



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 07:04 PM UTC

PDB ID : 9R8O / pdb_00009r8o
EMDB ID : EMD-53834
Title : Primed-state RyR1 in 0.05% POPC micelles, in complex with a nanobody and FKBP
Authors : Li, C.; Efremov, R.G.
Deposited on : 2025-05-16
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:

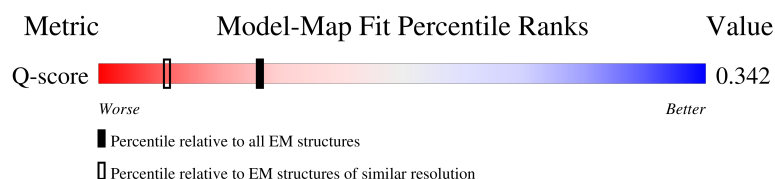
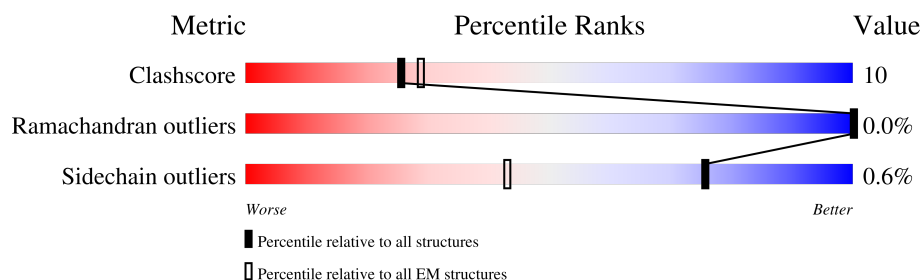
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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	A	126	
1	D	126	
1	G	126	
1	K	126	

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Mol	Chain	Length	Quality of chain
2	B	107	
2	E	107	
2	H	107	
2	L	107	
3	C	5027	
3	F	5027	
3	I	5027	
3	J	5027	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 145532 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	K	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
1	A	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	G	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	L	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	B	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	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

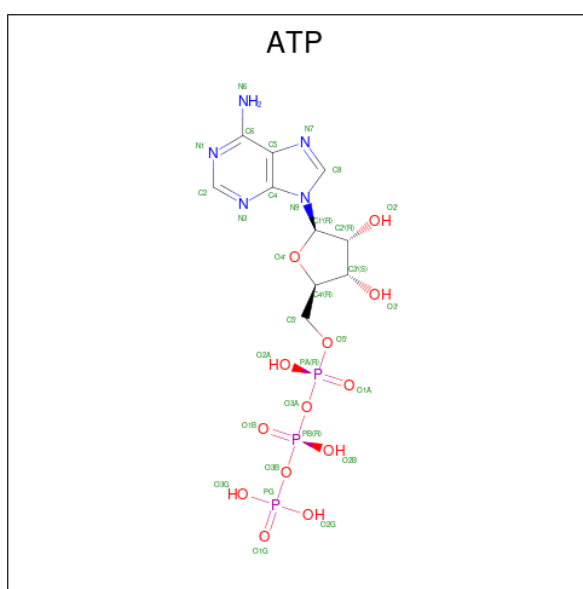
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	100	ASP	GLY	conflict	UNP Q8HYX6
B	100	ASP	GLY	conflict	UNP Q8HYX6
E	100	ASP	GLY	conflict	UNP Q8HYX6
H	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 3 is a protein called Ryanodine receptor 1.

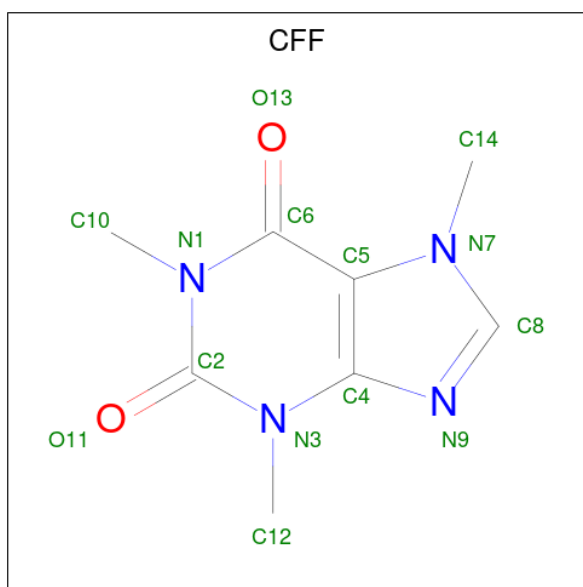
Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	4323	Total	C	N	O	S	0	0
			34214	21785	5897	6304	228		
3	C	4323	Total	C	N	O	S	0	0
			34214	21785	5897	6304	228		
3	F	4323	Total	C	N	O	S	0	0
			34214	21785	5897	6304	228		
3	I	4323	Total	C	N	O	S	0	0
			34214	21785	5897	6304	228		

- Molecule 4 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
4	J	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	I	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).

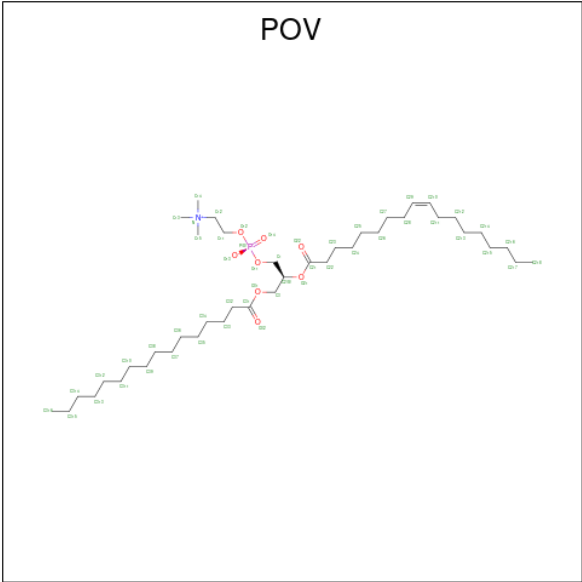


Mol	Chain	Residues	Atoms				AltConf
5	J	1	Total	C	N	O	0
			14	8	4	2	
5	C	1	Total	C	N	O	0
			14	8	4	2	
5	F	1	Total	C	N	O	0
			14	8	4	2	
5	I	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	J	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	
6	F	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	

- Molecule 7 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
7	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
7	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
7	J	1	Total	C	N	O	P	0
			26	16	1	8	1	
7	J	1	Total	C	N	O	P	0
			24	15	1	7	1	
7	J	1	Total	C	N	O	P	0
			34	24	1	8	1	
7	J	1	Total	C	N	O	P	0
			45	35	1	8	1	
7	J	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	J	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	J	1	Total	C				0
			13	13				
7	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	C	1	Total	C				0
			13	13				
7	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
7	C	1	Total	C	N	O	P	0
			44	34	1	8	1	
7	C	1	Total	C	N	O	P	0
			48	38	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total	C	N	O	P	0
			26	16	1	8	1	
7	C	1	Total	C	N	O	P	0
			24	15	1	7	1	
7	C	1	Total	C	N	O	P	0
			34	24	1	8	1	
7	C	1	Total	C	N	O	P	0
			48	38	1	8	1	
7	C	1	Total	C	N	O	P	0
			45	35	1	8	1	
7	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	F	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	F	1	Total	C				0
			13	13				
7	F	1	Total	C	N	O	P	0
			35	25	1	8	1	
7	F	1	Total	C	N	O	P	0
			44	34	1	8	1	
7	F	1	Total	C	N	O	P	0
			26	16	1	8	1	
7	F	1	Total	C	N	O	P	0
			24	15	1	7	1	
7	F	1	Total	C	N	O	P	0
			34	24	1	8	1	
7	F	1	Total	C	N	O	P	0
			48	38	1	8	1	
7	F	1	Total	C	N	O	P	0
			45	35	1	8	1	
7	F	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	I	1	Total	C	N	O	P	0
			48	38	1	8	1	
7	I	1	Total	C	N	O	P	0
			45	35	1	8	1	
7	I	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	I	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	I	1	Total	C				0
			13	13				

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Mol	Chain	Residues	Atoms					AltConf
7	I	1	Total	C	N	O	P	0
			35	25	1	8	1	
7	I	1	Total	C	N	O	P	0
			44	34	1	8	1	
7	I	1	Total	C	N	O	P	0
			26	16	1	8	1	
7	I	1	Total	C	N	O	P	0
			24	15	1	7	1	
7	I	1	Total	C	N	O	P	0
			34	24	1	8	1	

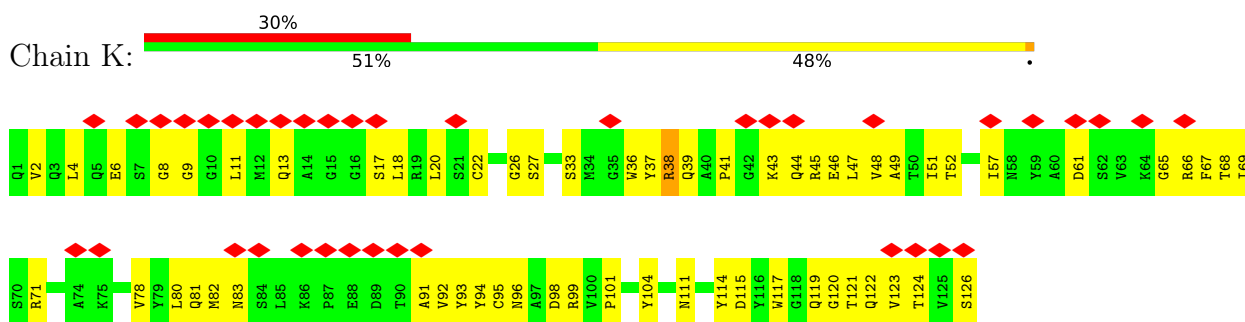
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	J	1	Total	Zn	0
			1	1	
8	C	1	Total	Zn	0
			1	1	
8	F	1	Total	Zn	0
			1	1	
8	I	1	Total	Zn	0
			1	1	

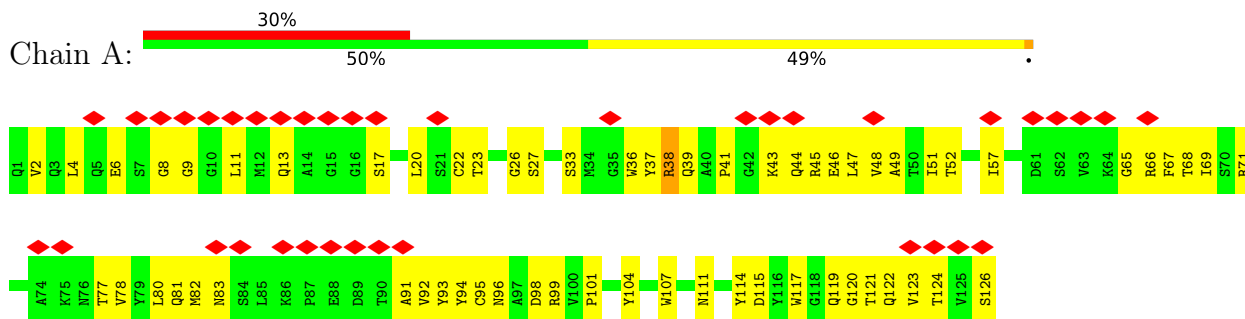
3 Residue-property plots [i](#)

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.

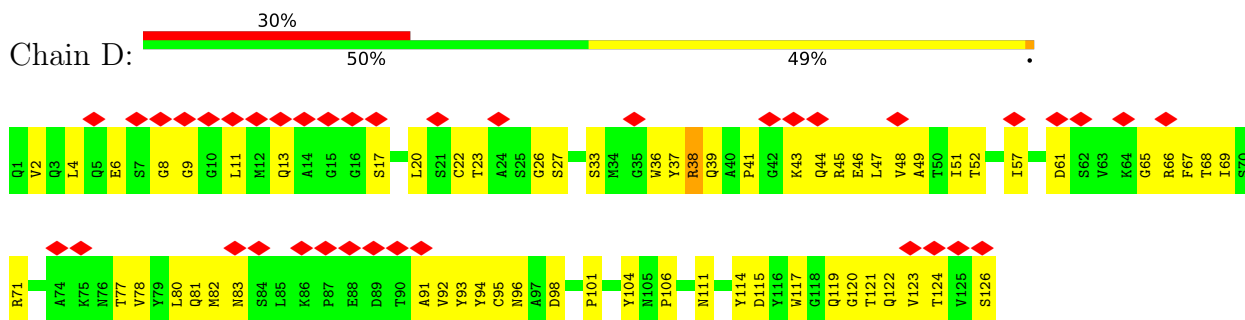
- Molecule 1: Nanobody 9657



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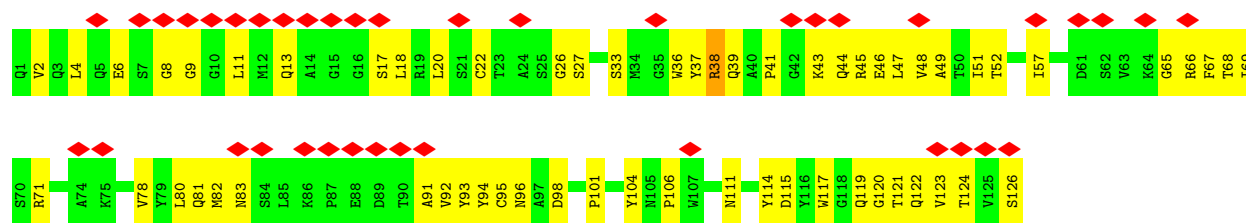


- Molecule 1: Nanobody 9657

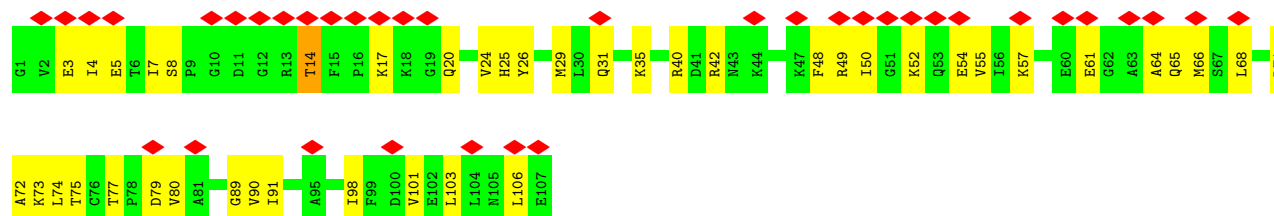


- Molecule 1: Nanobody 9657

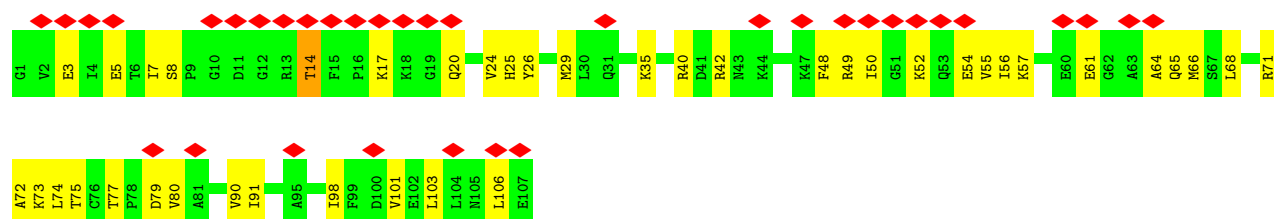




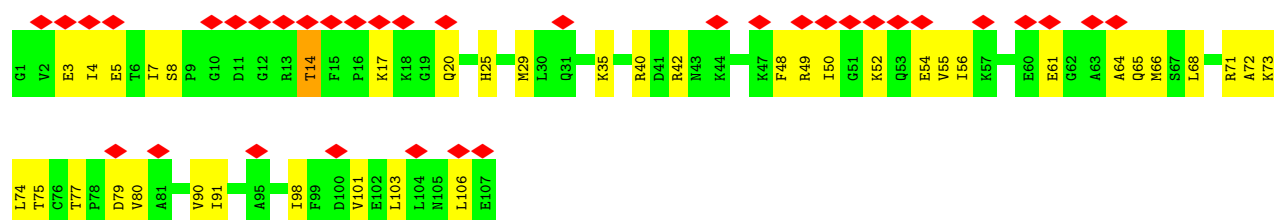
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



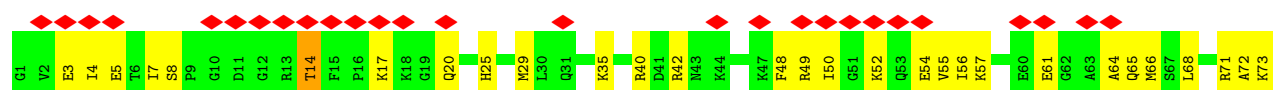
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

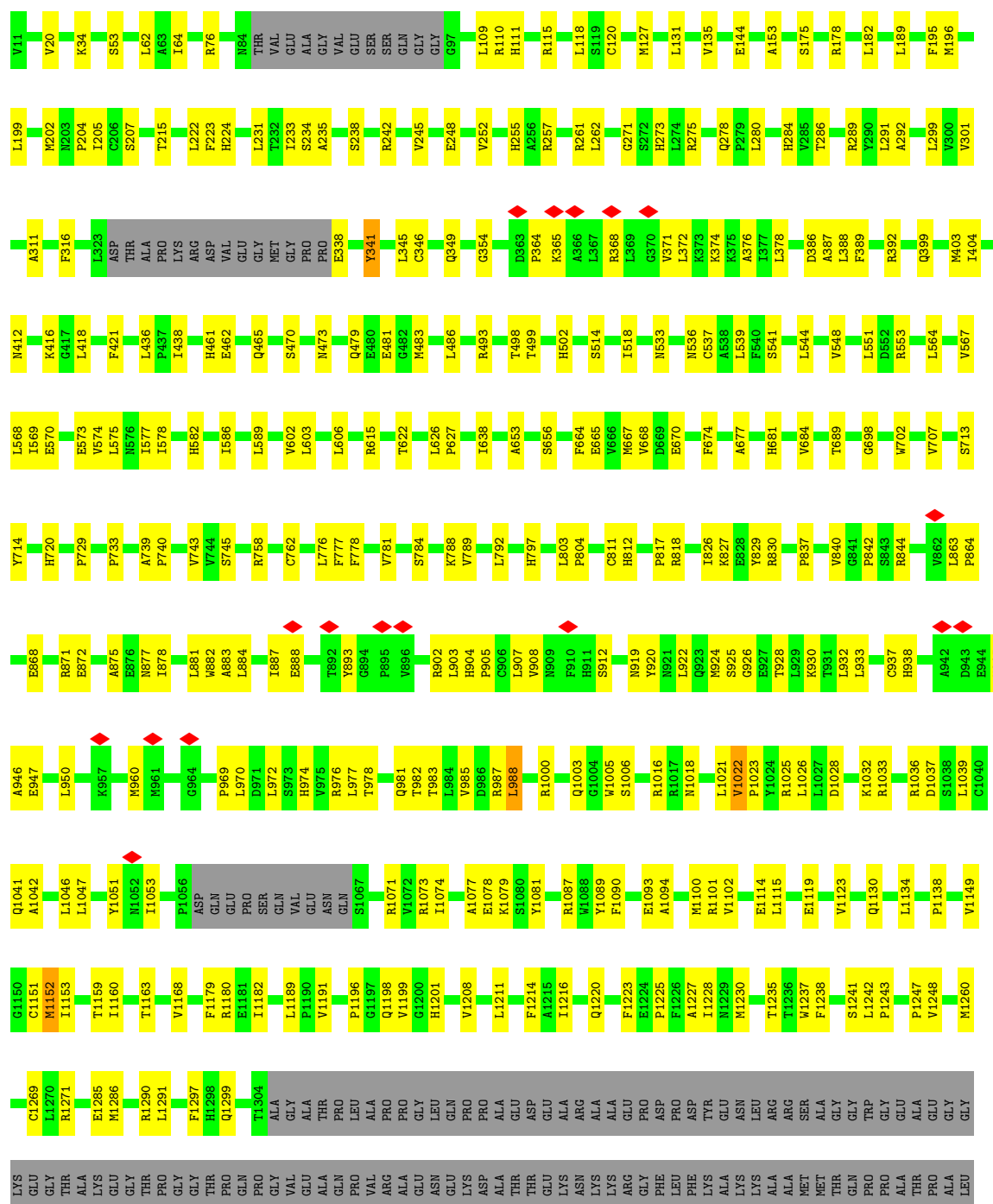


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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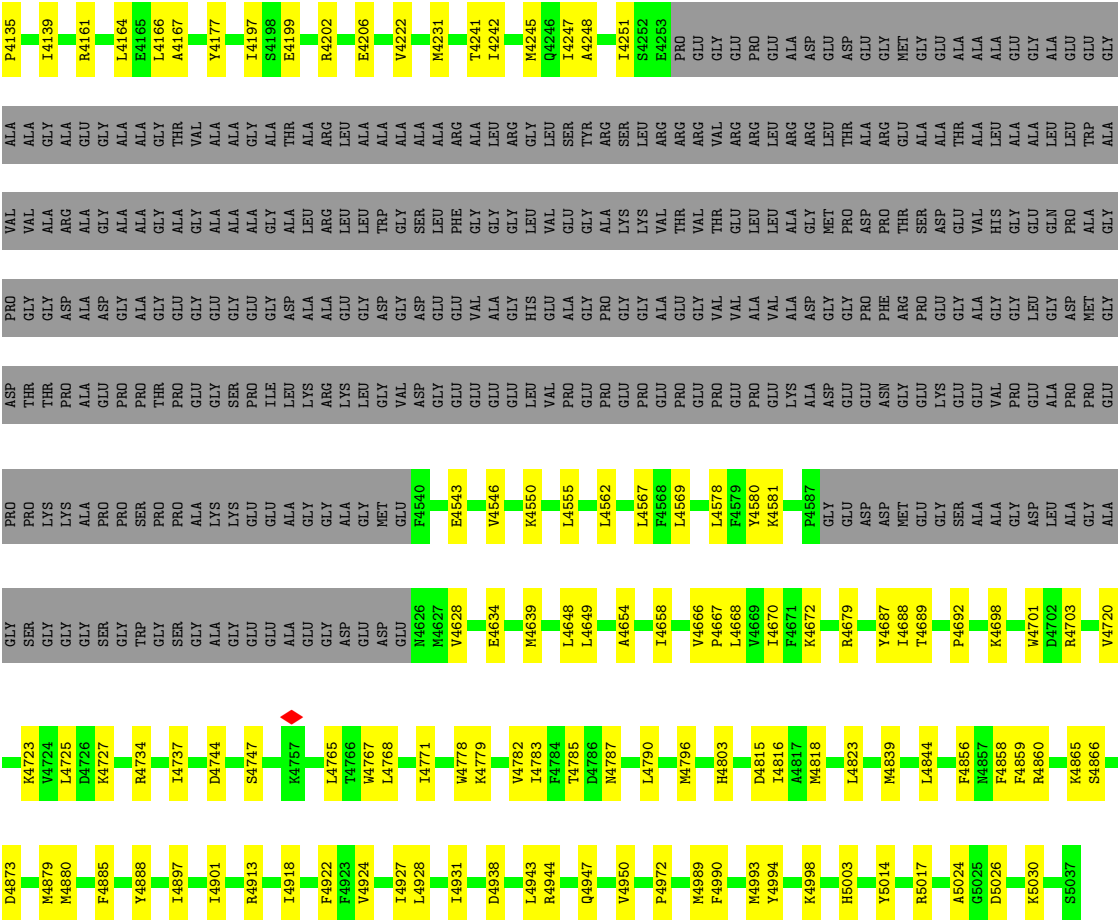


ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	Y2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	Q2864	V2865	T2866	L2867	S2868	P2869	E2870	L2871	Q2872	A2873	M2874	A2875	Q2876	Q2877	L2878	A2879	E2880	H2883	N2884	T2885	W2886	K2891	Q2892	E2893	L2894	E2895	A2896	L2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	V2905	V2906	P2907	Y2908	D2909
K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	P2797	S2798	E2799	K2800	D2801	K2802	E2803	I2804	Y2805	W2806	W2807	P2808	I2809	K2810	E2811	S2812	L2813	K2814	A2815	N2816	L2817	A2818	N2819	E2820	W2821	T2822	K2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLY	LYS	LYS	THR	LYS	ILE	SER	GLN	THR
R2624	R2625	L2626	V2627	F2628	D2629	V2630	A2637	K2638	M2639	P2640	L2641	K2642	L2643	L2644	T2645	N2646	K2647	Y2648	C2651	Y2654	Y2655	C2656	G2660	V2666	E2670	E2671	T2675	K2676	K2677	L2678	T2682	F2683	Y2696	K2697	M2698	M2700	P2701	C2702	L2703	I2706	L2710	P2711	P2712	K2722	ALA	GLU											
Q2525	F2526	L2527	R2531	A2534	S2535	L2536	M2546	A2547	L2559	P2560	L2561	T2562	T2563	K2564	C2565	E2573	H2574	A2575	I2577	M2578	V2579	D2580	S2581	M2582	L2583	R2588	T2596	Q2599	R2600	I2603	E2604	D2605	C2606	L2607	M2608	A2609	L2610	R2615	P2616	S2617	M2618	L2619	L2622	L2623													
PHE	GLY	GLU	PRO	PRO	GLU	GLU	I2414	L2418	G2419	H2420	A2421	I2422	M2423	L2424	L2429	I2430	D2431	T2453	R2454	R2458	S2459	L2460	D2465	L2466	V2467	G2468	I2469	S2470	L2472	P2473	D2482	G2483	K2489	M2490	S2491	A2492	S2501	Y2510	G2511	I2512	F2513	N2514	F2517	L2518	V2521	L2522											
R2248	M2250	L2257	L2285	Q2288	G2289	S2271	P2272	V2275	V2299	C2310	R2330	Y2331	L2332	V2346	N2349	R2355	R2359	K2360	P2361	R2369	G2372	I2380	E2381	I2384	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS																				
V2117	M2120	L2123	Q2127	Y2128	L2131	L2138	Y2142	P2146	L2156	E2157	C2158	L2162	L2166	E2175	M2178	L2179	L2182	Q2193	H2194	P2195	N2196	L2197	W2198	M2203	H2204	E2205	T2206	W2211	L2215	M2228	V2229	T2230	C2233	R2234	F2235	Y2238	I2242	S2243																			
H2041	Q2045	LEU	GLU	GLY	GLU	GLU	GLU	THR	SER	LEU	SER	LEU	ARG	ARG	SER	LEU	VAL	LYS	LYS	LYS	GLU	LYS	PRO	GLU	ALA	GLU	K2089	Q2095	E2096	L2097	V2098	M2101	V2102	W2103	R2104	S2113																					
D1690	Q1693	L1694	L1714	L1715	I1716	I1718	F1549	P1550	A1551	E1721	M1730	I1735	V1554	L1555	P1737	L1738	E1741	I1745	L1746	L1747	Q1598	M1599	L1600	M1601	P1602	V1603	F1782	V1783	A1784	A1785	L1786	P1787	ALA	ALA	GLY	VAL	VAL	E1793	I1802	P1803	L1804	R1808	L1815	L1819	R1680	V1681	E1885	V1839	P1840	G1525							
L1526	M1527	T1530	E1535	F1540	L1548	F1549	P1550	A1551	F1553	V1554	L1555	V1561	I1562	Q1563	F1564	L1595	Q1598	M1599	L1600	M1601	P1602	V1603	T1617	R1618	R1619	H1484	W1626	A1627	V1628	M1636	M1637	A1638	L1639	E1644	F1500	V1501	M1648	E1655	C1674	L1510	R1680	V1681	L1685	V1689													
PRO	ARG	PRO	HIS	ASP	VAL	VAL	PRO	ASP	Y1435	S1436	V1437	E1444	C1447	Q1448	V1449	M1462	N1463	F1464	R1470	A1471	P1472	T1475	M1476	V1483	H1484	S1485	S1486	N1491	M1494	G1497	G1498	D1499	V1500	V1501	Q1505	R1508	T1509	S1510	H1511	L1514	T1524	G1525															

