



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 03:10 PM UTC

PDB ID : 7VH6 / pdb_00007vh6
EMDB ID : EMD-31988
Title : Cryo-EM structure of the hexameric plasma membrane H⁺-ATPase in the active state (pH 6.0, BeF₃⁻, conformation 1, C1 symmetry)
Authors : Zhao, P.; Zhao, C.; Chen, D.; Yun, C.; Li, H.; Bai, L.
Deposited on : 2021-09-21
Resolution : 3.80 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

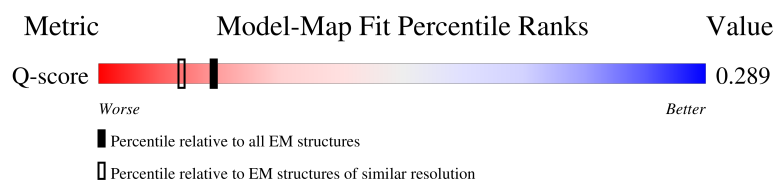
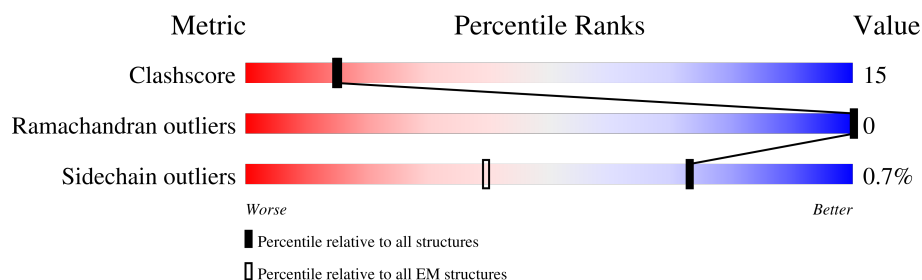
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	918	10% 60% 23% 16%
1	B	918	16% 60% 23% 16%
1	C	918	29% 60% 24% 16%
1	D	918	44% 60% 23% 16%

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Mol	Chain	Length	Quality of chain
1	E	918	
1	F	918	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BEF	A	1001	-	-	X	-
2	BEF	B	1001	-	-	X	-
2	BEF	C	1001	-	-	X	-
2	BEF	D	1001	-	-	X	-
2	BEF	E	1001	-	-	X	-
2	BEF	F	1001	-	-	X	-

2 Entry composition [i](#)

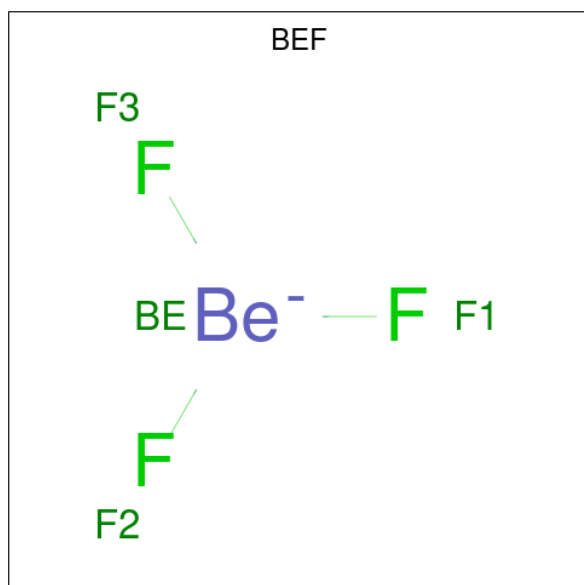
There are 3 unique types of molecules in this entry. The entry contains 38202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Plasma membrane ATPase 1.

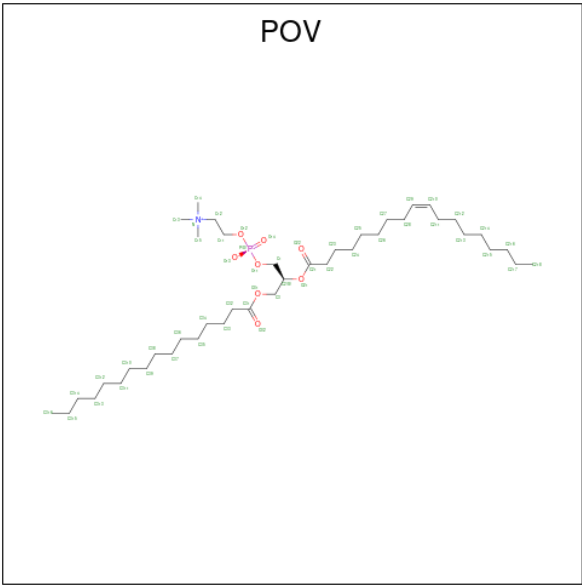
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	768	Total	C	N	O	S	0	0
			5869	3802	967	1073	27		
1	B	768	Total	C	N	O	S	0	0
			5869	3802	967	1073	27		
1	C	768	Total	C	N	O	S	0	0
			5869	3802	967	1073	27		
1	D	768	Total	C	N	O	S	0	0
			5869	3802	967	1073	27		
1	E	768	Total	C	N	O	S	0	0
			5869	3802	967	1073	27		
1	F	768	Total	C	N	O	S	0	0
			5869	3802	967	1073	27		

- Molecule 2 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	Be	F	0
			4	1	3	
2	B	1	Total	Be	F	0
			4	1	3	
2	C	1	Total	Be	F	0
			4	1	3	
2	D	1	Total	Be	F	0
			4	1	3	
2	E	1	Total	Be	F	0
			4	1	3	
2	F	1	Total	Be	F	0
			4	1	3	

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



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	

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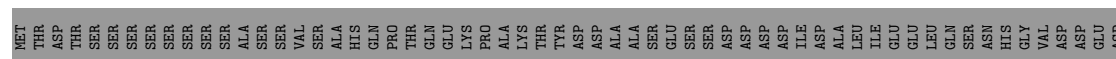
Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	

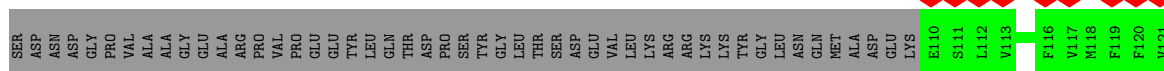
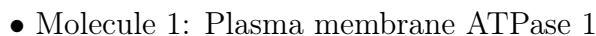
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Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	F	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	F	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	F	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	F	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	F	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	F	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	F	1	Total	C	N	O	P	0
			52	42	1	8	1	

Chain B:





V829	F830	D833	T840	S846	E847	N848	R857	T860	W861	V868	F872	E875	W876	D883	R884	G888	LYS	PRO	MET	LYS	GLU	LYS	LYS	SER	THR	ARG	SER	VAL	GLU	ASP	PHE	MET	ALA	ALA	MET	GLN	ARG	VAL	SER	THR	GLN	HIS	GLU	LYS	THR														
L702	L708	I712	L717	I722	V723	I727	L734	A737	V738	D739	P747	V748	K749	W750	W751	L752	W756	I760	L766	A767	I768	L772	T773	T776	W777	V778	L779	P780	K781	G782	G783	Q786	M791	L797	Q798	L799	S800	L801	N804	W805	I809																		
V618	V619	E620	I621	L622	Q623	N624	R625	G626	Y627	D634	G635	V636	N637	D638	K643	K644	T647	A650	V651	E652	G653	A654	T655	D656	A657	A658	R659	A662	D663	I664	V665	A668	L674	L678	R682	Q683	I684	F685	H686	R687	H688	Y694	R695	I696	A697	L698	S699	L700	H701										
G528	V529	C532	N533	D534	P535	P536	R537	Q542	T543	V544	S545	R548	H549	L550	G551	V554	A561	V562	G563	I564	E567	R570	L574	N580	A581	E582	R583	L584	G585	L586	G587	G588	GLY	GLY	ASP	MET	PRO	G594	S595	E596	D605	A608	E609	V610	K615	Y616	R617												
E468	R469	I470	V471	C472	V473	K474	G475	A476	P477	L478	F479	V480	L481	K482	T483	V484	E485	E486	D487	H488	P489	I490	P491	E492	D493	Y494	H495	E496	R497	Y498	E499	N500	K501	V502	A503	E504	L505	A506	S507	R508	G509	F510	R511	A512	L513	G514	V515	A516	R517	K518	R519	G520	E521	G522	H523	N524	E525	I526	L527
T407	A408	C409	L410	A411	A412	S413	R414	K415	K416	K417	G418	L419	D420	A421	I422	D423	K424	L427	K428	S429	L430	K431	Q432	Y433	P434	K435	A436	K437	D438	A439	L440	T441	K442	Y443	K444	V445	L446	E447	F448	H449	P450	F451	D452	P453	V454	S455	K456	K457	V458	T459	A460	V461	V462	E463	S464	P465	E466	G467	
R315	T316	N317	G318	I319	I322	T326	I332	V336	V342	K346	A347	V348	V360	L363	S364	A365	I366	E367	L375	C376	S377	D378	K379	T380	G381	T382	L383	T384	K385	N386	K387	L388	S389	L390	H391	E392	P393	Y394	T395	V396	E397	G398	V399	S400	P401	D402	D403	L404	M405	L406									
S228	A229	S234	L235	A236	V237	D238	K239	H240	Y241	G242	D243	Q244	T245	F246	S247	S248	R253	G254	E255	F257	V260	T261	G264	ASP	ASN	T267	R271	N277	K278	A279	A280	G281	G282	Q283	F286	T287	L290	G294	L297	L306	L307	V308	W309	C312	F313	Y314													
F144	L150	D170	E171	L172	K173	LYS	THR	LEU	ALA	M178	T179	A180	V181	V182	I183	R184	D185	G186	Q187	G256	V189	E190	I191	P192	A193	V196	V197	P198	G199	D200	I201	L202	Q203	L204	E205	D206	G207	T208	P211	T212	D213	G214	R215	I216	V217	T218	E219	D220	C221	Q224	I225	D226	Q227						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63661	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POV, BEF

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	0.28	1/5989 (0.0%)	0.55	4/8141 (0.0%)
1	B	0.28	1/5989 (0.0%)	0.55	4/8141 (0.0%)
1	C	0.28	1/5989 (0.0%)	0.55	4/8141 (0.0%)
1	D	0.28	1/5989 (0.0%)	0.55	4/8141 (0.0%)
1	E	0.28	1/5989 (0.0%)	0.55	4/8141 (0.0%)
1	F	0.28	1/5989 (0.0%)	0.55	4/8141 (0.0%)
All	All	0.28	6/35934 (0.0%)	0.55	24/48846 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	PRO	CG-CD	-10.91	1.13	1.50
1	F	198	PRO	CG-CD	-10.91	1.13	1.50
1	D	198	PRO	CG-CD	-10.90	1.13	1.50
1	E	198	PRO	CG-CD	-10.89	1.13	1.50
1	A	198	PRO	CG-CD	-10.89	1.13	1.50

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	PRO	N-CD-CG	-12.83	83.96	103.20
1	A	198	PRO	N-CD-CG	-12.82	83.97	103.20
1	F	198	PRO	N-CD-CG	-12.81	83.98	103.20
1	E	198	PRO	N-CD-CG	-12.81	83.99	103.20
1	B	198	PRO	N-CD-CG	-12.80	84.00	103.20

There are no chirality outliers.

