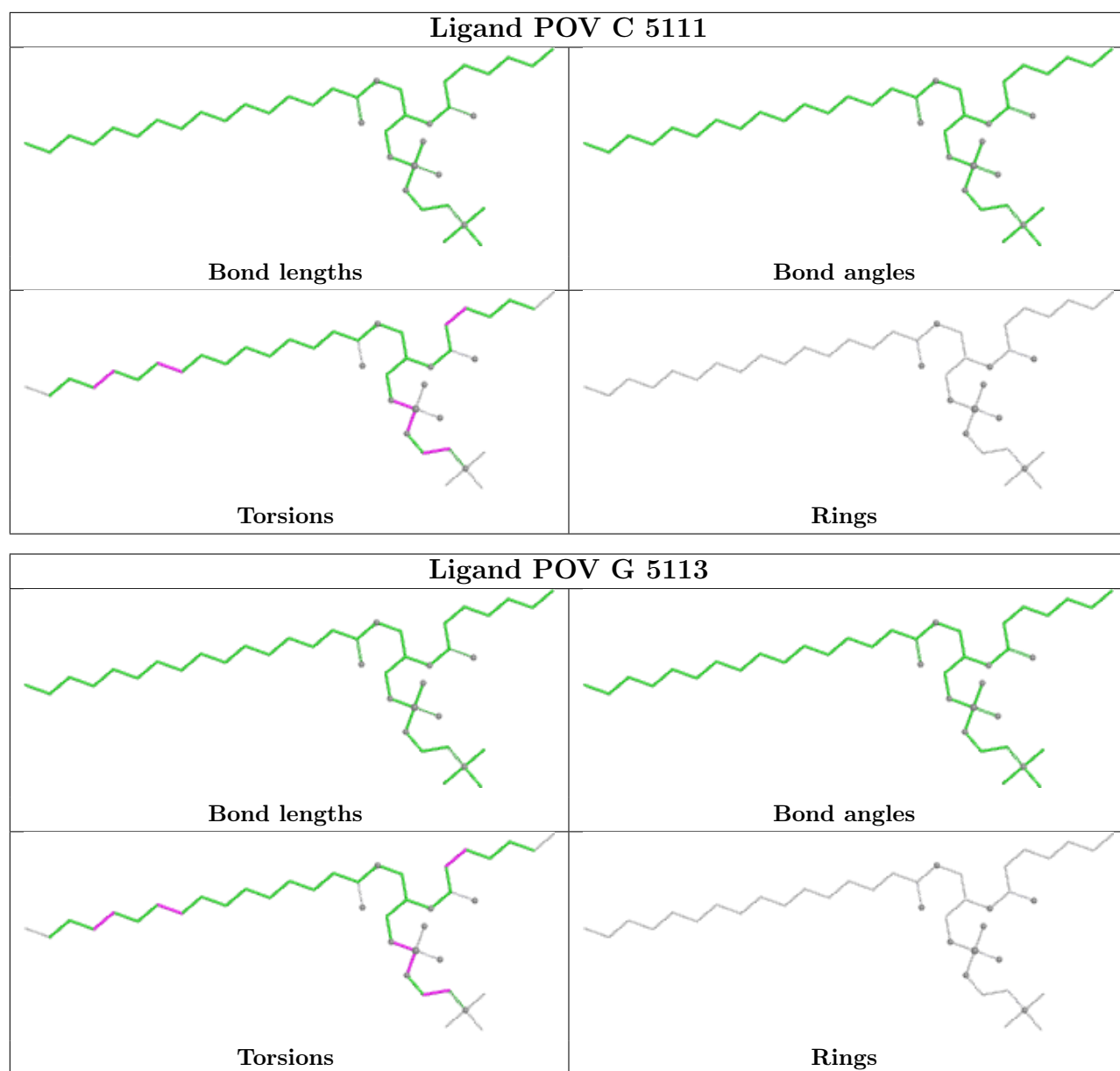
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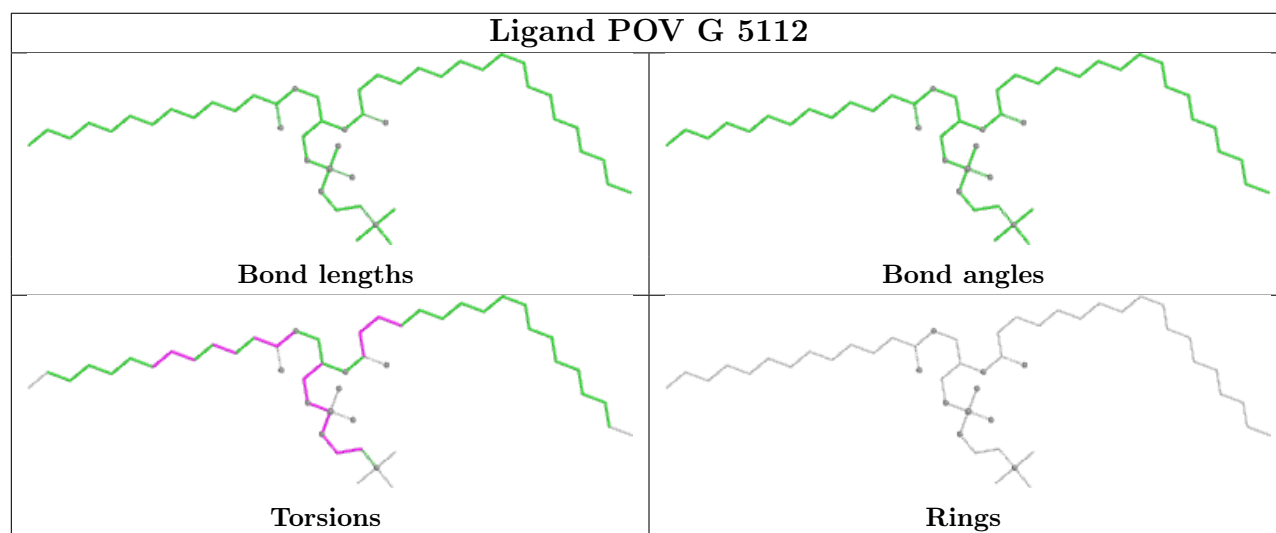
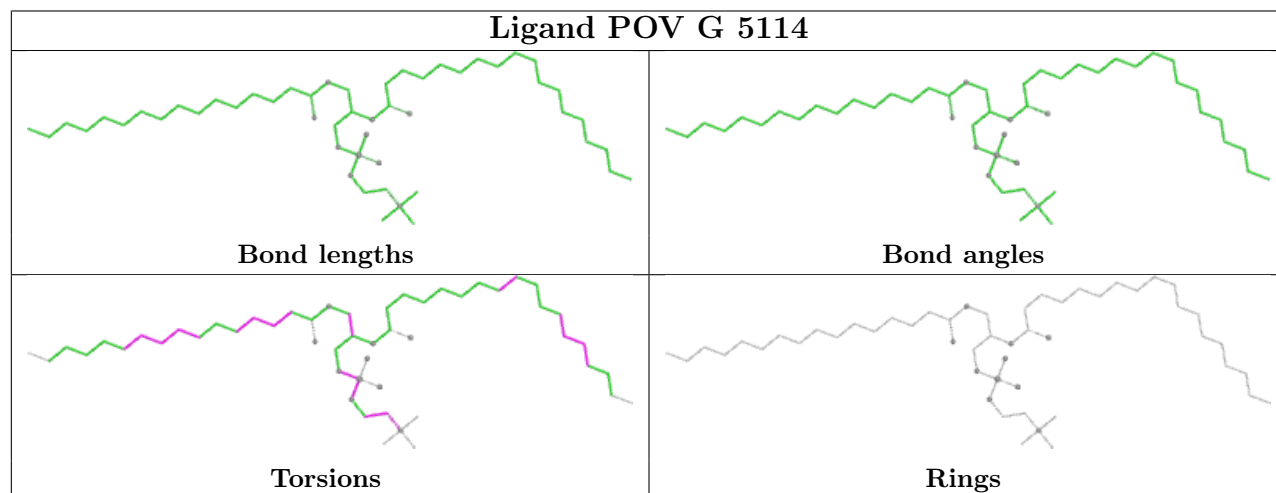
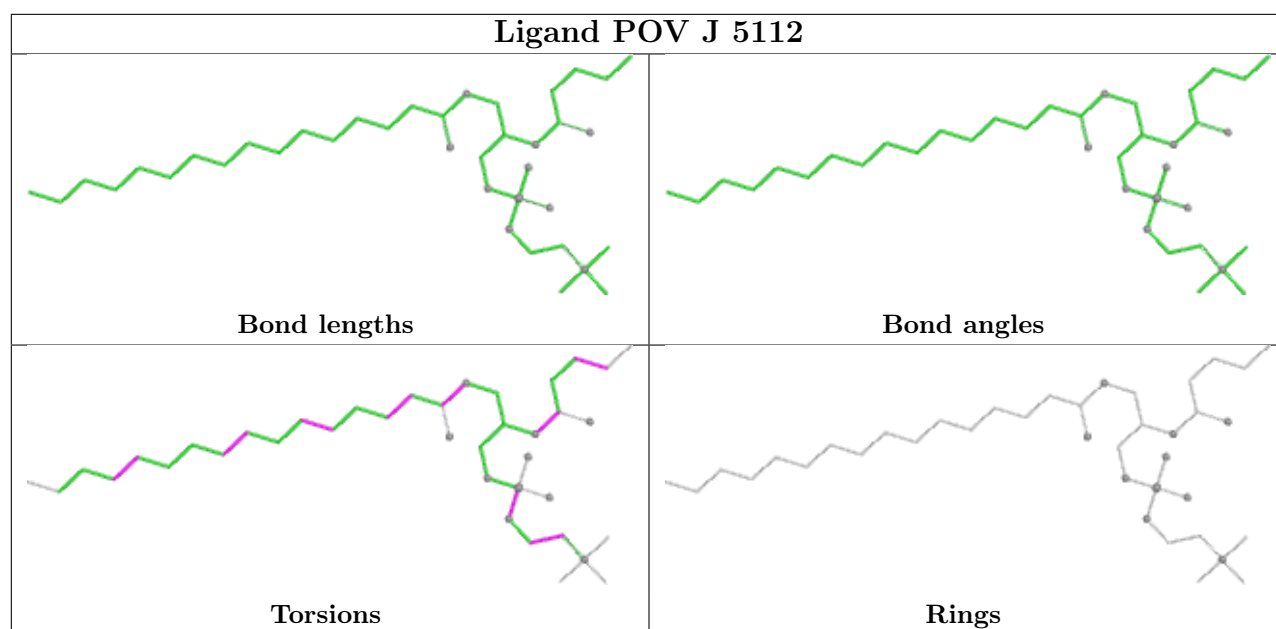
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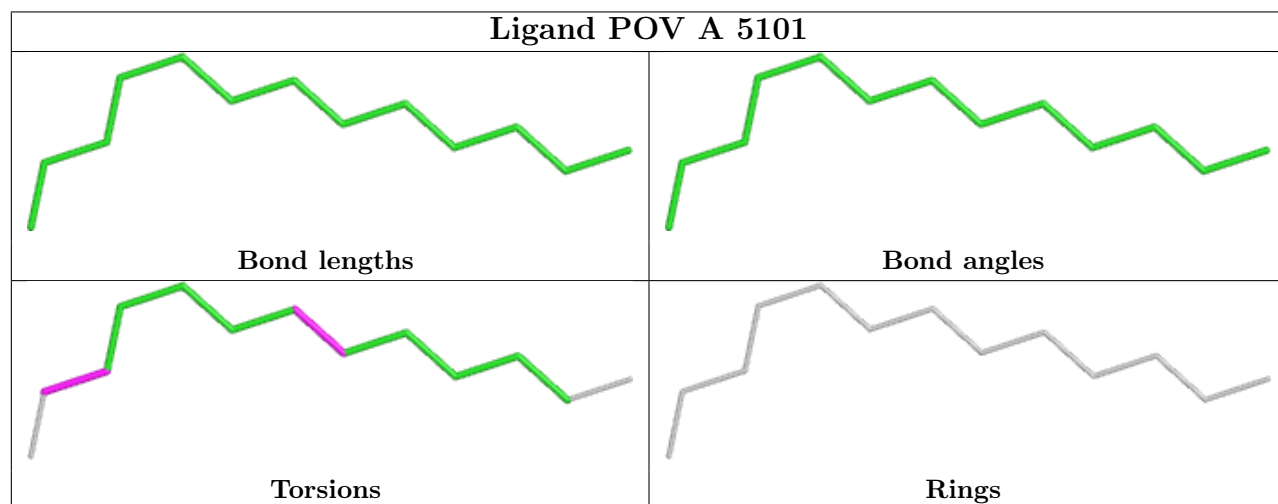
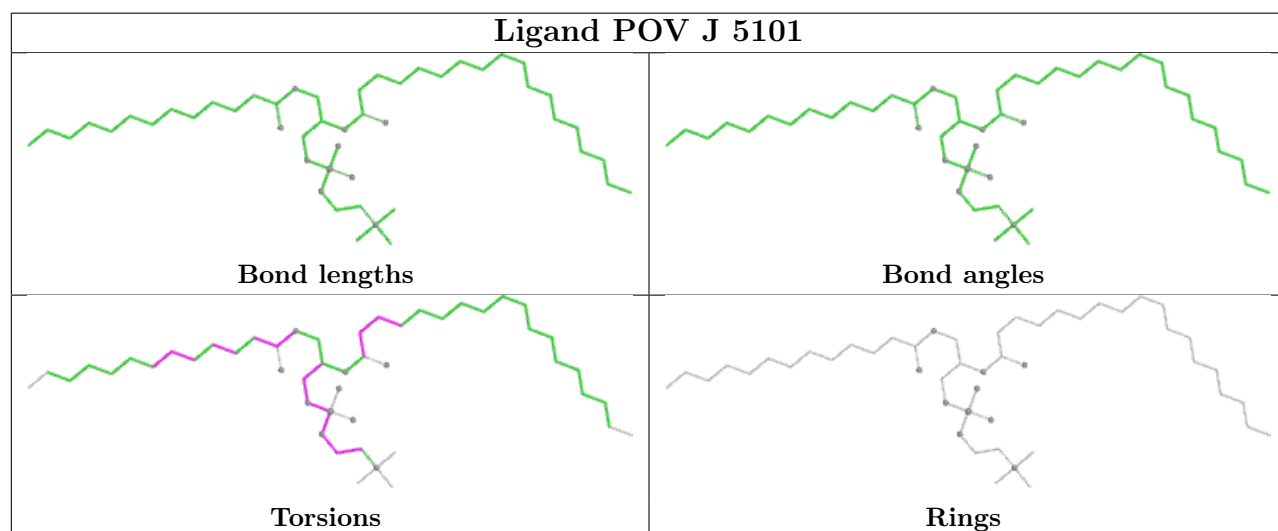
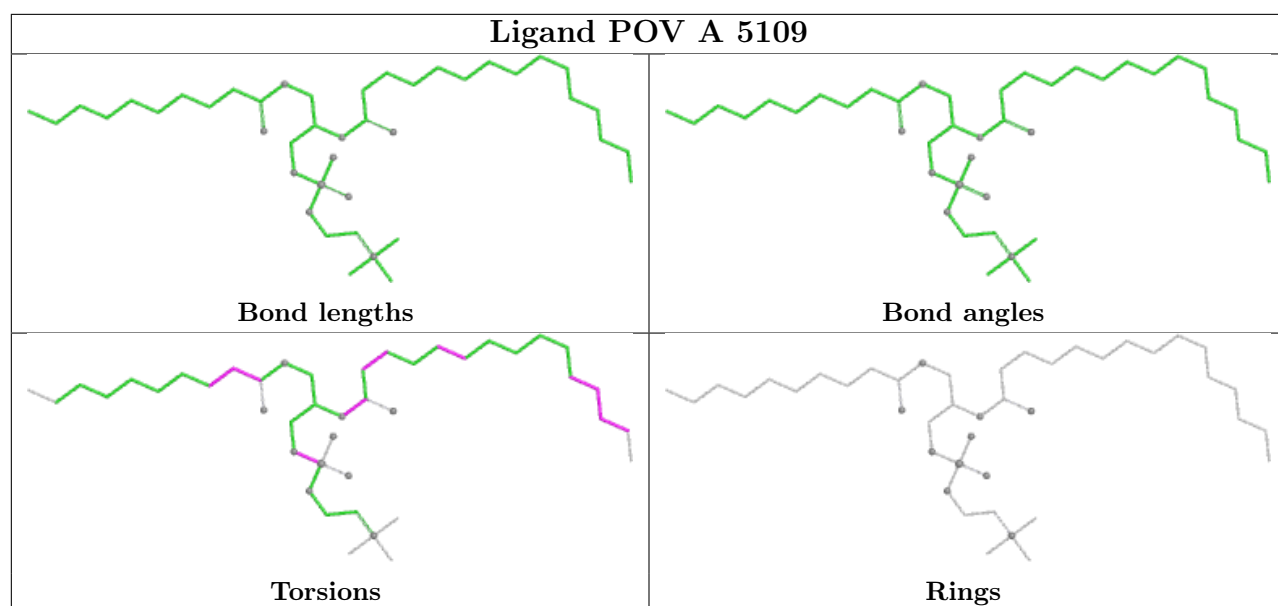
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	5113	POV	1	0
4	G	5107	POV	1	0
4	A	5116	POV	1	0
4	A	5115	POV	3	0