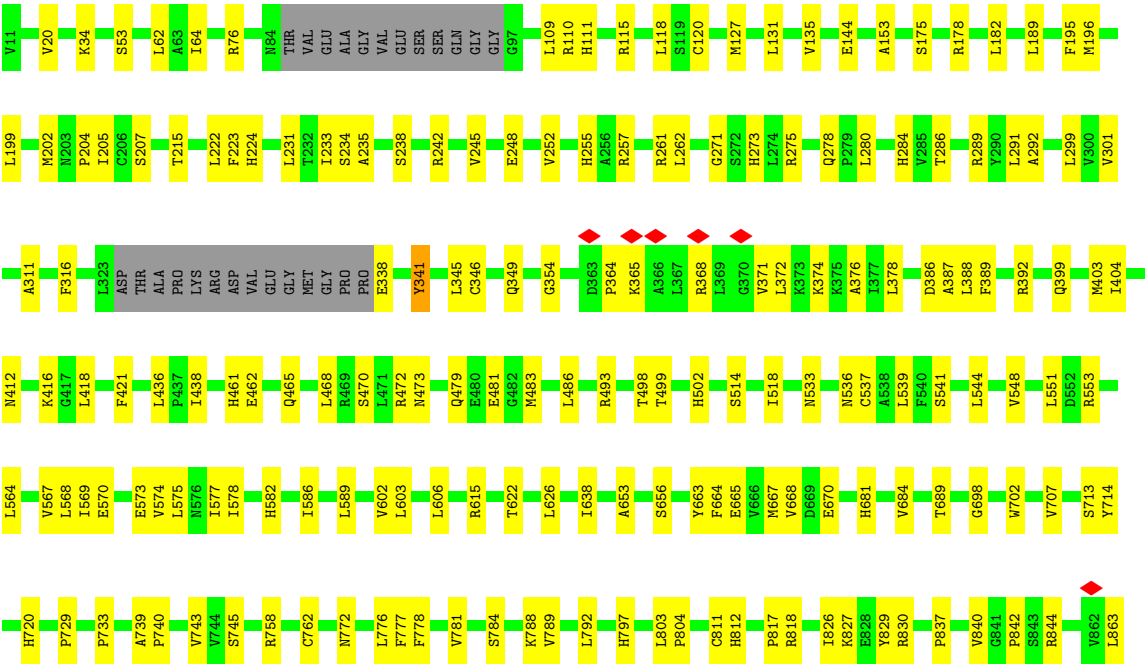


A2609	L2610	R2615	P2616	S2617	M2618	L2619	L2622	L2623	R2624	R2626	V2627	F2628	D2629	V2630	A2637	K2638	M2639	P2640	L2641	K2642	L2643	L2644	L2645	N2646	H2647	Y2648	C2651	Y2654	Y2655	C2656	G2660	V2666	E2670	E2671	T2675	R2676	K2677	L2678	L2682	F2683	Y2696	R2697	M2698	A2699	M2700	P2701	C2702																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G2511	L2512	E2513	N2514	F2517	L2518	V2521	L2522	G2525	F2526	L2527	R2531	A2534	S2535	L2536	M2546	S2547	L2559	F2560	L2561	L2562	T2563	K2564	C2565	L2568	F2569	E2573	H2574	R2575	A2576	L2577	M2578	V2579	D2580	S2581	N2582	L2583	R2588	T2596	Q2599	R2600	L2603	S2491	V2605	L2606	M2608																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
D2393	G2394	P2395	GLY	VAL	ARG	ARG	ARG	ARG	HIS	PHE	GLY	GLU	GLU	PRO	GLU	N2414	L2418	G2419	H2420	A2421	L2422	T2423	L2429	I2430	D2431	I2453	R2454	R2458	S2459	L2460	V2467	G2468	L2469	I2470	S2471	L2472	P2473	D2482	G2483	K2489	M2490	A2492	S2501	Y2510																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
V2229	T2230	C2233	R2234	F2235	Y2238	L2242	S2243	R2248	S2249	M2250	L2257	L2265	Q2268	G2269	S2270	T2271	P2272	V2275	L2276	E2285	V2289	C2310	M2324	P2325	R2330	T2331	L2332	V2346	N2349	R2355	R2359	K2360	P2361	R2369	G2372	T2380	E2381	L2384																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
E2025	R2028	L2031	Q2032	Q2036	D2037	H2041	Q2045	LEU	GLY	GLY	GLY	GLY	GLY	PRO	GLY	GLY	GLY	THR	SER	LEU	SER	SER	ARG	LEU	ARG	SER	LEU	LEU	GLY	THR	VAL	ARG	LEU	VAL	LYS	L2183	H2194	P2195	N2196	L2197	M2198	M2203	H2204	E2205	T2206	M2211	L2215	M2228																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
E1835	V1839	P1840	V1845	I1853	L1854	G1855	D1856	E1857	L1714	L1715	I1716	S1717	I1718	E1721	M1730	I1736	V1736	P1737	L1738	E1741	I1745	T1746	L1747	R1758	P1773	F1782	V1783	A1784	L1785	L1786	P1787	ALA	GLY	VAL	ALA	E1793	T1802	F1803	L1804	R1808	L1815																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
LYS	GLU	GLU	GLU	ALA	PRO	GLU	GLY	LYS	ASP	L1922	G1925	L1926	M1929	K1930	L1931	M1865	V1870	Q1938	M1939	L1943	E1944	L1958	A1959	A1960	R1964	Y1965	Q1970	R1974	L1979	L1980	M1981	R1982	E1990	P2001	P2002	Q2005	L2010	H2011	F2012	K2013	C2021																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
E1655	V1819	E1835	V1839	P1840	V1845	I1853	F1854	G1855	D1856	E1857	L1714	L1715	I1716	S1717	I1718	E1721	M1730	I1736	V1736	P1737	L1738	E1741	I1745	T1746	L1747	R1758	P1773	F1782	V1783	A1784	L1785	L1786	P1787	ALA	GLY	VAL	ALA	E1793	T1802	F1803	L1804	R1808	L1815																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
I1509	S1510	H1511	L1514	T1524	G1526	L1526	M1527	T1530	Q1693	L1694	L1714	L1715	I1716	S1717	I1718	E1721	M1730	I1736	V1736	P1737	L1738	E1741	I1745	T1746	L1747	R1758	P1773	F1782	V1783	A1784	L1785	L1786	P1787	ALA	GLY	VAL	ALA	E1793	T1802	F1803	L1804	R1808	L1815																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
ALA	THR	ALA	LEU	PRO	ARG	LEU	PRO	VAL	VAL	PRO	THR	GLY	THR	THR	PRO	GLN	PRO	GLY	VAL	GLY	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	

V9989	L3817	L3654	L3542	L3424	V3284	E3184	P3085	V2966	T2901	LYS	S2776	L2703
V9995	K3821	E3655	E3547	N3428	R3287	L3186	V3088	M2967	H2902	LYS	Y2777	L2706
F9996	A3834	S3656	V3549	E3432	A3295	R3187	V3089	D2968	P2903	THR	G2778	L2710
M4000	L3842	V3661	R3550	F3442	L3296	R3196	A3099	S2970	L2905	ARG	E2779	P2711
K4014	L3854	H3667	E3551	F3459	F3297	L3197	S3100	Q2971	V2906	LYS	N2780	P2712
L4017	E3854	S3668	F3552	V3464	A3298	A3198	E3101	F2972	P2907	ILE	N2781	
L4018	M3858	F3669	L3553	I3464	C3304	A3200	D3102	D2973	T2909	GLN	D2782	K2722
L4019	V3859	R3672	Q3560	I3470	E3304	M3201	E3104	L2977	D2909	THR	E2783	ALA
Q4020	N3860	Q3683	D3585	M3467	H3311	P3202	K3105	V2980	T2911	ALA	E2784	GLU
D4022	E3861	E3684	E3590	L3470	L3312	V3203	V3107	V2981	T2912	LYS	E2785	LYS
M4023	G3863	E3691	K3591	K3475	L3315	L3210	R3111	R2985	A2913	THR	K2786	ALA
M4026	T3864	E3687	E3592	S3475	L3316	Y3213	GLY	V2986	K2914	PRO	T2787	THR
M4034	V3865	V3690	I3592	S3475	L3320	N3214	LYS	E2987	E2915	ARG	H2788	ASP
G4038	I3866	K3694	V3593	S3475	I3329	S3217	SER	H2991	GLY	GLU	P2789	ALA
E4056	N3867	L3710	R3594	S3475	D3330	Y3219	VAL	E2987	A2917	GLY	M2790	GLY
M4057	M3875	D3719	V3596	S3475	I3332	K3222	GLN	E2987	D2918	GLY	L2791	W2734
I4058	F3885	M3723	F3604	S3475	A3336	E3226	LYS	E2987	R2919	GLY	R2792	F2735
L4059	Q3889	A3724	E3607	S3475	K3356	E3226	GLY	E2987	R2920	GLY	P2793	D2736
L4068	L3890	Y3725	F3612	S3475	A3359	I3229	VAL	E2987	E2921	GLY	Y2794	P2737
V4072	H3895	Y3725	T3612	S3475	V3340	L3232	GLY	E2987	K2922	GLY	K2795	R2738
V4081	Q3900	M3729	LYS	S3475	A3342	L3232	GLY	E2987	Q2924	GLY	F2797	V2740
V4087	I3916	A3730	LYS	S3475	Q3343	V3236	GLY	E2987	E2925	GLY	S2798	E2741
L4088	T3919	H3734	ALA	S3475	P3344	V3236	GLY	E2987	L2926	GLY	E2799	T2742
S4089	S3929	E3740	TRP	S3475	I3345	M3239	GLY	E2987	K2928	GLY	K2800	L2743
K4090	I3930	ASN	LYS	S3475	V3244	P3244	GLY	E2987	E2932	GLY	D2801	N2744
M4096	Y3936	GLY	LEU	S3475	V3245	V3245	GLY	E2987	M2932	GLY	K2802	V2745
M4097	Y3936	GLY	LEU	S3475	L3249	L3249	GLY	E2987	Q2931	GLY	E2803	I2746
Q4100	Q3945	GLY	LEU	S3475	M3250	M3250	GLY	E2987	Y2935	GLY	I2804	I2747
T4104	F3951	GLY	LEU	S3475	I3253	I3253	GLY	E2987	A2936	GLY	Y2805	P2748
G4105	M3955	GLY	LEU	S3475	R3262	Y3263	GLY	E2987	E2934	GLY	R2806	E2749
I4108	N3955	R3762	ALA	S3475	T3264	T3264	GLY	E2987	G2934	GLY	W2807	K2750
Q4109	Q3960	S3768	VAL	S3475	P3267	H3268	GLY	E2987	Y2936	GLY	P2808	L2751
F4110	L3965	R3769	ALA	S3475	H3268	V3269	GLY	E2987	A2937	GLY	I2809	D2752
L4111	T3966	L3770	CYS	S3475	V3269	I3270	GLY	E2987	T2938	GLY	K2810	S2753
L4112	E3967	H3771	PHE	S3475	G3390	I3270	GLY	E2987	R2939	GLY	E2811	F2754
D4118	Y3968	H3771	ARG	S3475	E3391	L3175	GLY	E2987	GLY	GLY	S2812	I2755
Y4118	I3969	G3788	MET	S3475	V3394	L3175	GLY	E2987	L2946	GLY	L2813	I2756
M4122	Q3970	E3788	T3639	S3475	R3395	L3274	GLY	E2987	D2947	GLY	A2814	K2757
A4129	N3976	M3793	Y3642	S3475	R3395	L3277	GLY	E2987	E2952	GLY	A2815	F2758
	L3980	I3804	C3650	S3475	V3400	L3281	GLY	E2987	F2957	GLY	M2816	A2759
		L3805		S3475	A3407		GLY	E2987		GLY	I2817	E2760
				S3475			GLY	E2987		GLY	W2819	E2764
				S3475			GLY	E2987		GLY	E2820	K2765
				S3475			GLY	E2987		GLY	W2821	W2766
				S3475			GLY	E2987		GLY	L2823	A2767
				S3475			GLY	E2987		GLY	E2824	F2768
				S3475			GLY	E2987		GLY	K2825	K2770
				S3475			GLY	E2987		GLY	I2771	I2772
				S3475			GLY	E2987		GLY	R2827	W2773
				S3475			GLY	E2987		GLY	E2828	N2774
				S3475			GLY	E2987		GLY	G2829	W2775
				S3475			GLY	E2987		GLY	E2830	
				S3475			GLY	E2987		GLY	GLU	
				S3475			GLY	E2987		GLY	ARG	
				S3475			GLY	E2987		GLY	THR	
				S3475			GLY	E2987		GLY	GLU	



● Molecule 3: Ryanodine receptor 1













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	4.014	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.066	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	479.136, 479.136, 479.136	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.426, 1.426, 1.426	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, CA, CFF, POV, 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	0.26	0/987	0.66	1/1340 (0.1%)
1	D	0.26	0/987	0.66	1/1340 (0.1%)
1	G	0.26	0/987	0.66	1/1340 (0.1%)
1	K	0.26	0/987	0.66	1/1340 (0.1%)
2	B	0.22	0/834	0.62	0/1123
2	E	0.22	0/834	0.62	0/1123
2	H	0.22	0/834	0.62	0/1123
2	L	0.22	0/834	0.62	0/1123
3	C	0.15	0/34990	0.39	1/47426 (0.0%)
3	F	0.15	0/34990	0.39	1/47426 (0.0%)
3	I	0.15	0/34990	0.39	1/47426 (0.0%)
3	J	0.15	0/34990	0.39	1/47426 (0.0%)
All	All	0.16	0/147244	0.41	8/199556 (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	A	0	1
1	D	0	1
1	G	0	1
1	K	0	1
All	All	0	4

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(°)
1	G	48	VAL	N-CA-C	-5.94	103.50	110.21
1	D	48	VAL	N-CA-C	-5.92	103.52	110.21
1	A	48	VAL	N-CA-C	-5.90	103.54	110.21
1	K	48	VAL	N-CA-C	-5.89	103.55	110.21
3	J	4122	MET	CB-CG-SD	5.57	129.41	112.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	LYS	Peptide
1	D	43	LYS	Peptide
1	G	43	LYS	Peptide
1	K	43	LYS	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	A	967	0	916	41	0
1	D	967	0	916	40	0
1	G	967	0	916	41	0
1	K	967	0	916	43	0
2	B	818	0	824	25	0
2	E	818	0	824	24	0
2	H	818	0	824	25	0
2	L	818	0	824	29	0
3	C	34214	0	33622	691	0
3	F	34214	0	33622	683	0
3	I	34214	0	33622	680	0
3	J	34214	0	33622	687	0
4	C	31	0	12	0	0
4	F	31	0	12	0	0
4	I	31	0	12	0	0
4	J	31	0	12	0	0
5	C	14	0	10	0	0
5	F	14	0	10	0	0
5	I	14	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	14	0	10	0	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	C	385	0	508	24	0
7	F	337	0	437	22	0
7	I	337	0	437	21	0
7	J	289	0	366	18	0
8	C	1	0	0	0	0
8	F	1	0	0	0	0
8	I	1	0	0	0	0
8	J	1	0	0	0	0
All	All	145532	0	143284	2972	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 2972 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:F:2759:ALA:HB1	3:F:2806:ARG:HB2	1.57	0.86
3:J:2759:ALA:HB1	3:J:2806:ARG:HB2	1.57	0.85
3:I:2759:ALA:HB1	3:I:2806:ARG:HB2	1.57	0.84
3:C:2759:ALA:HB1	3:C:2806:ARG:HB2	1.57	0.84
3:F:3036:LYS:HD3	3:F:3076:ASP:HB3	1.62	0.82

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	124/126 (98%)	111 (90%)	11 (9%)	2 (2%)	7	31
1	D	124/126 (98%)	111 (90%)	11 (9%)	2 (2%)	7	31
1	G	124/126 (98%)	111 (90%)	11 (9%)	2 (2%)	7	31
1	K	124/126 (98%)	111 (90%)	11 (9%)	2 (2%)	7	31
2	B	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
2	E	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
2	H	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
2	L	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
3	C	4287/5027 (85%)	4191 (98%)	96 (2%)	0	100	100
3	F	4287/5027 (85%)	4190 (98%)	97 (2%)	0	100	100
3	I	4287/5027 (85%)	4190 (98%)	97 (2%)	0	100	100
3	J	4287/5027 (85%)	4190 (98%)	97 (2%)	0	100	100
All	All	18064/21040 (86%)	17605 (98%)	451 (2%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	49	ALA
1	A	49	ALA
1	D	49	ALA
1	G	49	ALA
1	K	44	GLN

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	104/104 (100%)	103 (99%)	1 (1%)	68	76
1	D	104/104 (100%)	102 (98%)	2 (2%)	50	68
1	G	104/104 (100%)	103 (99%)	1 (1%)	68	76
1	K	104/104 (100%)	102 (98%)	2 (2%)	50	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	88/88 (100%)	86 (98%)	2 (2%)	44	66
2	E	88/88 (100%)	86 (98%)	2 (2%)	44	66
2	H	88/88 (100%)	86 (98%)	2 (2%)	44	66
2	L	88/88 (100%)	86 (98%)	2 (2%)	44	66
3	C	3690/4270 (86%)	3670 (100%)	20 (0%)	81	83
3	F	3690/4270 (86%)	3671 (100%)	19 (0%)	81	83
3	I	3690/4270 (86%)	3672 (100%)	18 (0%)	81	83
3	J	3690/4270 (86%)	3671 (100%)	19 (0%)	81	83
All	All	15528/17848 (87%)	15438 (99%)	90 (1%)	76	81

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	2211	MET
2	H	80	VAL
3	F	2577	ILE
3	F	3734	HIS
3	I	1022	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 151 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	138	GLN
3	I	3927	GLN
3	I	495	ASN
3	I	1590	GLN
3	I	5031	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
7	POV	C	5109	-	25,25,51	0.80	1 (4%)	29,32,59	0.66	0
7	POV	C	5106	-	34,34,51	0.58	0	40,42,59	0.61	0
7	POV	F	5108	-	25,25,51	0.80	1 (4%)	29,32,59	0.66	0
7	POV	F	5114	-	31,31,51	0.62	0	37,39,59	0.57	0
7	POV	F	5101	-	35,35,51	0.59	0	41,43,59	0.51	0
7	POV	J	5111	-	31,31,51	0.62	0	37,39,59	0.57	0
7	POV	I	5103	-	31,31,51	0.62	0	37,39,59	0.57	0
5	CFF	J	5102	-	15,15,15	0.51	0	23,23,23	0.72	1 (4%)
4	ATP	F	5103	-	32,33,33	0.28	0	48,52,52	0.39	0
7	POV	F	5109	-	23,23,51	0.66	0	28,30,59	0.65	0
7	POV	I	5102	-	44,44,51	0.53	0	50,52,59	0.50	0
7	POV	C	5111	-	33,33,51	0.60	0	39,41,59	0.53	0
7	POV	C	5115	-	31,31,51	0.62	0	37,39,59	0.57	0
7	POV	I	5105	-	12,12,51	0.23	0	11,11,59	0.25	0
7	POV	J	5106	-	25,25,51	0.80	1 (4%)	29,32,59	0.66	0
7	POV	I	5110	-	43,43,51	0.54	0	49,51,59	0.50	0
7	POV	C	5107	-	43,43,51	0.54	0	49,51,59	0.50	0
7	POV	C	5113	-	47,47,51	0.52	0	53,55,59	0.49	0
5	CFF	I	5107	-	15,15,15	0.51	0	23,23,23	0.72	1 (4%)
7	POV	C	5114	-	44,44,51	0.53	0	50,52,59	0.50	0
7	POV	J	5110	-	44,44,51	0.53	0	50,52,59	0.50	0
7	POV	J	5108	-	33,33,51	0.60	0	39,41,59	0.53	0
7	POV	I	5109	-	34,34,51	0.58	0	40,42,59	0.61	0
7	POV	C	5110	-	23,23,51	0.66	0	28,30,59	0.65	0
5	CFF	C	5104	-	15,15,15	0.51	0	23,23,23	0.72	1 (4%)
7	POV	C	5108	-	47,47,51	0.52	0	53,55,59	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	POV	I	5111	-	25,25,51	0.80	1 (4%)	29,32,59	0.66	0
7	POV	F	5102	-	12,12,51	0.23	0	11,11,59	0.25	0
4	ATP	I	5106	-	32,33,33	0.28	0	48,52,52	0.39	0
7	POV	F	5106	-	34,34,51	0.58	0	40,42,59	0.61	0
7	POV	F	5107	-	43,43,51	0.54	0	49,51,59	0.50	0
7	POV	C	5102	-	12,12,51	0.23	0	11,11,59	0.25	0
7	POV	J	5105	-	43,43,51	0.54	0	49,51,59	0.50	0
7	POV	I	5112	-	23,23,51	0.66	0	28,30,59	0.65	0
7	POV	J	5112	-	35,35,51	0.59	0	41,43,59	0.51	0
7	POV	I	5101	-	47,47,51	0.52	0	53,55,59	0.49	0
7	POV	J	5113	-	12,12,51	0.23	0	11,11,59	0.25	0
7	POV	J	5107	-	23,23,51	0.66	0	28,30,59	0.65	0
5	CFF	F	5104	-	15,15,15	0.51	0	23,23,23	0.72	1 (4%)
7	POV	C	5101	-	35,35,51	0.59	0	41,43,59	0.51	0
4	ATP	C	5103	-	32,33,33	0.28	0	48,52,52	0.39	0
7	POV	J	5104	-	34,34,51	0.58	0	40,42,59	0.61	0
7	POV	F	5110	-	33,33,51	0.60	0	39,41,59	0.54	0
7	POV	F	5112	-	47,47,51	0.52	0	53,55,59	0.49	0
7	POV	I	5113	-	33,33,51	0.60	0	39,41,59	0.54	0
4	ATP	J	5101	-	32,33,33	0.28	0	48,52,52	0.39	0
7	POV	I	5104	-	35,35,51	0.59	0	41,43,59	0.51	0
7	POV	F	5113	-	44,44,51	0.53	0	50,52,59	0.50	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
7	POV	C	5109	-	-	10/28/28/55	-
7	POV	C	5106	-	-	10/38/38/55	-
7	POV	F	5108	-	-	10/28/28/55	-
7	POV	F	5114	-	-	9/35/35/55	-
7	POV	F	5101	-	-	13/39/39/55	-
7	POV	J	5111	-	-	9/35/35/55	-
7	POV	I	5103	-	-	9/35/35/55	-
4	ATP	F	5103	-	-	2/22/38/38	0/3/3/3
5	CFF	J	5102	-	-	-	0/2/2/2
7	POV	F	5109	-	-	2/26/26/55	-
7	POV	I	5102	-	-	11/48/48/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	POV	C	5111	-	-	8/37/37/55	-
7	POV	C	5115	-	-	9/35/35/55	-
7	POV	I	5105	-	-	0/10/10/55	-
7	POV	J	5106	-	-	10/28/28/55	-
7	POV	I	5110	-	-	12/47/47/55	-
7	POV	C	5107	-	-	12/47/47/55	-
7	POV	C	5113	-	-	13/51/51/55	-
5	CFF	I	5107	-	-	-	0/2/2/2
7	POV	C	5114	-	-	11/48/48/55	-
7	POV	J	5110	-	-	11/48/48/55	-
7	POV	J	5108	-	-	8/37/37/55	-
7	POV	I	5109	-	-	10/38/38/55	-
7	POV	C	5110	-	-	2/26/26/55	-
7	POV	I	5111	-	-	10/28/28/55	-
7	POV	C	5108	-	-	13/51/51/55	-
5	CFF	C	5104	-	-	-	0/2/2/2
7	POV	F	5102	-	-	0/10/10/55	-
4	ATP	I	5106	-	-	2/22/38/38	0/3/3/3
7	POV	F	5106	-	-	10/38/38/55	-
7	POV	F	5107	-	-	12/47/47/55	-
7	POV	C	5102	-	-	0/10/10/55	-
7	POV	J	5105	-	-	12/47/47/55	-
7	POV	I	5112	-	-	2/26/26/55	-
7	POV	J	5112	-	-	13/39/39/55	-
7	POV	I	5101	-	-	13/51/51/55	-
7	POV	J	5113	-	-	0/10/10/55	-
7	POV	J	5107	-	-	2/26/26/55	-
7	POV	C	5101	-	-	13/39/39/55	-
5	CFF	F	5104	-	-	-	0/2/2/2
4	ATP	C	5103	-	-	2/22/38/38	0/3/3/3
7	POV	J	5104	-	-	10/38/38/55	-
7	POV	F	5110	-	-	8/37/37/55	-
7	POV	F	5112	-	-	13/51/51/55	-
7	POV	I	5113	-	-	8/37/37/55	-
4	ATP	J	5101	-	-	2/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	POV	I	5104	-	-	13/39/39/55	-
7	POV	F	5113	-	-	11/48/48/55	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	5109	POV	O21-C2	-2.55	1.43	1.46
7	J	5106	POV	O21-C2	-2.54	1.43	1.46
7	F	5108	POV	O21-C2	-2.54	1.43	1.46
7	I	5111	POV	O21-C2	-2.54	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	5102	CFF	C12-N3-C2	2.25	121.25	117.33
5	C	5104	CFF	C12-N3-C2	2.25	121.25	117.33
5	I	5107	CFF	C12-N3-C2	2.25	121.25	117.33
5	F	5104	CFF	C12-N3-C2	2.25	121.25	117.33

There are no chirality outliers.

5 of 360 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	5104	POV	C11-O12-P-O11
7	J	5104	POV	C11-O12-P-O13
7	J	5104	POV	C11-O12-P-O14
7	J	5104	POV	O12-C11-C12-N
7	J	5105	POV	C1-O11-P-O14

There are no ring outliers.