There are no planarity outliers.

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	5869	0	5973	185	0
1	B	5869	0	5973	184	0
1	C	5869	0	5973	200	0
1	D	5869	0	5973	194	0
1	E	5869	0	5973	176	0
1	F	5869	0	5973	191	0
2	A	4	0	0	3	0
2	B	4	0	0	3	0
2	C	4	0	0	3	0
2	D	4	0	0	3	0
2	E	4	0	0	3	0
2	F	4	0	0	3	0
3	A	572	0	900	67	0
3	B	468	0	736	48	0
3	C	468	0	734	58	0
3	D	520	0	818	55	0
3	E	468	0	736	45	0
3	F	468	0	736	45	0
All	All	38202	0	40498	1173	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 15.

The worst 5 of 1173 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:C:400:SER:O	1:C:404:LEU:HG	1.23	1.32
1:F:400:SER:O	1:F:404:LEU:HG	1.21	1.30
1:D:400:SER:O	1:D:404:LEU:HG	1.23	1.29
1:B:400:SER:O	1:B:404:LEU:HG	1.24	1.28
1:F:315:ARG:NE	3:F:1002:POV:O13	1.67	1.28

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	760/918 (83%)	734 (97%)	26 (3%)	0	100	100
1	B	760/918 (83%)	734 (97%)	26 (3%)	0	100	100
1	C	760/918 (83%)	734 (97%)	26 (3%)	0	100	100
1	D	760/918 (83%)	734 (97%)	26 (3%)	0	100	100
1	E	760/918 (83%)	734 (97%)	26 (3%)	0	100	100
1	F	760/918 (83%)	734 (97%)	26 (3%)	0	100	100
All	All	4560/5508 (83%)	4404 (97%)	156 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	622/752 (83%)	618 (99%)	4 (1%)	78	79
1	B	622/752 (83%)	617 (99%)	5 (1%)	73	76
1	C	622/752 (83%)	616 (99%)	6 (1%)	68	74
1	D	622/752 (83%)	618 (99%)	4 (1%)	78	79
1	E	622/752 (83%)	618 (99%)	4 (1%)	78	79
1	F	622/752 (83%)	618 (99%)	4 (1%)	78	79
All	All	3732/4512 (83%)	3705 (99%)	27 (1%)	73	77

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	435	LYS
1	D	433	TYR
1	F	400	SER
1	D	400	SER
1	D	435	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	154	ASN
1	F	386	ASN
1	E	391	HIS
1	E	701	HIS
1	F	613	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

63 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	E	1002	-	51,51,51	1.23	4 (7%)	57,59,59	1.14	2 (3%)
3	POV	F	1010	3	51,51,51	1.24	6 (11%)	57,59,59	1.16	2 (3%)
2	BEF	F	1001	-	0,3,3	-	-	-	-	-
3	POV	A	1010	-	51,51,51	1.24	4 (7%)	57,59,59	1.17	4 (7%)
3	POV	E	1004	-	51,51,51	1.24	5 (9%)	57,59,59	1.08	2 (3%)
3	POV	B	1008	3	51,51,51	1.24	5 (9%)	57,59,59	1.26	3 (5%)
3	POV	E	1009	-	51,51,51	1.22	4 (7%)	57,59,59	1.18	3 (5%)
3	POV	F	1005	-	51,51,51	1.22	4 (7%)	57,59,59	1.20	2 (3%)
3	POV	F	1008	-	51,51,51	1.22	5 (9%)	57,59,59	1.22	3 (5%)
3	POV	A	1012	-	51,51,51	1.22	5 (9%)	57,59,59	1.19	3 (5%)
3	POV	D	1010	-	51,51,51	1.21	4 (7%)	57,59,59	1.18	3 (5%)
2	BEF	A	1001	-	0,3,3	-	-	-	-	-
3	POV	B	1005	-	51,51,51	1.22	5 (9%)	57,59,59	1.12	2 (3%)
3	POV	C	1009	-	51,51,51	1.21	4 (7%)	57,59,59	1.20	3 (5%)
3	POV	B	1010	-	51,51,51	1.21	4 (7%)	57,59,59	1.19	3 (5%)
3	POV	A	1005	-	51,51,51	1.22	5 (9%)	57,59,59	1.18	3 (5%)
3	POV	C	1003	-	51,51,51	1.26	5 (9%)	57,59,59	1.18	2 (3%)
3	POV	F	1004	-	51,51,51	1.22	5 (9%)	57,59,59	1.18	3 (5%)
3	POV	F	1006	3	51,51,51	1.26	6 (11%)	57,59,59	1.26	4 (7%)
3	POV	B	1009	-	51,51,51	1.22	4 (7%)	57,59,59	1.15	3 (5%)
3	POV	E	1010	3	51,51,51	1.23	5 (9%)	57,59,59	1.16	2 (3%)
3	POV	C	1002	-	51,51,51	1.23	4 (7%)	57,59,59	1.11	2 (3%)
3	POV	C	1004	-	51,51,51	1.22	5 (9%)	57,59,59	1.12	2 (3%)
3	POV	E	1005	-	51,51,51	1.21	4 (7%)	57,59,59	1.18	4 (7%)
3	POV	A	1006	-	51,51,51	1.22	4 (7%)	57,59,59	1.19	2 (3%)
3	POV	B	1004	-	51,51,51	1.24	4 (7%)	57,59,59	1.21	3 (5%)
3	POV	C	1005	-	51,51,51	1.21	4 (7%)	57,59,59	1.19	3 (5%)
3	POV	A	1004	-	51,51,51	1.22	5 (9%)	57,59,59	1.11	2 (3%)
3	POV	D	1005	-	51,51,51	1.21	4 (7%)	57,59,59	1.19	3 (5%)
3	POV	B	1002	3	51,51,51	1.24	6 (11%)	57,59,59	1.16	2 (3%)
3	POV	D	1008	-	51,51,51	1.22	4 (7%)	57,59,59	1.16	3 (5%)
3	POV	F	1002	-	51,51,51	1.23	5 (9%)	57,59,59	1.17	2 (3%)
3	POV	A	1003	-	51,51,51	1.24	5 (9%)	57,59,59	1.21	2 (3%)
3	POV	C	1007	3	51,51,51	1.25	6 (11%)	57,59,59	1.27	3 (5%)
2	BEF	C	1001	-	0,3,3	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	F	1009	-	51,51,51	1.21	4 (7%)	57,59,59	1.15	3 (5%)
3	POV	D	1007	3	51,51,51	1.25	6 (11%)	57,59,59	1.25	3 (5%)
2	BEF	E	1001	-	0,3,3	-	-	-	-	-
3	POV	F	1003	-	51,51,51	1.22	5 (9%)	57,59,59	1.12	2 (3%)
3	POV	D	1011	3	51,51,51	1.22	5 (9%)	57,59,59	1.17	2 (3%)
2	BEF	B	1001	-	0,3,3	-	-	-	-	-
3	POV	A	1002	-	51,51,51	1.24	4 (7%)	57,59,59	1.15	3 (5%)
3	POV	E	1008	-	51,51,51	1.23	4 (7%)	57,59,59	1.14	2 (3%)
3	POV	B	1007	-	51,51,51	1.22	4 (7%)	57,59,59	1.19	2 (3%)
3	POV	C	1010	3	51,51,51	1.22	5 (9%)	57,59,59	1.19	2 (3%)
3	POV	D	1006	-	51,51,51	1.22	5 (9%)	57,59,59	1.22	2 (3%)
3	POV	A	1008	-	51,51,51	1.22	4 (7%)	57,59,59	1.14	2 (3%)
3	POV	E	1007	3	51,51,51	1.25	6 (11%)	57,59,59	1.25	3 (5%)
3	POV	D	1004	-	51,51,51	1.21	5 (9%)	57,59,59	1.16	2 (3%)
3	POV	D	1009	-	51,51,51	1.21	5 (9%)	57,59,59	1.22	3 (5%)
3	POV	C	1008	-	51,51,51	1.22	4 (7%)	57,59,59	1.18	3 (5%)
3	POV	D	1003	-	51,51,51	1.27	6 (11%)	57,59,59	1.17	3 (5%)
3	POV	B	1003	-	51,51,51	1.22	4 (7%)	57,59,59	1.18	3 (5%)
3	POV	A	1007	3	51,51,51	1.25	6 (11%)	57,59,59	1.24	3 (5%)
3	POV	C	1006	-	51,51,51	1.21	4 (7%)	57,59,59	1.23	3 (5%)
3	POV	A	1011	3	51,51,51	1.24	6 (11%)	57,59,59	1.14	2 (3%)
3	POV	B	1006	-	51,51,51	1.22	5 (9%)	57,59,59	1.18	3 (5%)
3	POV	D	1002	-	51,51,51	1.24	4 (7%)	57,59,59	1.11	3 (5%)
3	POV	E	1006	-	51,51,51	1.22	4 (7%)	57,59,59	1.18	3 (5%)
3	POV	A	1009	-	51,51,51	1.21	4 (7%)	57,59,59	1.18	3 (5%)
3	POV	E	1003	-	51,51,51	1.25	6 (11%)	57,59,59	1.16	3 (5%)
2	BEF	D	1001	-	0,3,3	-	-	-	-	-
3	POV	F	1007	-	51,51,51	1.23	4 (7%)	57,59,59	1.16	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	E	1002	-	-	25/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	F	1010	3	-	24/55/55/55	-
3	POV	A	1010	-	-	26/55/55/55	-
3	POV	B	1008	3	-	21/55/55/55	-
3	POV	E	1009	-	-	23/55/55/55	-
3	POV	F	1005	-	-	26/55/55/55	-
3	POV	F	1008	-	-	20/55/55/55	-
3	POV	A	1012	-	-	21/55/55/55	-
3	POV	D	1010	-	-	22/55/55/55	-
3	POV	B	1005	-	-	24/55/55/55	-
3	POV	C	1009	-	-	23/55/55/55	-
3	POV	B	1010	-	-	22/55/55/55	-
3	POV	A	1005	-	-	26/55/55/55	-
3	POV	C	1003	-	-	25/55/55/55	-
3	POV	F	1004	-	-	27/55/55/55	-
3	POV	F	1006	3	-	21/55/55/55	-
3	POV	B	1009	-	-	28/55/55/55	-
3	POV	E	1010	3	-	24/55/55/55	-
3	POV	C	1002	-	-	27/55/55/55	-
3	POV	C	1004	-	-	22/55/55/55	-
3	POV	E	1005	-	-	26/55/55/55	-
3	POV	A	1006	-	-	27/55/55/55	-
3	POV	B	1004	-	-	24/55/55/55	-
3	POV	C	1005	-	-	27/55/55/55	-
3	POV	A	1004	-	-	23/55/55/55	-
3	POV	D	1005	-	-	25/55/55/55	-
3	POV	B	1002	3	-	26/55/55/55	-
3	POV	D	1008	-	-	29/55/55/55	-
3	POV	F	1002	-	-	26/55/55/55	-
3	POV	A	1003	-	-	23/55/55/55	-
3	POV	C	1007	3	-	23/55/55/55	-
3	POV	F	1009	-	-	22/55/55/55	-
3	POV	D	1007	3	-	23/55/55/55	-
3	POV	F	1003	-	-	24/55/55/55	-
3	POV	D	1011	3	-	22/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	E	1008	-	-	25/55/55/55	-
3	POV	A	1002	-	-	26/55/55/55	-
3	POV	B	1007	-	-	27/55/55/55	-
3	POV	C	1010	3	-	22/55/55/55	-
3	POV	D	1006	-	-	28/55/55/55	-
3	POV	A	1008	-	-	27/55/55/55	-
3	POV	E	1007	3	-	19/55/55/55	-
3	POV	D	1004	-	-	24/55/55/55	-
3	POV	D	1009	-	-	21/55/55/55	-
3	POV	C	1008	-	-	24/55/55/55	-
3	POV	D	1003	-	-	25/55/55/55	-
3	POV	B	1003	-	-	30/55/55/55	-
3	POV	A	1007	3	-	22/55/55/55	-
3	POV	C	1006	-	-	27/55/55/55	-
3	POV	A	1011	3	-	21/55/55/55	-
3	POV	B	1006	-	-	27/55/55/55	-
3	POV	D	1002	-	-	26/55/55/55	-
3	POV	E	1006	-	-	26/55/55/55	-
3	POV	A	1009	-	-	24/55/55/55	-
3	POV	E	1003	-	-	26/55/55/55	-
3	POV	E	1004	-	-	26/55/55/55	-
3	POV	F	1007	-	-	31/55/55/55	-