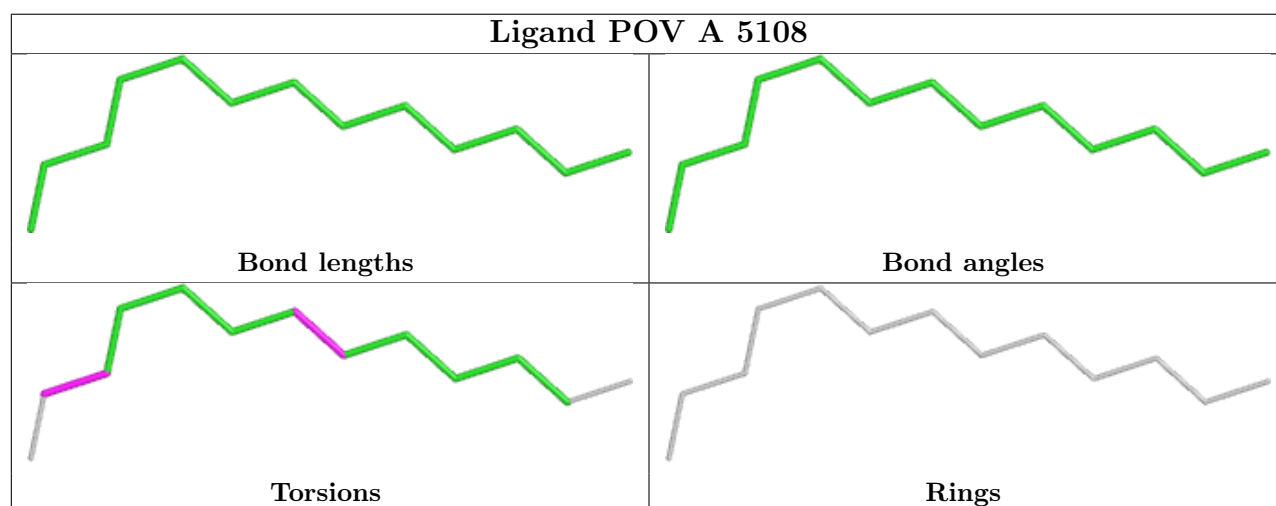
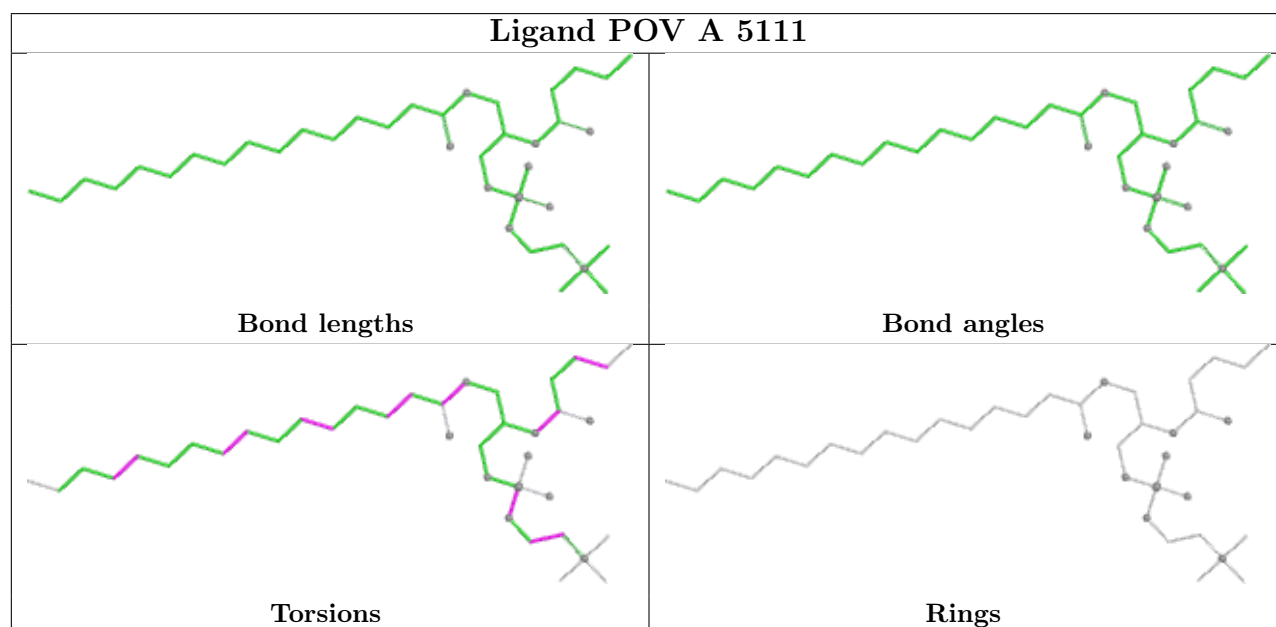
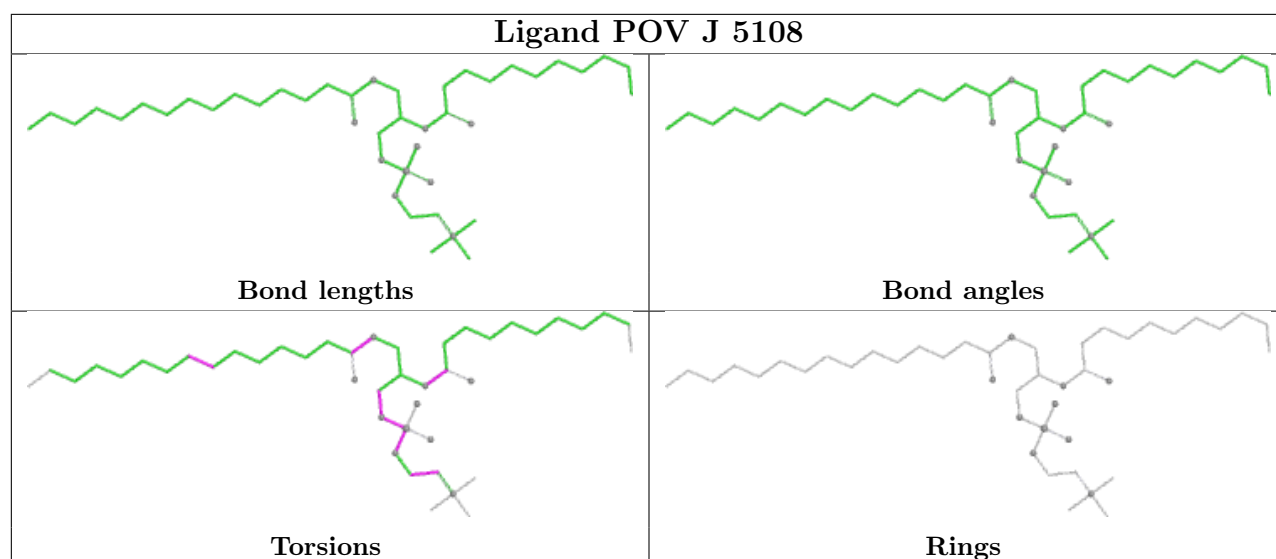
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