39 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	5109	POV	2	0
7	C	5106	POV	2	0
7	F	5108	POV	2	0
7	F	5114	POV	1	0
7	F	5101	POV	3	0
7	J	5111	POV	1	0
7	F	5109	POV	3	0

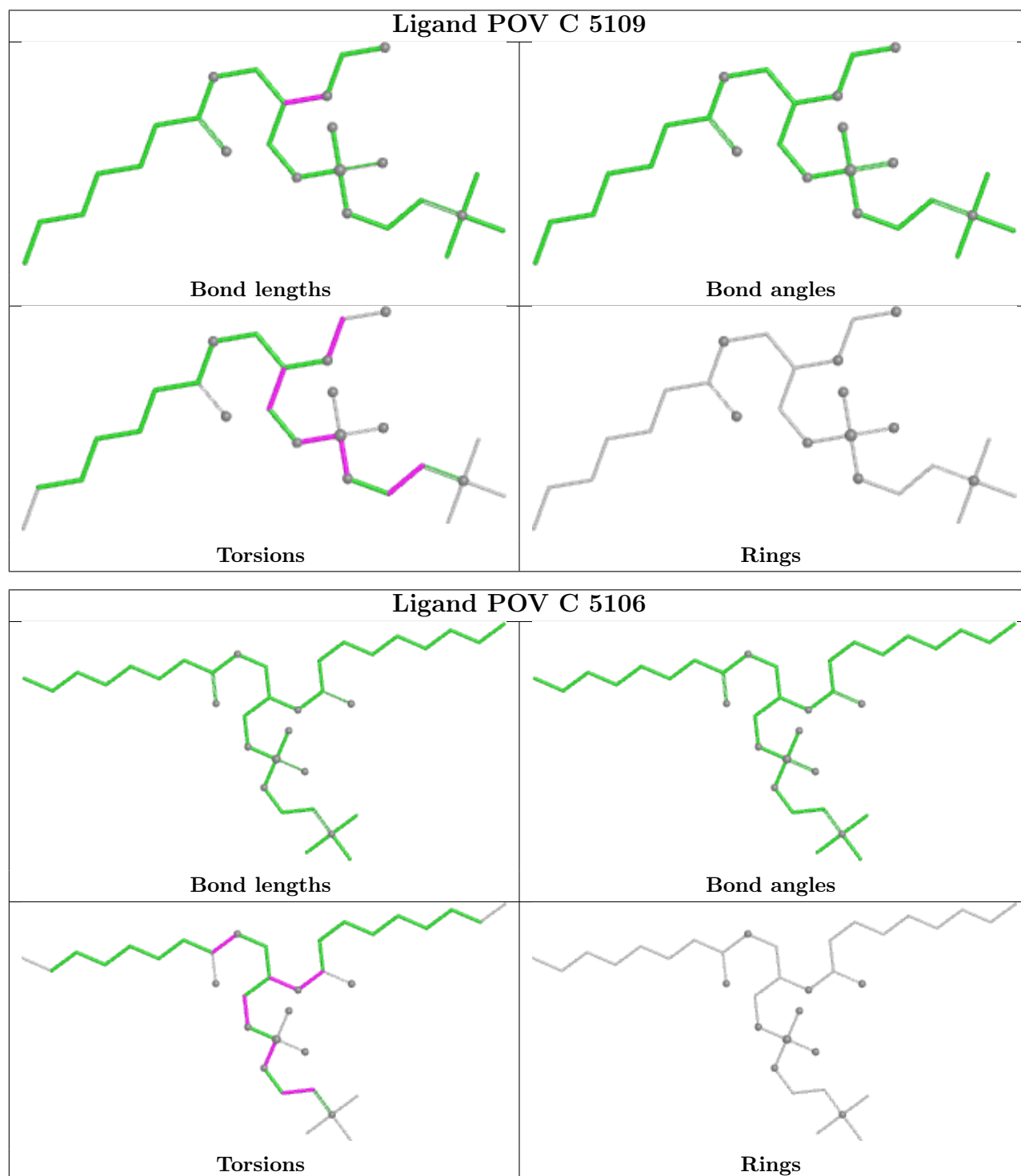
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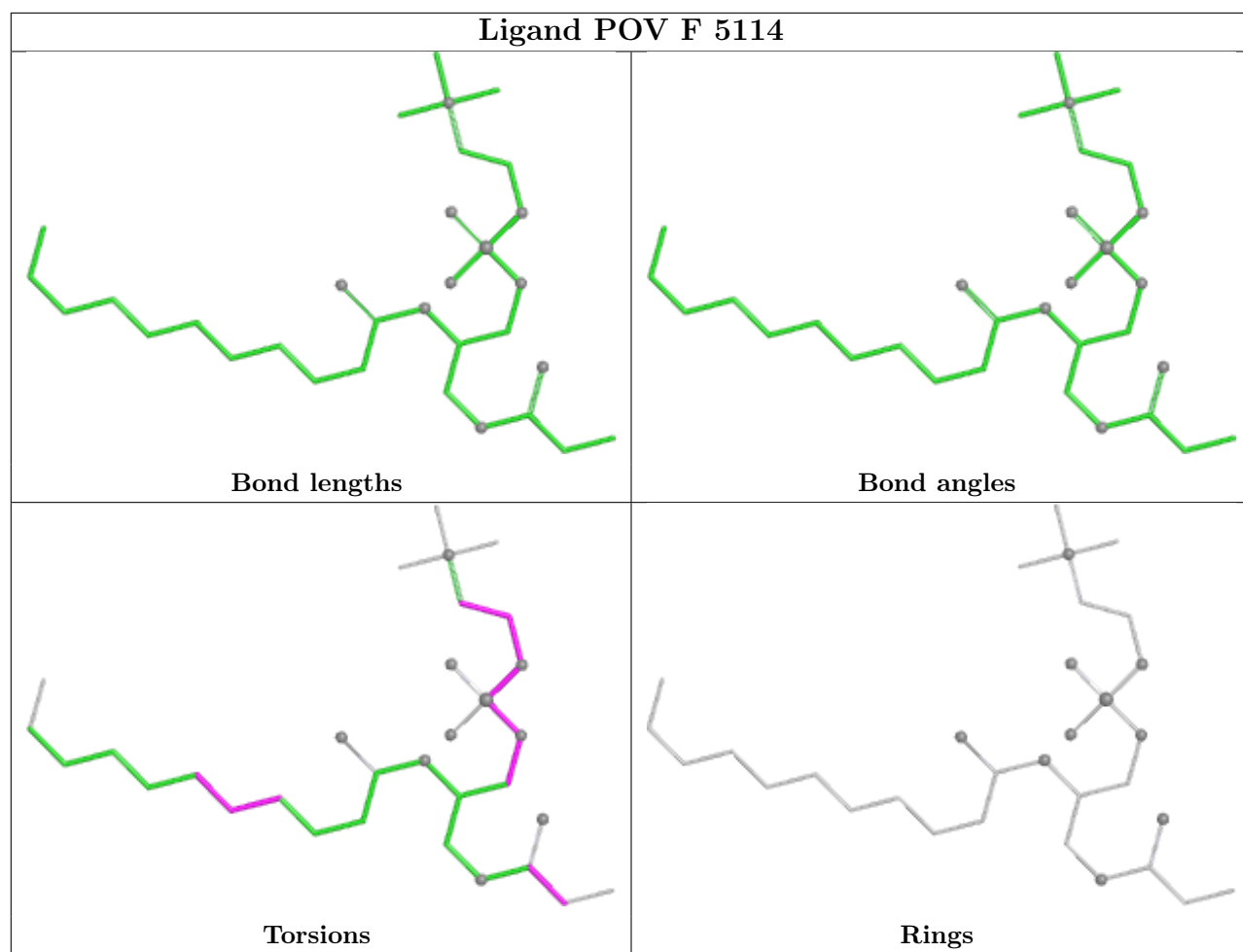
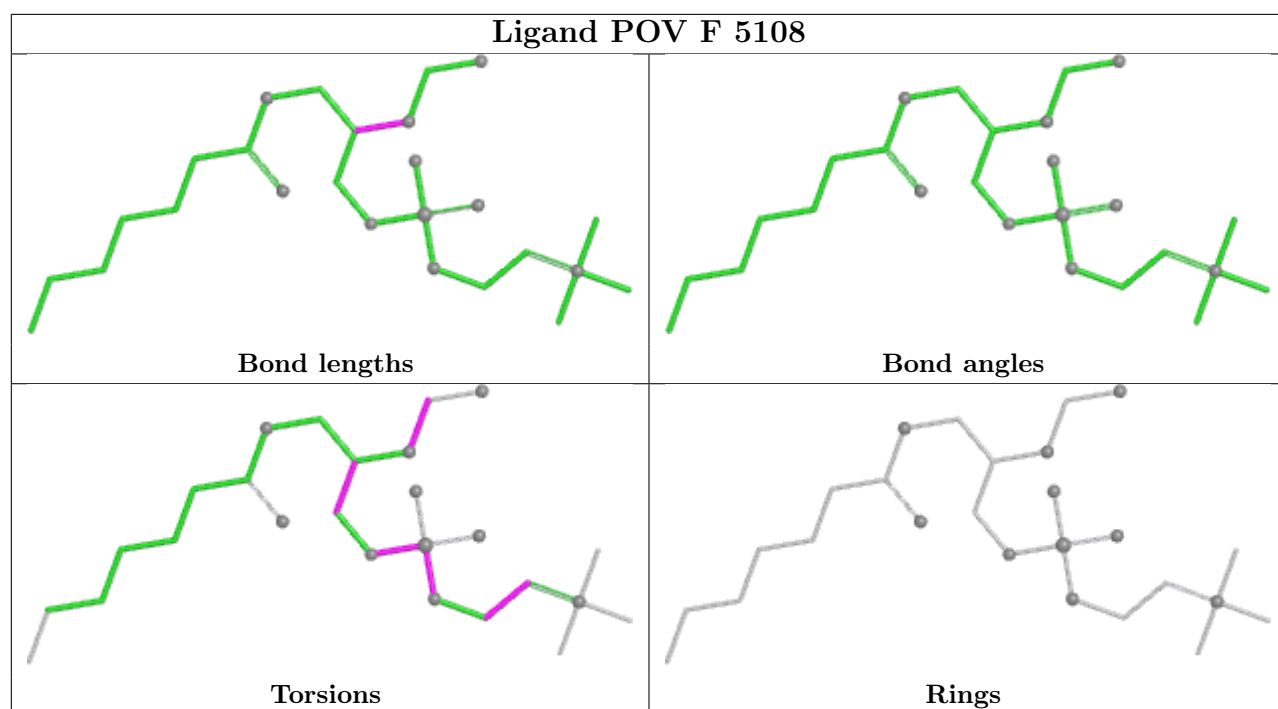
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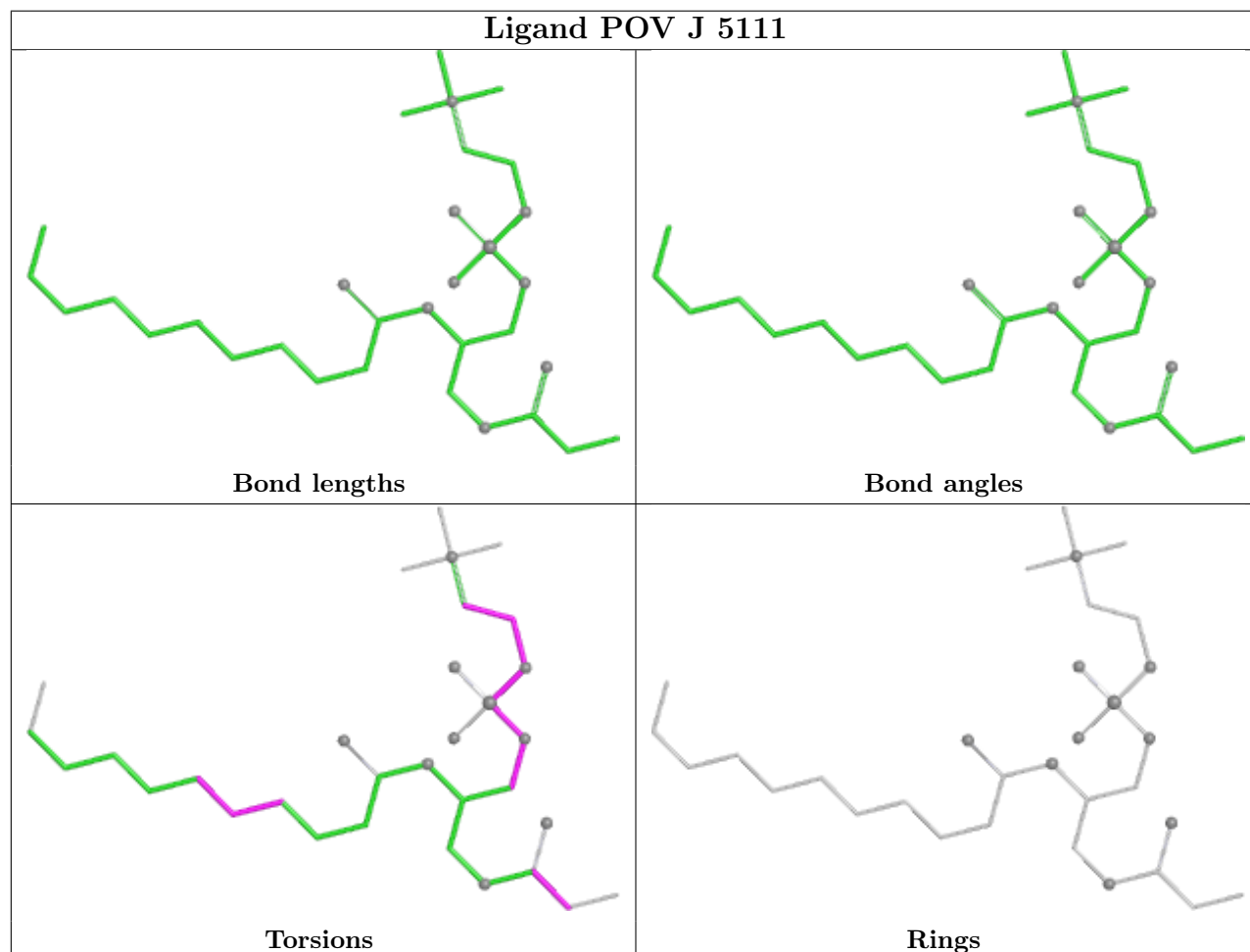
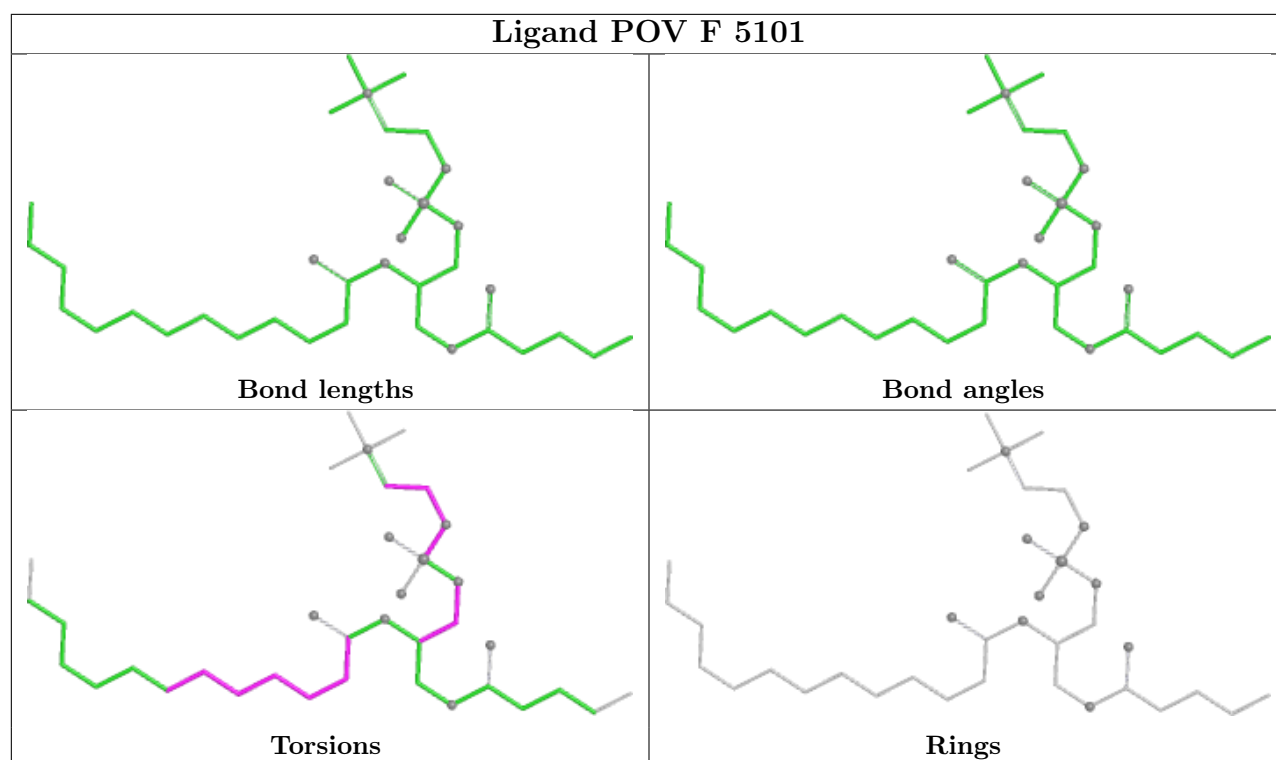
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	5102	POV	2	0
7	C	5111	POV	4	0
7	C	5115	POV	1	0
7	I	5105	POV	1	0
7	J	5106	POV	2	0
7	I	5110	POV	4	0
7	C	5107	POV	4	0
7	C	5113	POV	3	0
7	C	5114	POV	2	0
7	J	5110	POV	2	0
7	J	5108	POV	4	0
7	I	5109	POV	2	0
7	C	5110	POV	3	0
7	C	5108	POV	3	0
7	I	5111	POV	2	0
7	F	5102	POV	1	0
7	F	5106	POV	1	0
7	F	5107	POV	4	0
7	C	5102	POV	1	0
7	J	5105	POV	3	0
7	I	5112	POV	3	0
7	J	5112	POV	3	0
7	I	5101	POV	3	0
7	J	5113	POV	1	0
7	J	5107	POV	3	0
7	C	5101	POV	3	0
7	J	5104	POV	1	0
7	F	5110	POV	4	0
7	F	5112	POV	3	0
7	I	5113	POV	4	0
7	I	5104	POV	2	0
7	F	5113	POV	2	0

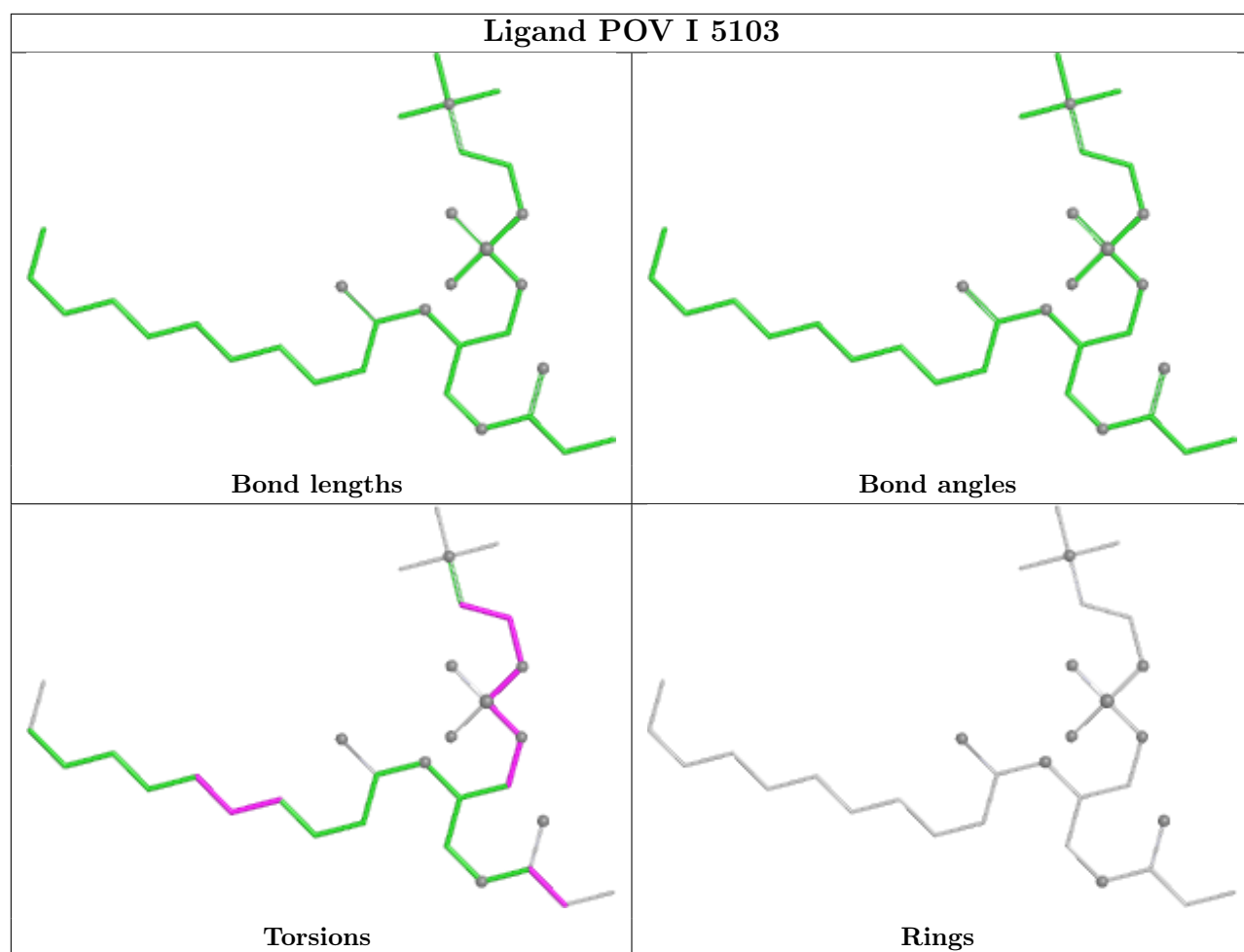
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

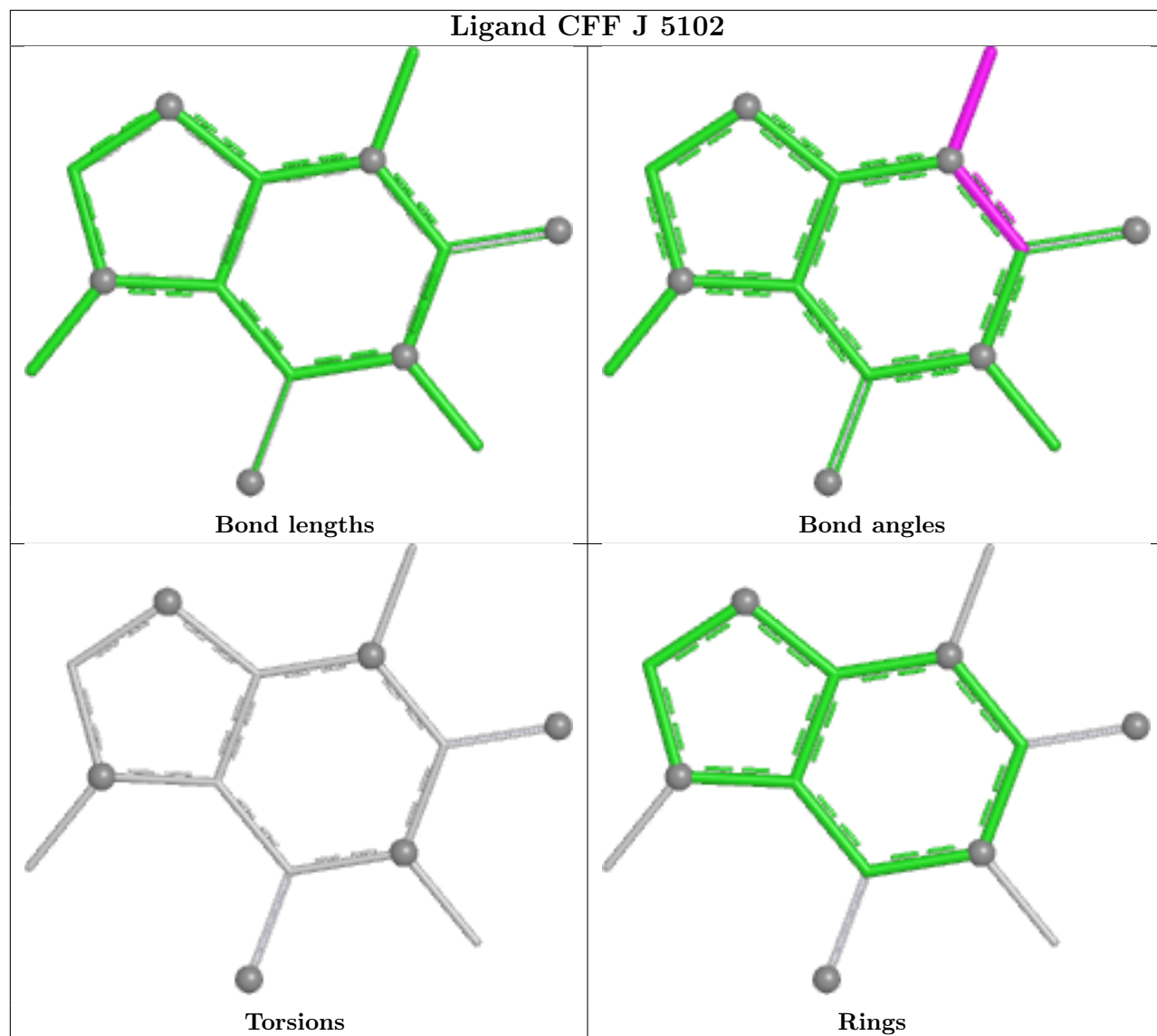
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