The worst 5 of 268 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1004	POV	O31-C31	3.84	1.44	1.33
3	D	1003	POV	O31-C31	3.82	1.44	1.33
3	D	1002	POV	O31-C31	3.79	1.44	1.33
3	C	1003	POV	O31-C31	3.79	1.44	1.33
3	A	1005	POV	O31-C31	3.78	1.44	1.33

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1006	POV	O21-C21-C22	5.06	122.43	111.48
3	E	1007	POV	O21-C21-C22	4.86	122.00	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	1007	POV	O21-C21-C22	4.79	121.85	111.48
3	D	1007	POV	O21-C21-C22	4.78	121.81	111.48
3	C	1007	POV	O21-C21-C22	4.72	121.69	111.48

There are no chirality outliers.

5 of 1401 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	POV	C1-O11-P-O14
3	A	1003	POV	C12-C11-O12-P
3	A	1004	POV	C1-O11-P-O13
3	A	1005	POV	C22-C21-O21-C2
3	A	1006	POV	C1-O11-P-O14

There are no ring outliers.

63 monomers are involved in 305 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1002	POV	11	0
3	F	1010	POV	5	0
2	F	1001	BEF	3	0
3	A	1010	POV	14	0
3	E	1004	POV	5	0
3	B	1008	POV	3	0
3	E	1009	POV	3	0
3	F	1005	POV	9	0
3	F	1008	POV	3	0
3	A	1012	POV	5	0
3	D	1010	POV	4	0
2	A	1001	BEF	3	0
3	B	1005	POV	6	0
3	C	1009	POV	5	0
3	B	1010	POV	6	0
3	A	1005	POV	5	0
3	C	1003	POV	8	0
3	F	1004	POV	8	0
3	F	1006	POV	4	0
3	B	1009	POV	2	0
3	E	1010	POV	5	0
3	C	1002	POV	12	0
3	C	1004	POV	14	0