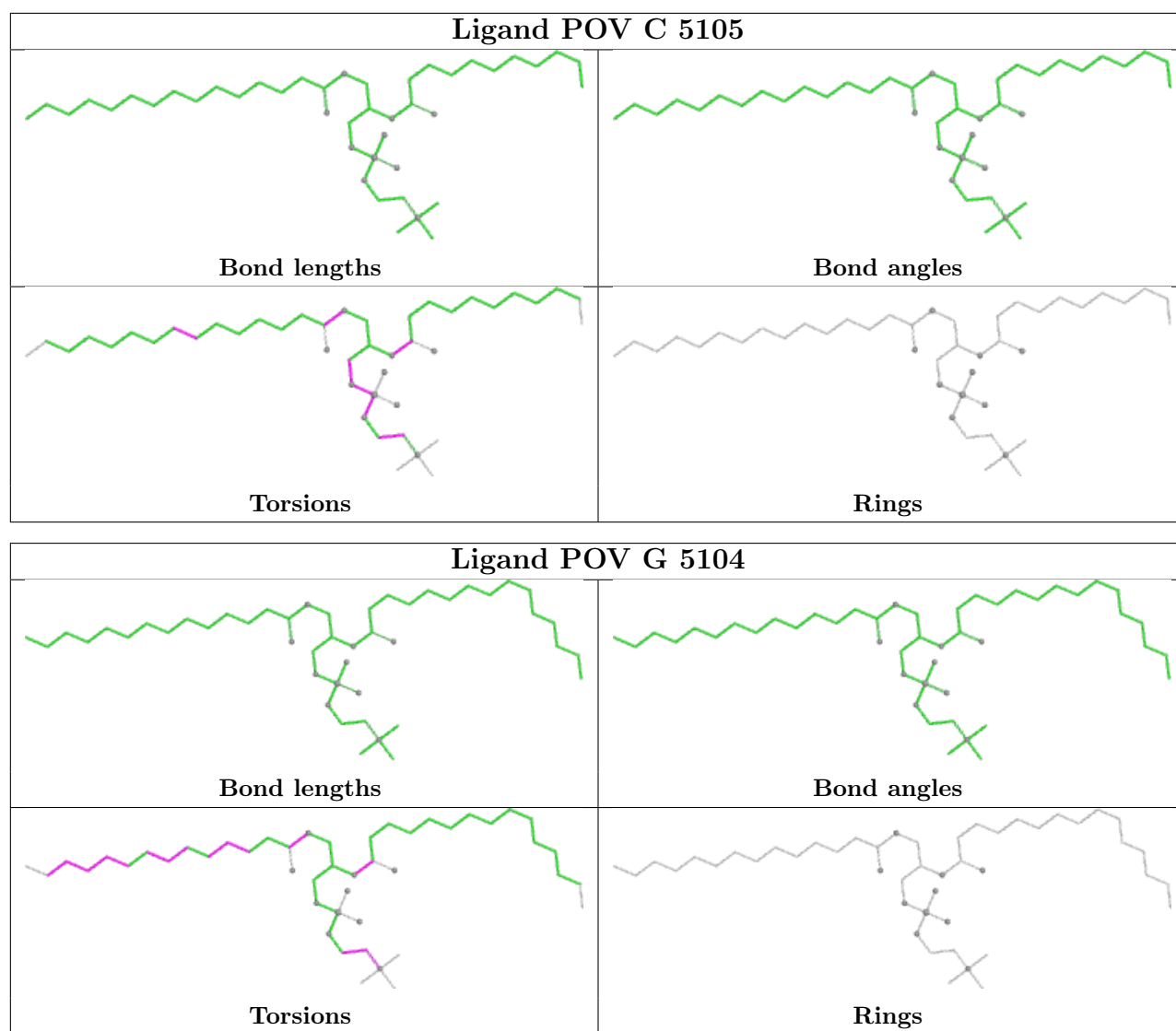


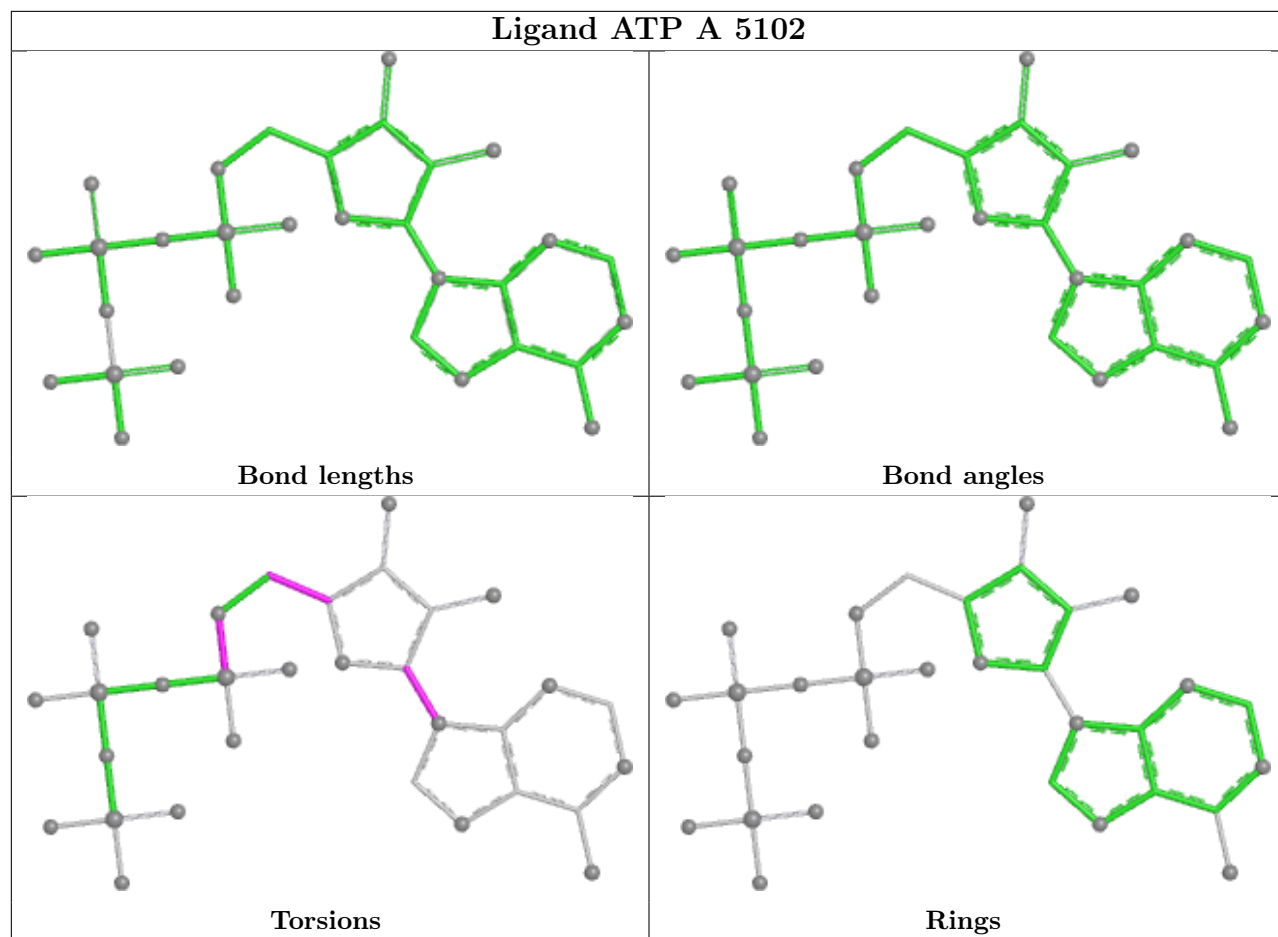


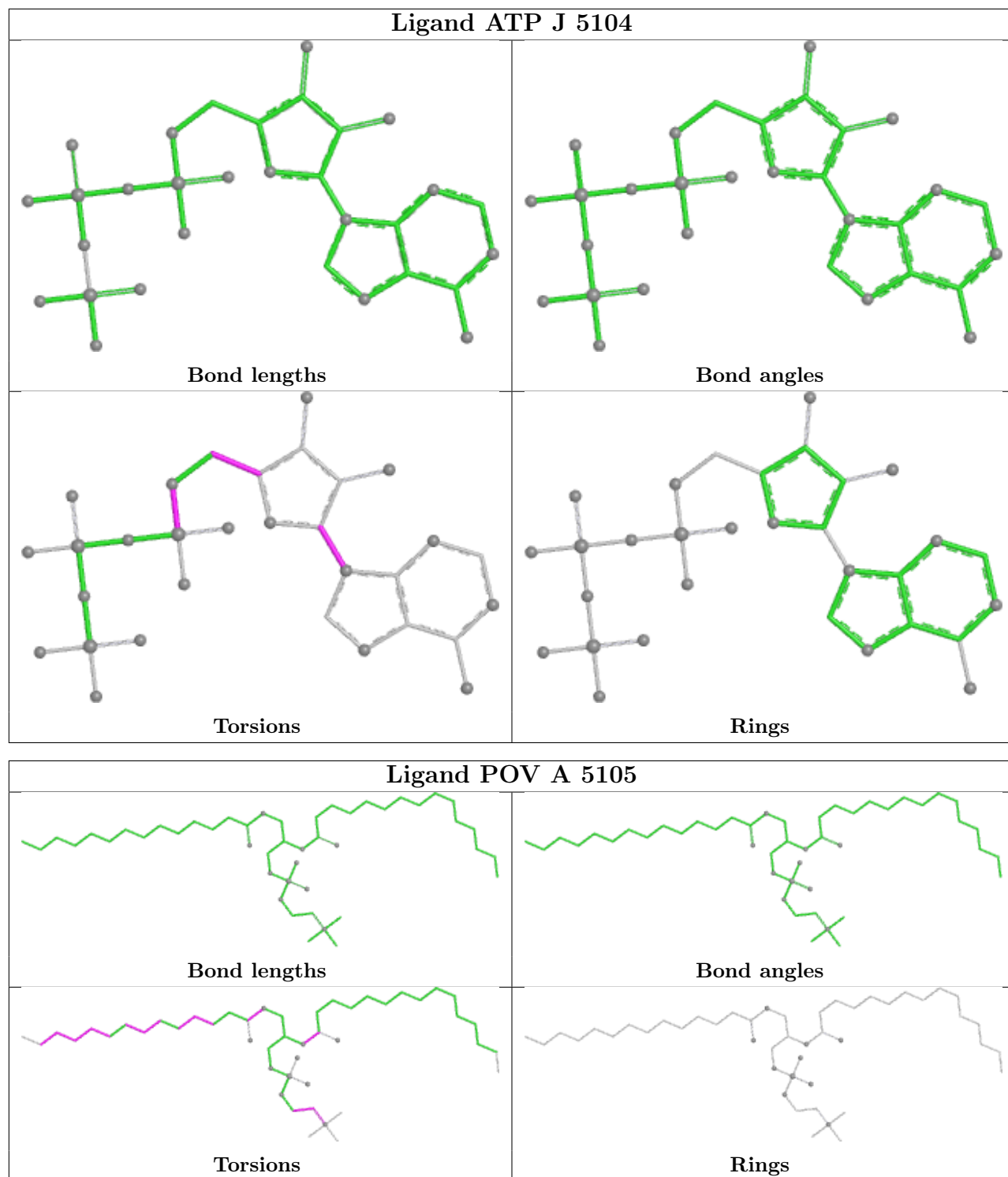


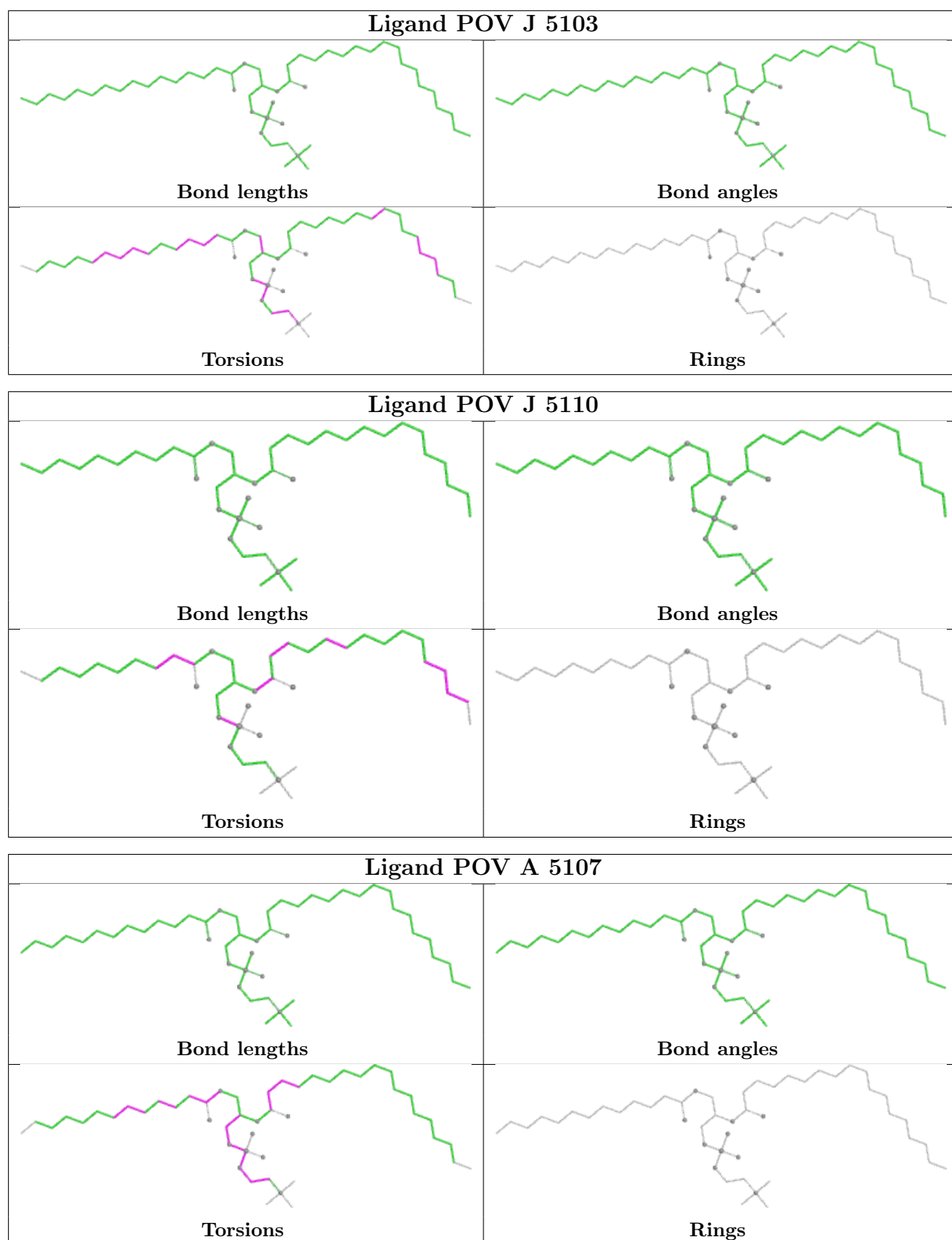


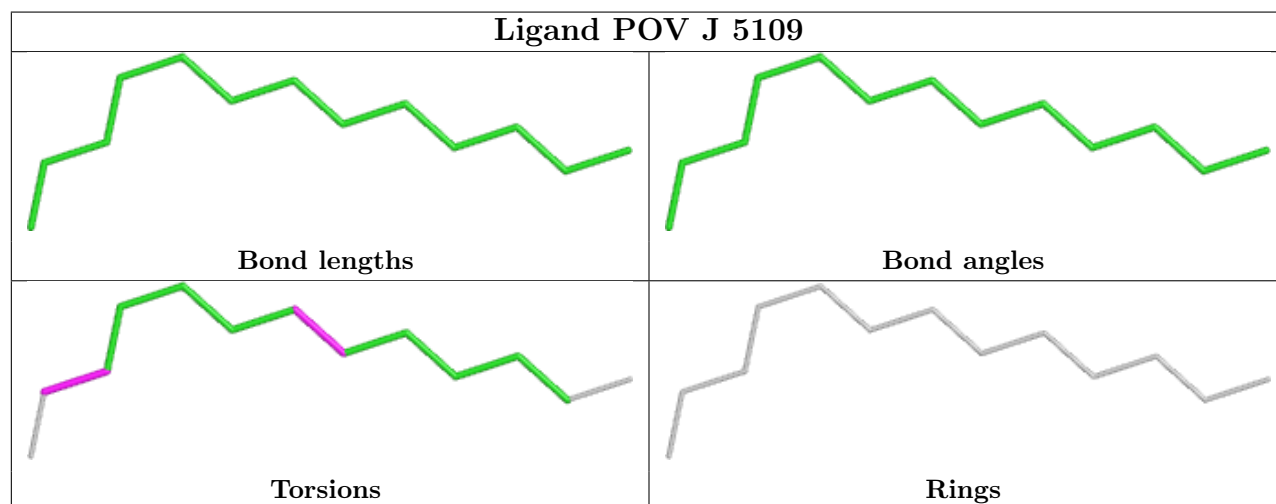
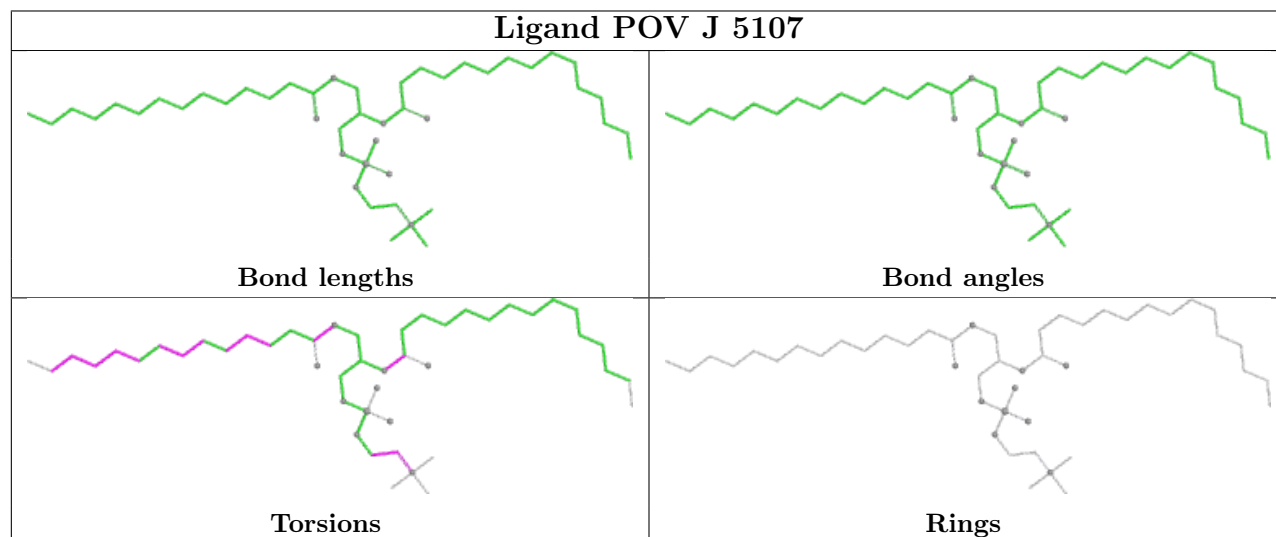
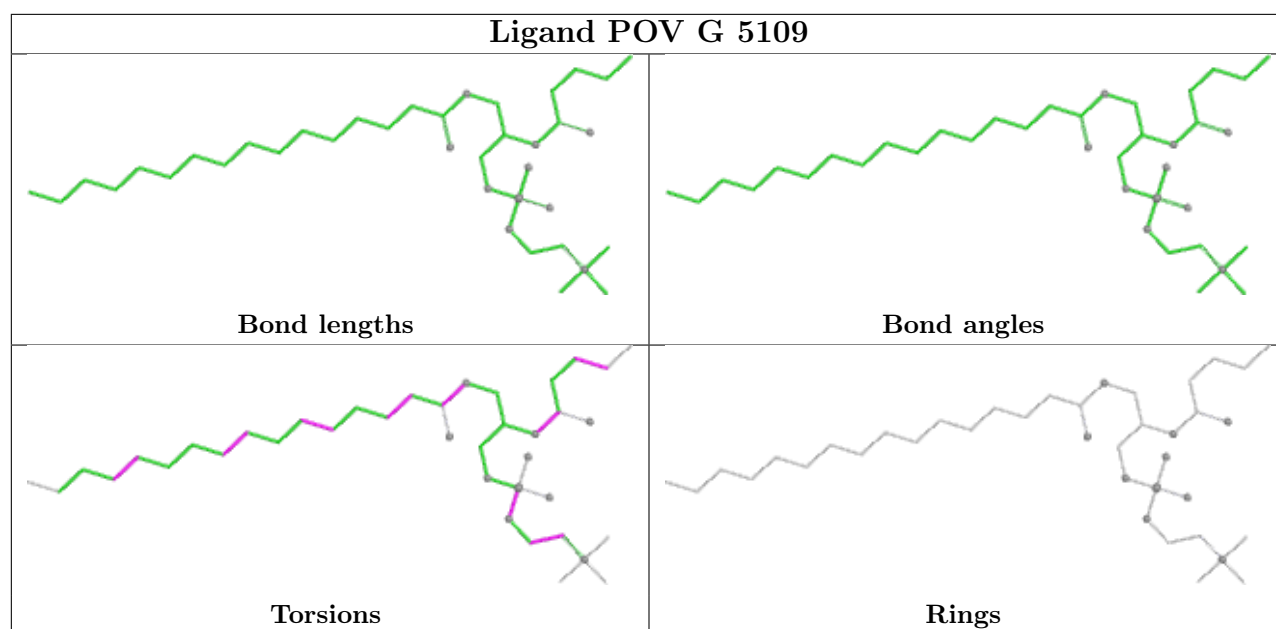