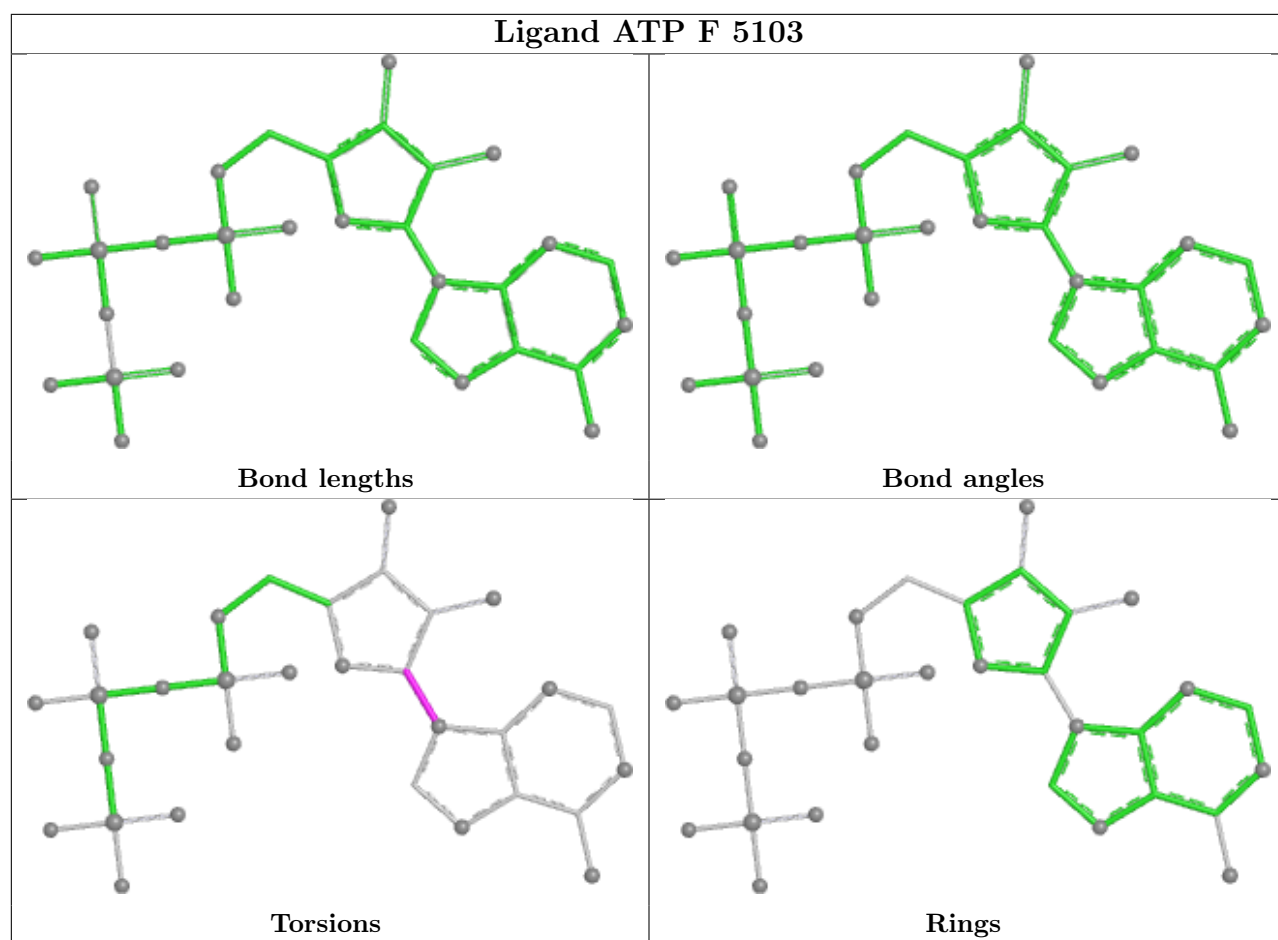


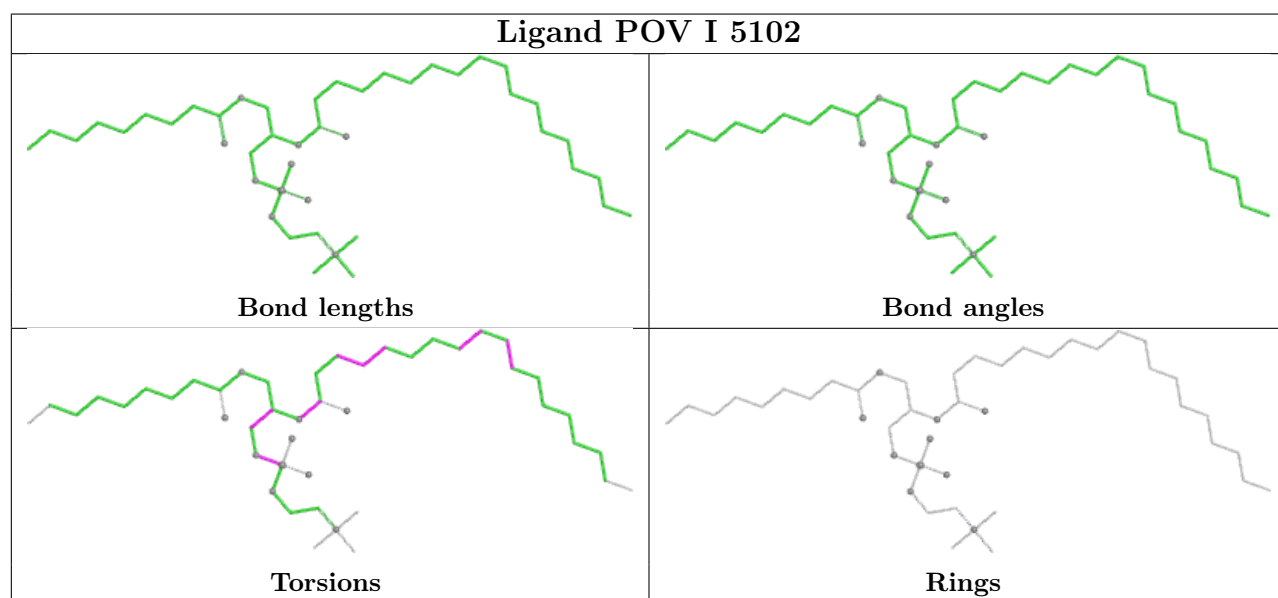
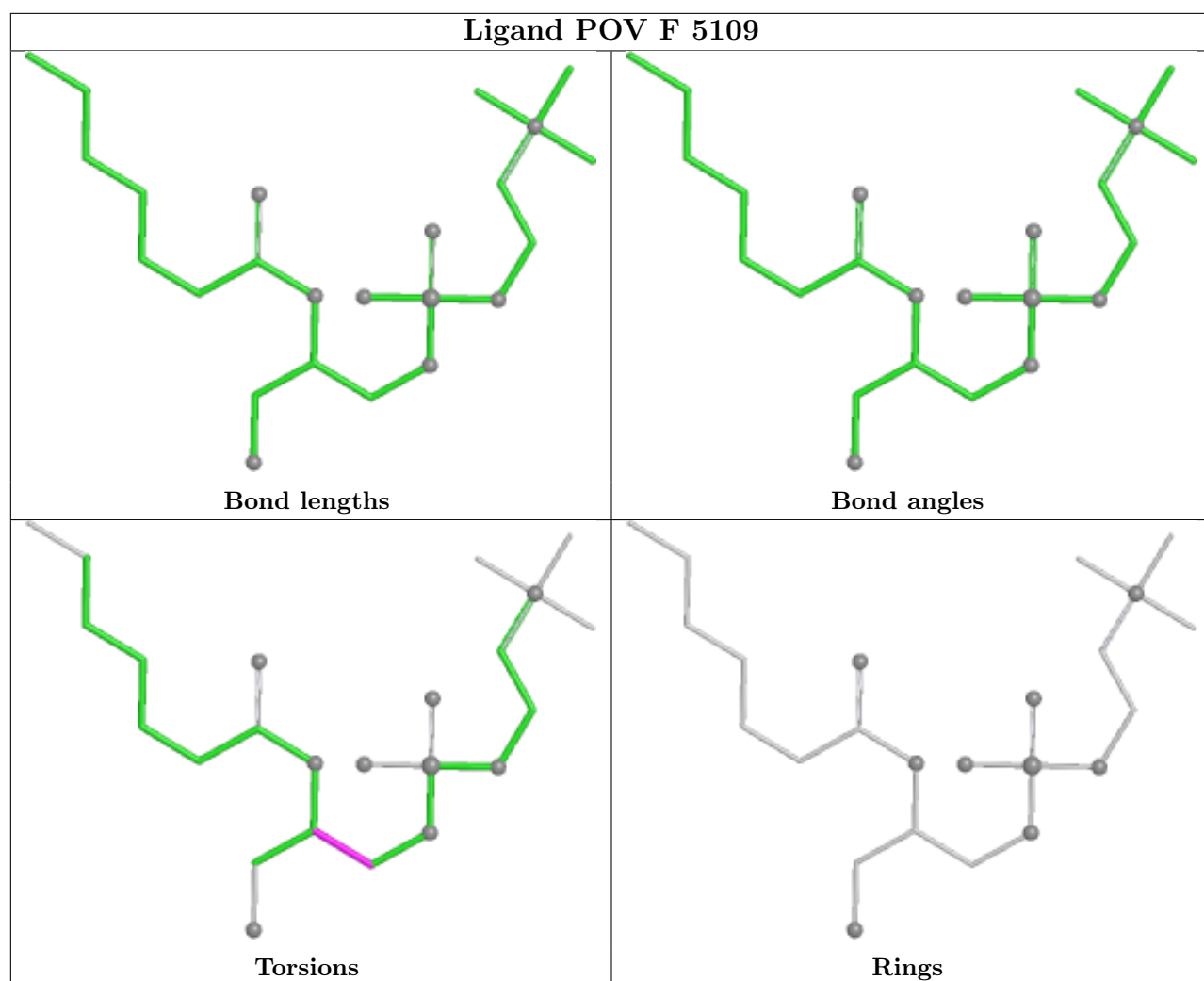


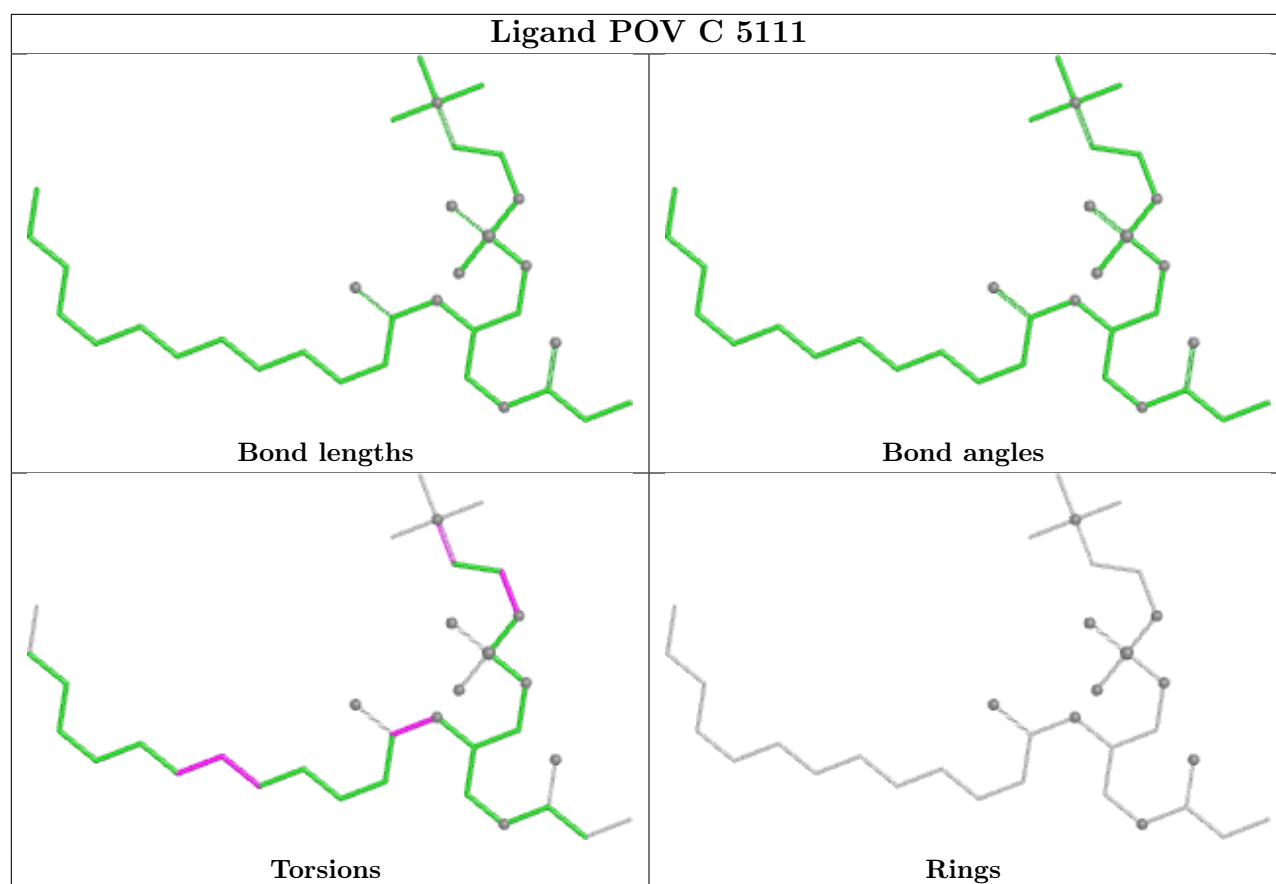


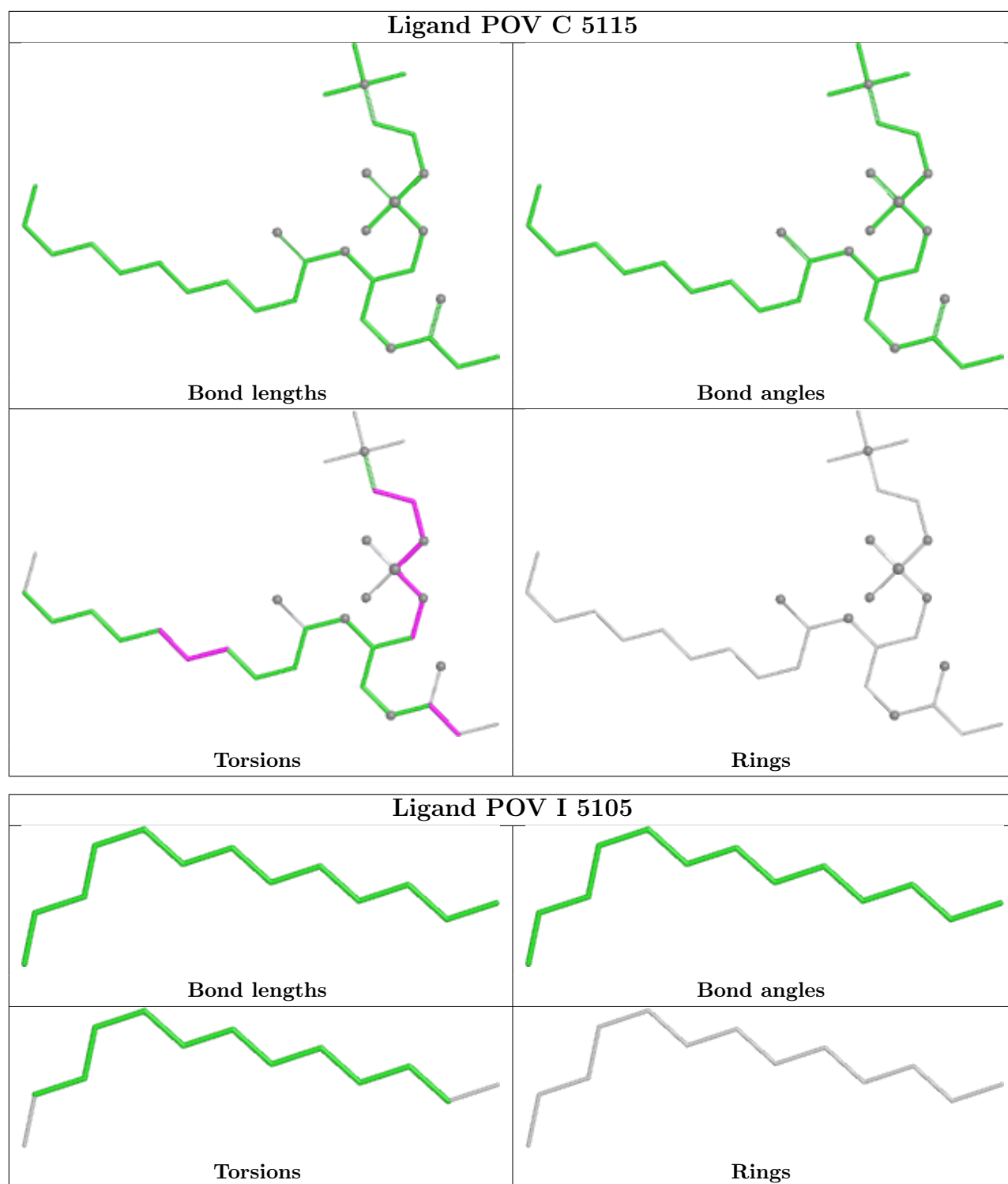


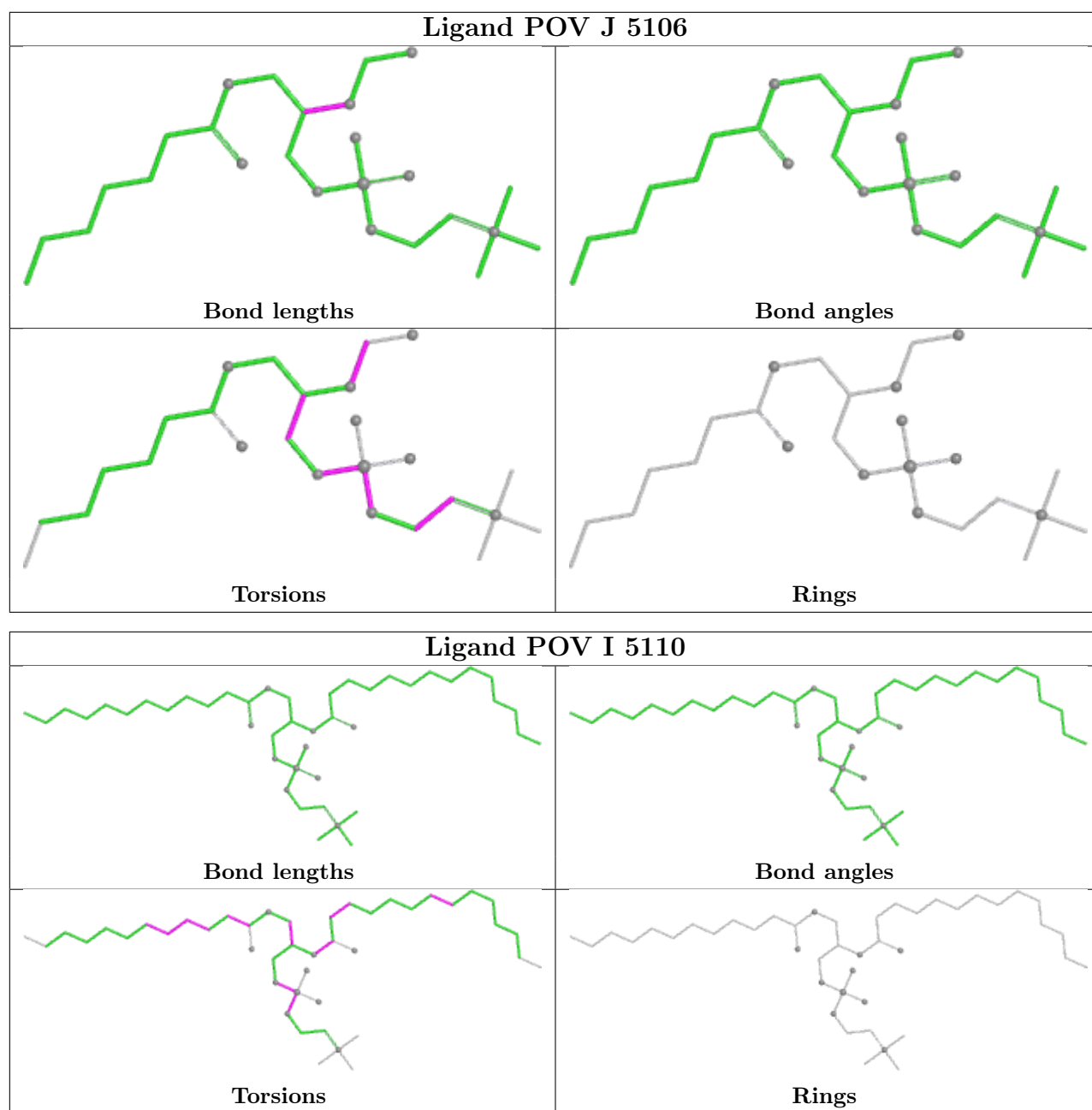


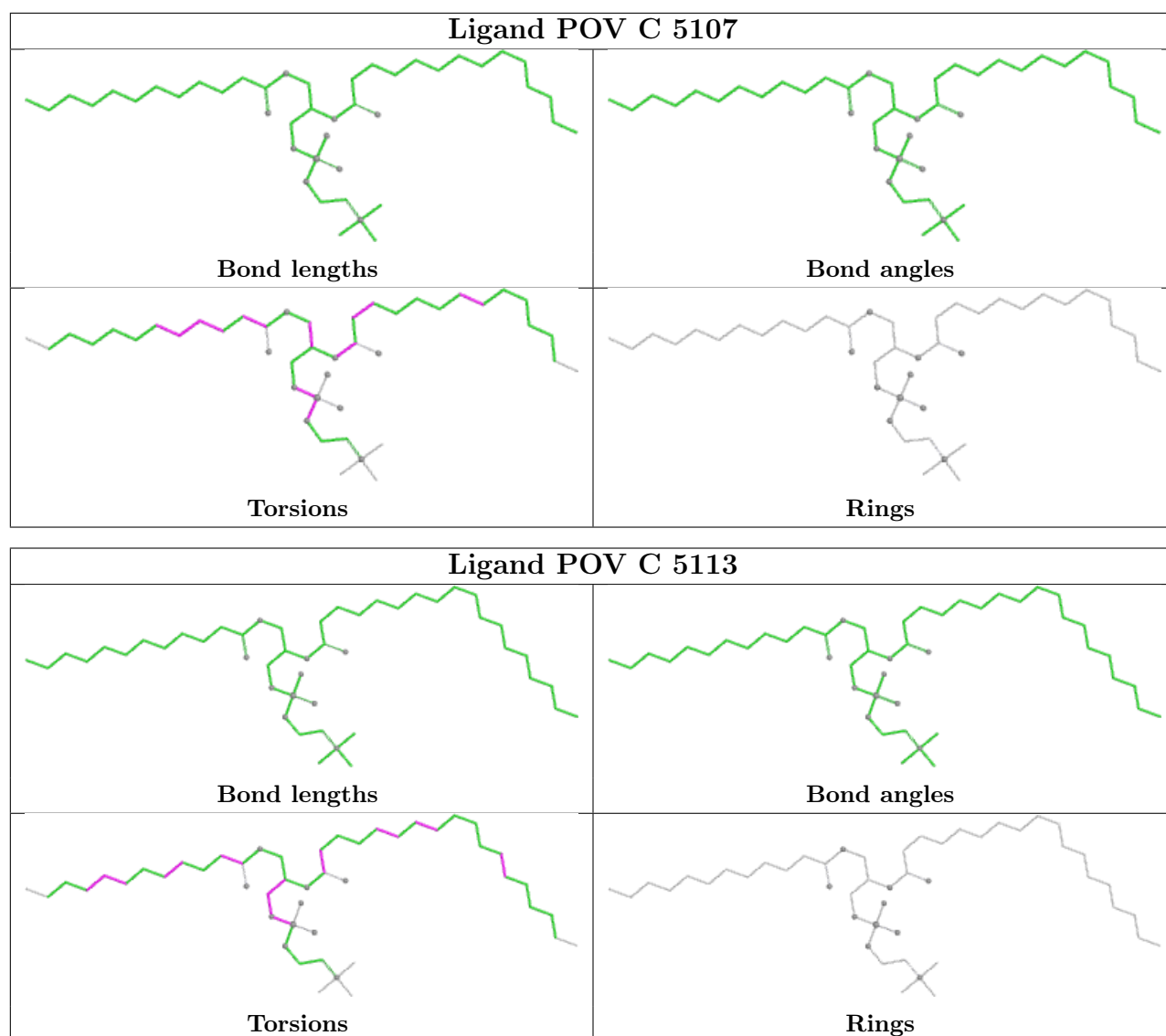


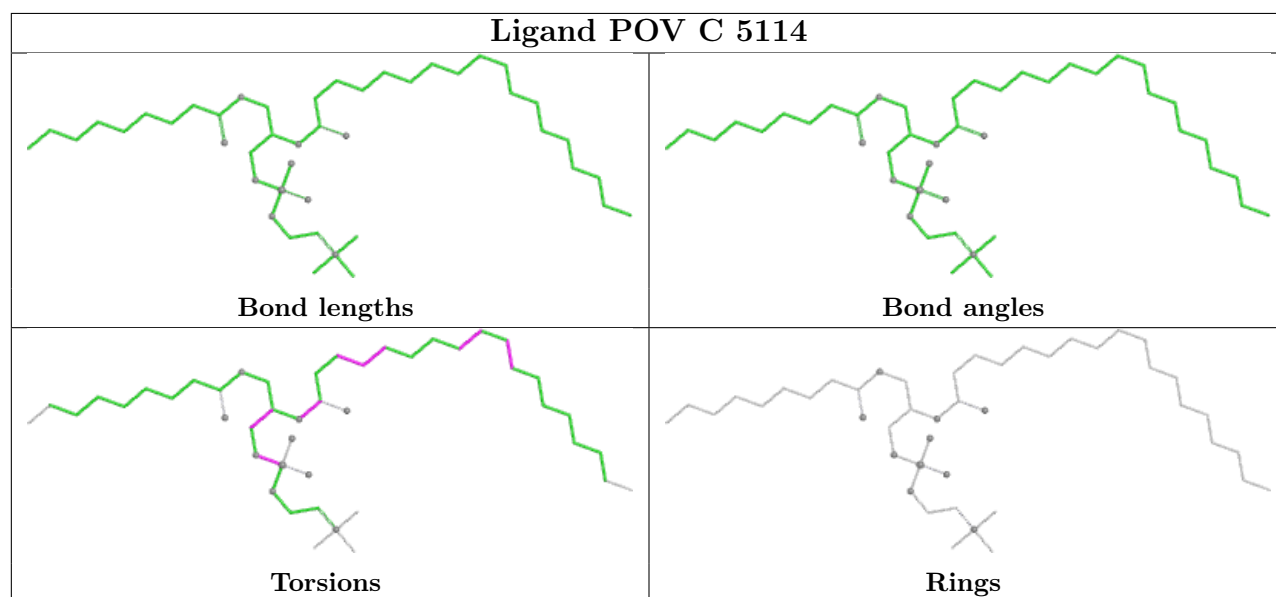
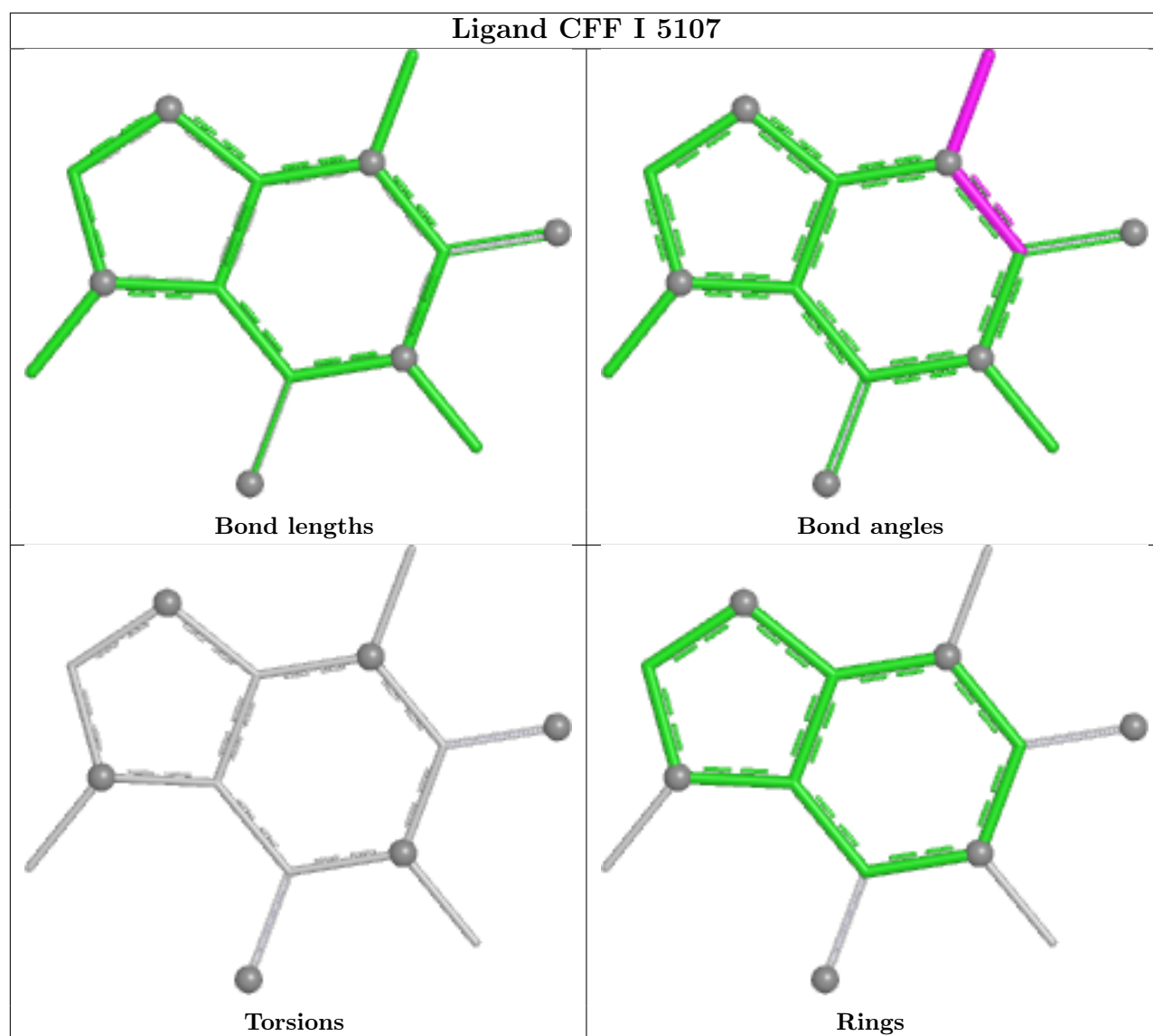