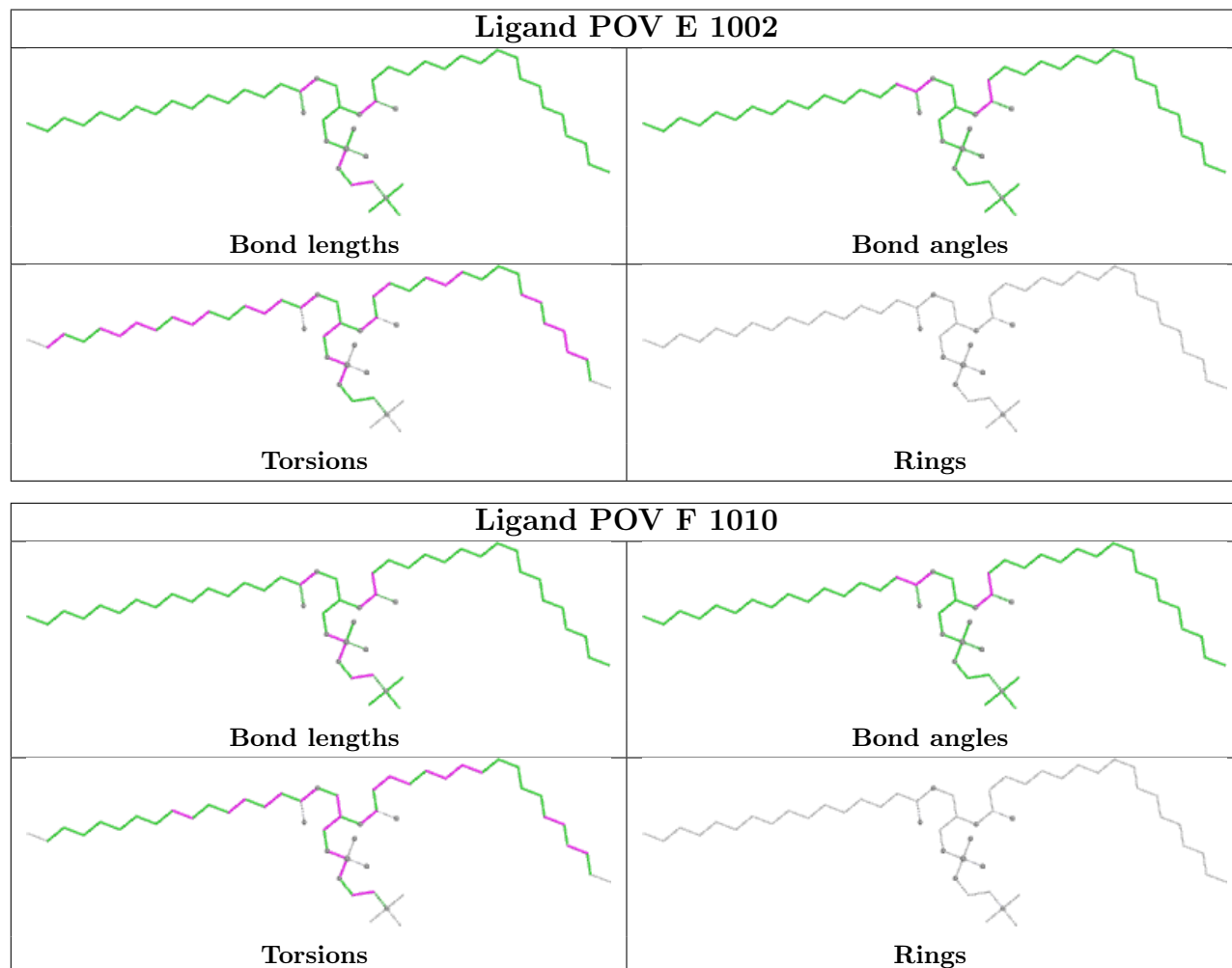
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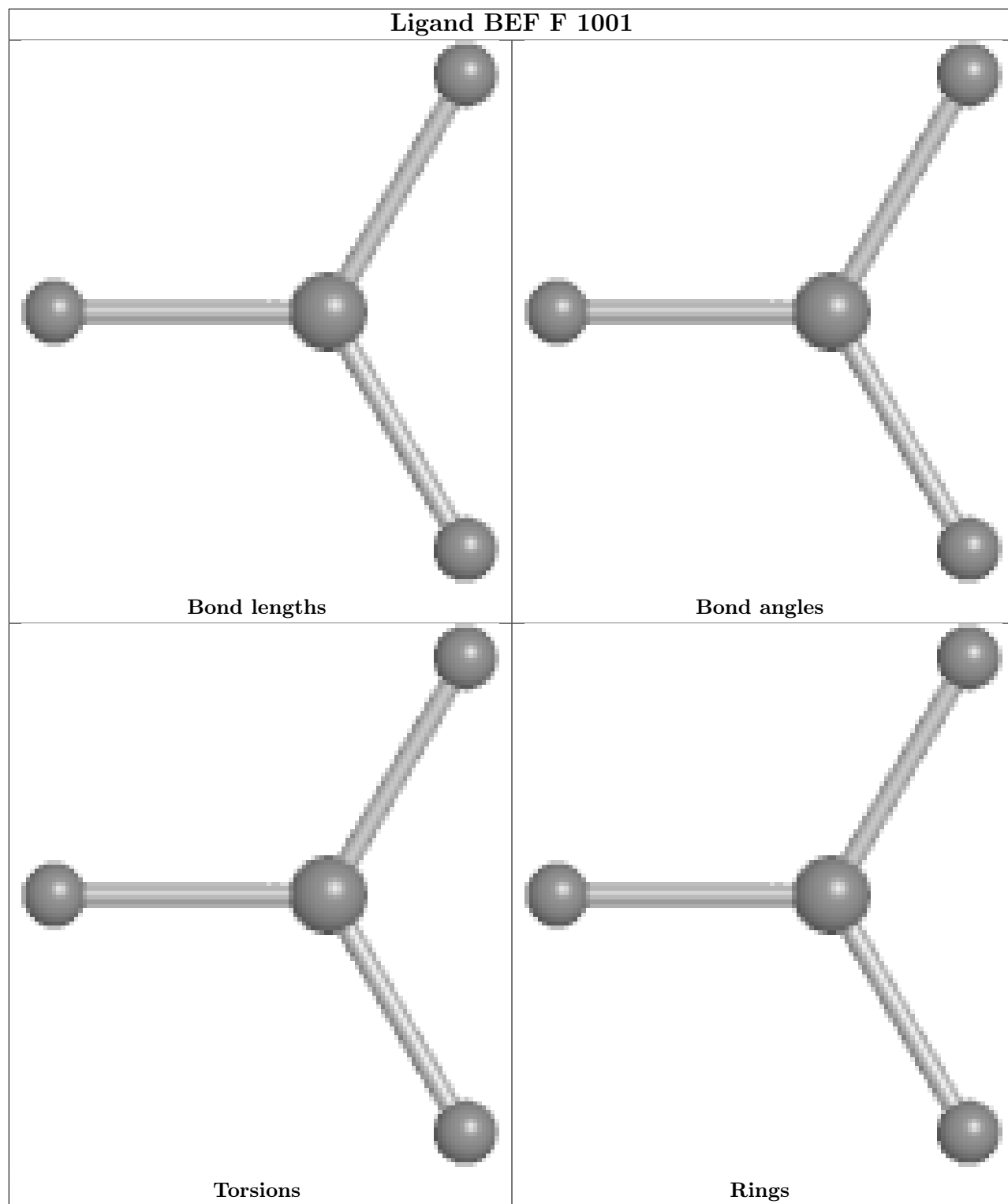
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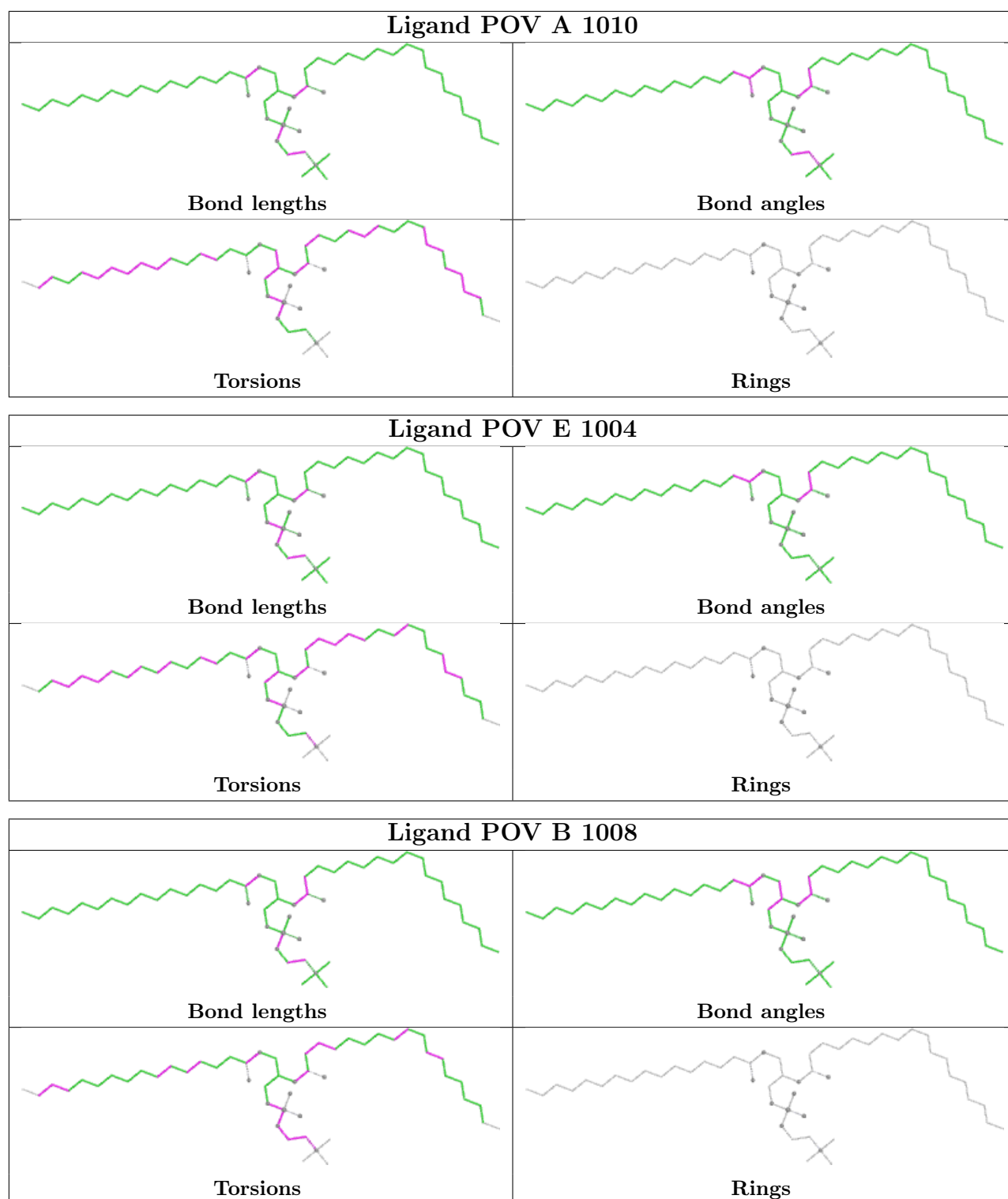
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1005	POV	7	0
3	A	1006	POV	6	0
3	B	1004	POV	9	0
3	C	1005	POV	7	0
3	A	1004	POV	7	0
3	D	1005	POV	8	0
3	B	1002	POV	6	0
3	D	1008	POV	2	0
3	F	1002	POV	10	0
3	A	1003	POV	9	0
3	C	1007	POV	4	0
2	C	1001	BEF	3	0
3	F	1009	POV	6	0
3	D	1007	POV	5	0
2	E	1001	BEF	3	0
3	F	1003	POV	7	0
3	D	1011	POV	4	0
2	B	1001	BEF	3	0
3	A	1002	POV	13	0
3	E	1008	POV	3	0
3	B	1007	POV	6	0
3	C	1010	POV	4	0
3	D	1006	POV	4	0
3	A	1008	POV	4	0
3	E	1007	POV	4	0
3	D	1004	POV	14	0
3	D	1009	POV	3	0
3	C	1008	POV	5	0
3	D	1003	POV	8	0
3	B	1003	POV	10	0
3	A	1007	POV	5	0
3	C	1006	POV	8	0
3	A	1011	POV	6	0
3	B	1006	POV	8	0
3	D	1002	POV	11	0
3	E	1006	POV	4	0
3	A	1009	POV	1	0
3	E	1003	POV	8	0
2	D	1001	BEF	3	0
3	F	1007	POV	4	0

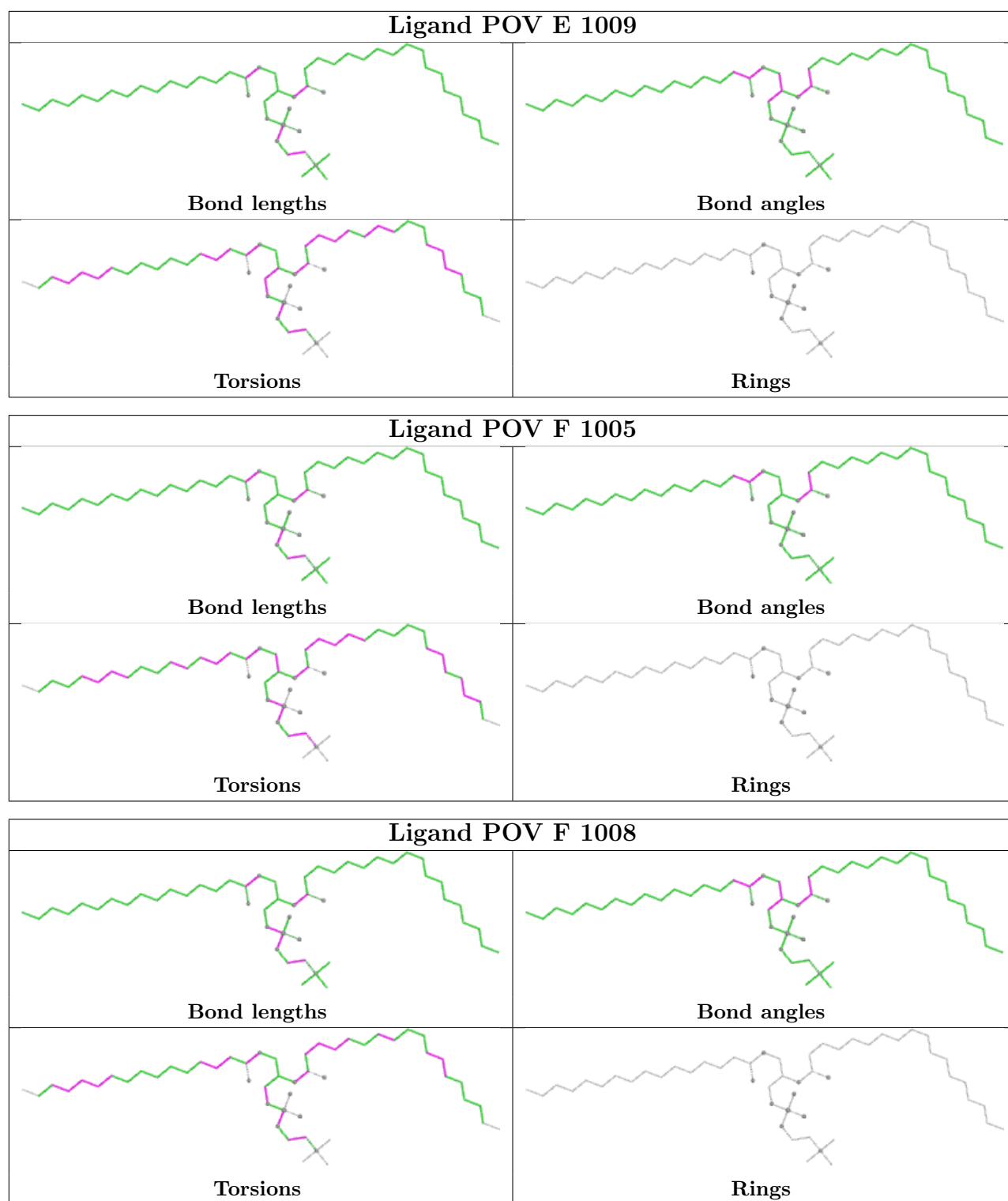
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