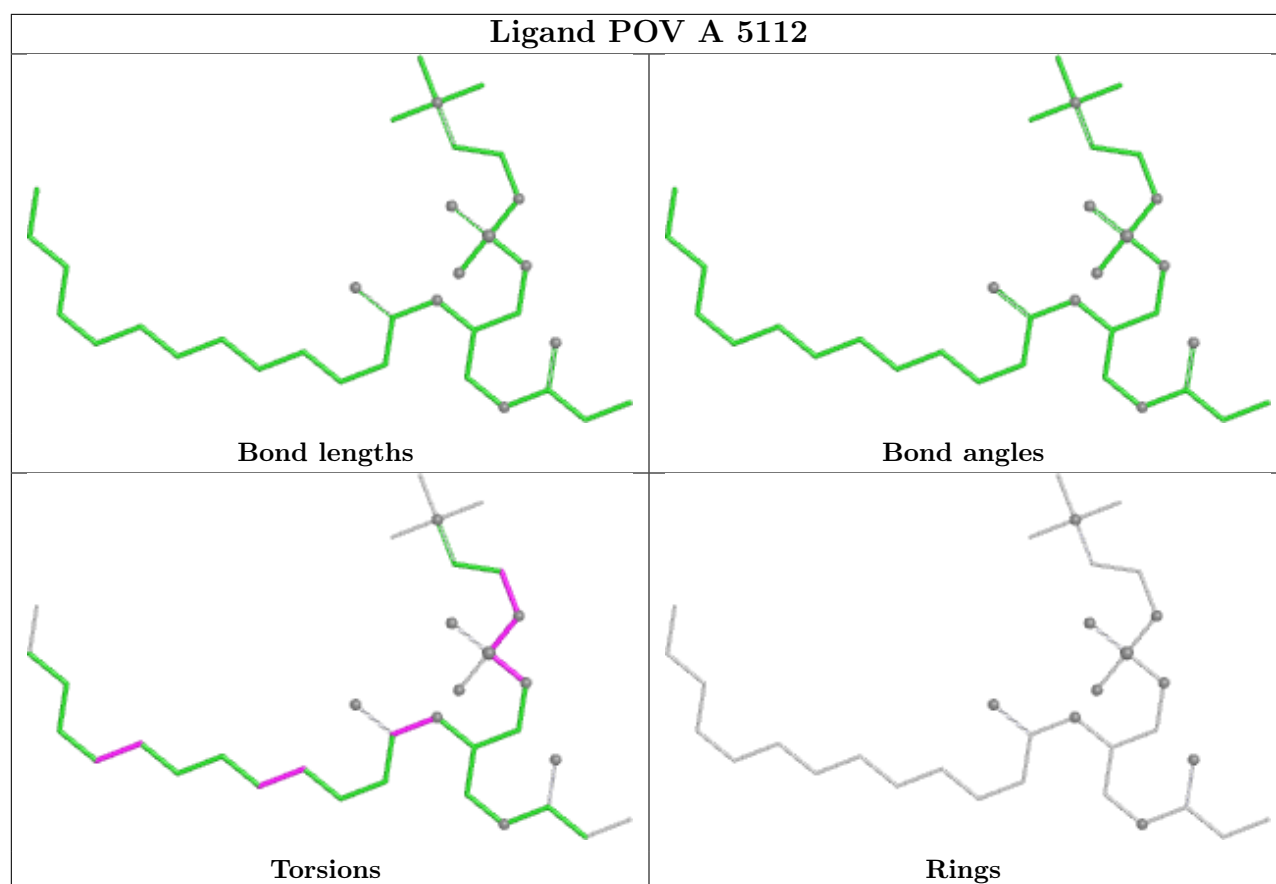


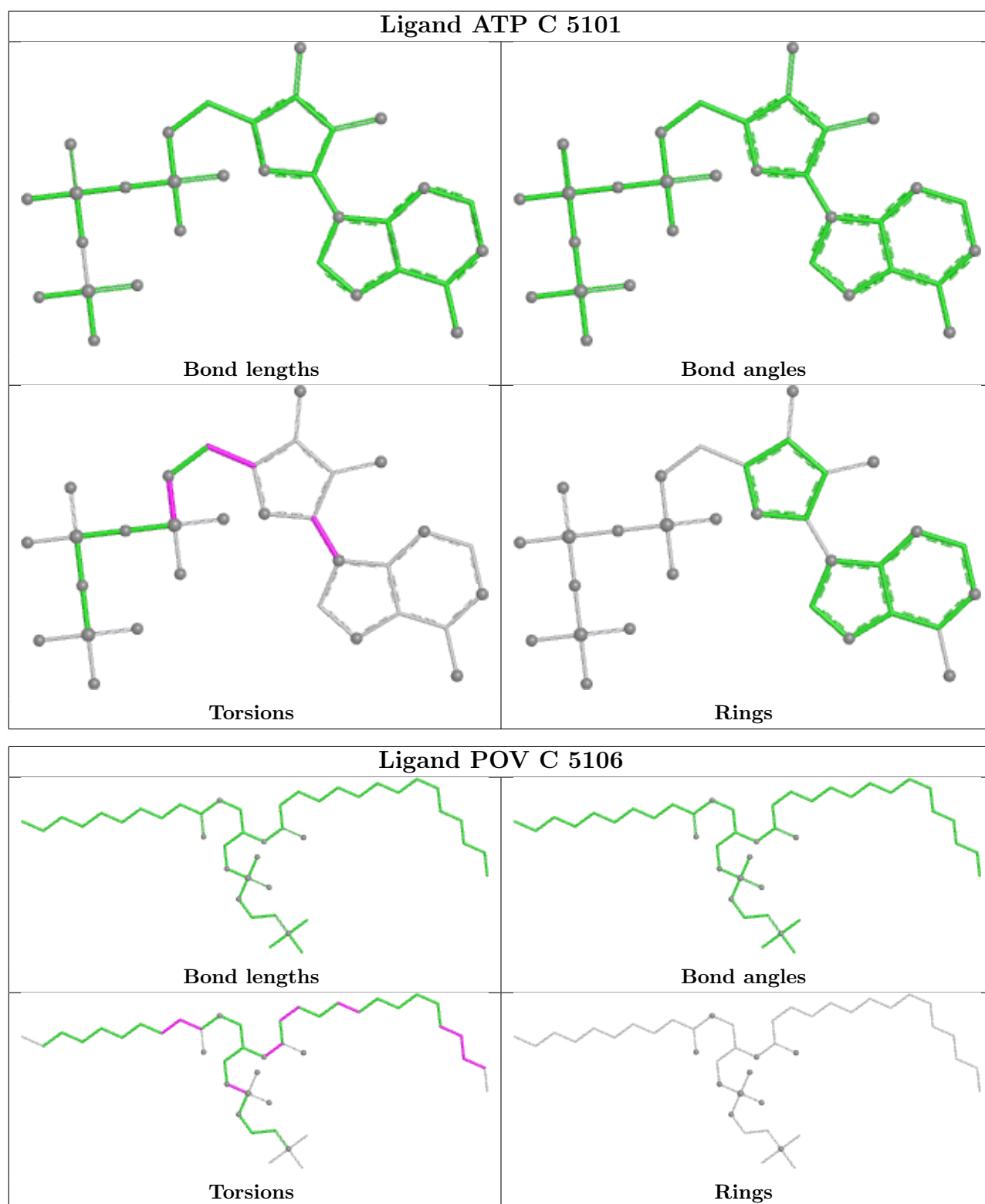


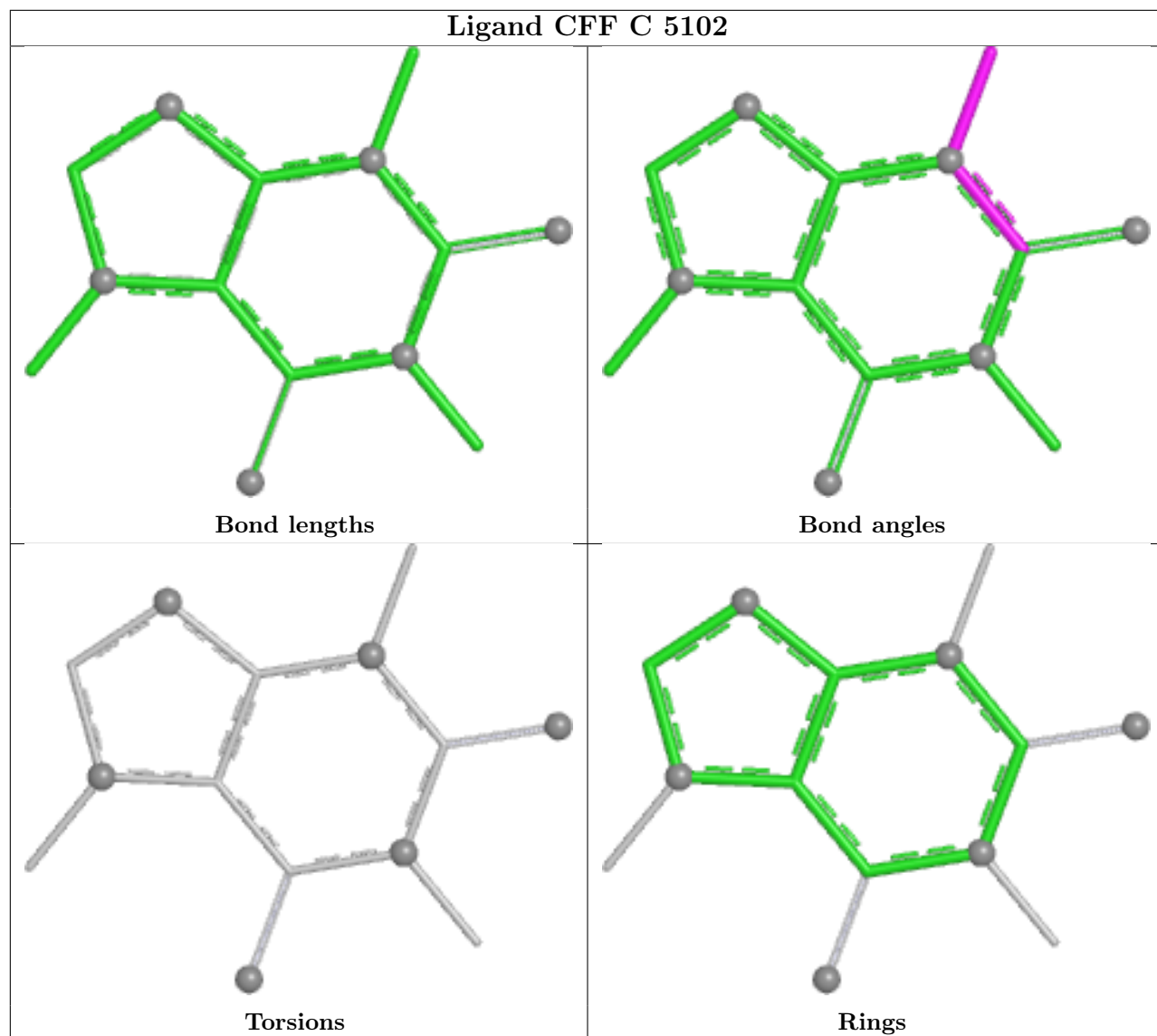


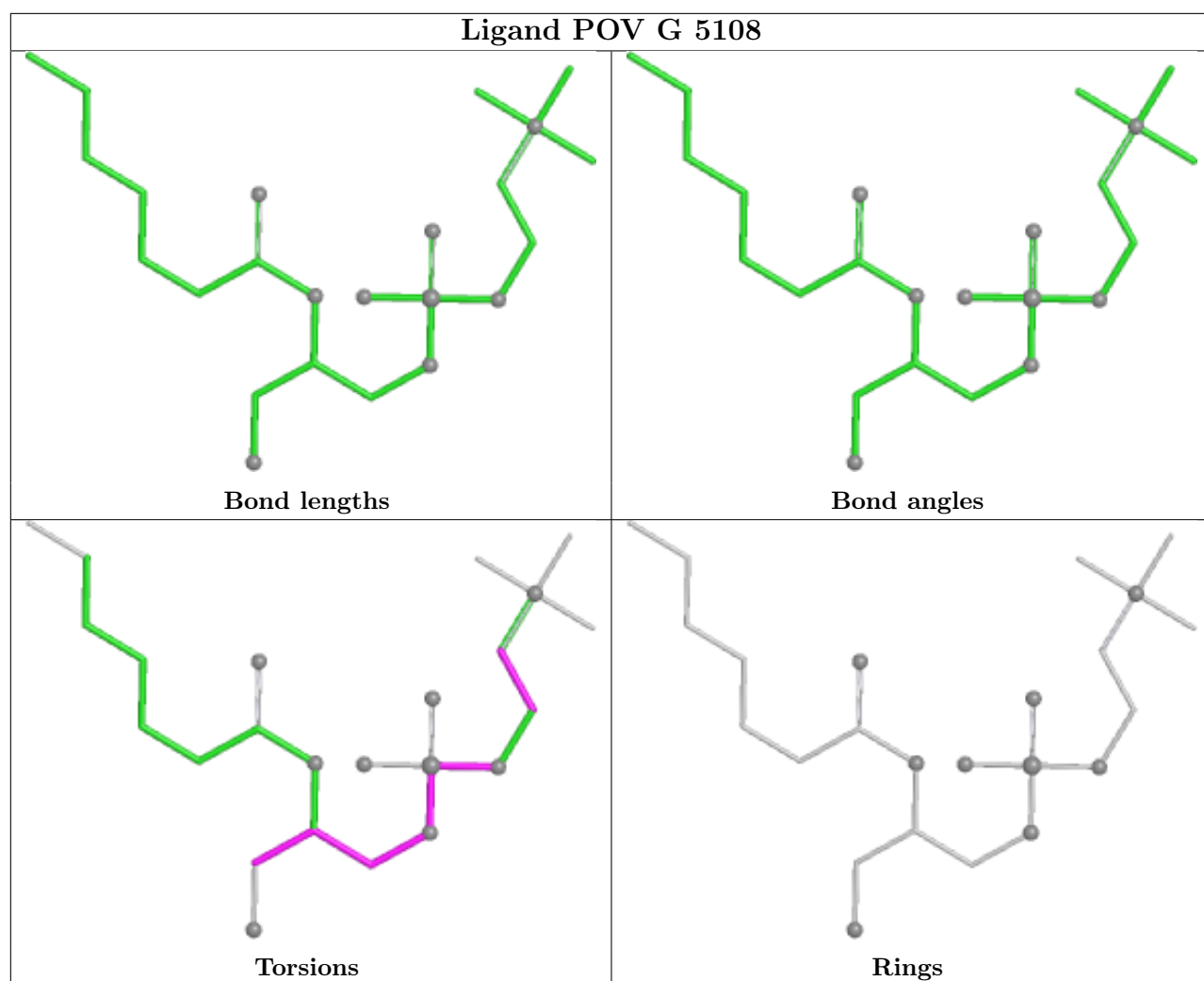


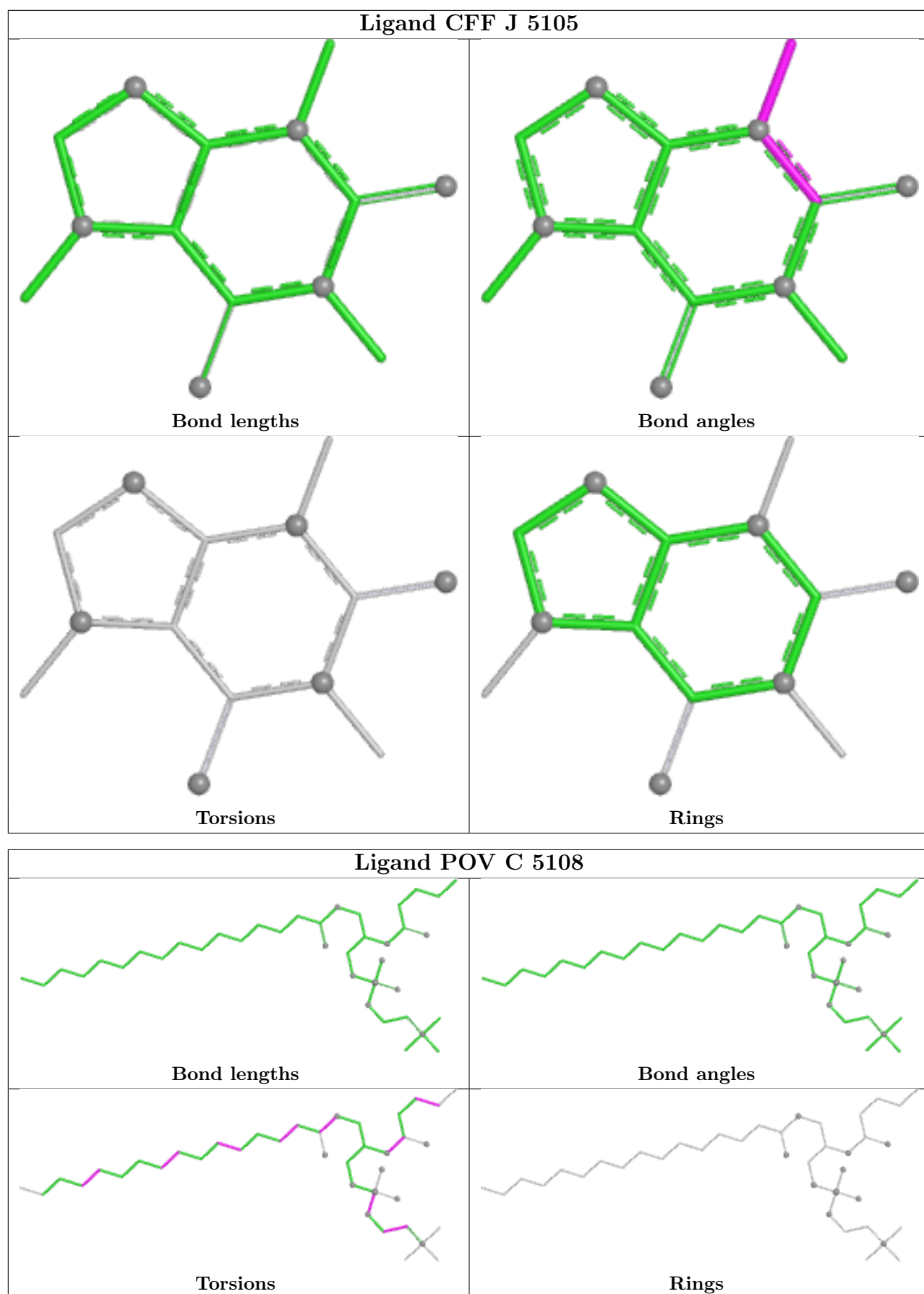


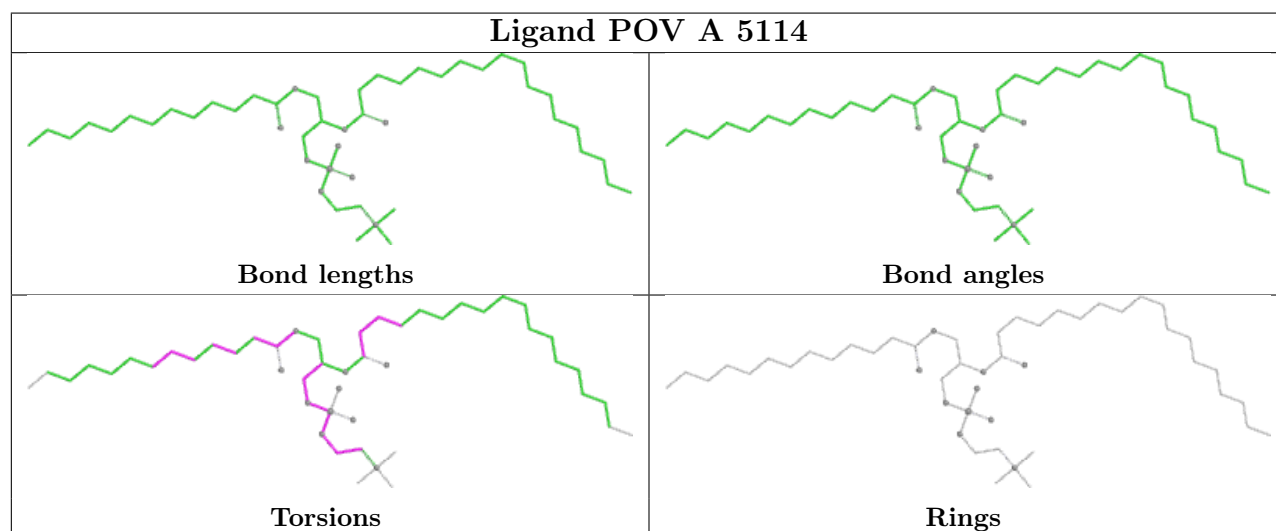
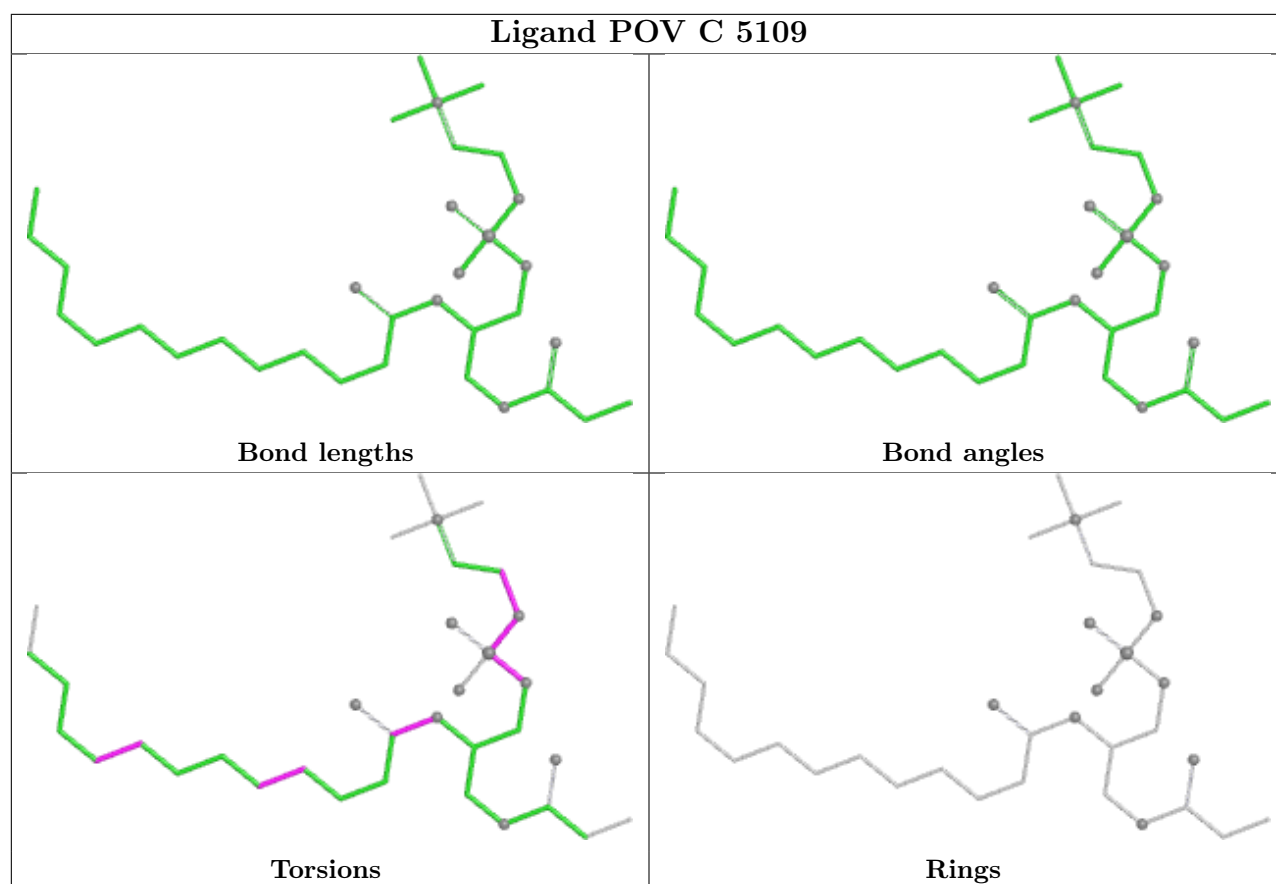


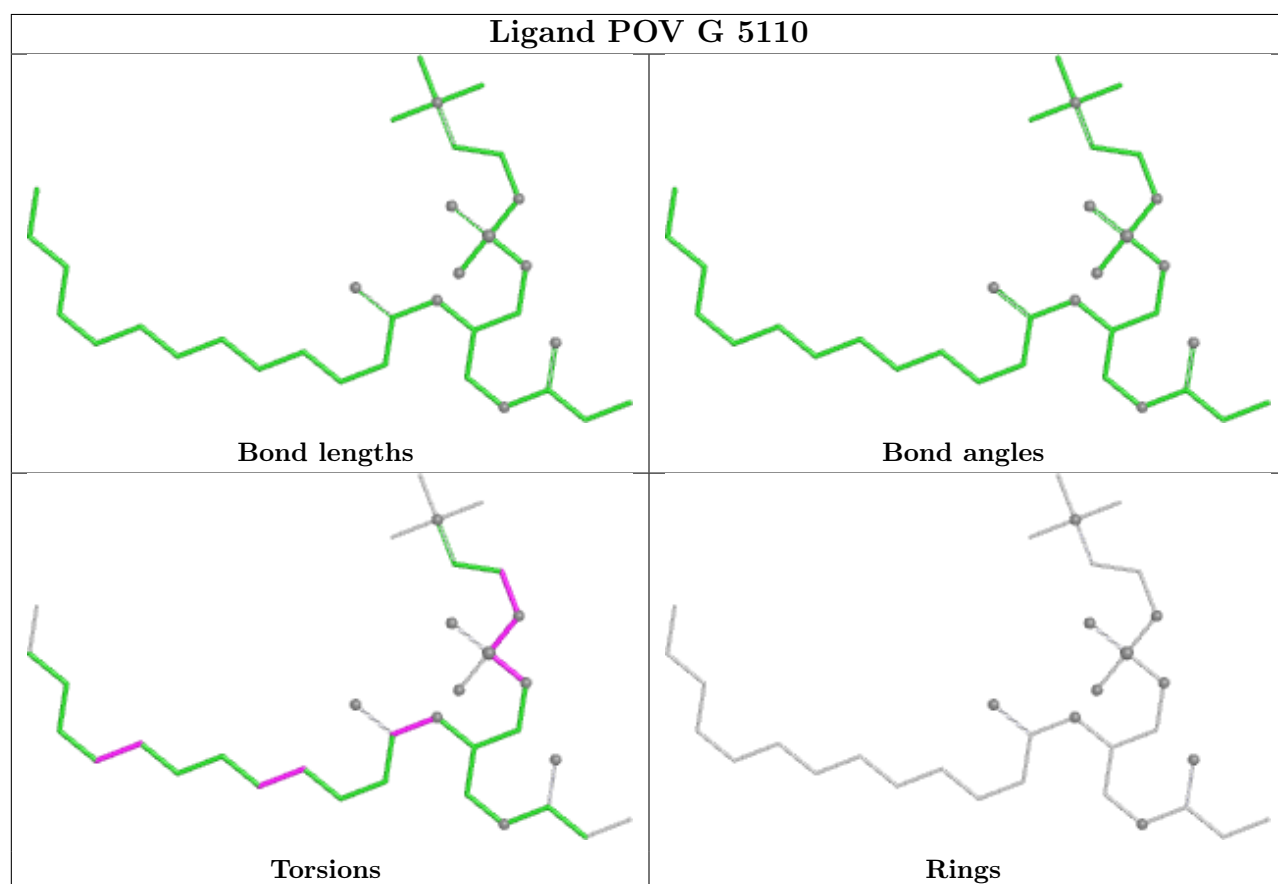
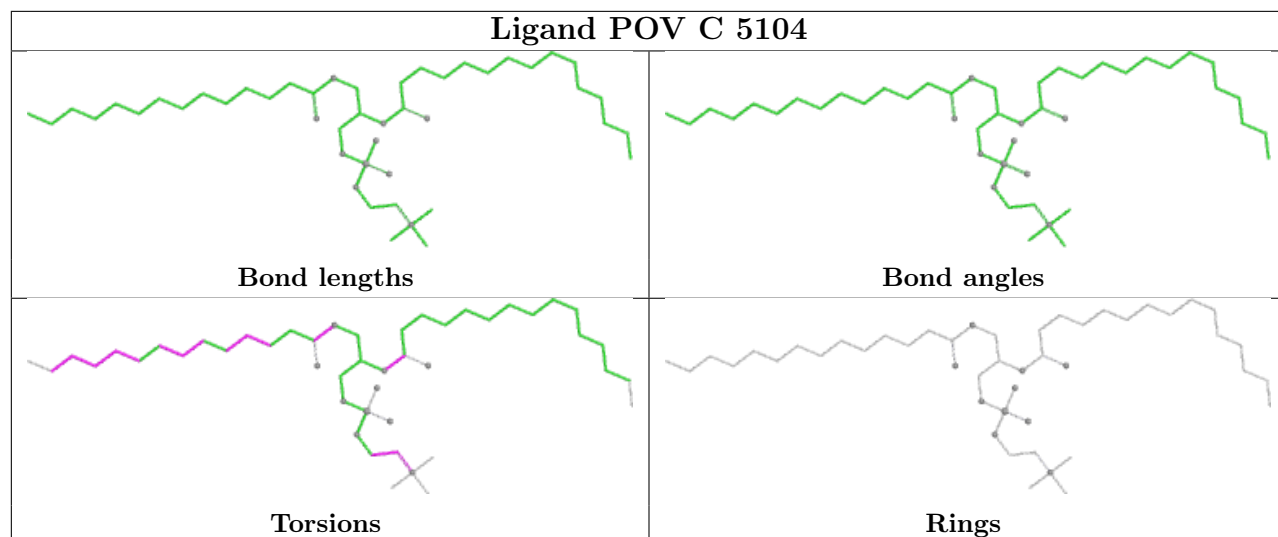