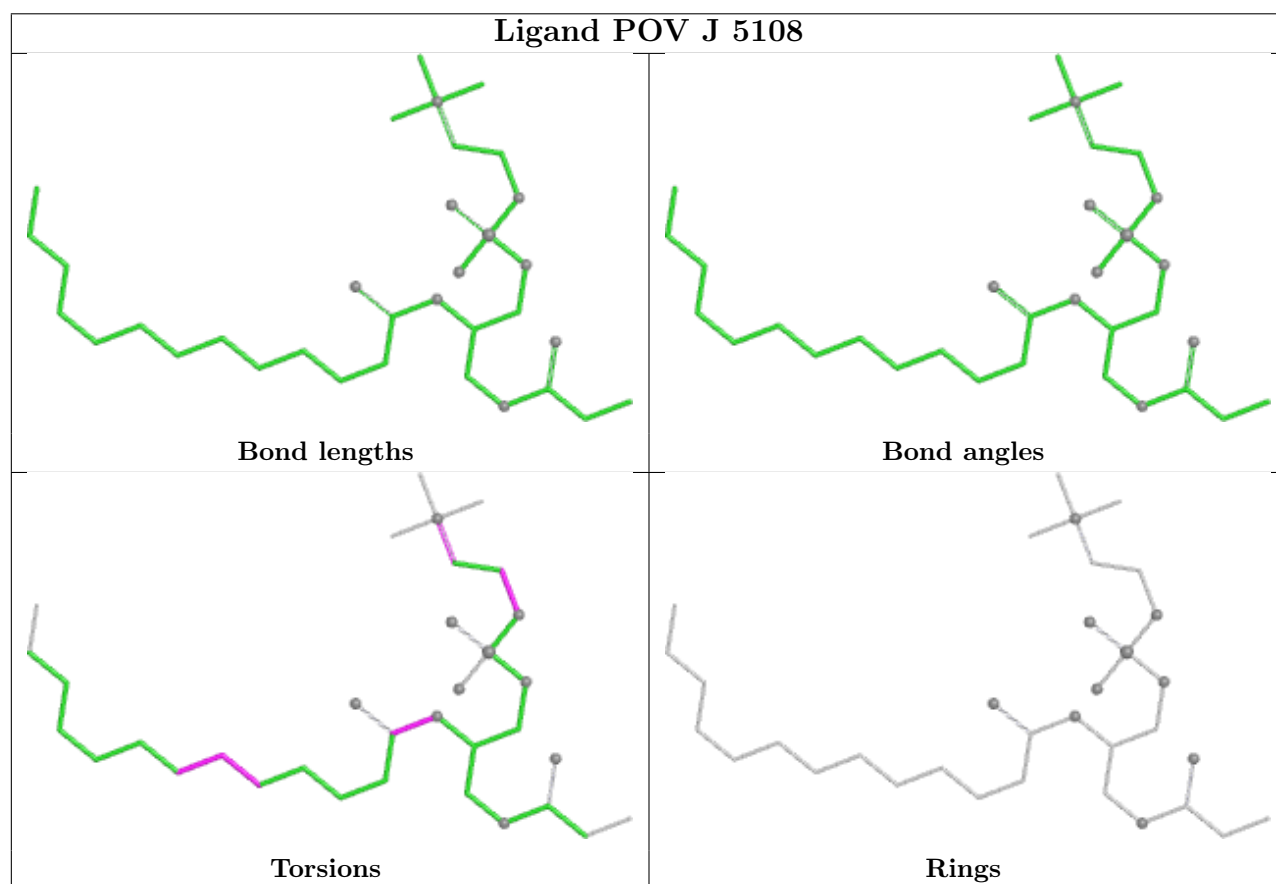
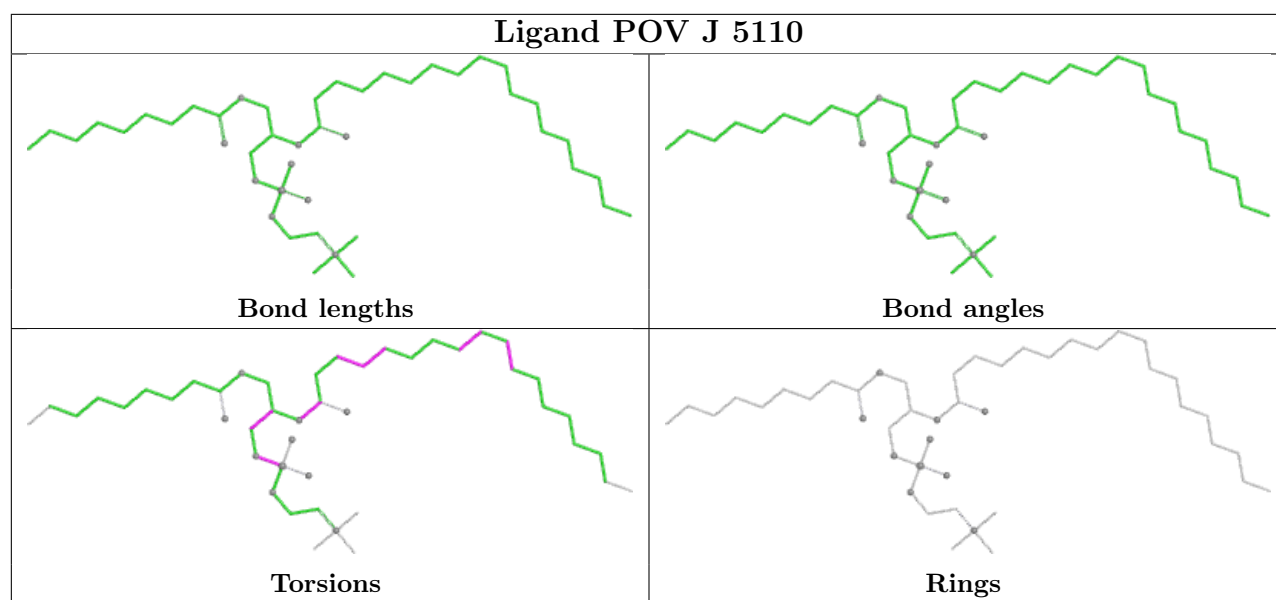


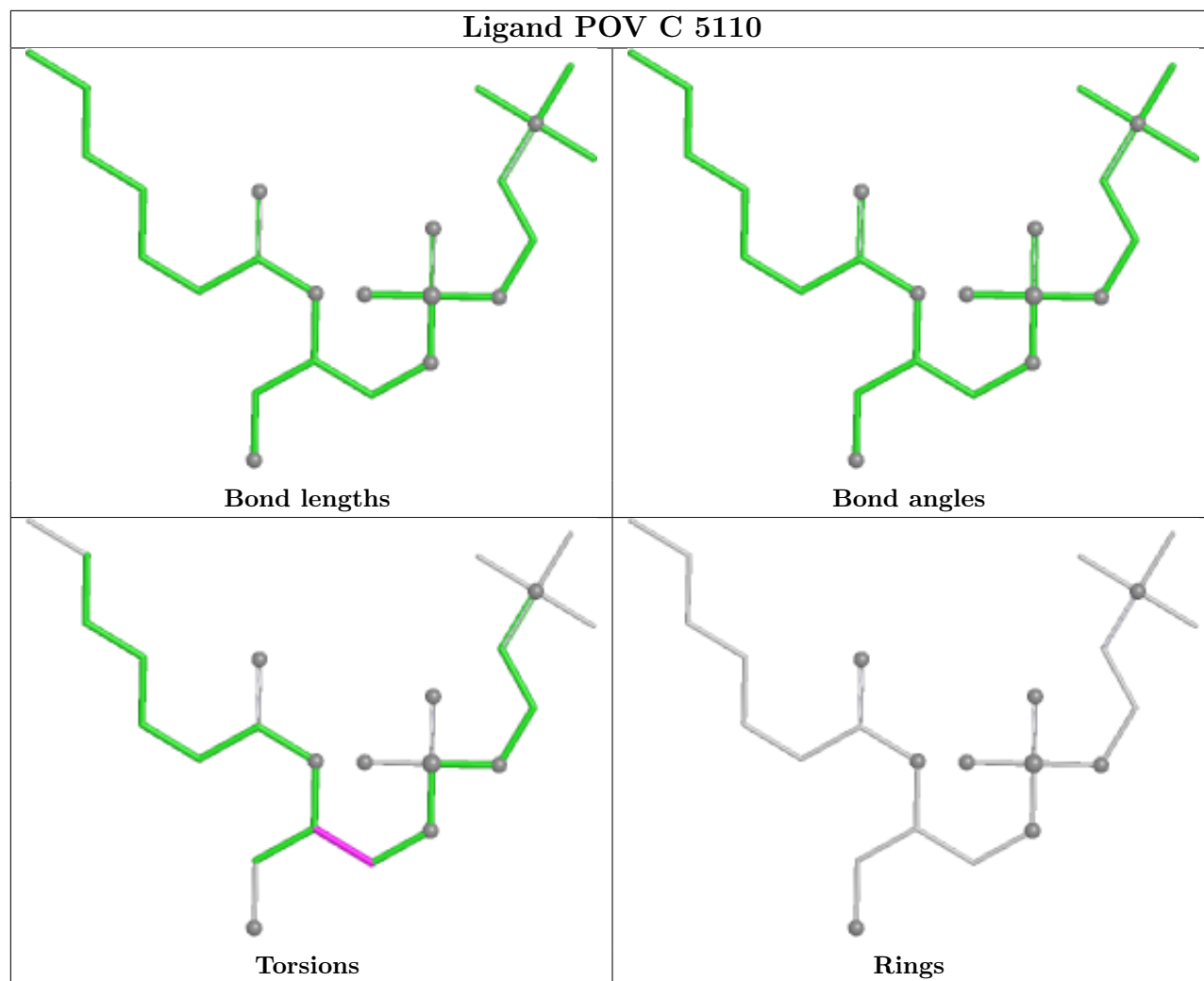
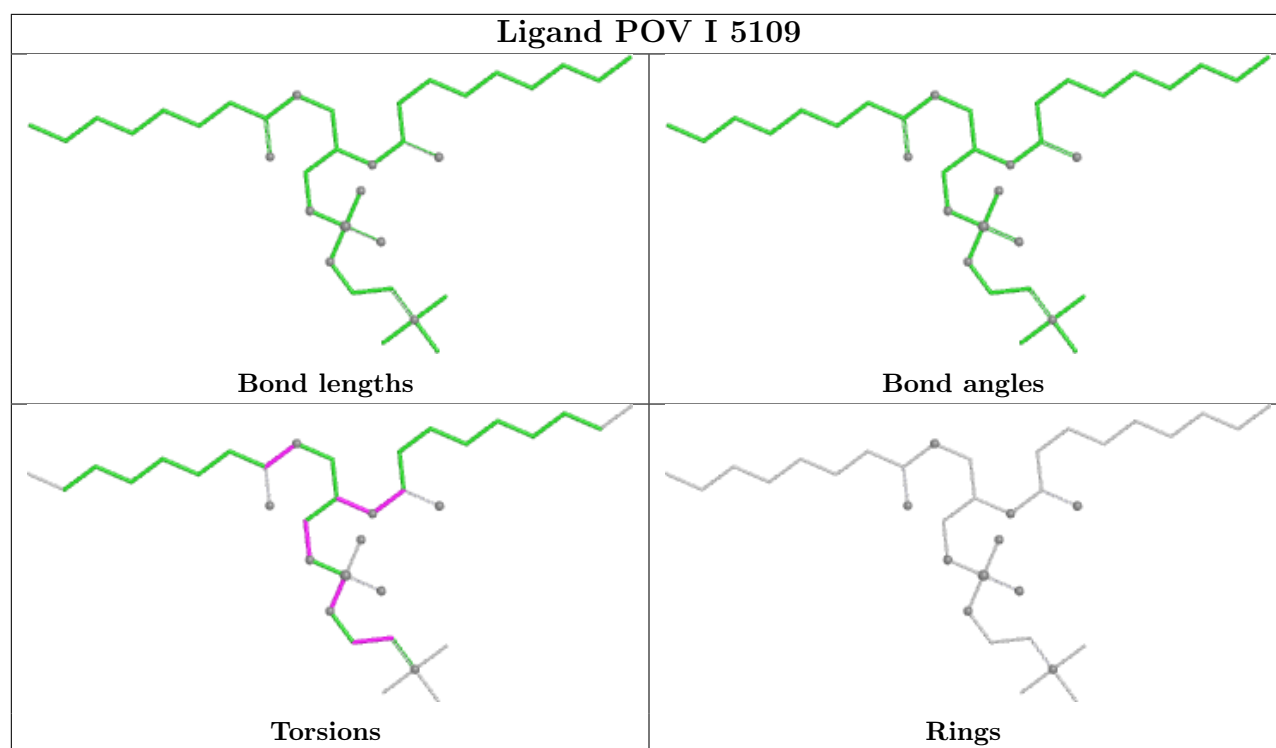


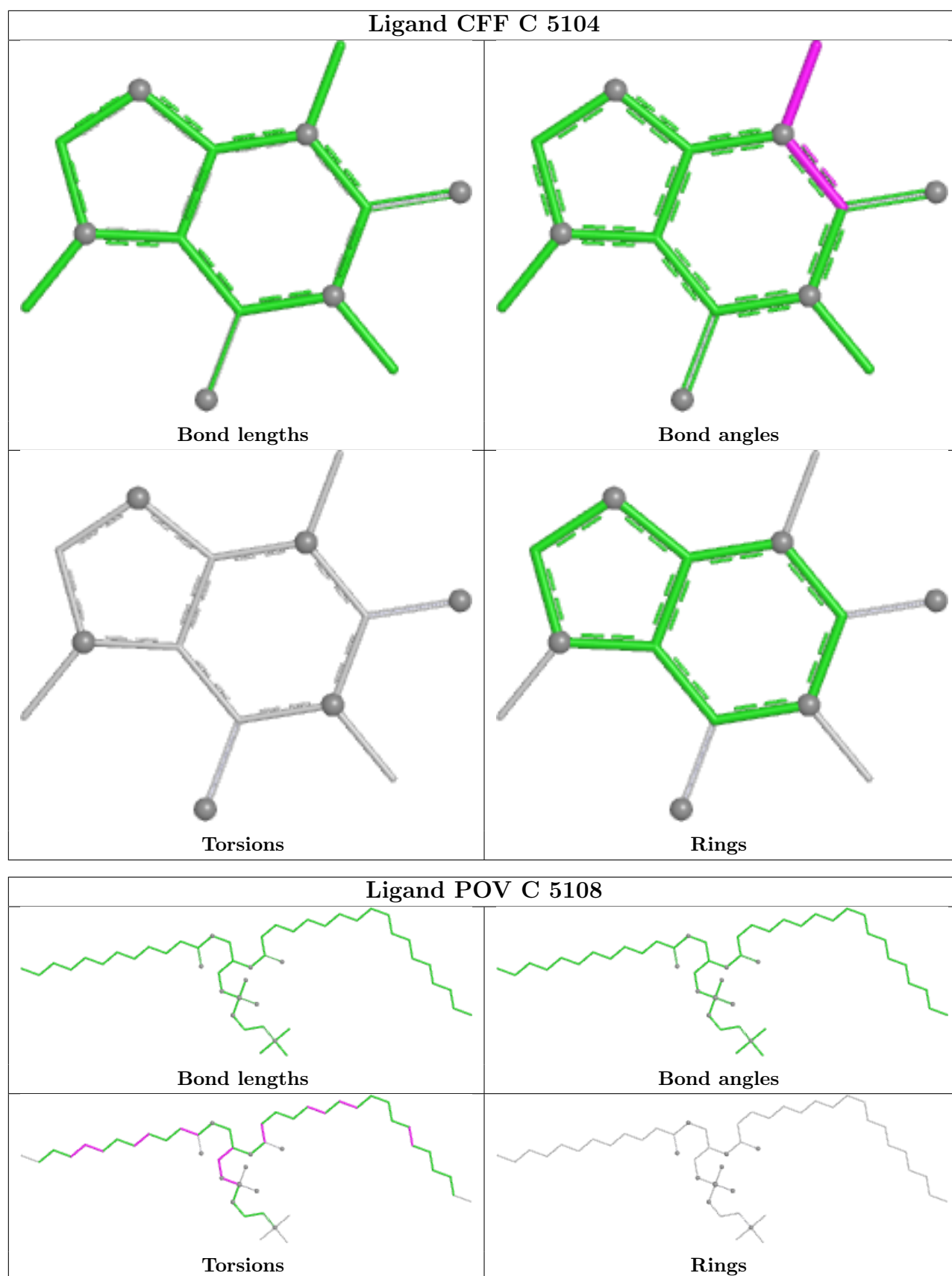


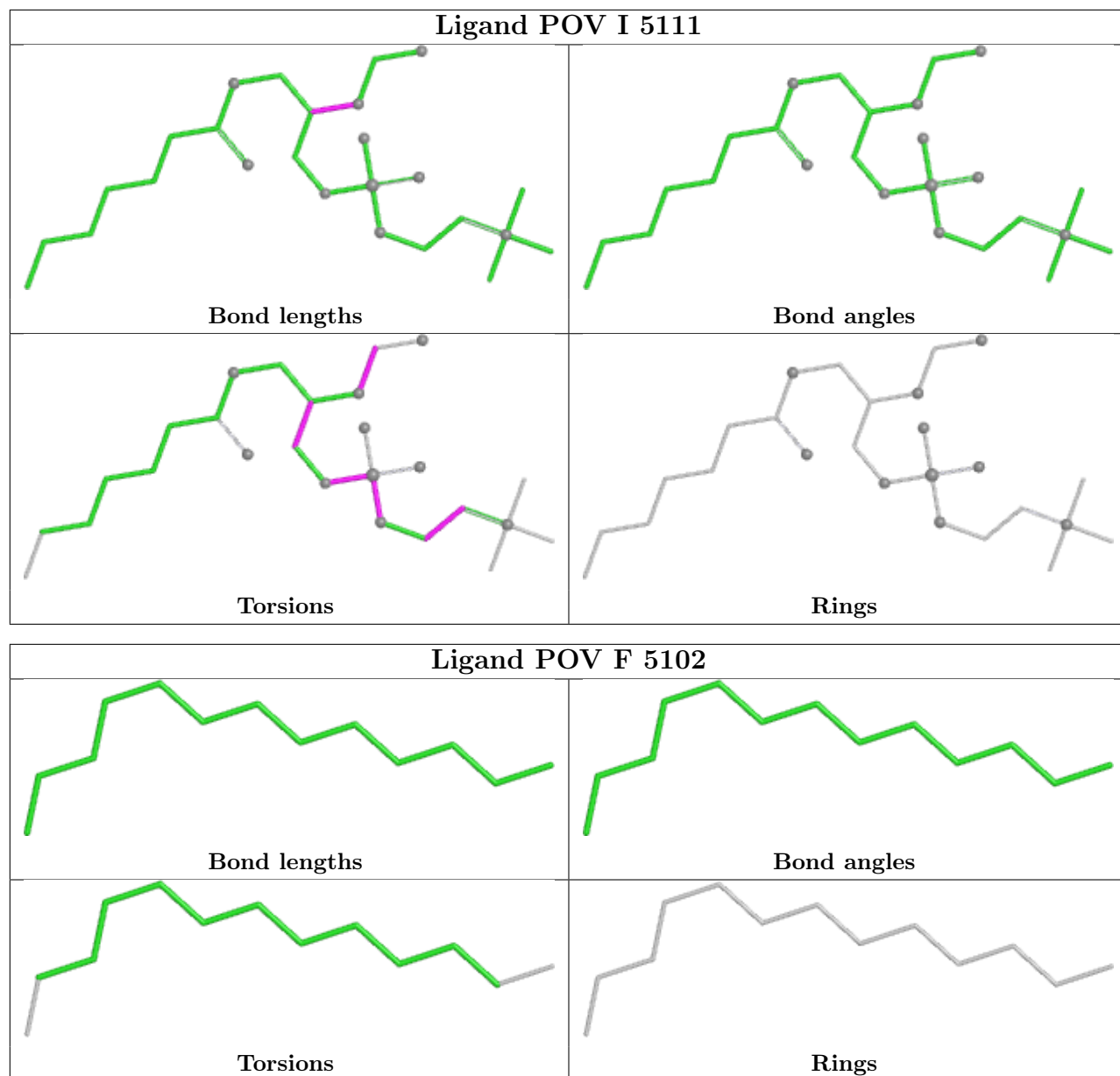


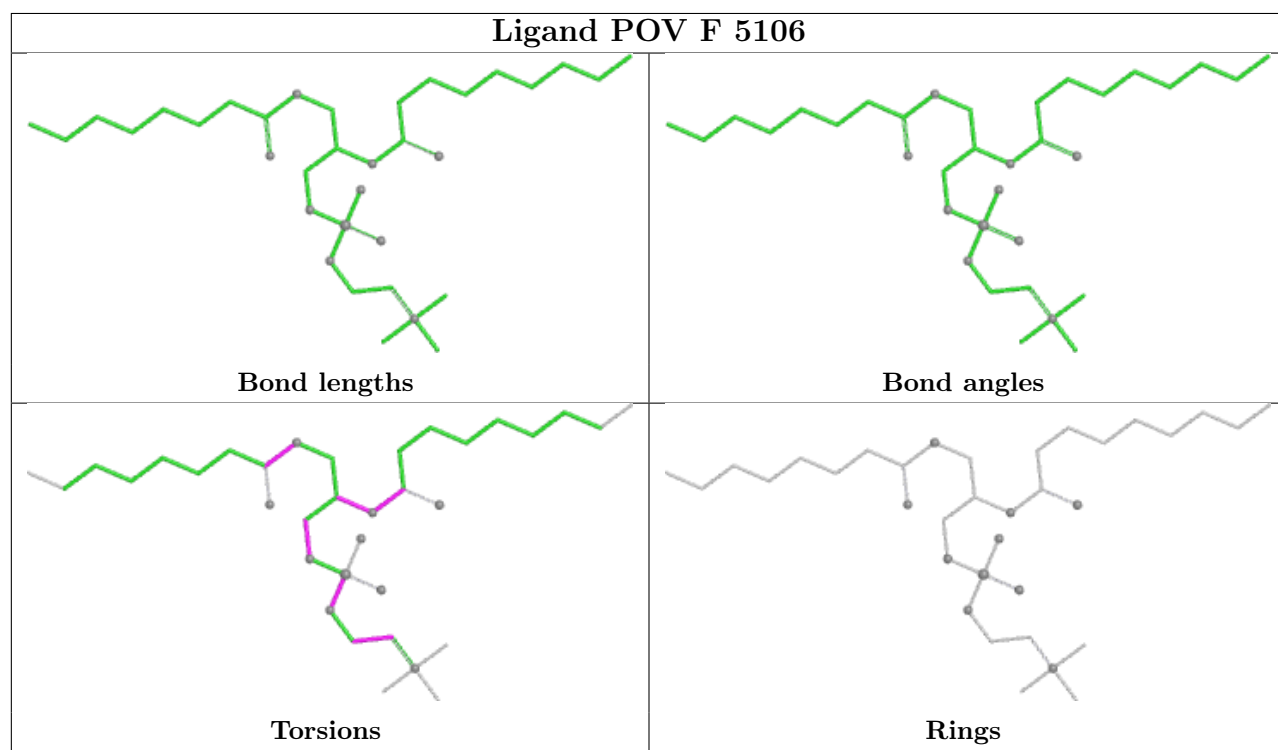
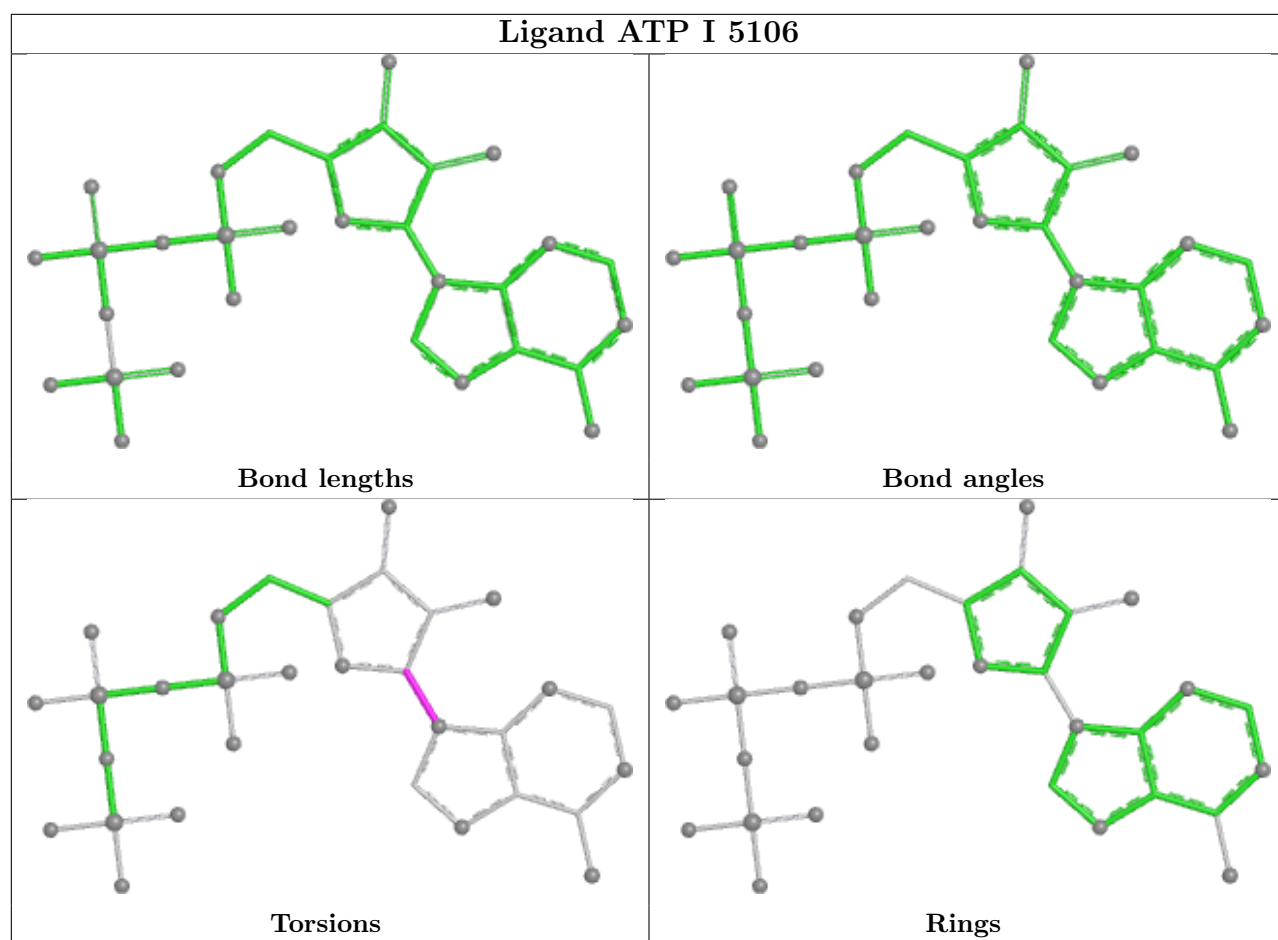