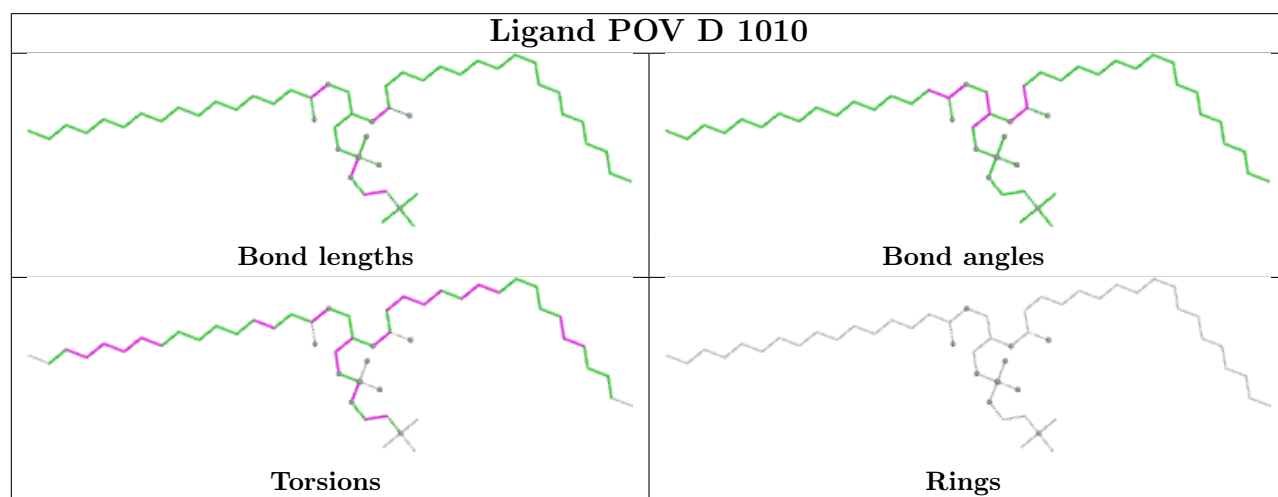
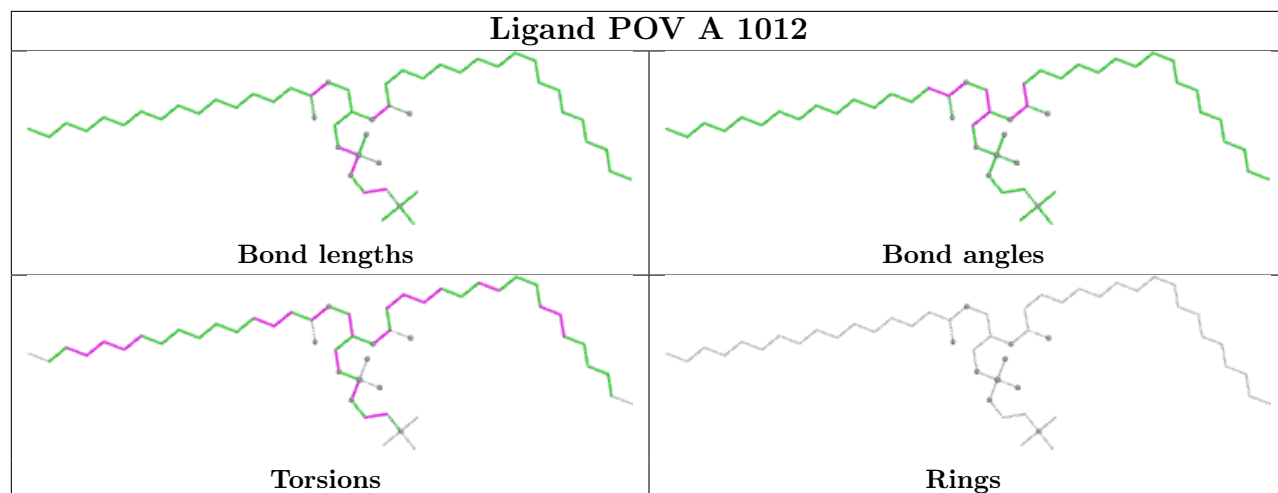
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