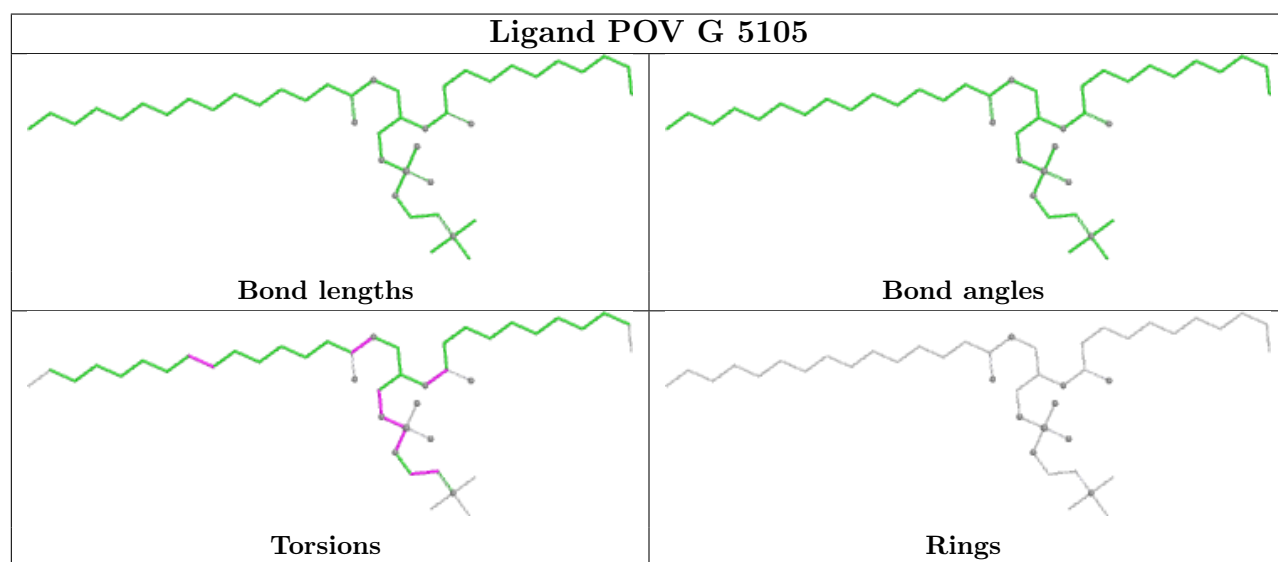
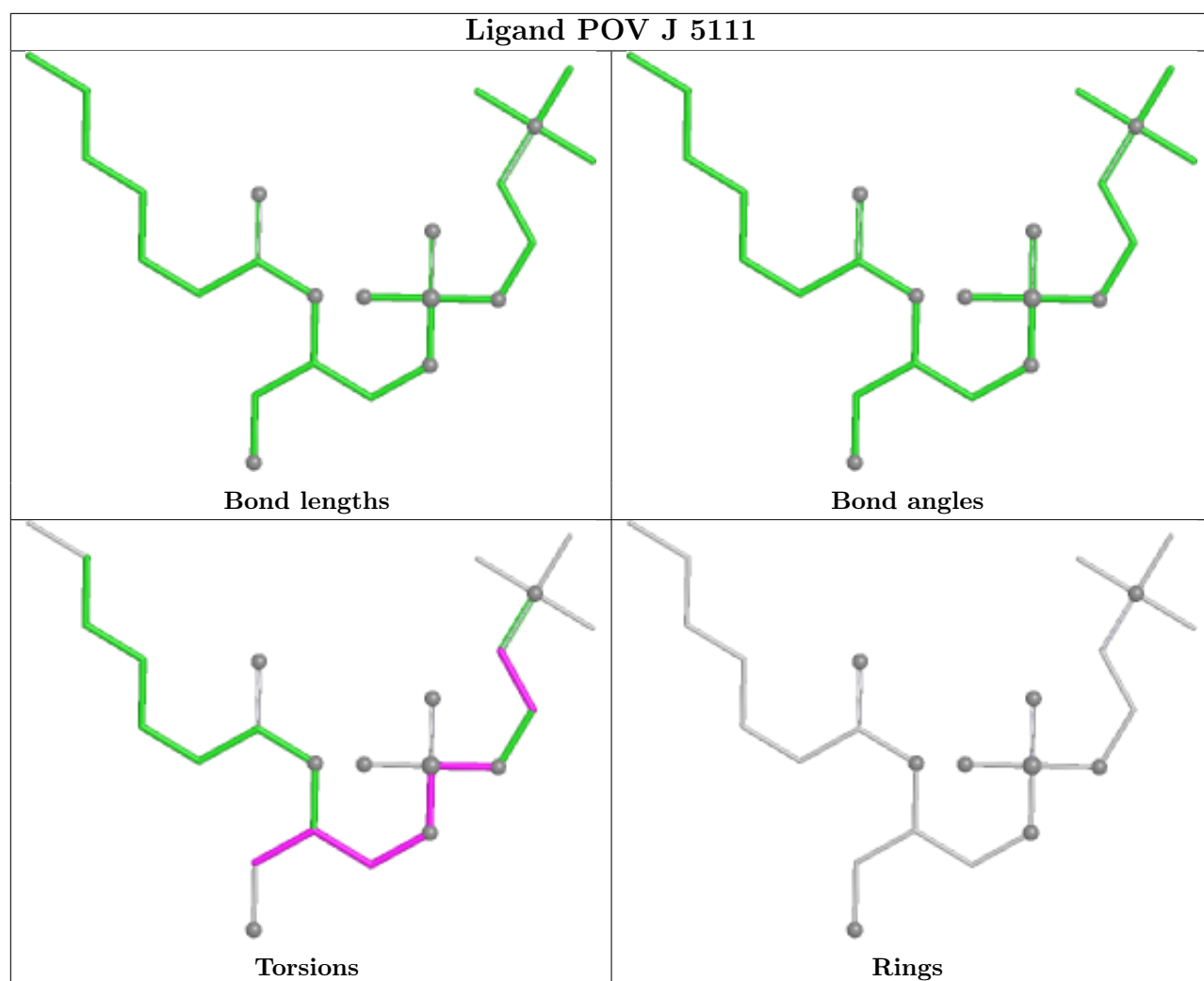


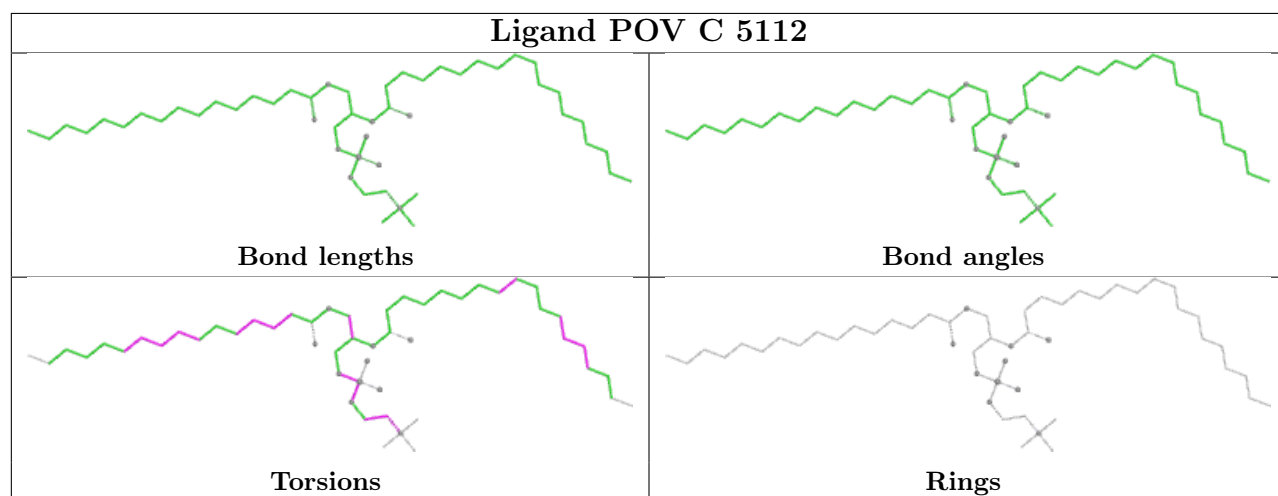
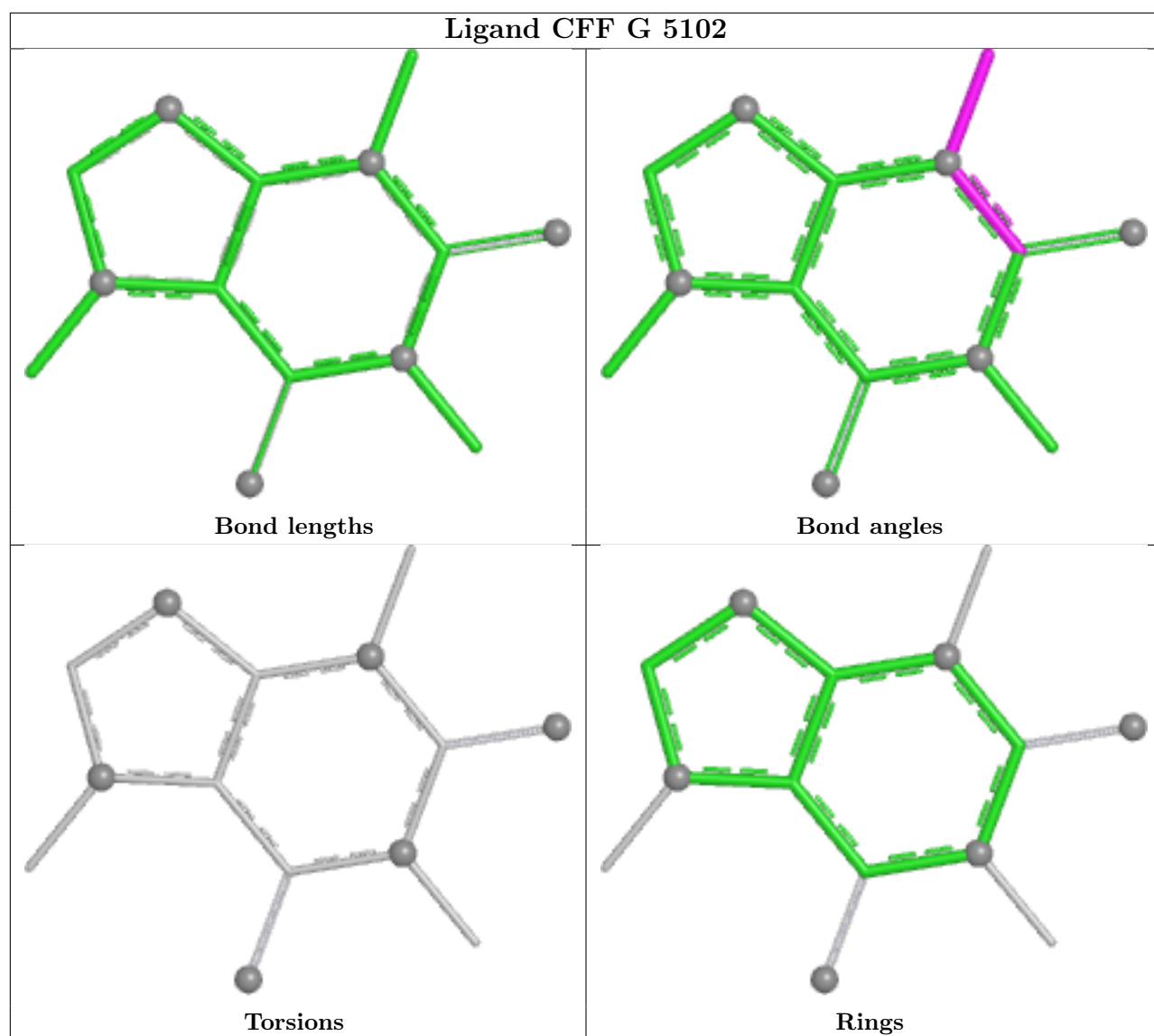


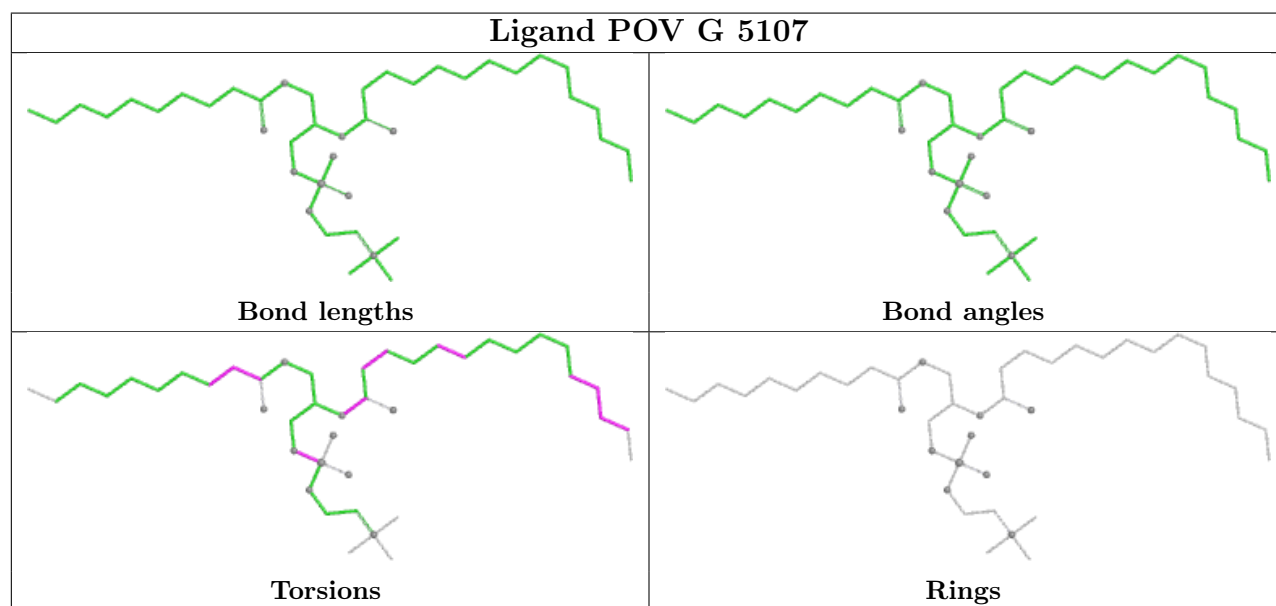
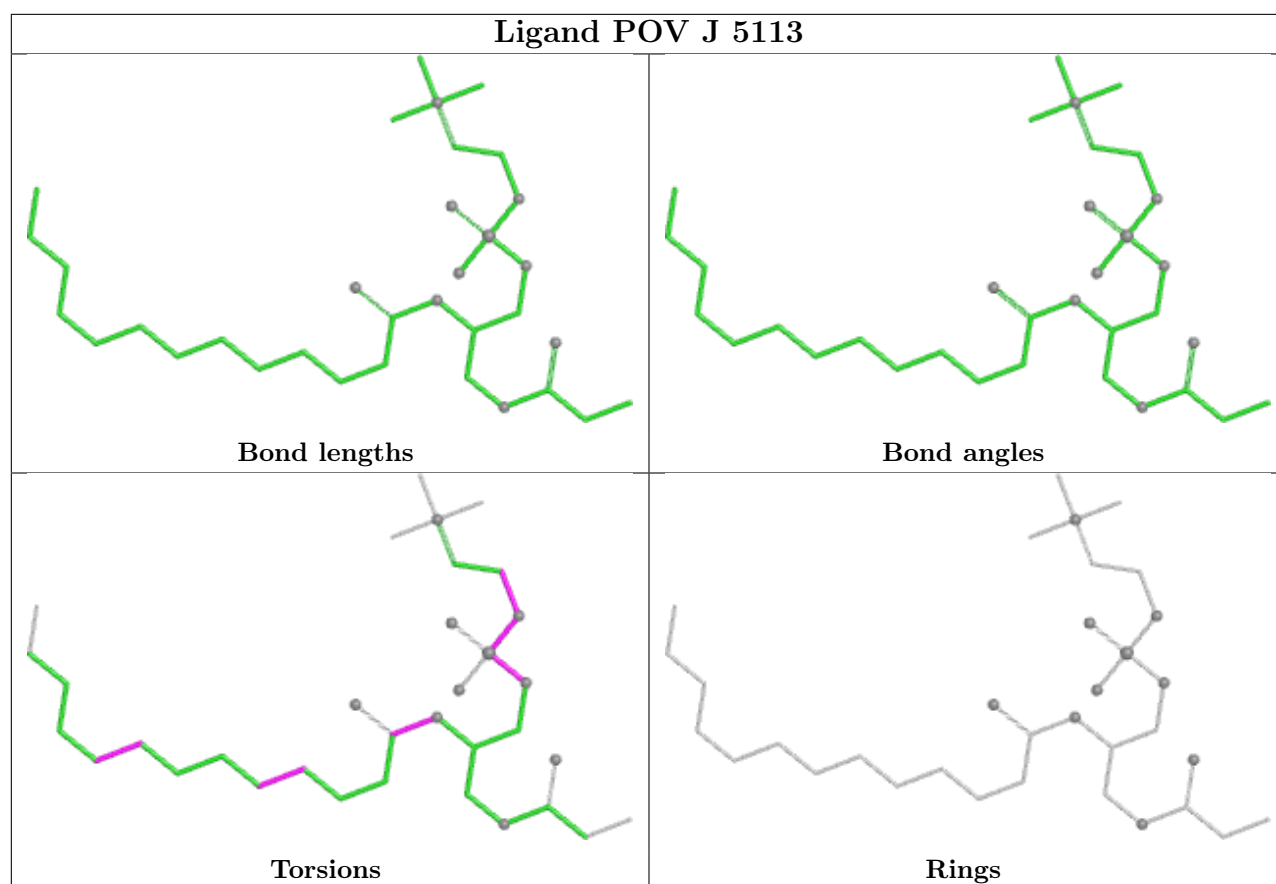