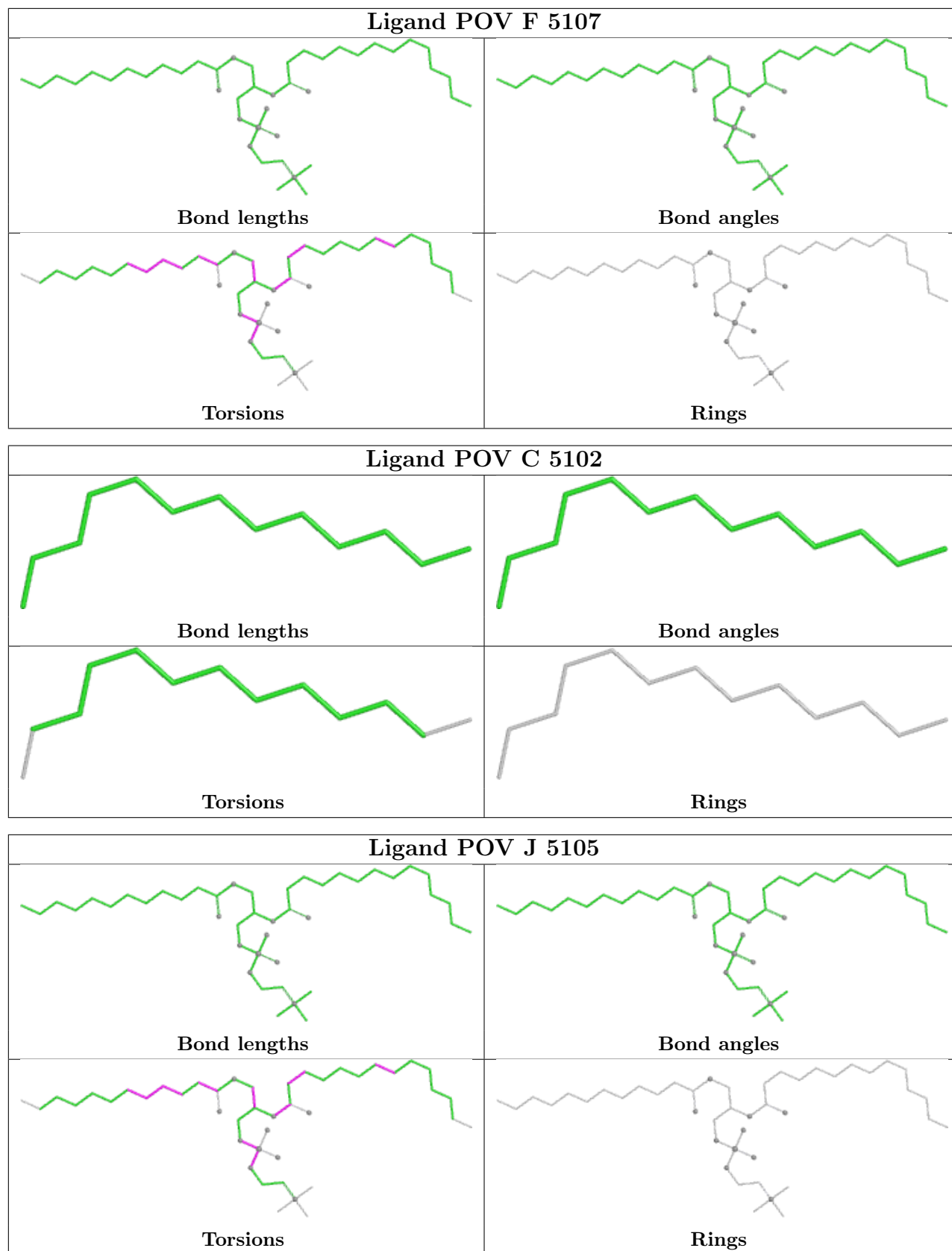


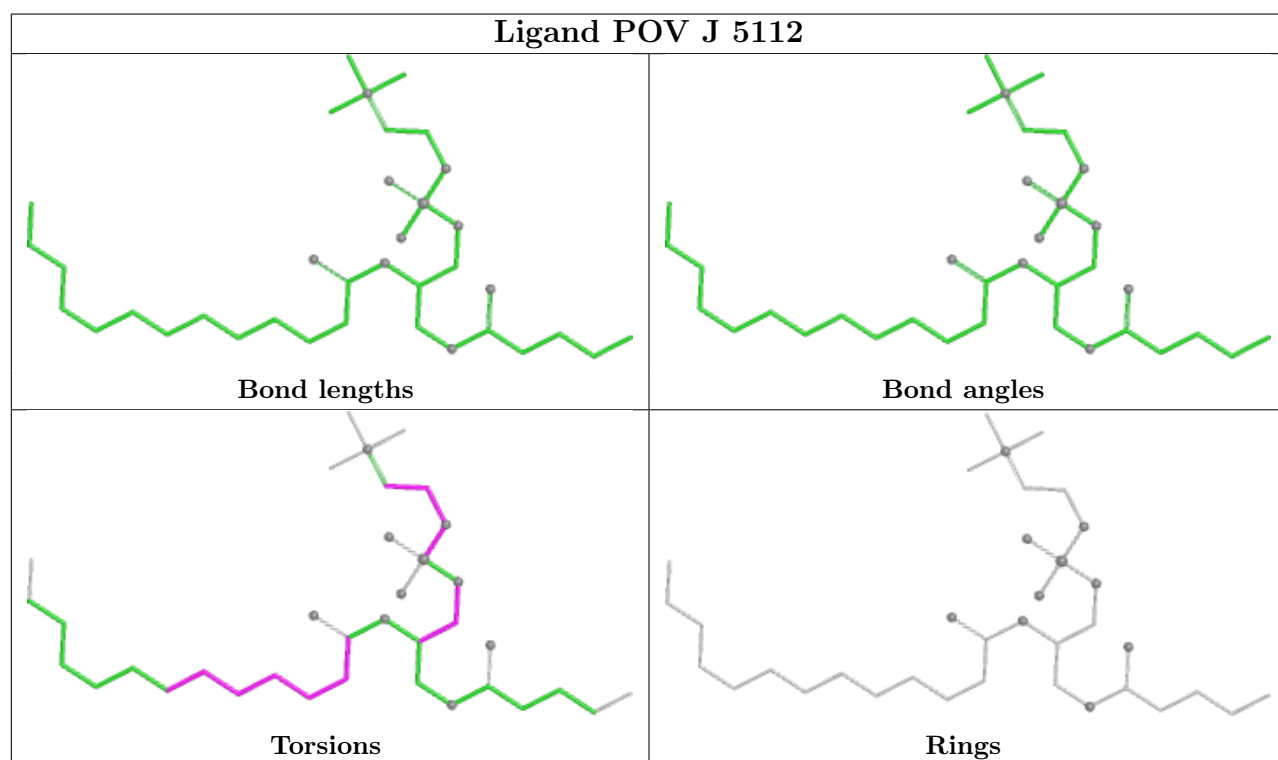
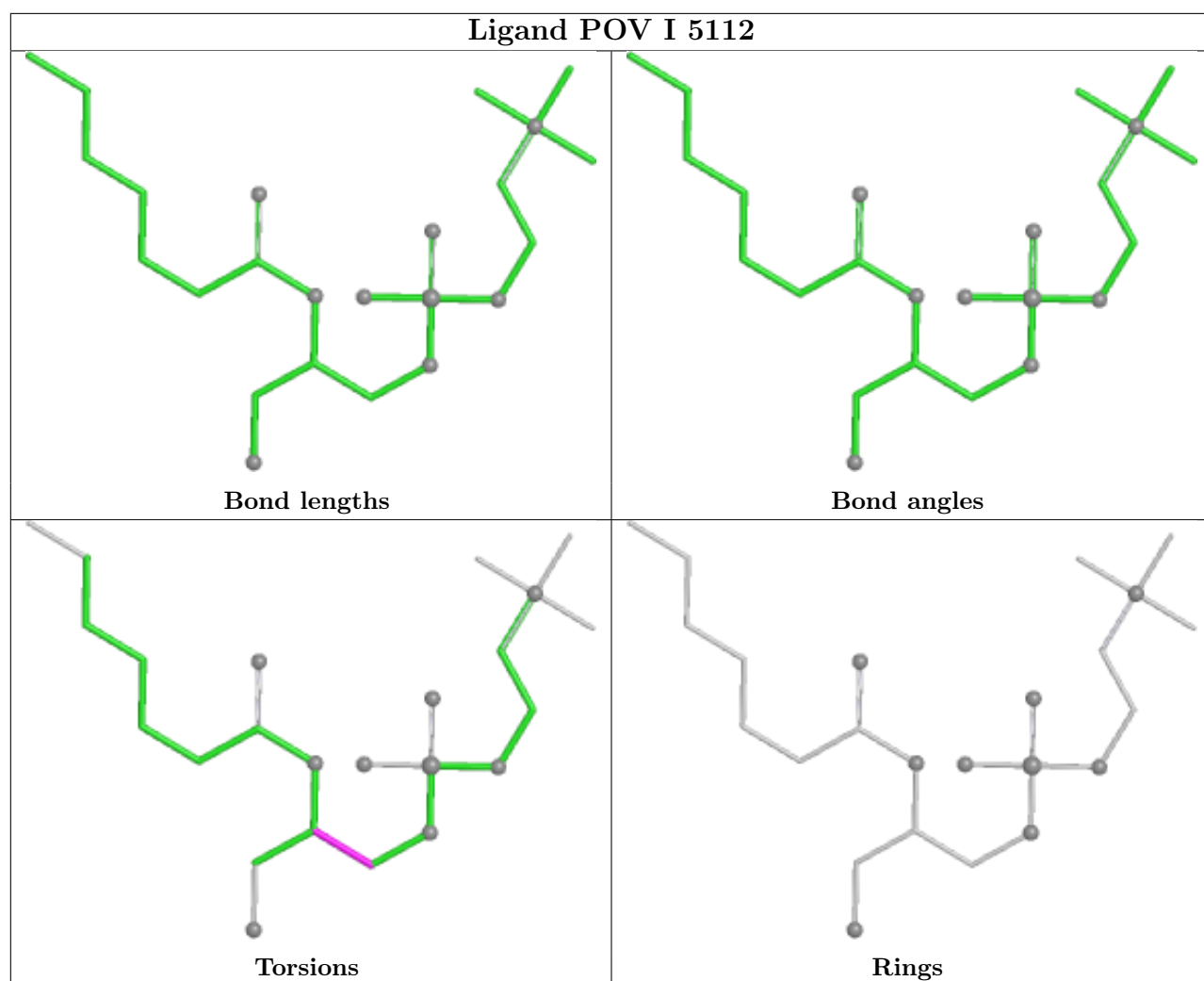