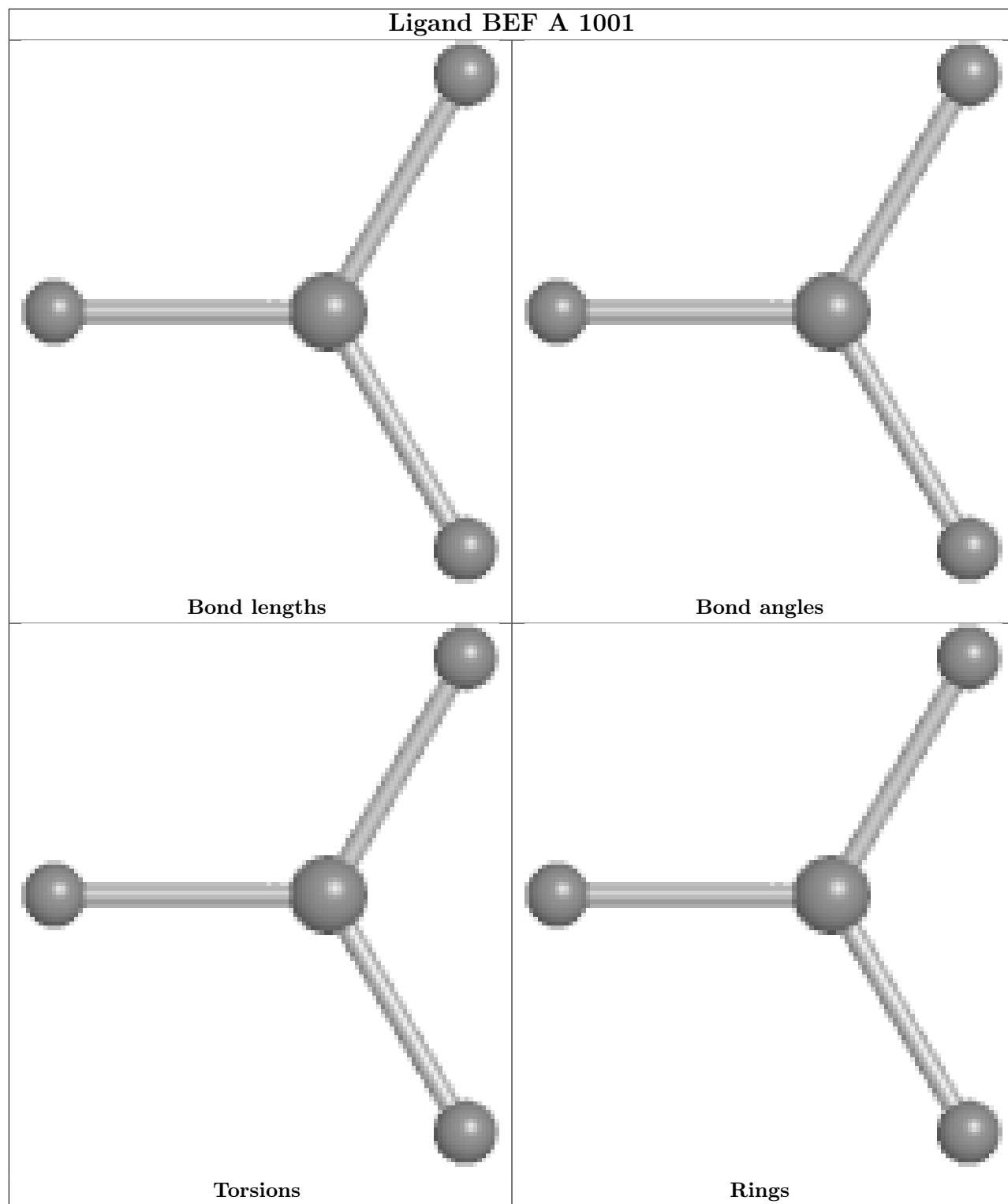


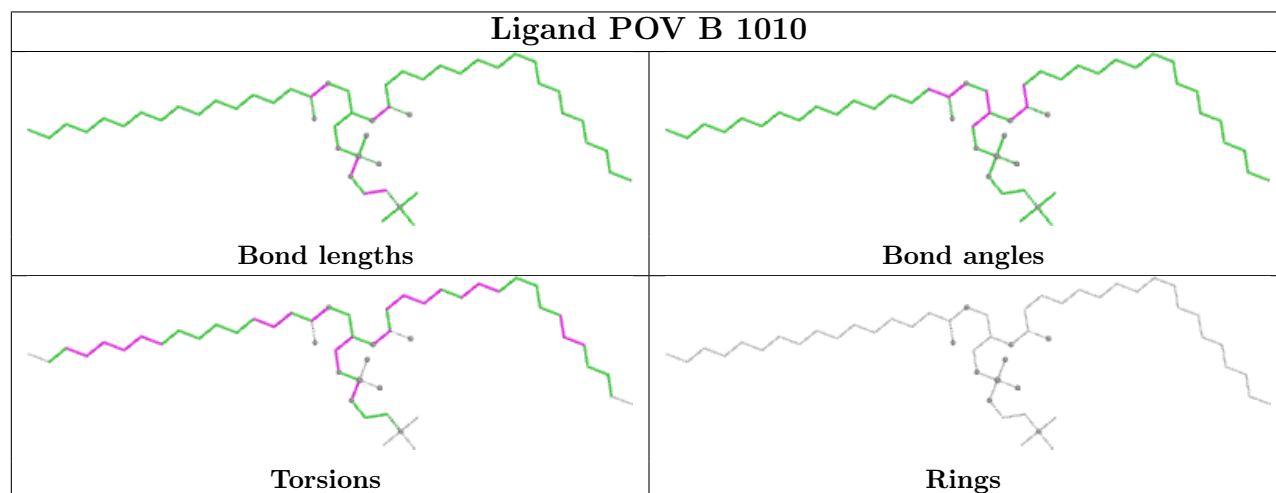
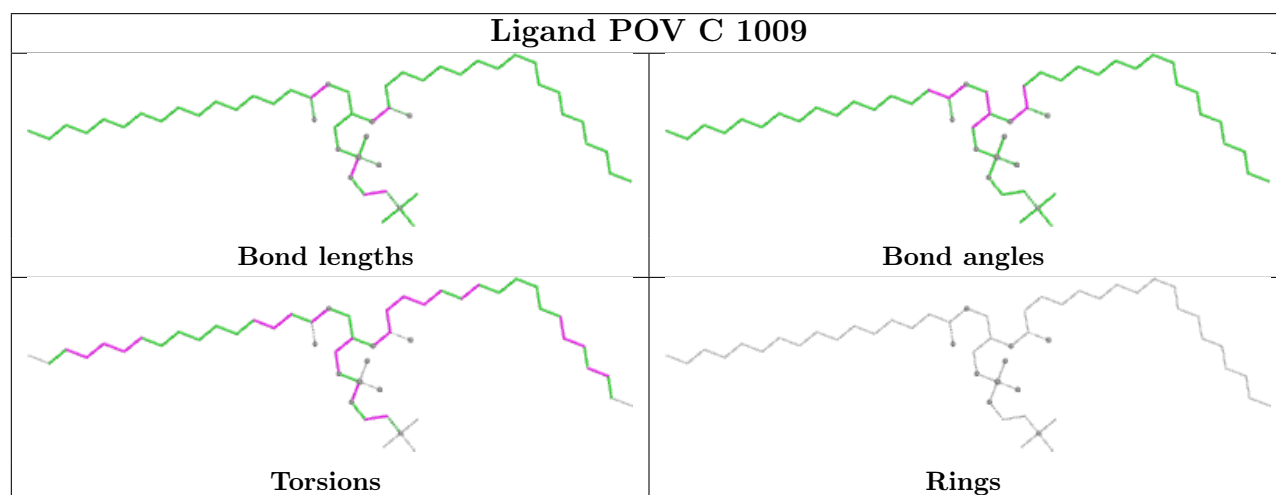
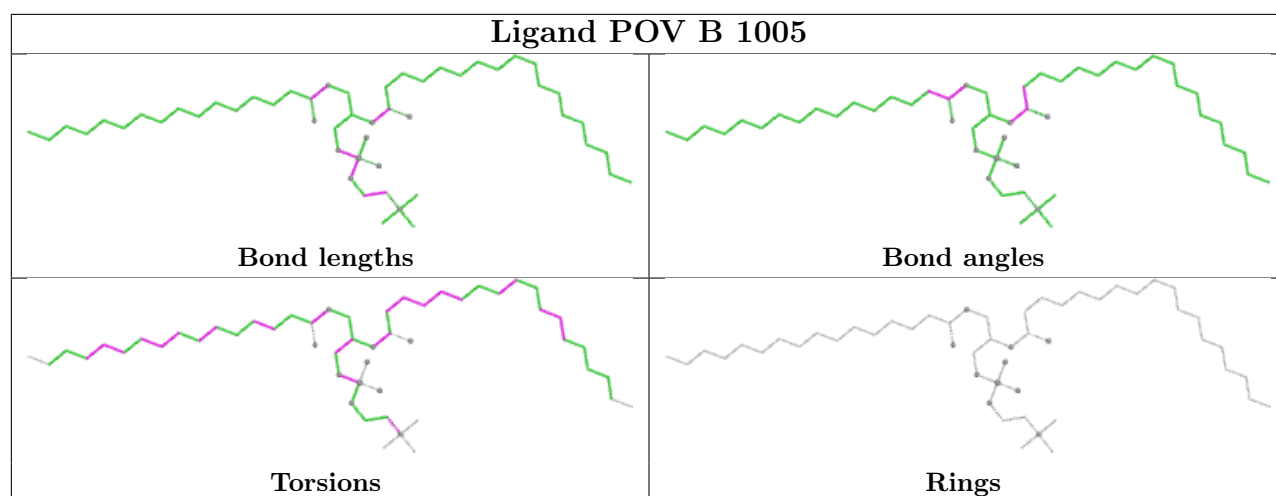