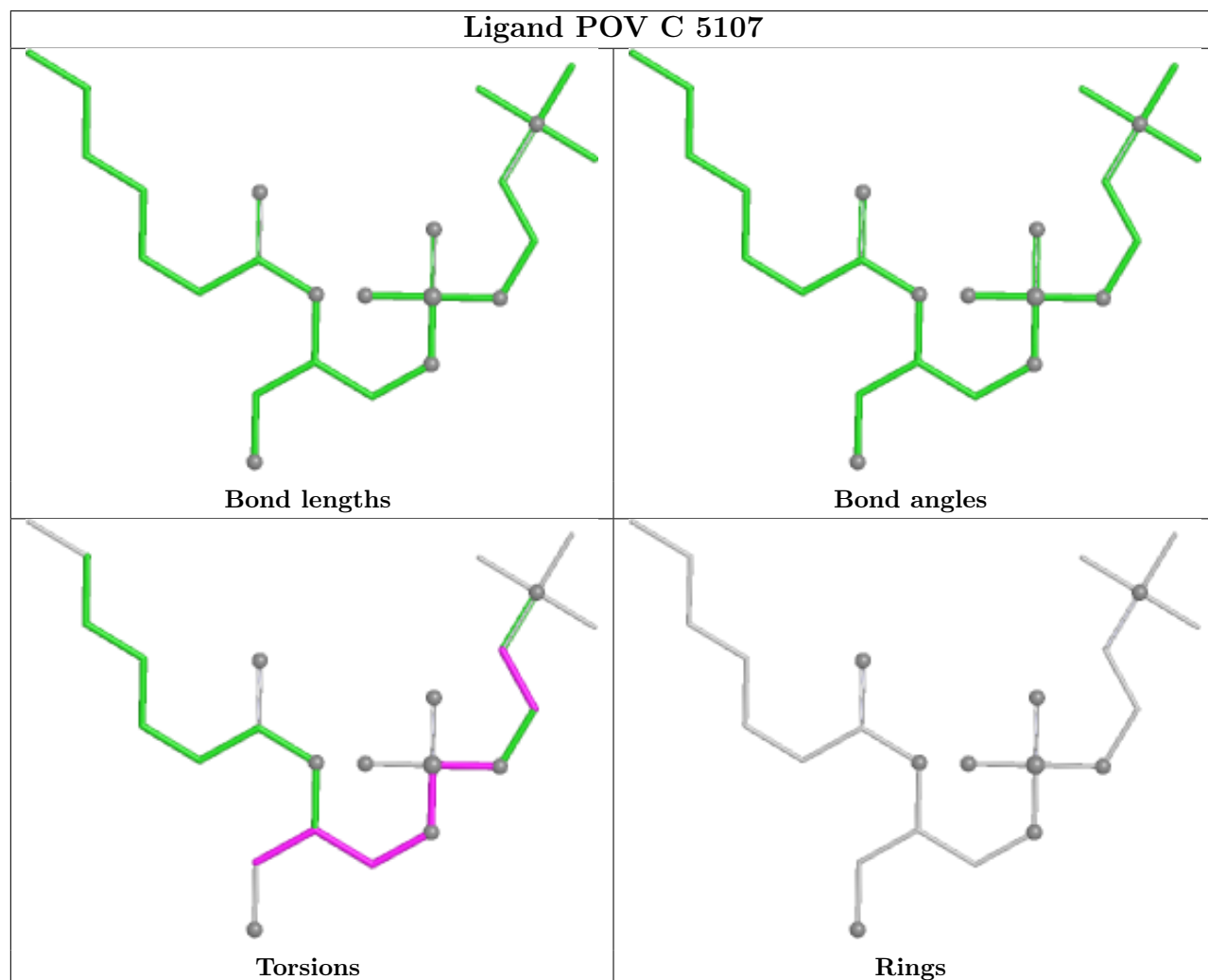
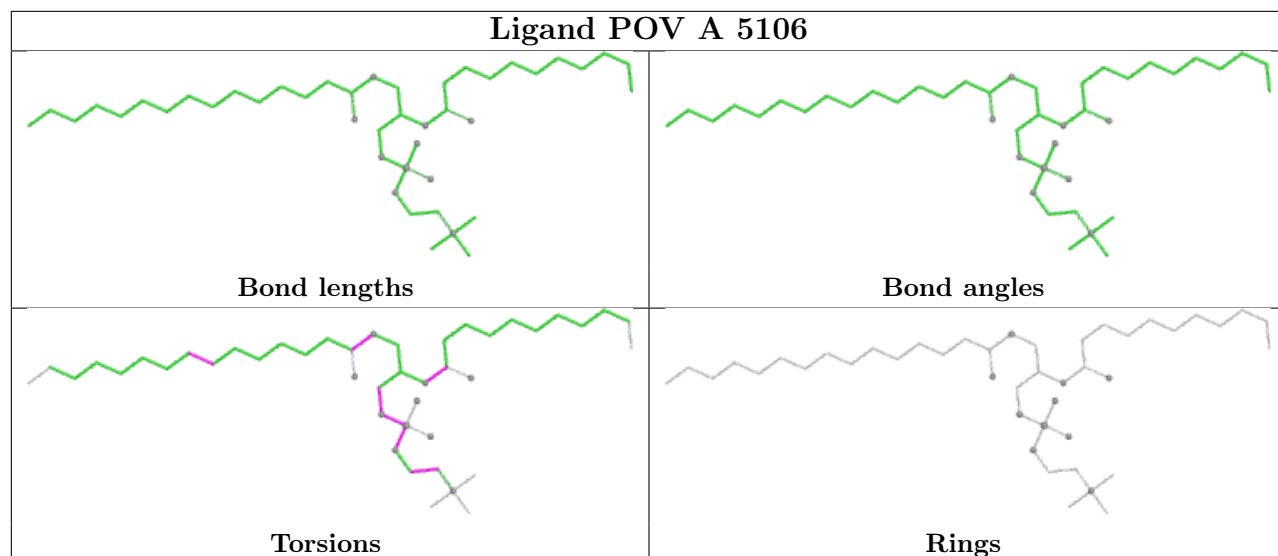


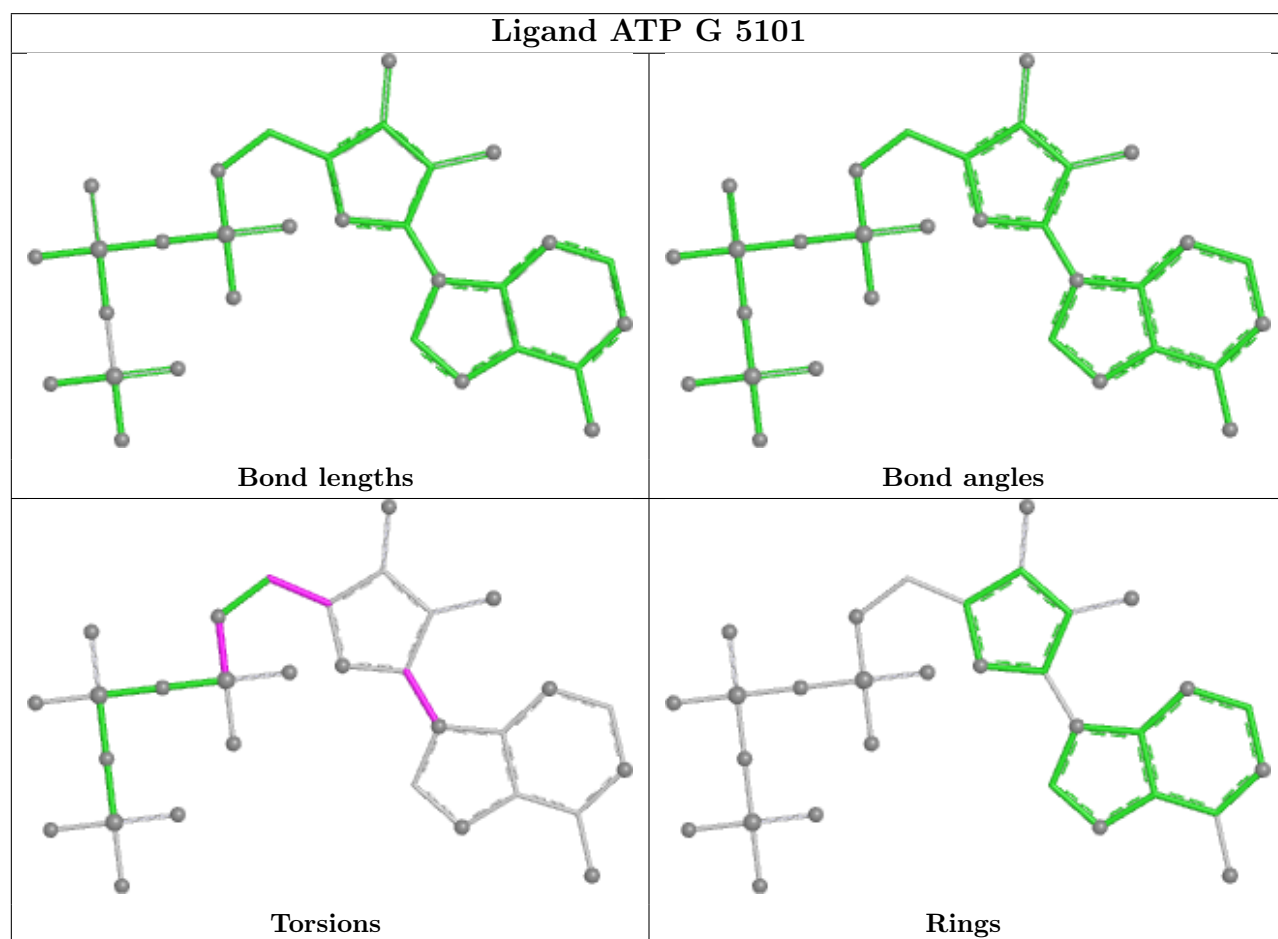
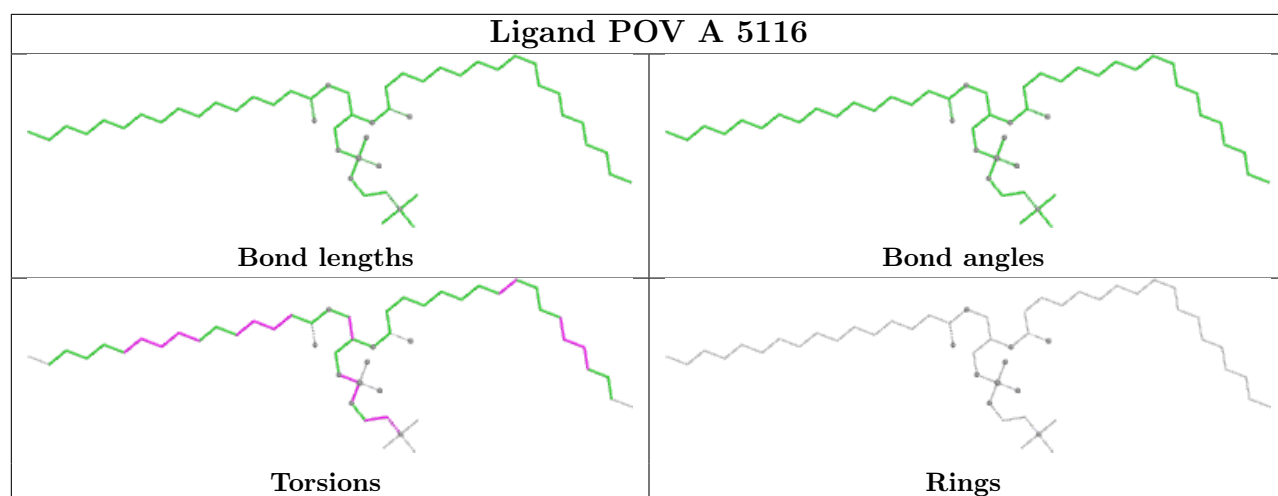


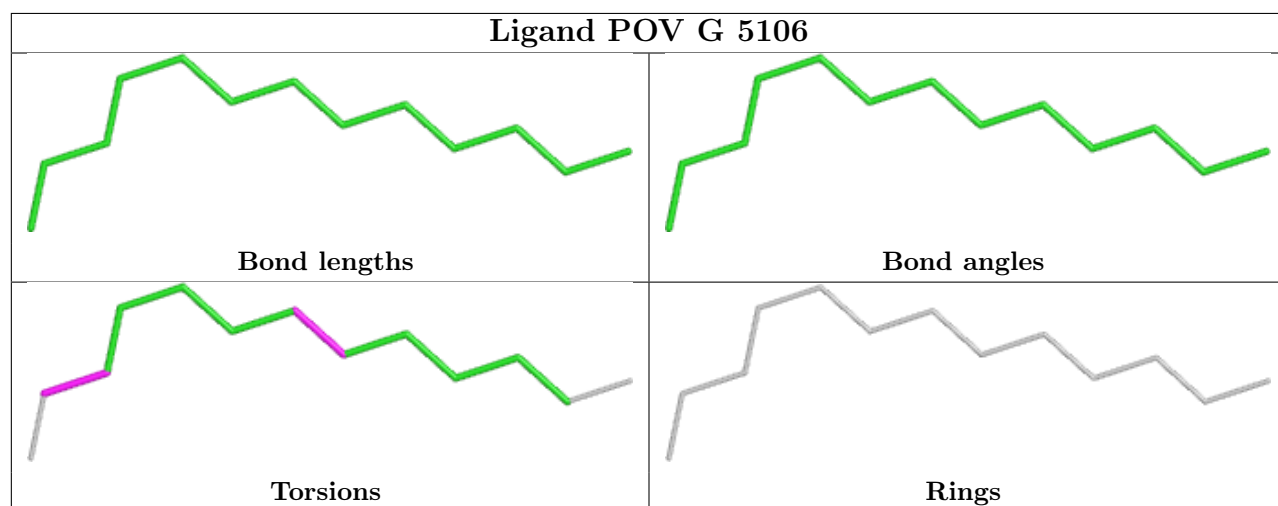
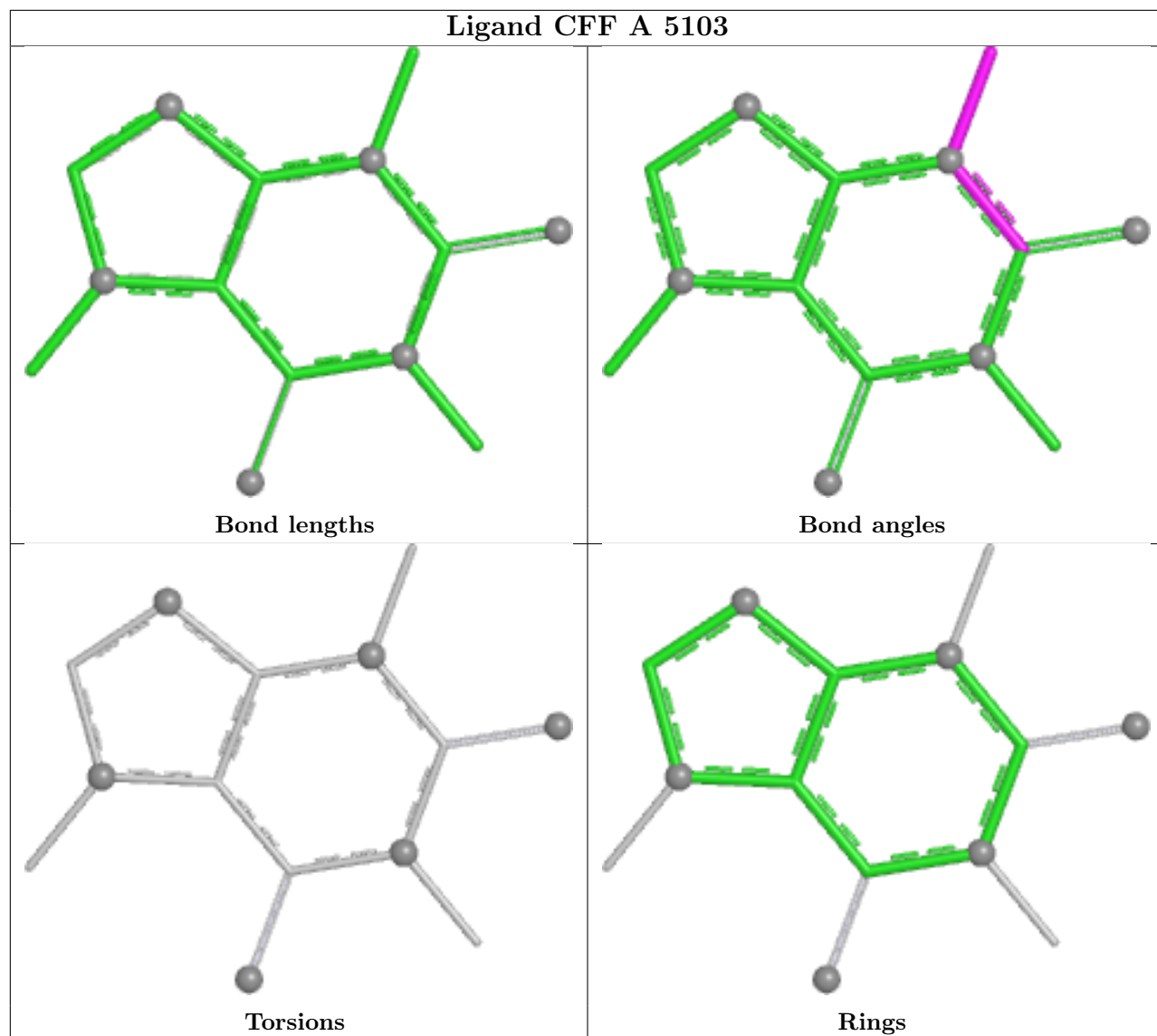