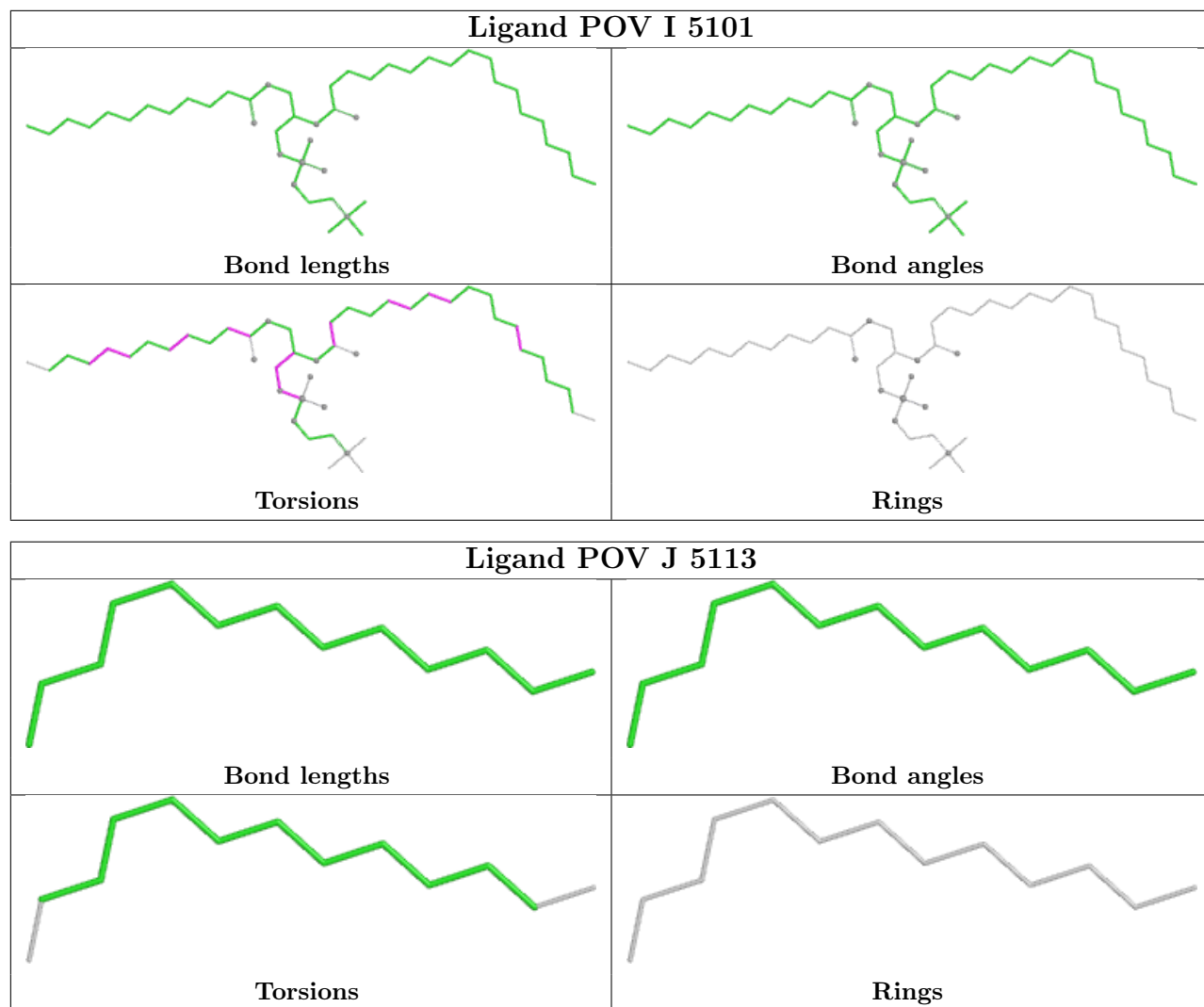


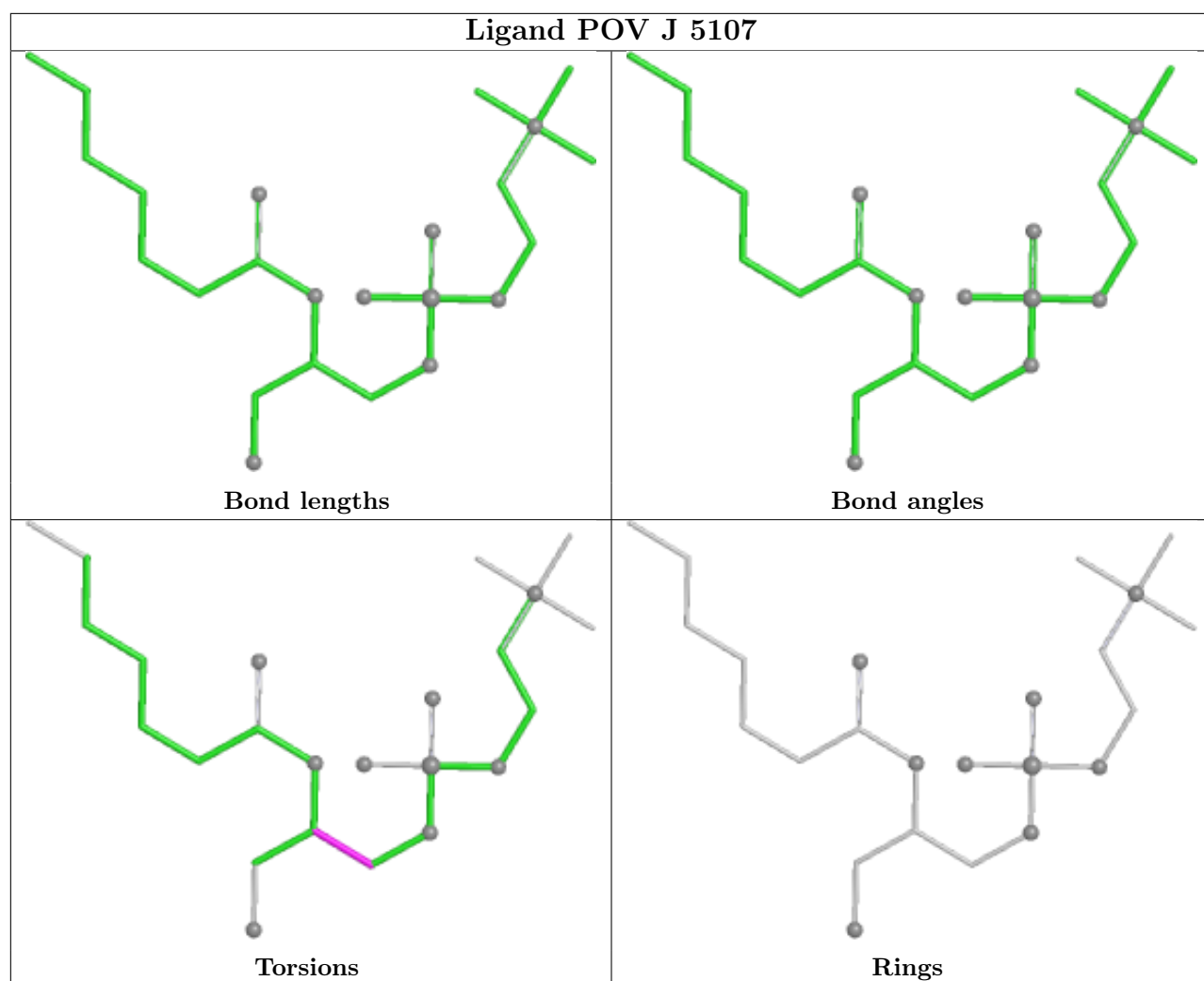


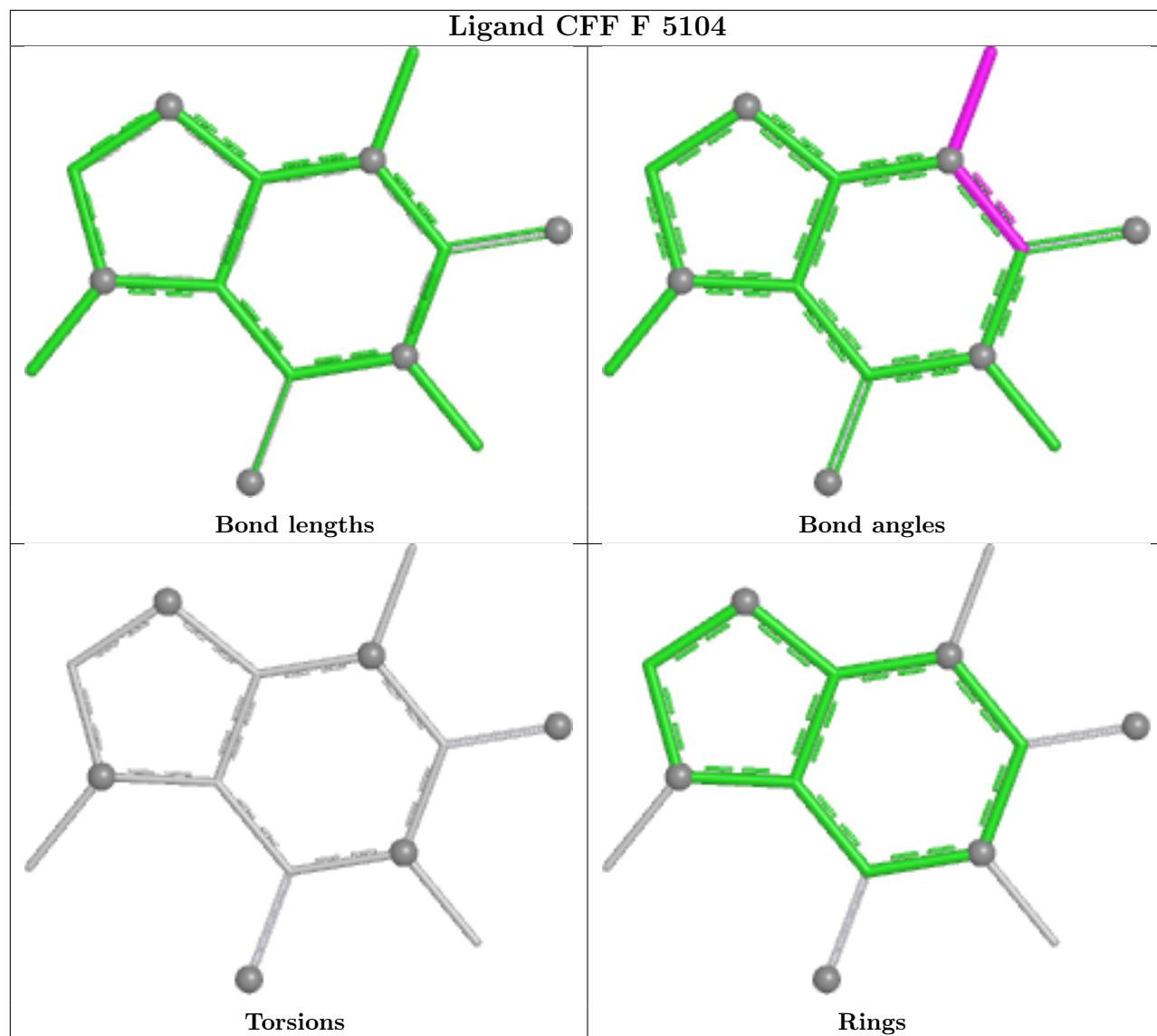


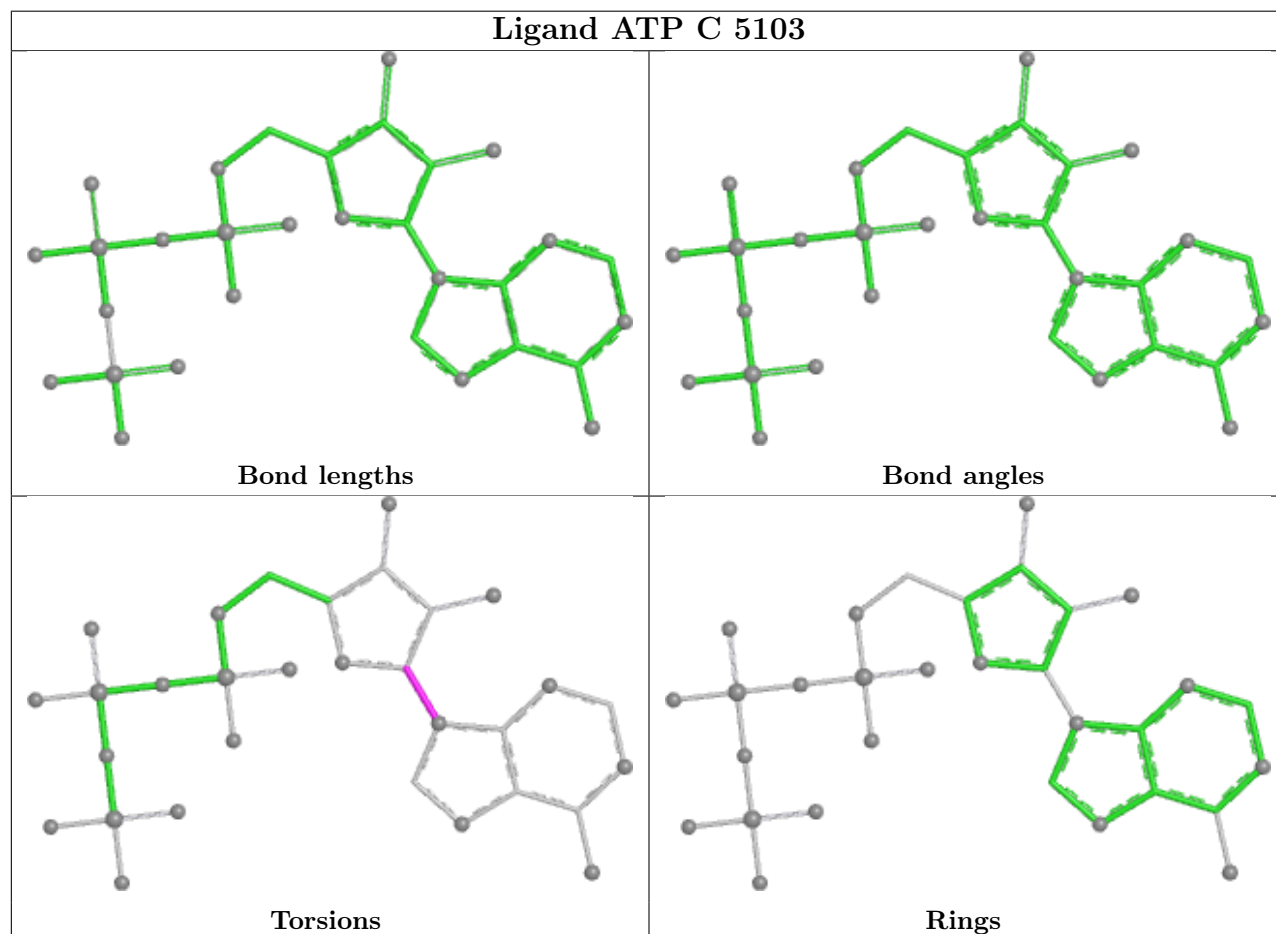
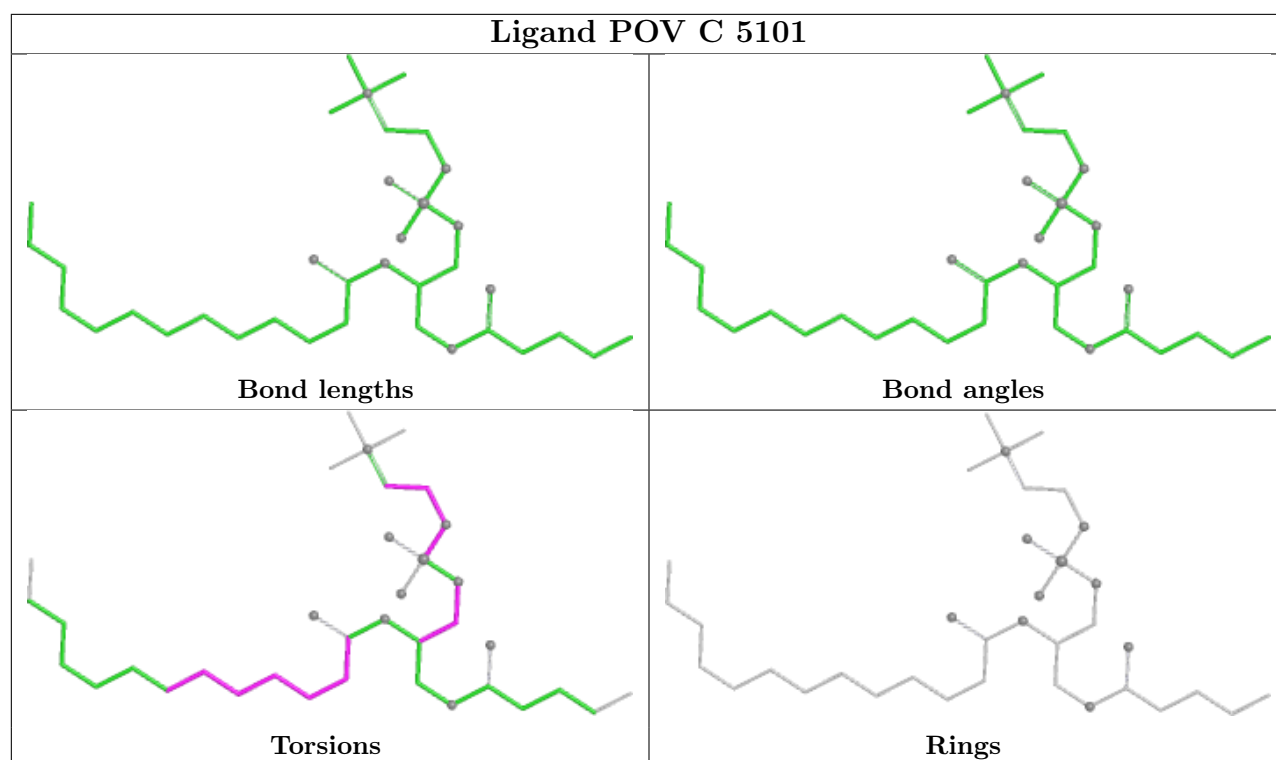


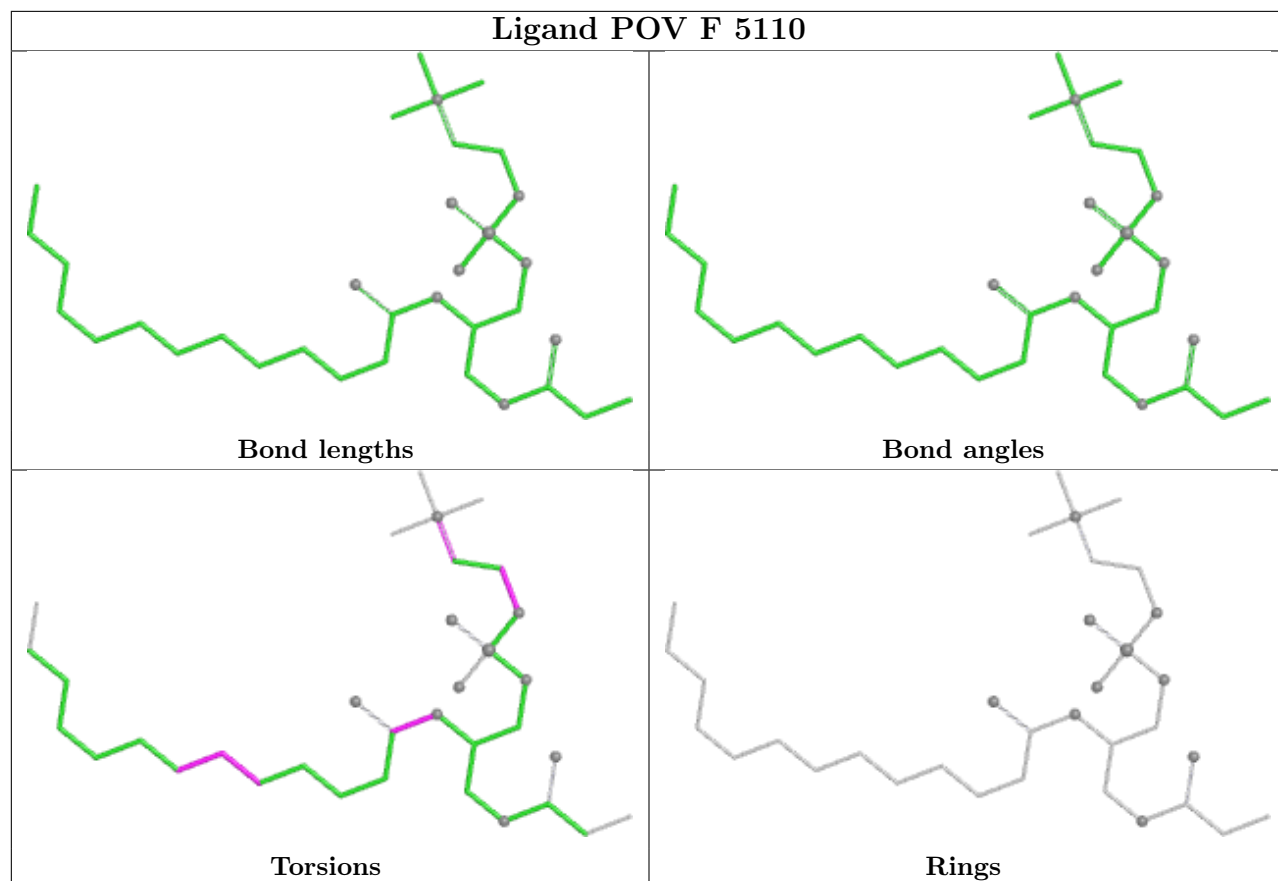
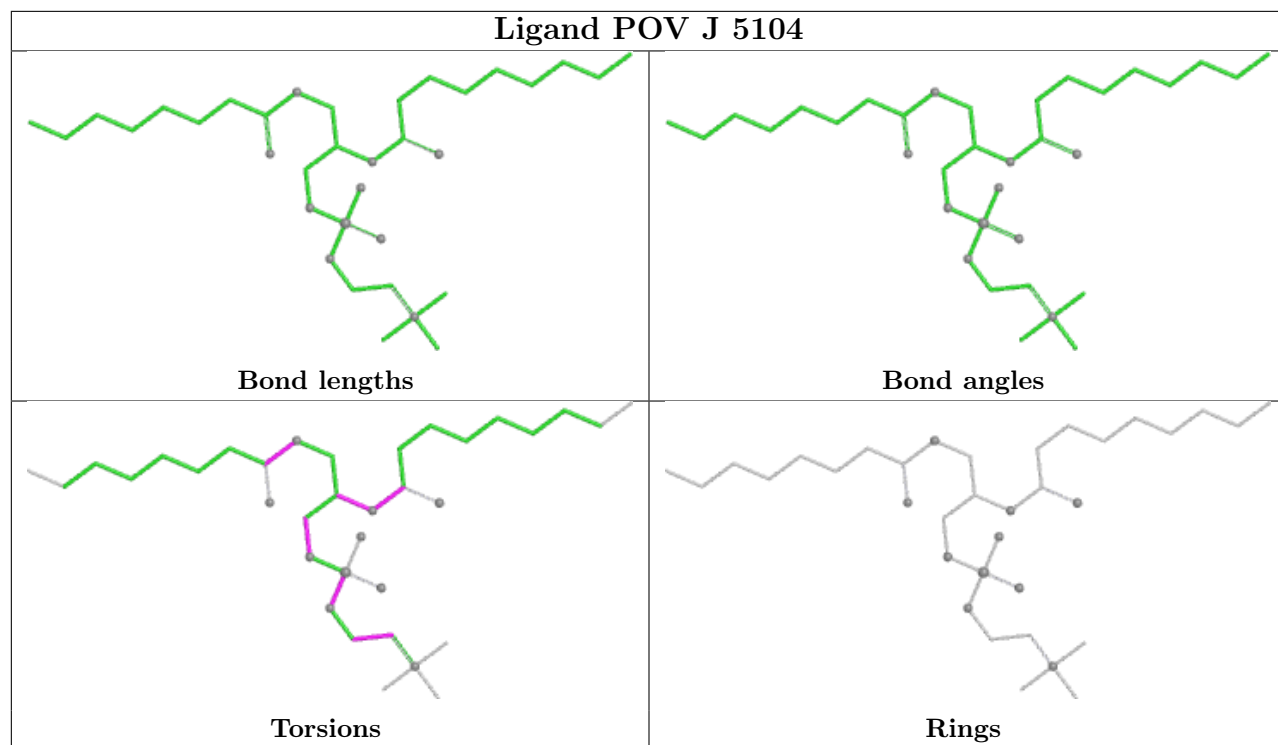


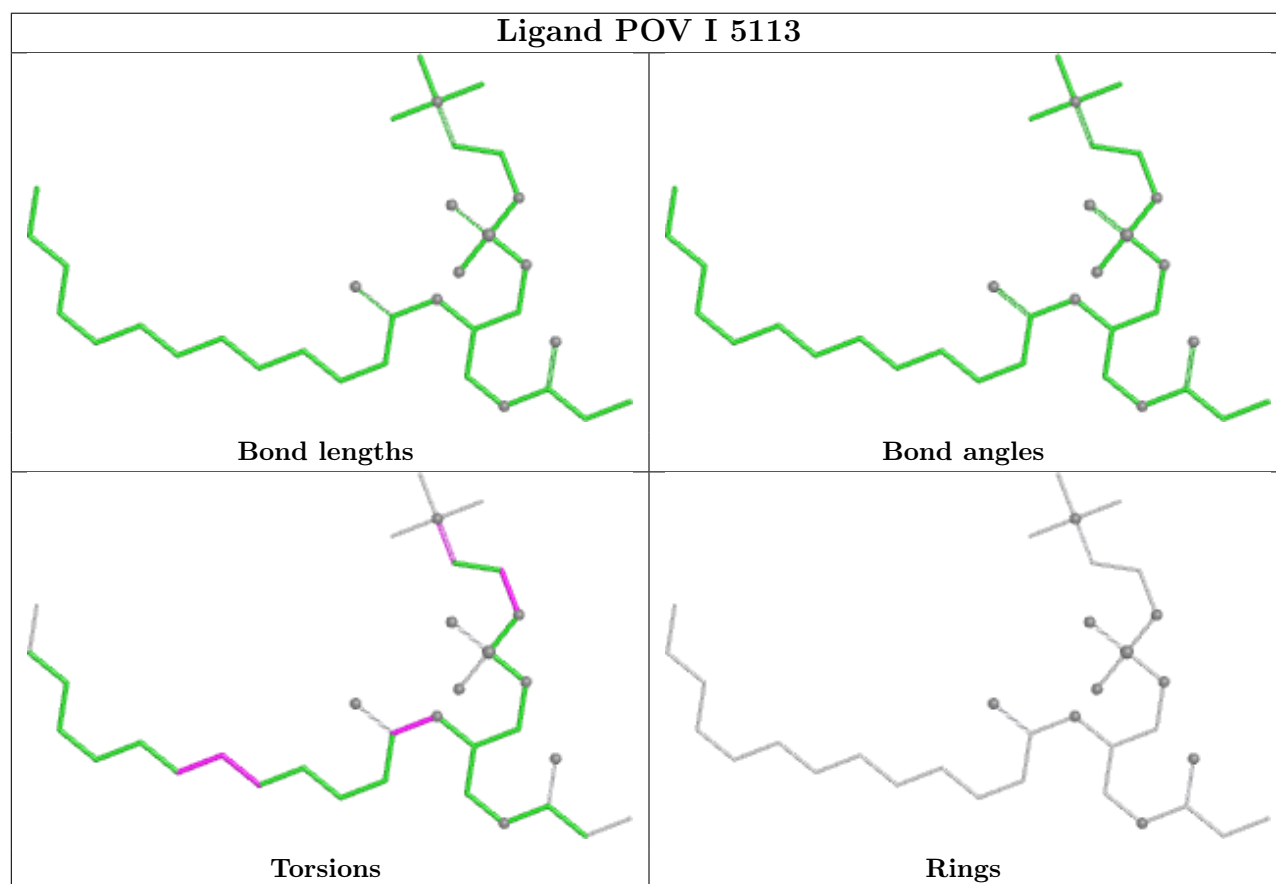
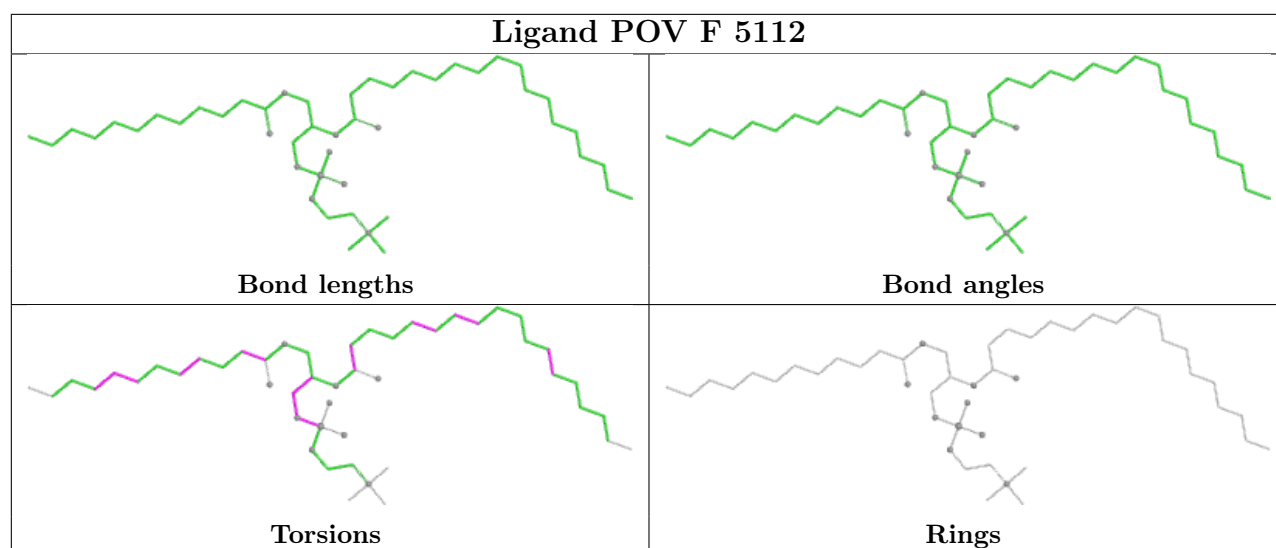


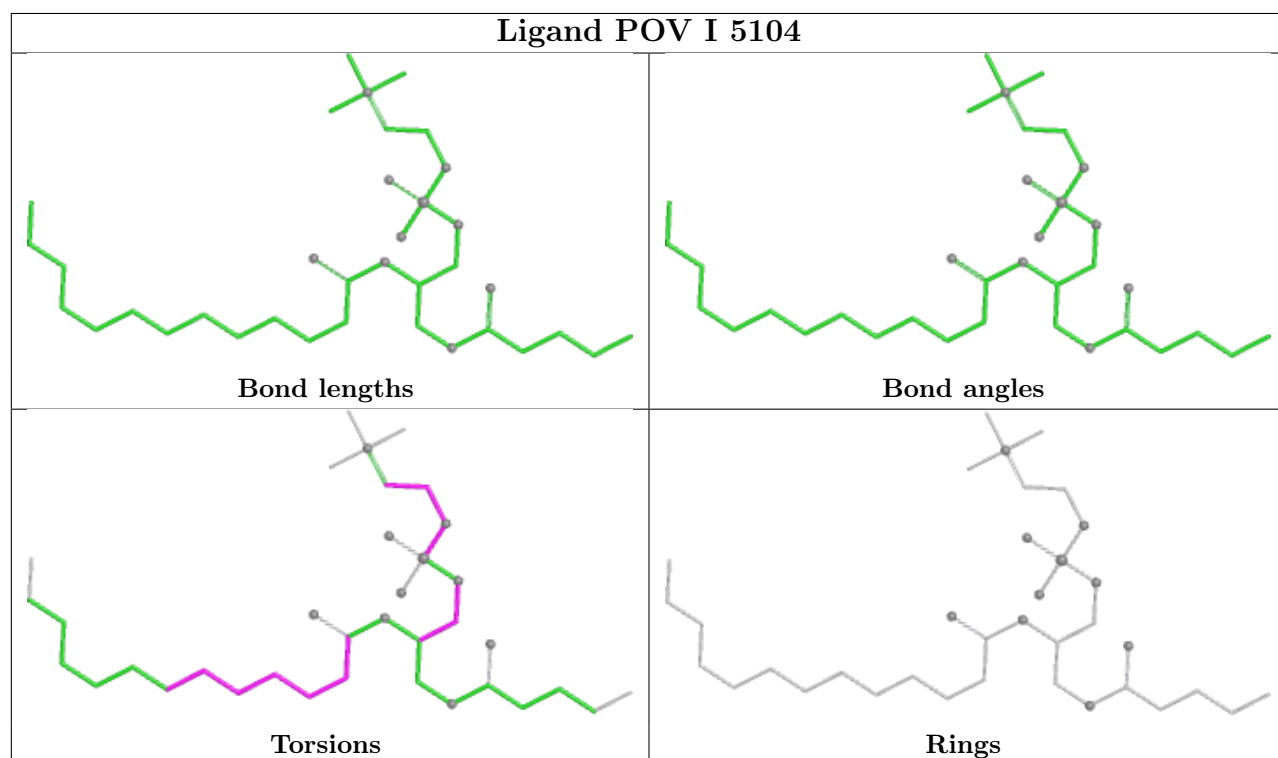
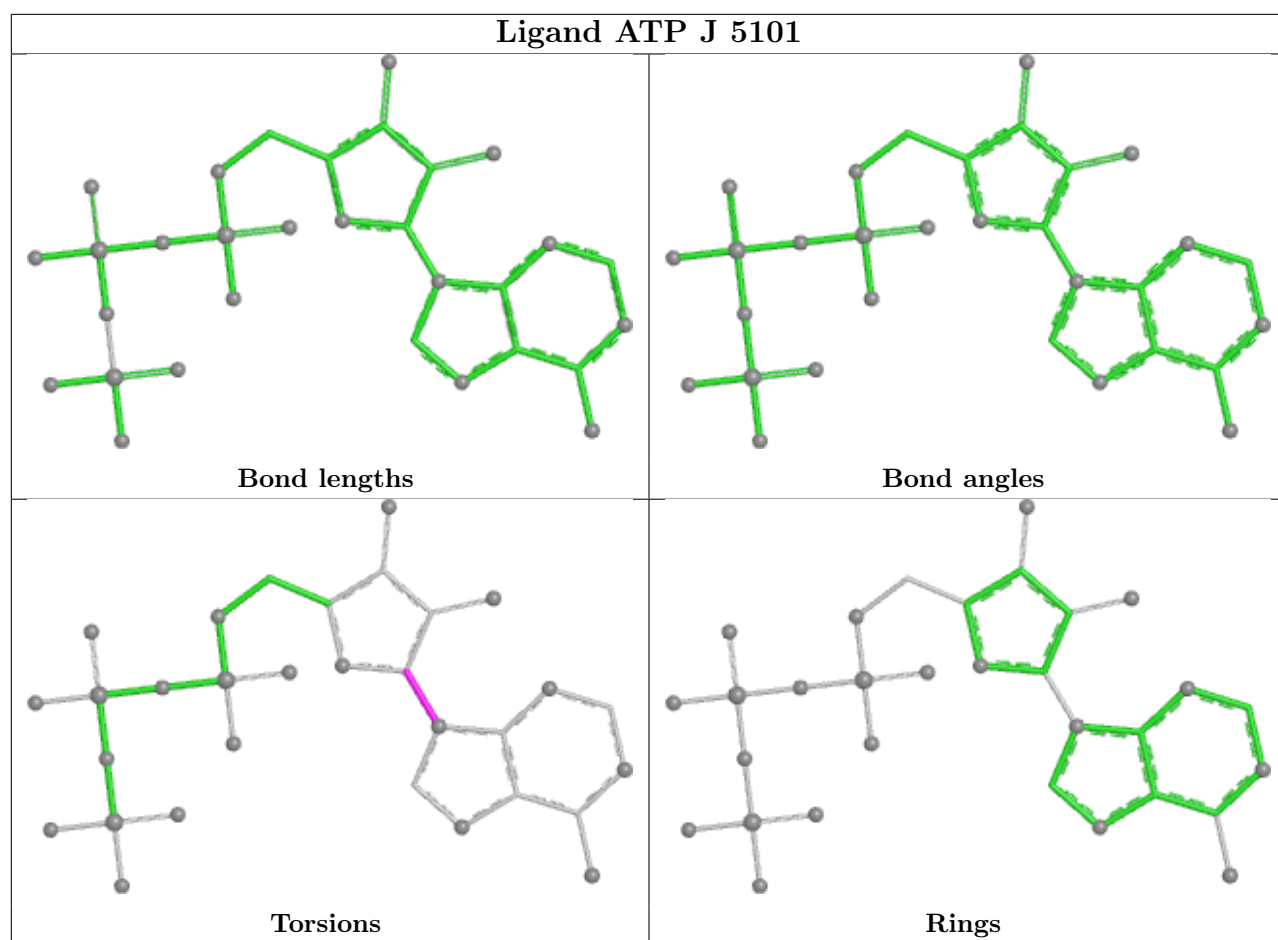


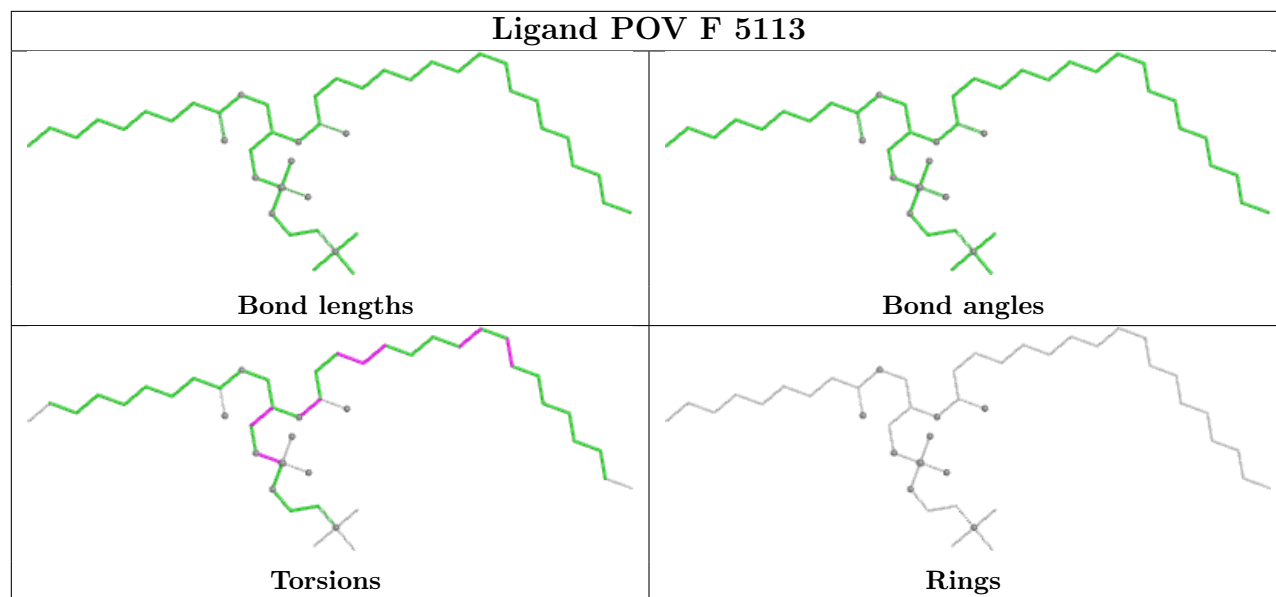












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

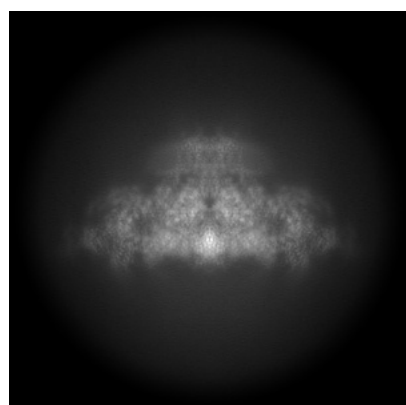
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53834. These allow visual inspection of the internal detail of the map and identification of artifacts.