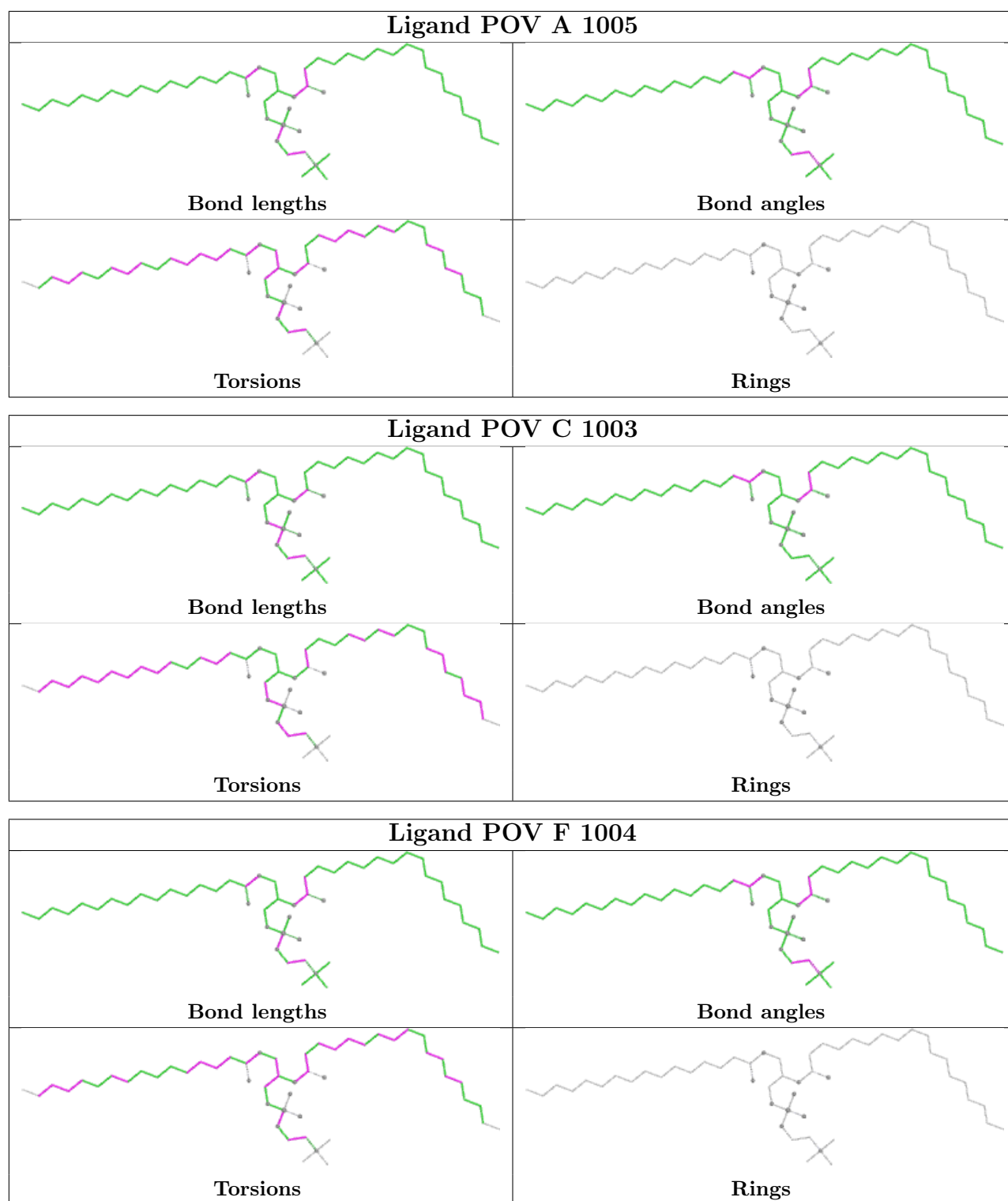


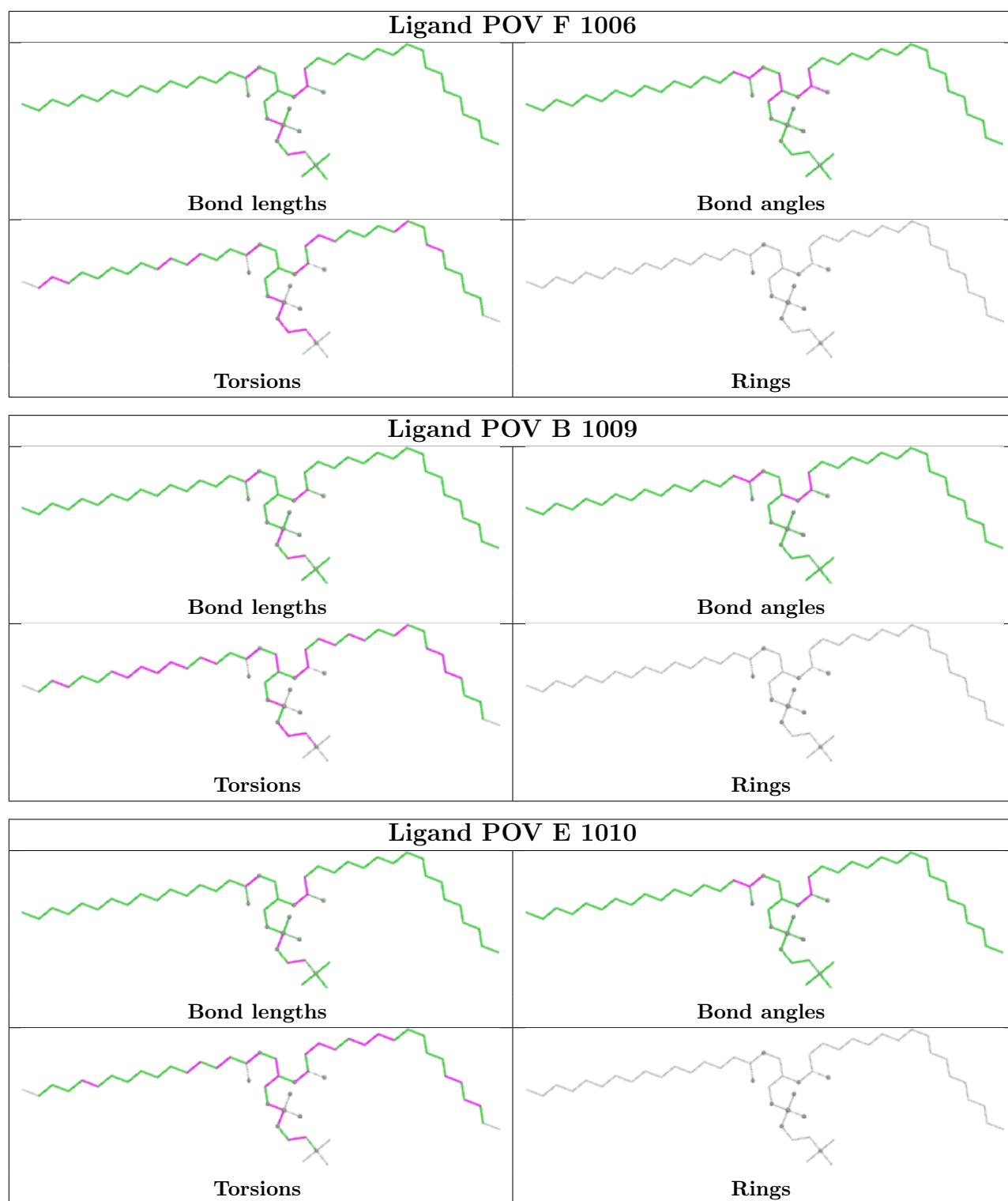


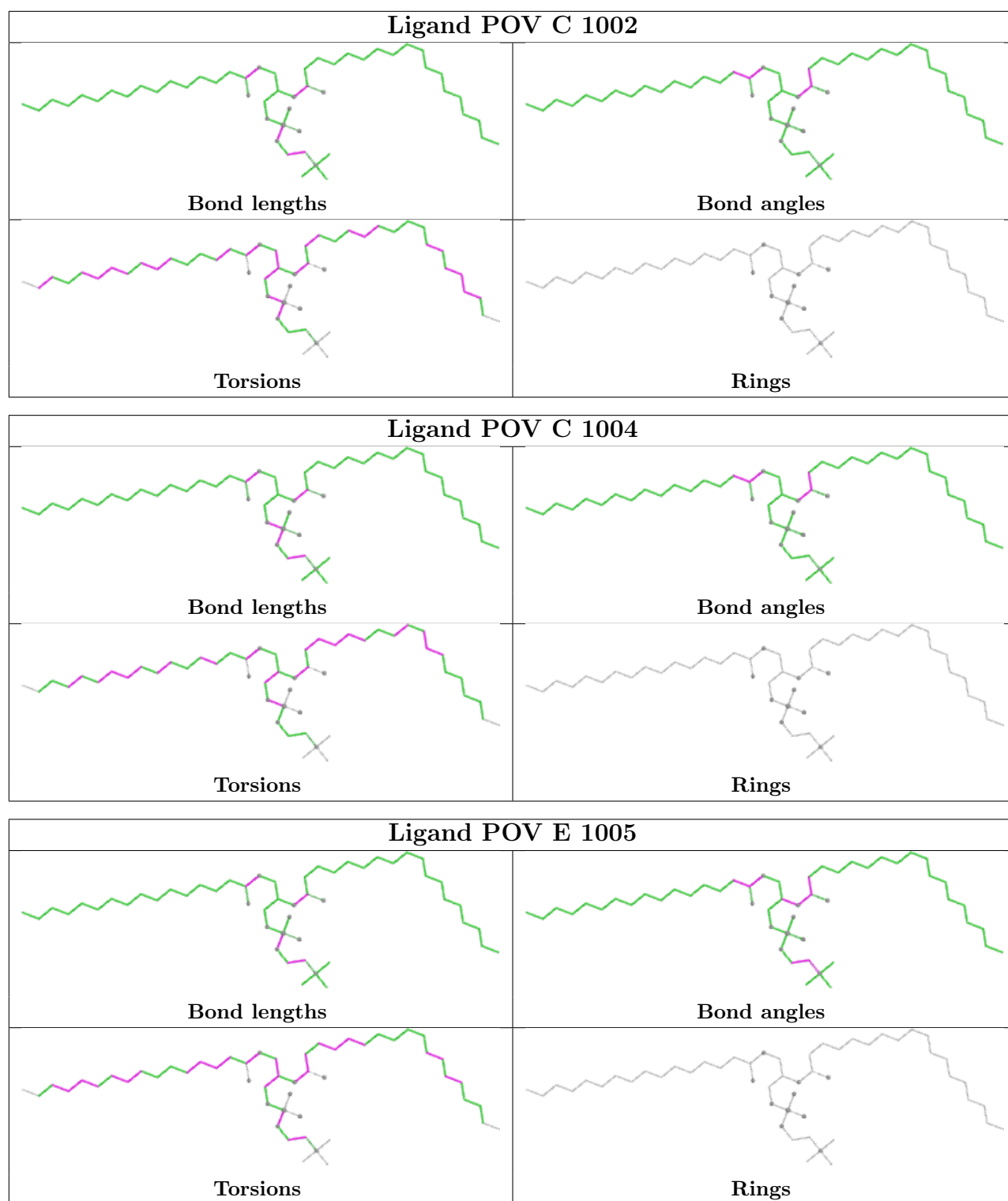


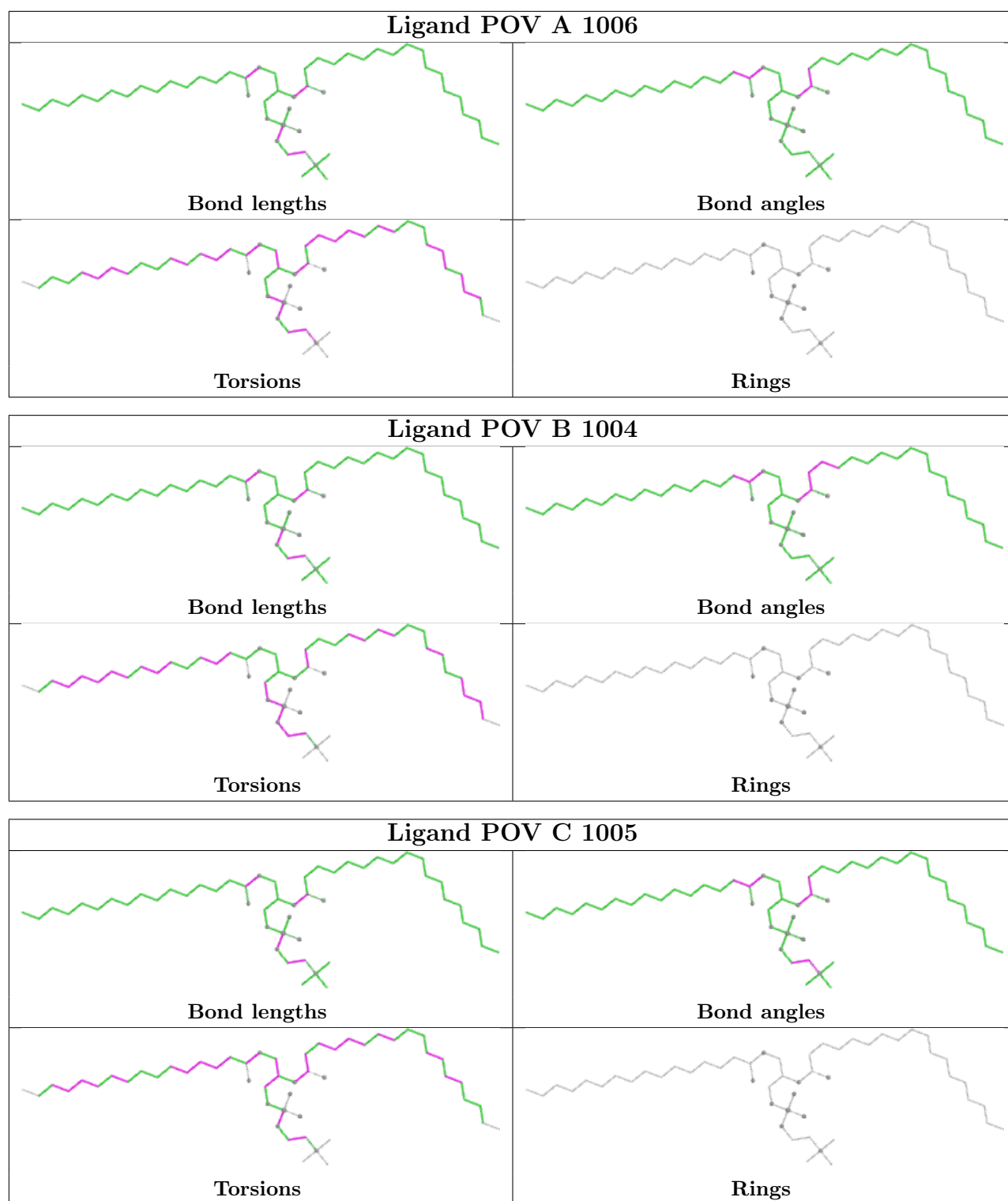