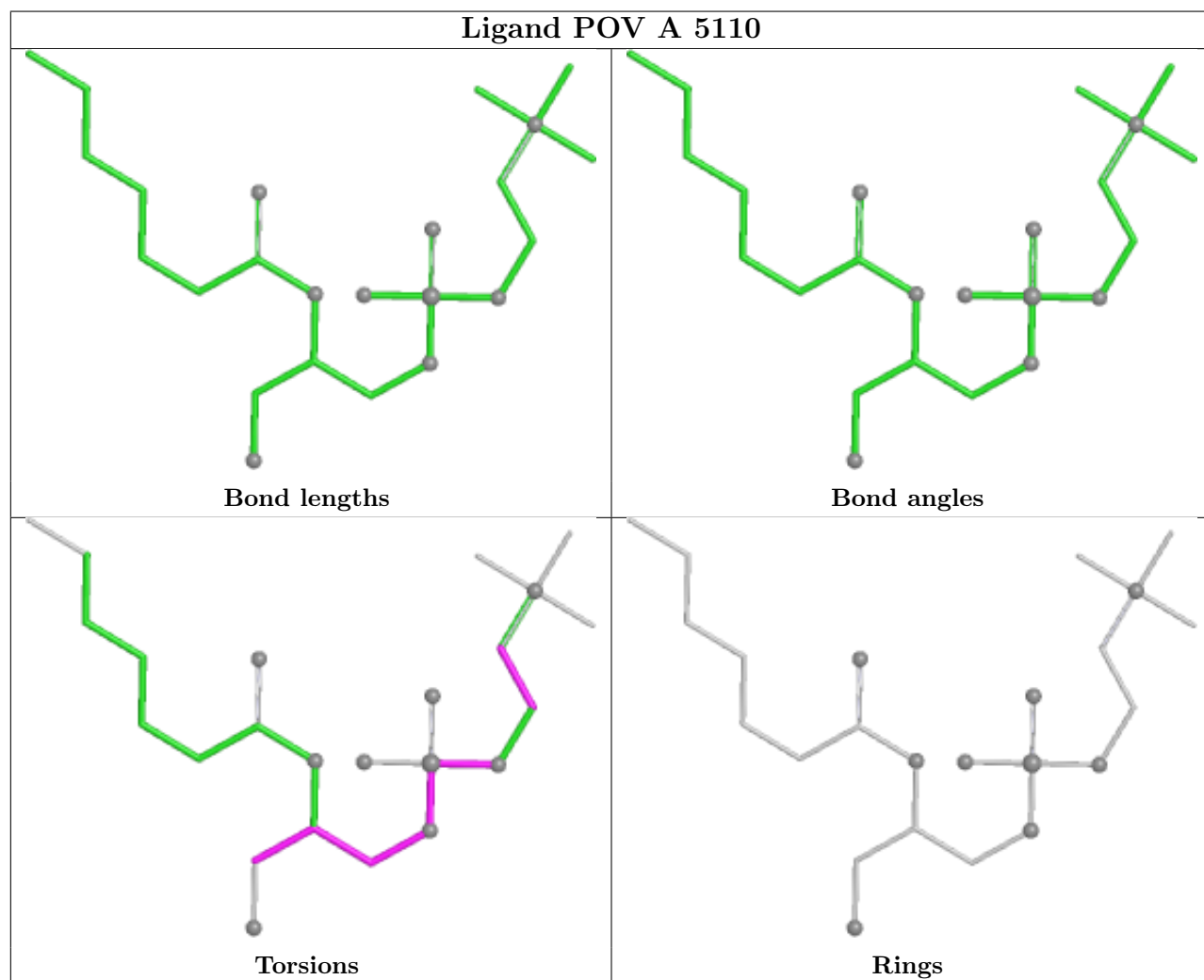
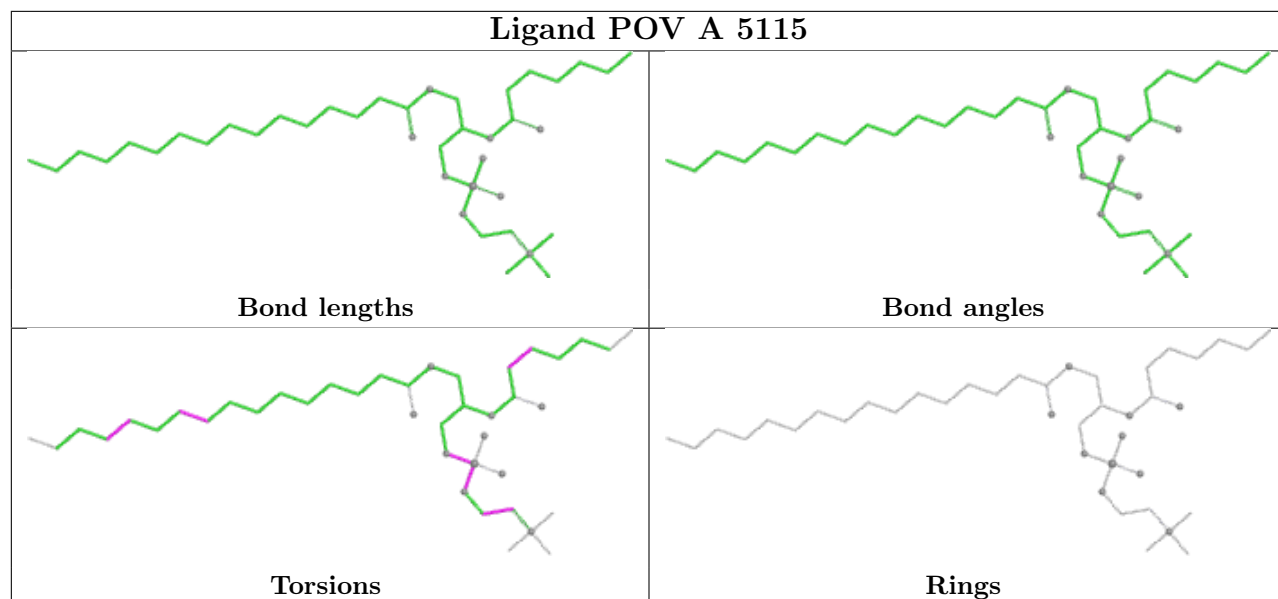












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

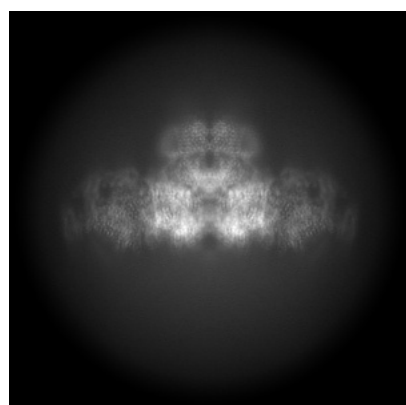
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52091. These allow visual inspection of the internal detail of the map and identification of artifacts.

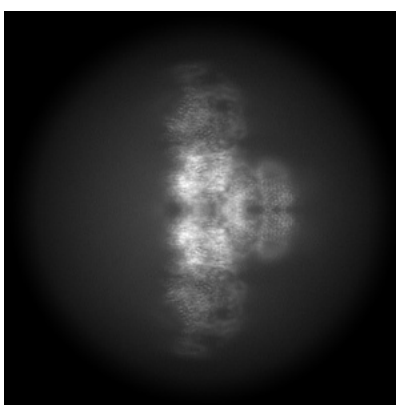
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

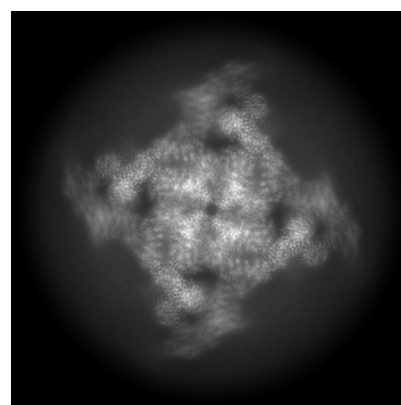
6.1.1 Primary map



X



Y

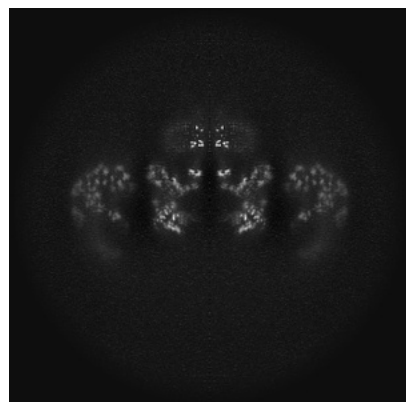


Z

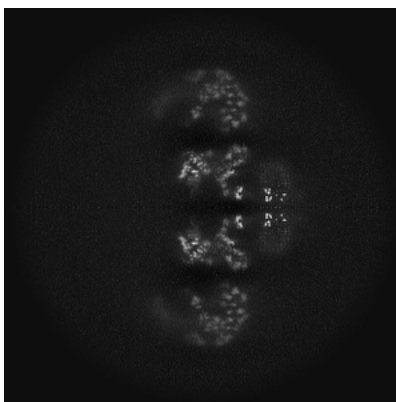
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

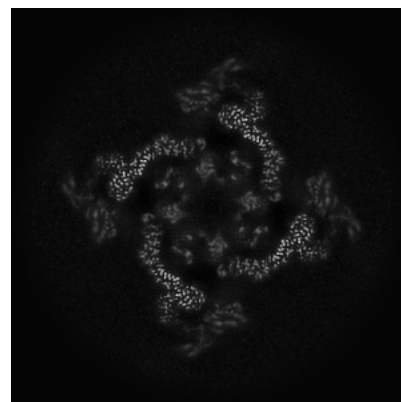
6.2.1 Primary map



X Index: 168



Y Index: 168

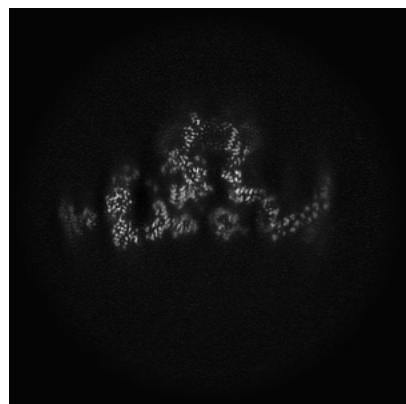


Z Index: 168

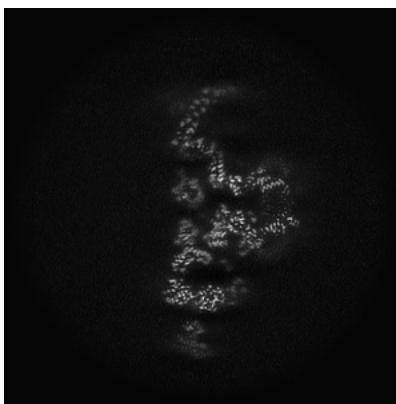
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

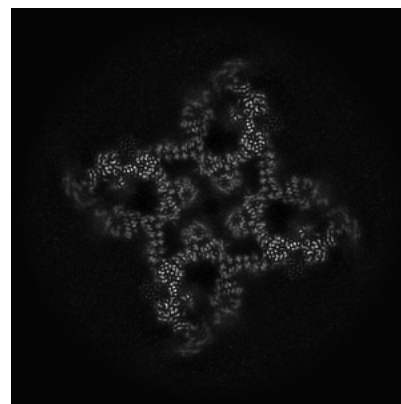
6.3.1 Primary map



X Index: 149



Y Index: 187

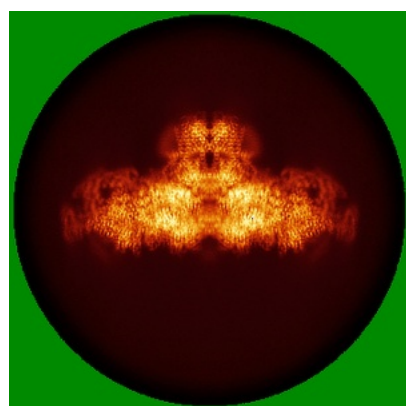


Z Index: 159

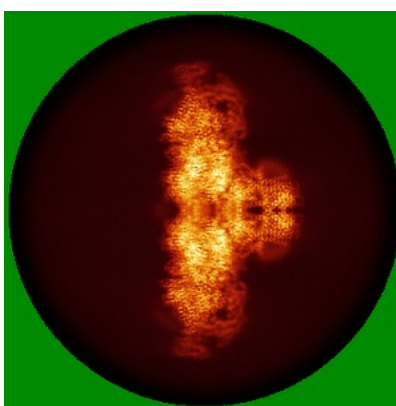
The images above show the largest variance slices of the map in three orthogonal directions.

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

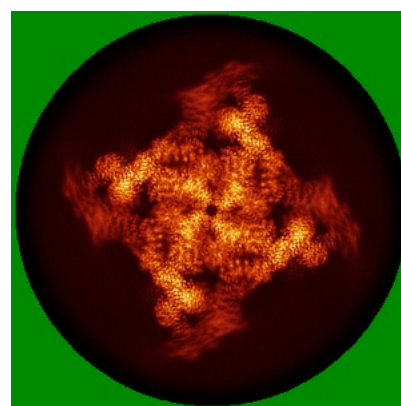
6.4.1 Primary map



X



Y

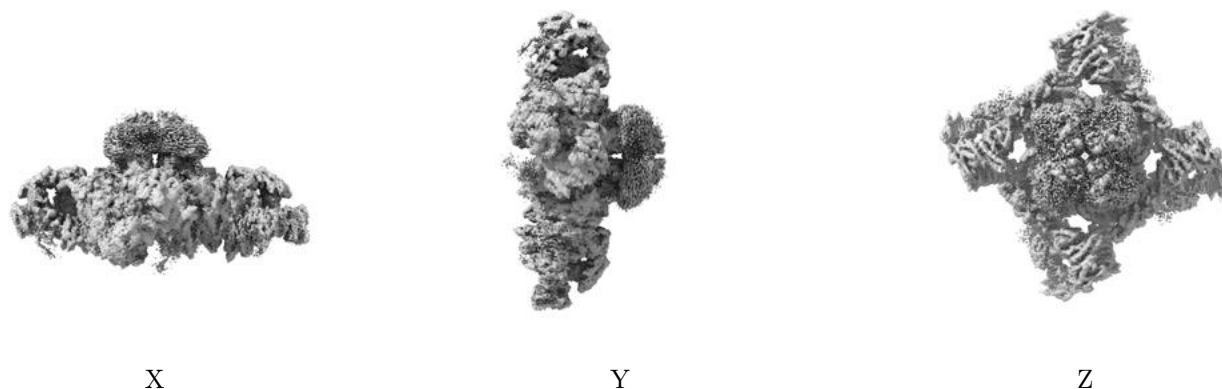


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

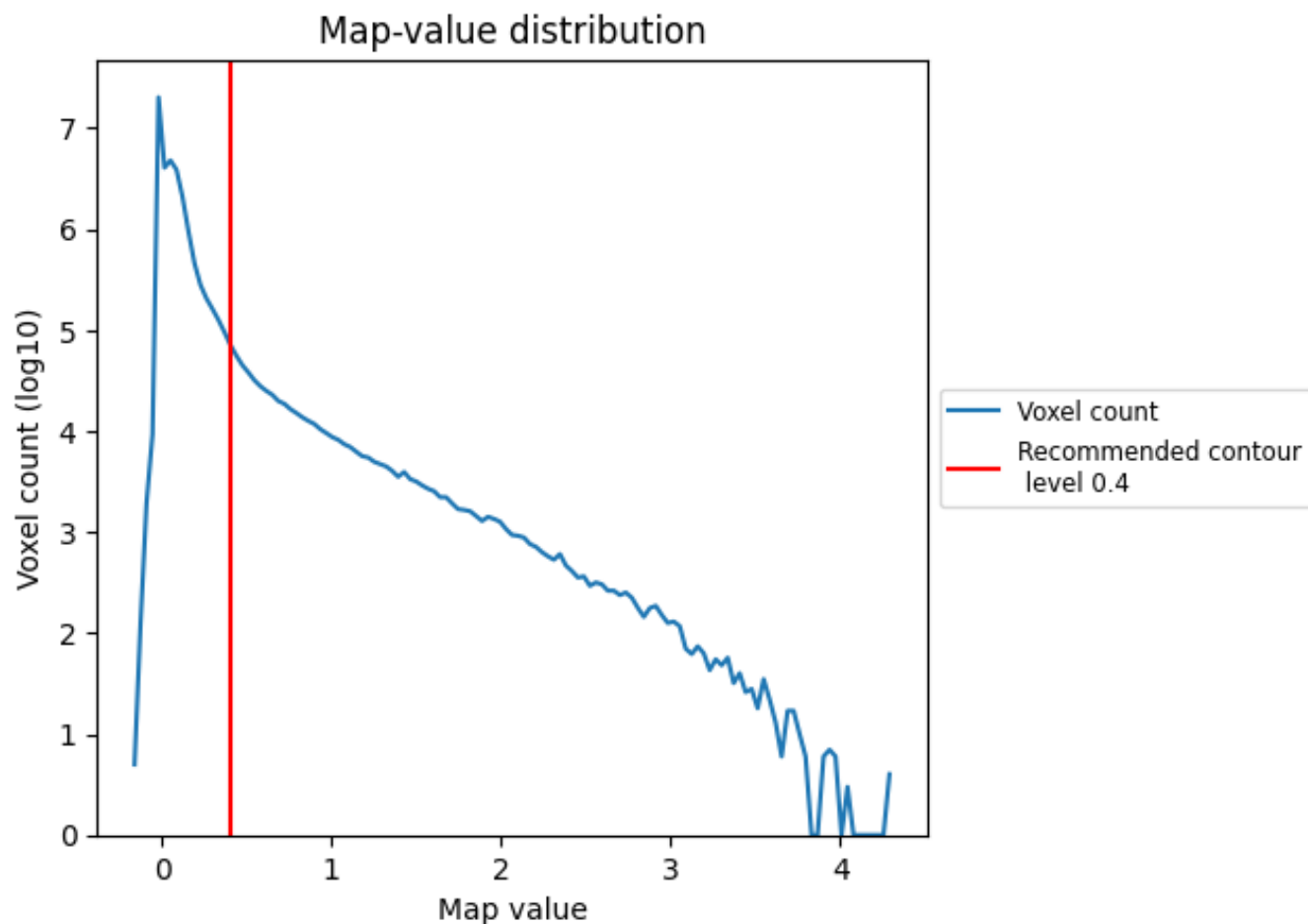
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