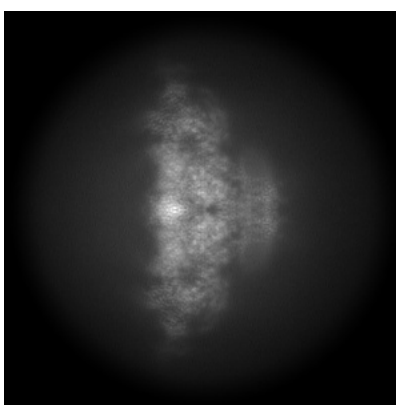
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

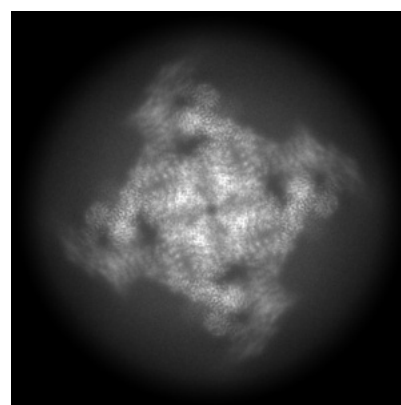
6.1.1 Primary map



X



Y

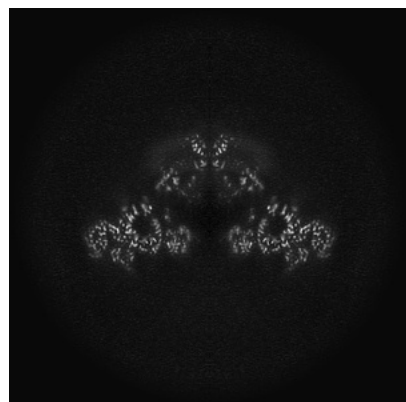


Z

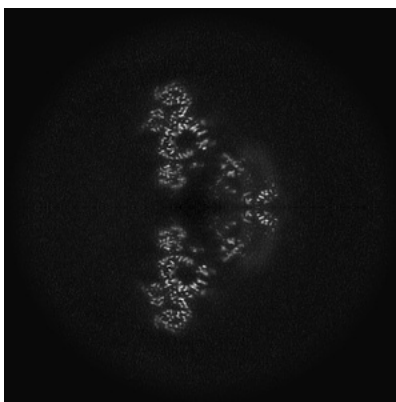
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

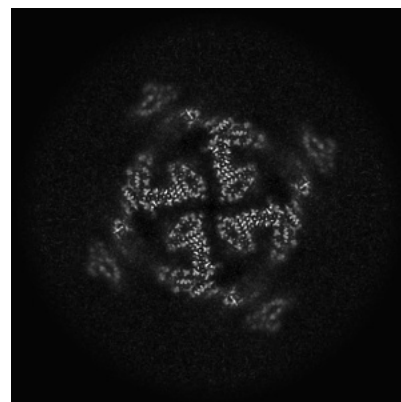
6.2.1 Primary map



X Index: 168



Y Index: 168

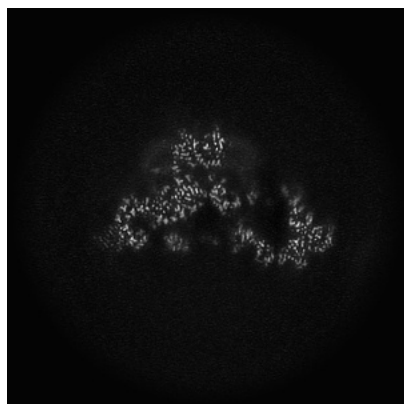


Z Index: 168

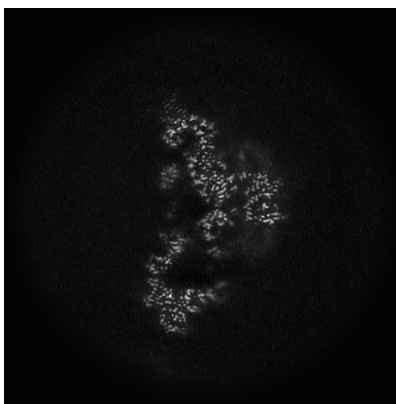
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

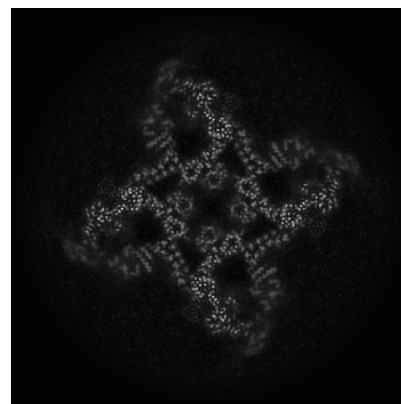
6.3.1 Primary map



X Index: 157



Y Index: 157

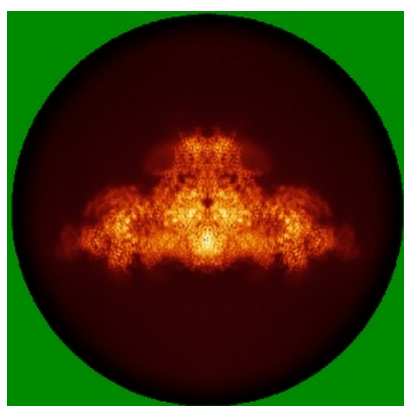


Z Index: 144

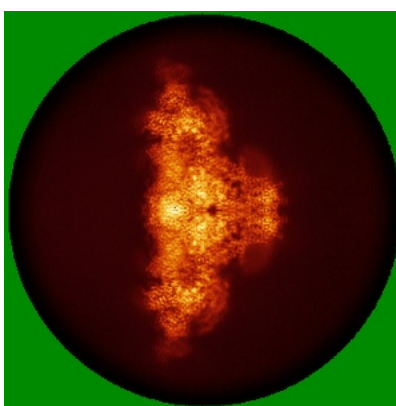
The images above show the largest variance slices of the map in three orthogonal directions.

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

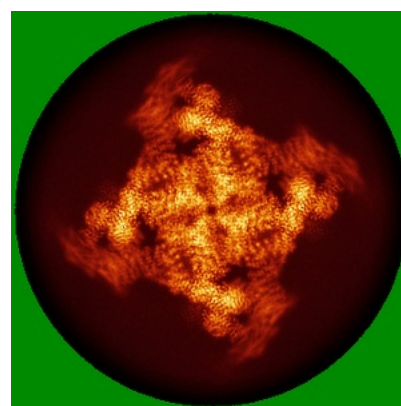
6.4.1 Primary map



X



Y



Z

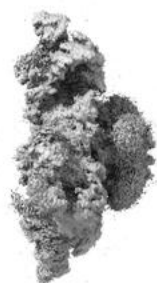
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

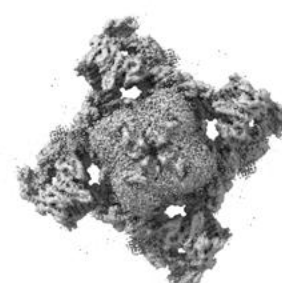
6.5.1 Primary map



X



Y



Z

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.

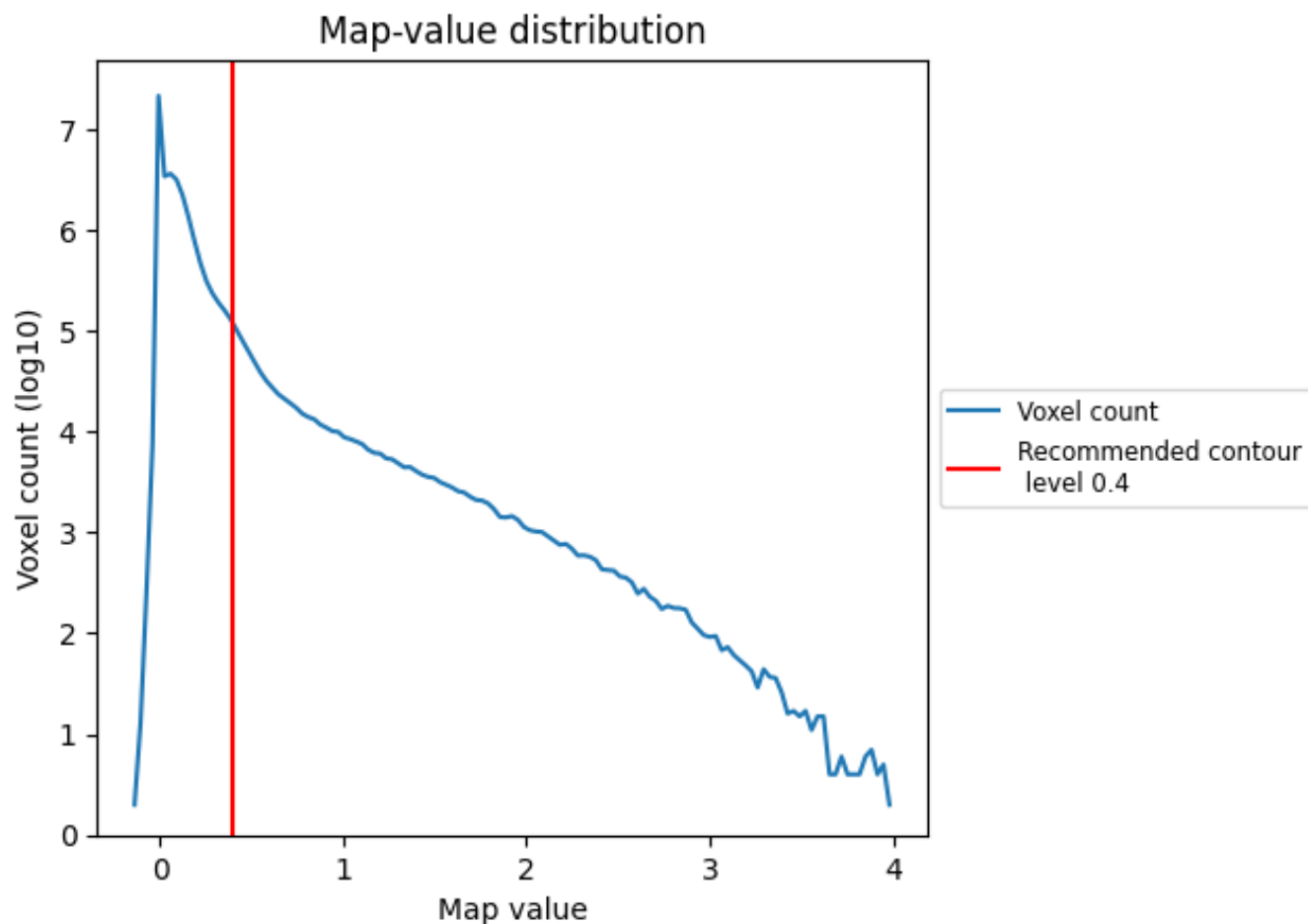
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

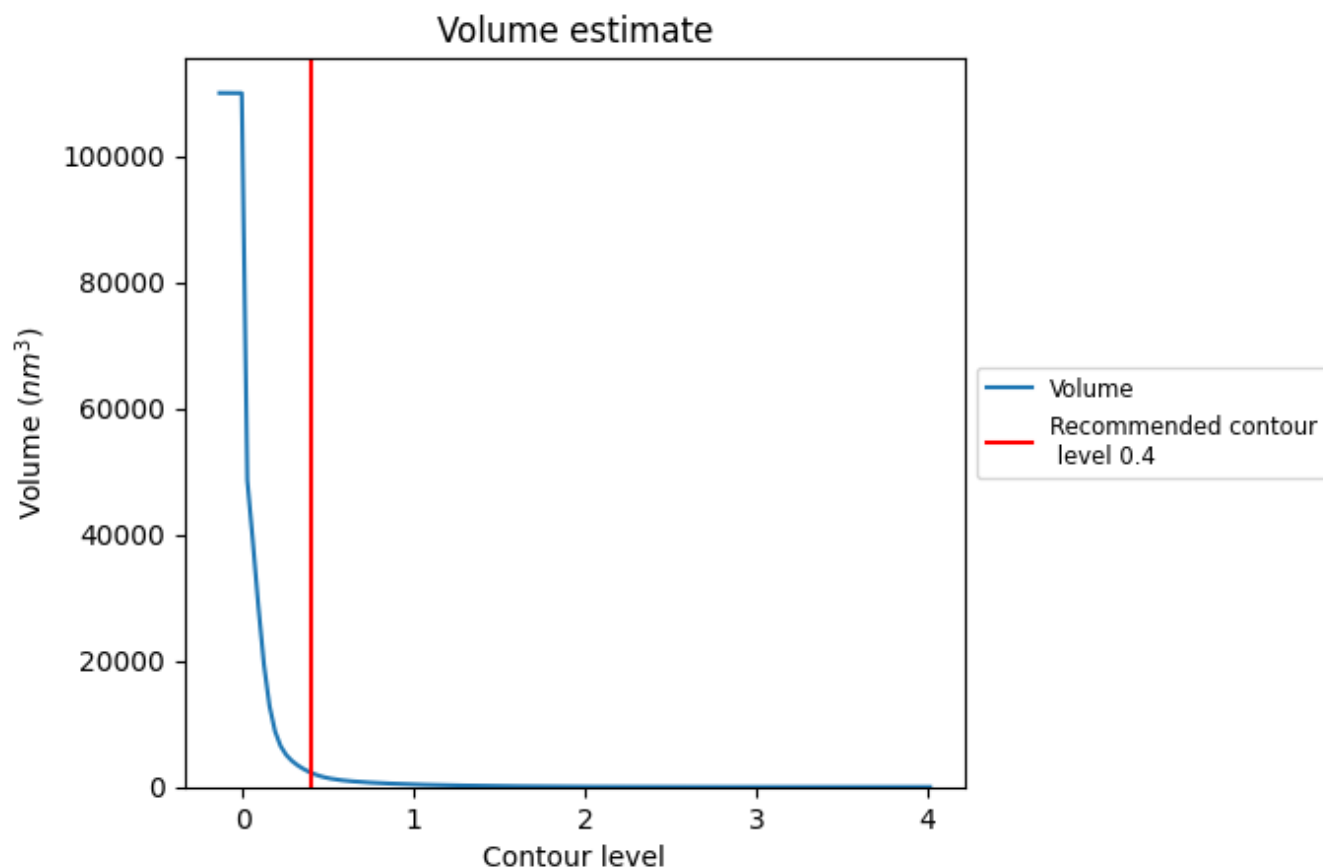
This section contains the results of statistical analysis of the map.

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.

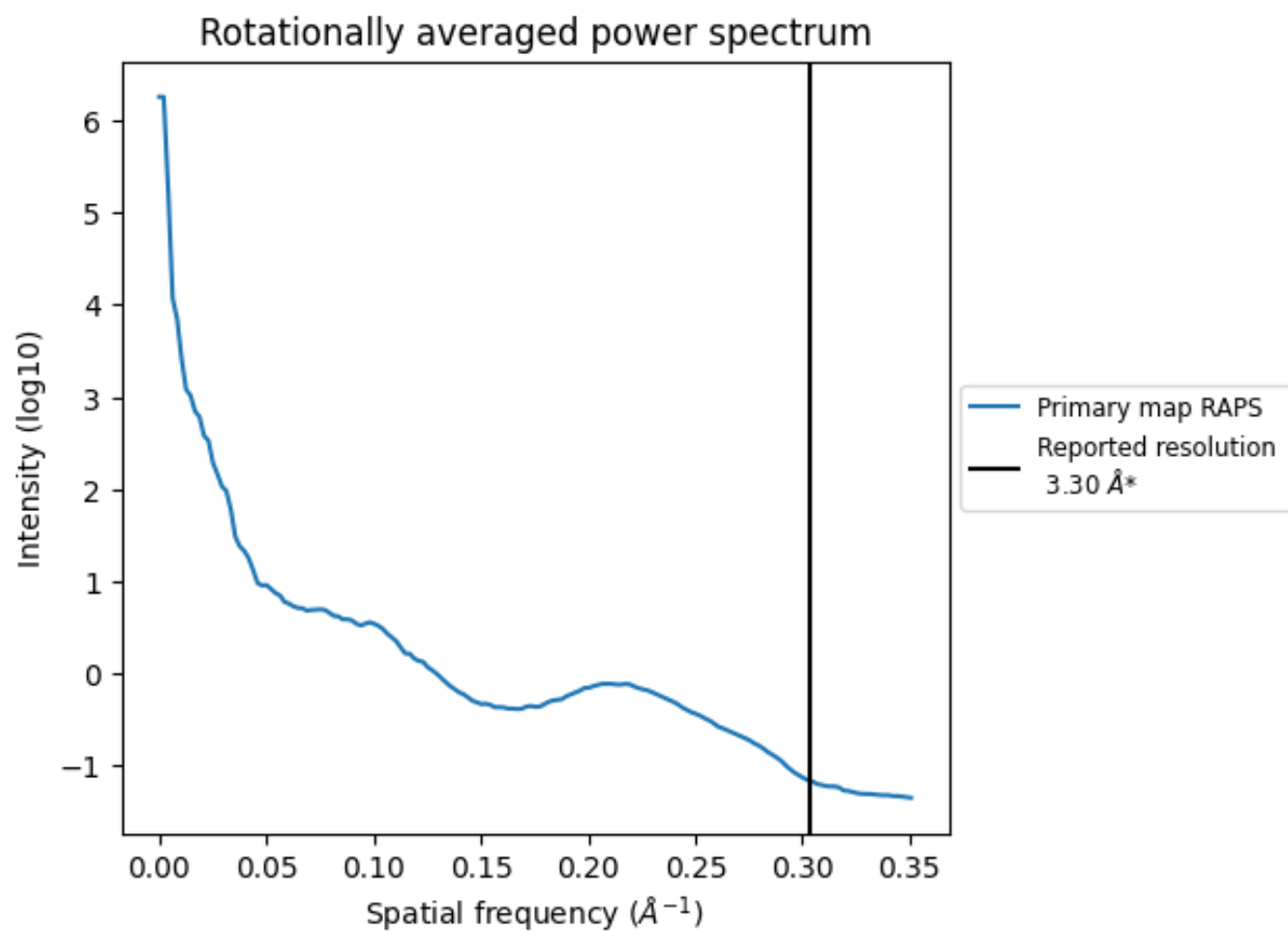
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2246 nm³; this corresponds to an approximate mass of 2029 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

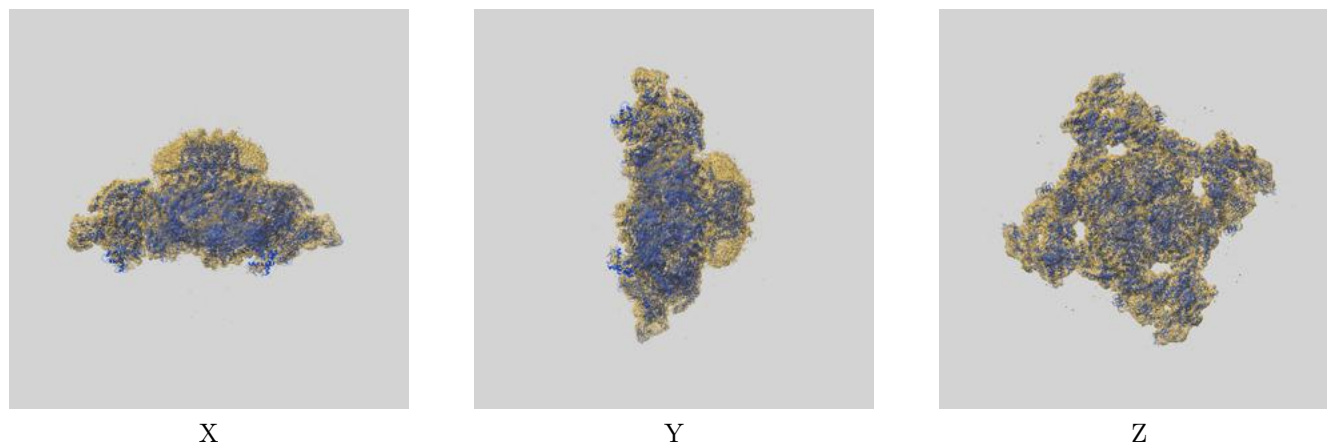
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

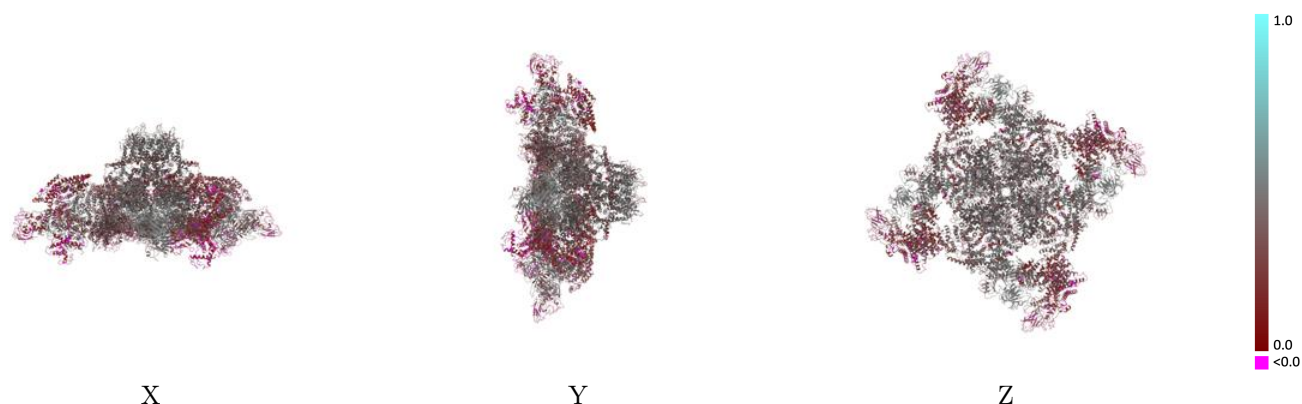
This section contains information regarding the fit between EMDB map EMD-53834 and PDB model 9R8O. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



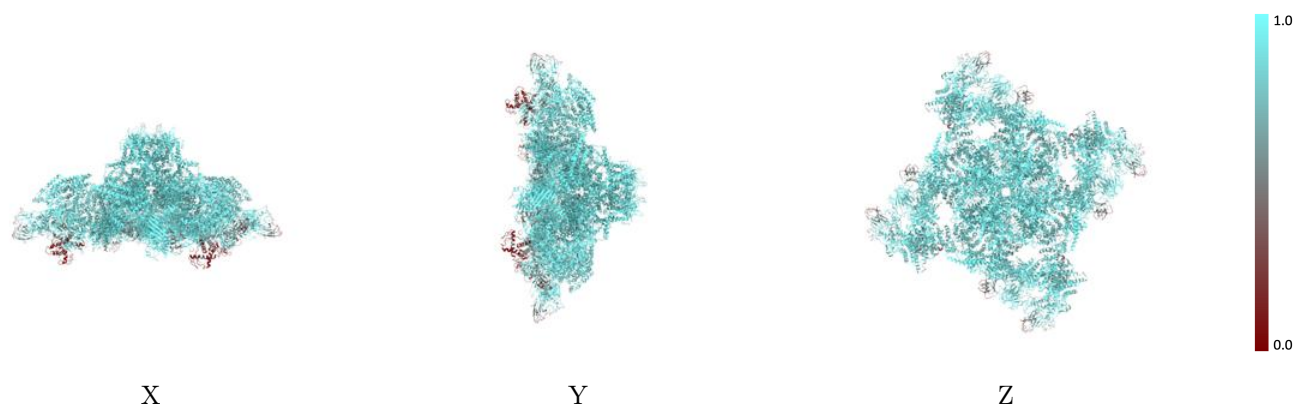
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



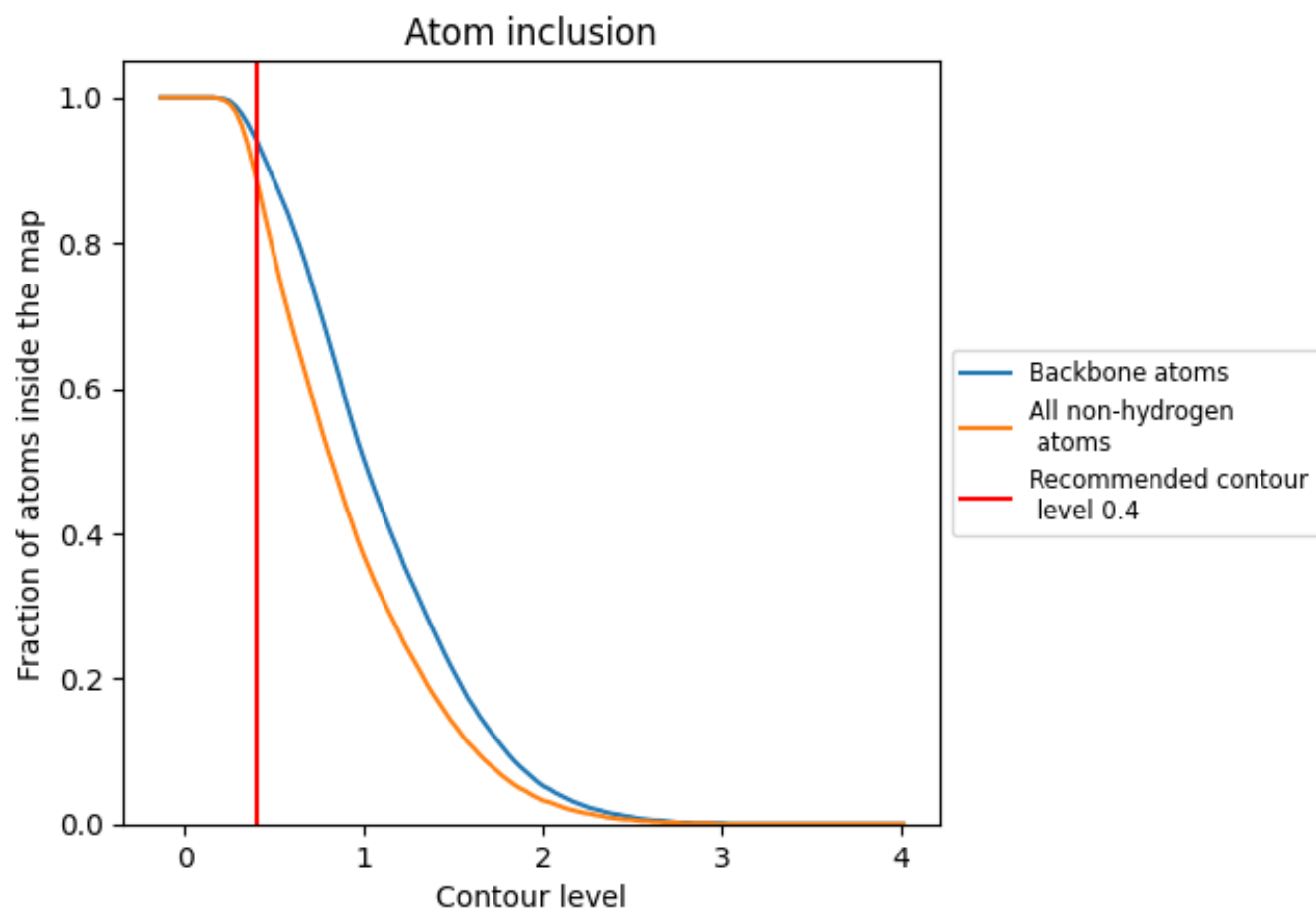
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8890	0.3420
A	0.6020	0.1580
B	0.5360	0.3510
C	0.9060	0.3460
D	0.5960	0.1580
E	0.5270	0.3530
F	0.9050	0.3470
G	0.5950	0.1570
H	0.5360	0.3530
I	0.9050	0.3470
J	0.9050	0.3460
K	0.6020	0.1640
L	0.5240	0.3530