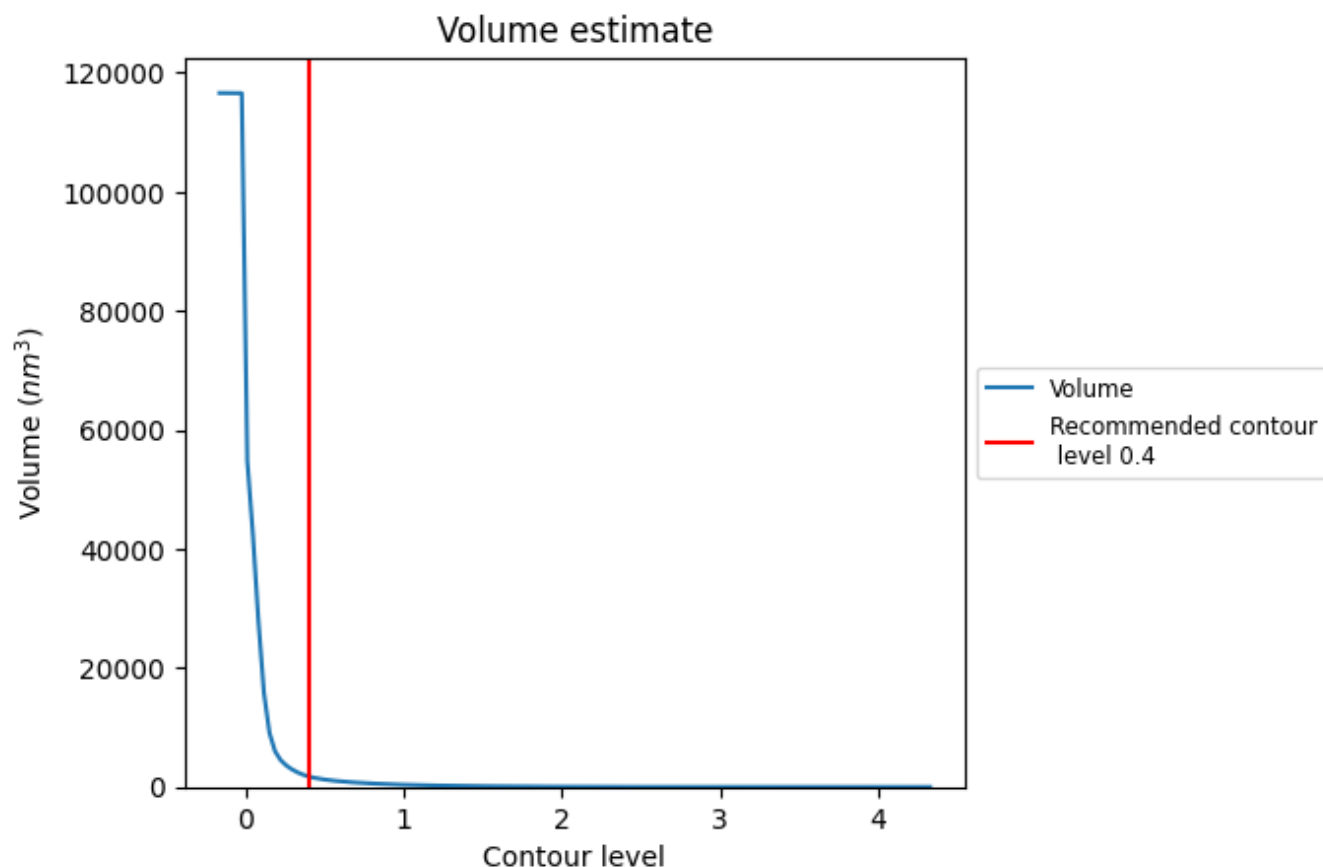
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

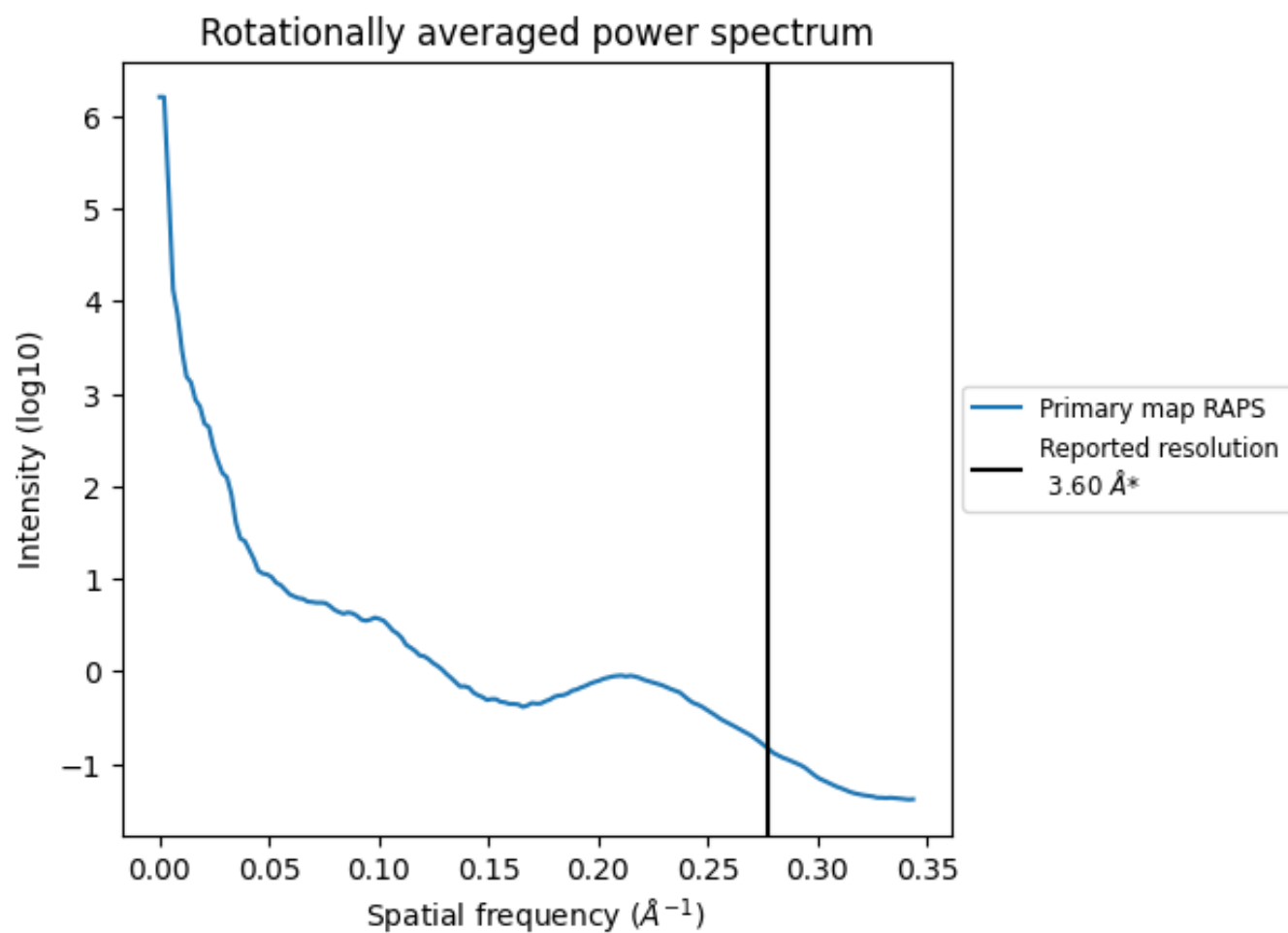
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1771 nm³; this corresponds to an approximate mass of 1600 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 0.278 Å⁻¹

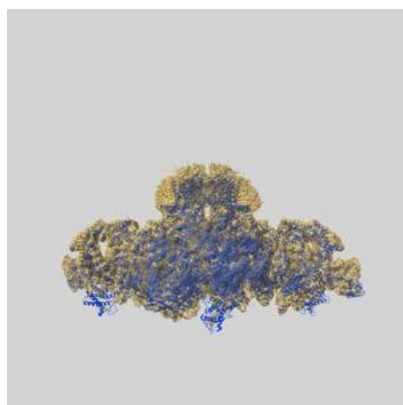
8 Fourier-Shell correlation

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

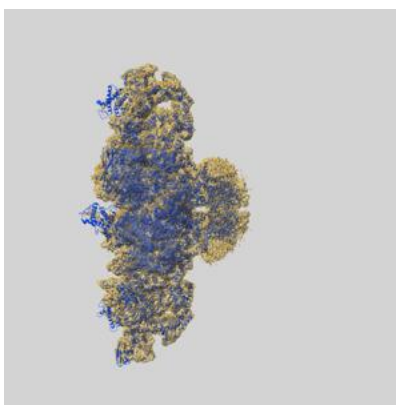
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52091 and PDB model 9HEQ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

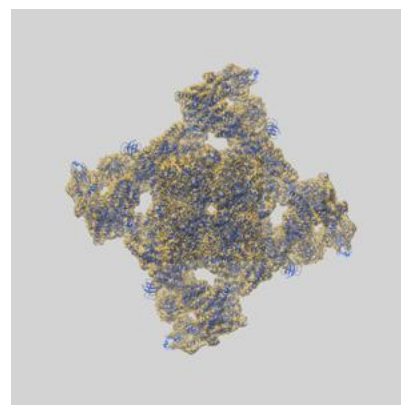
9.1 Map-model overlay [i](#)



X



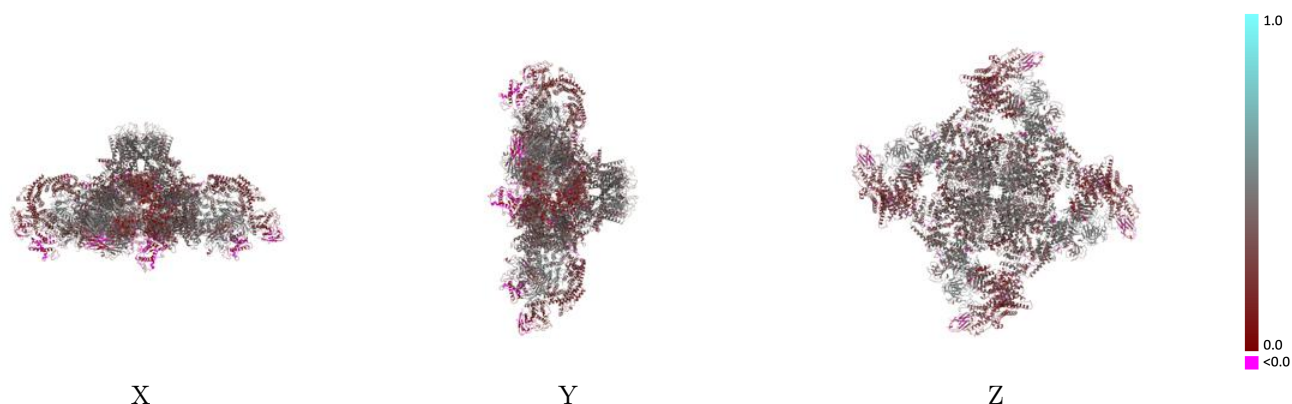
Y



Z

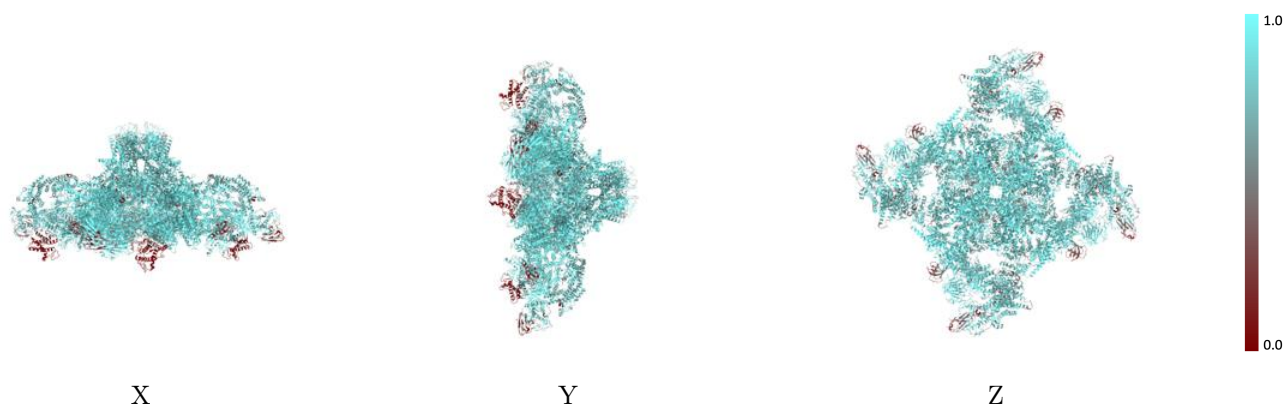
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



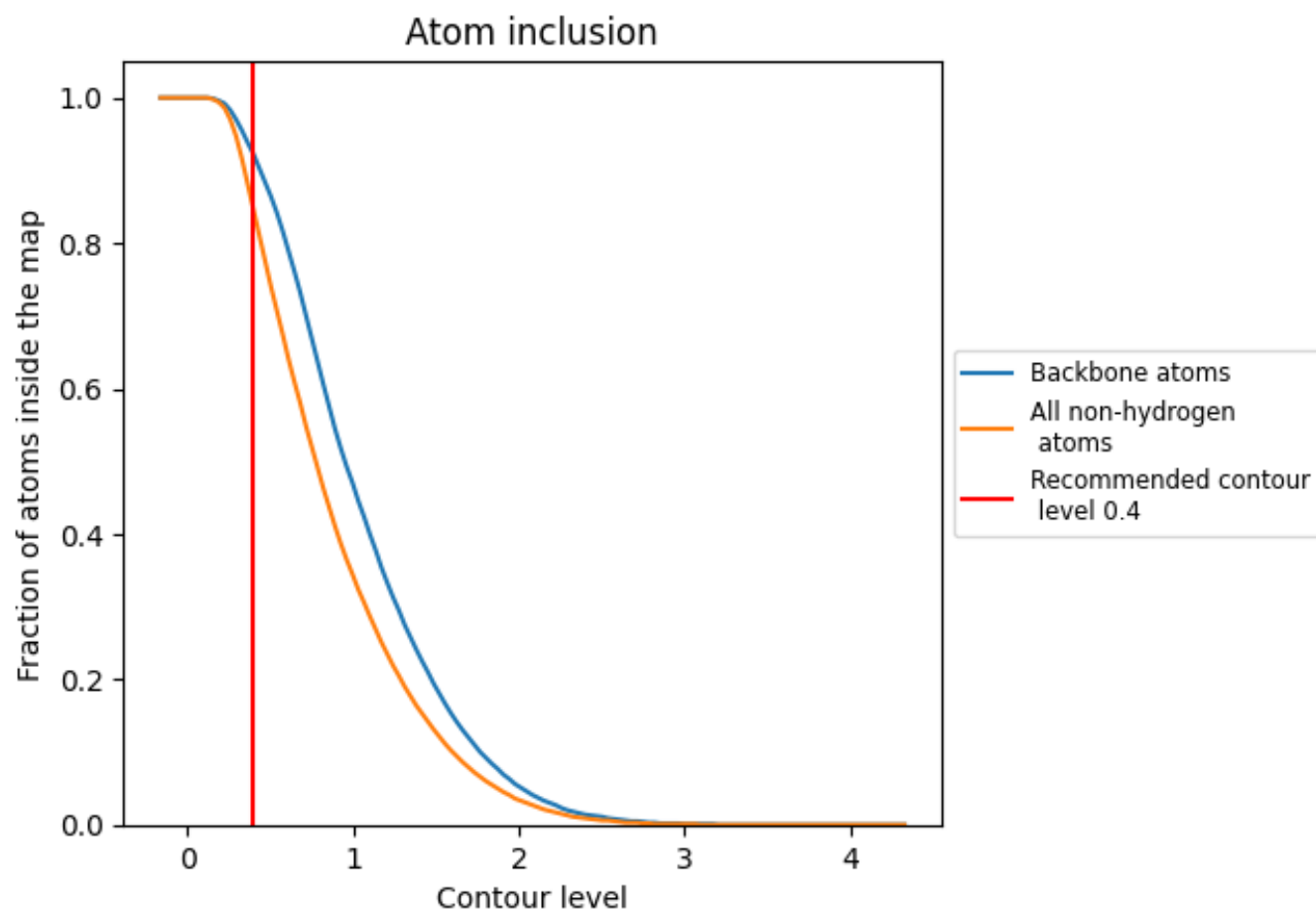
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8450	<div></div> 0.3410
A	<div></div> 0.8670	<div></div> 0.3470
B	<div></div> 0.4180	<div></div> 0.1050
C	<div></div> 0.8660	<div></div> 0.3460
D	<div></div> 0.4210	<div></div> 0.1080
E	<div></div> 0.3950	<div></div> 0.3530
F	<div></div> 0.4000	<div></div> 0.3520
G	<div></div> 0.8680	<div></div> 0.3470
H	<div></div> 0.4240	<div></div> 0.1080
I	<div></div> 0.4030	<div></div> 0.3580
J	<div></div> 0.8680	<div></div> 0.3470
K	<div></div> 0.4190	<div></div> 0.1100
L	<div></div> 0.3970	<div></div> 0.3560