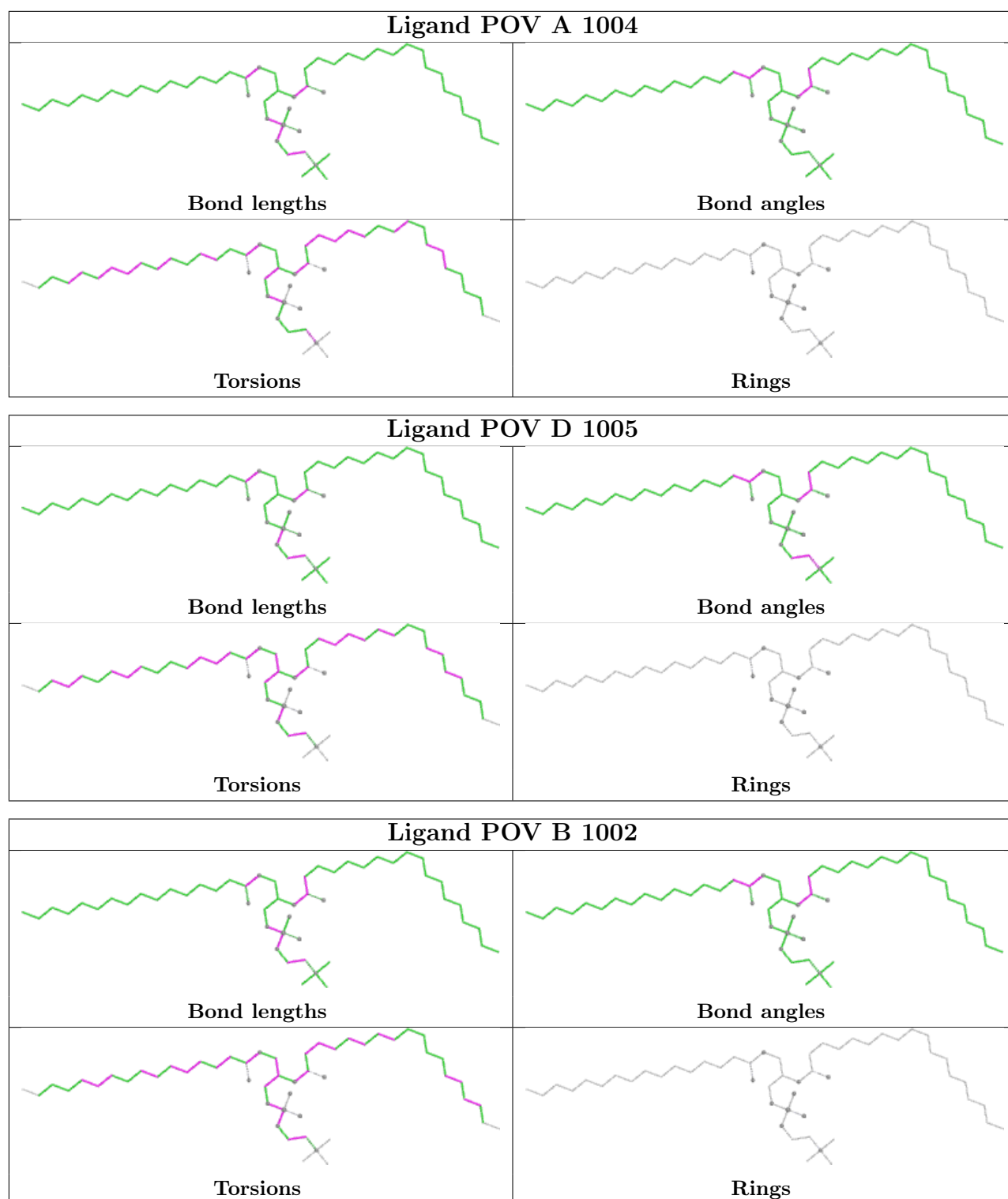


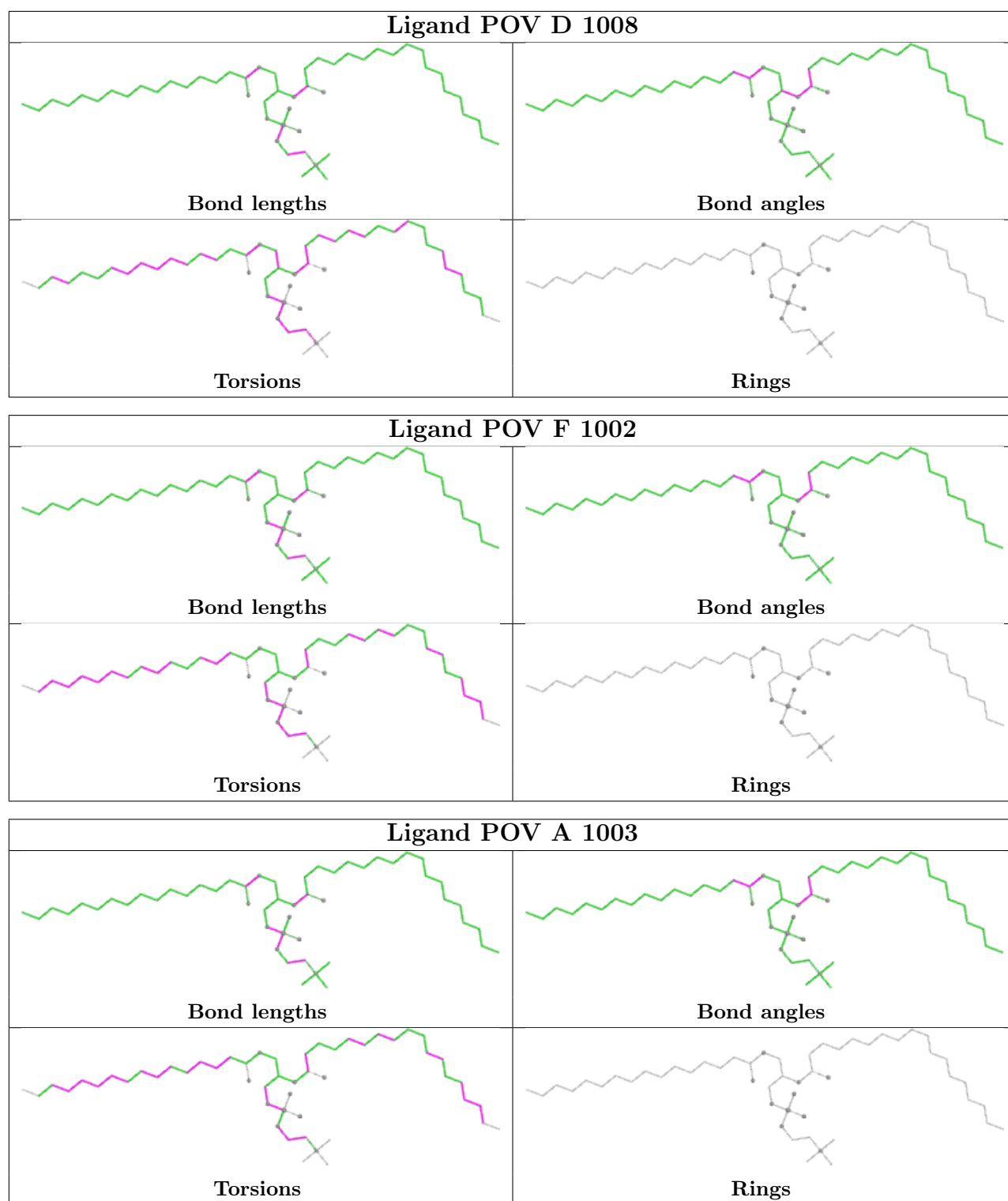


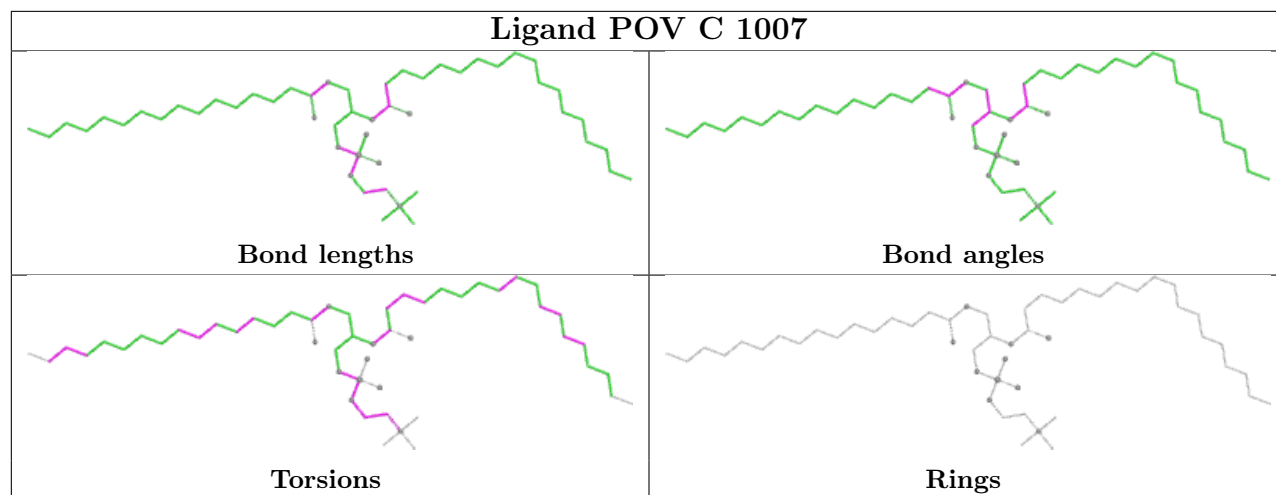


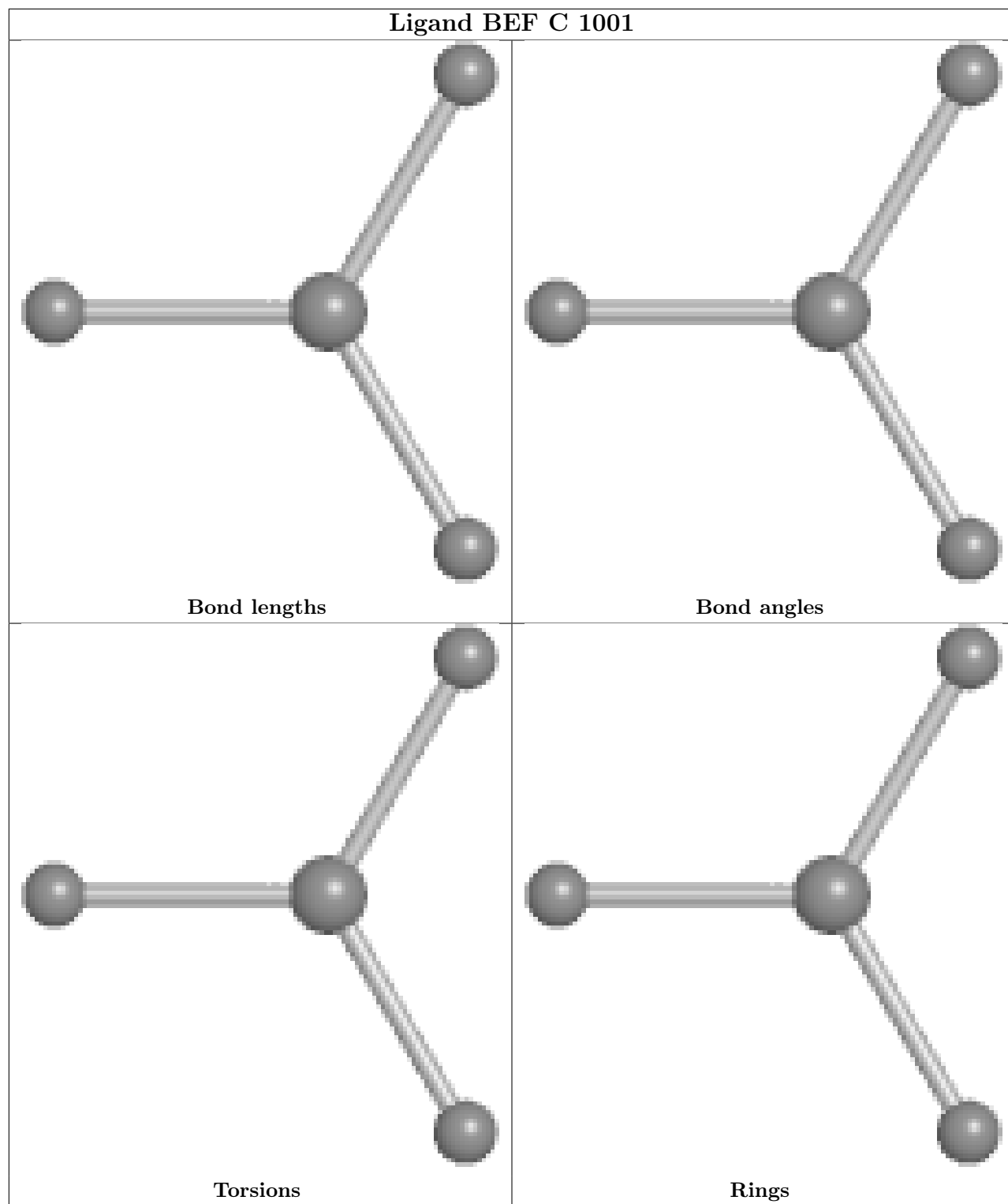


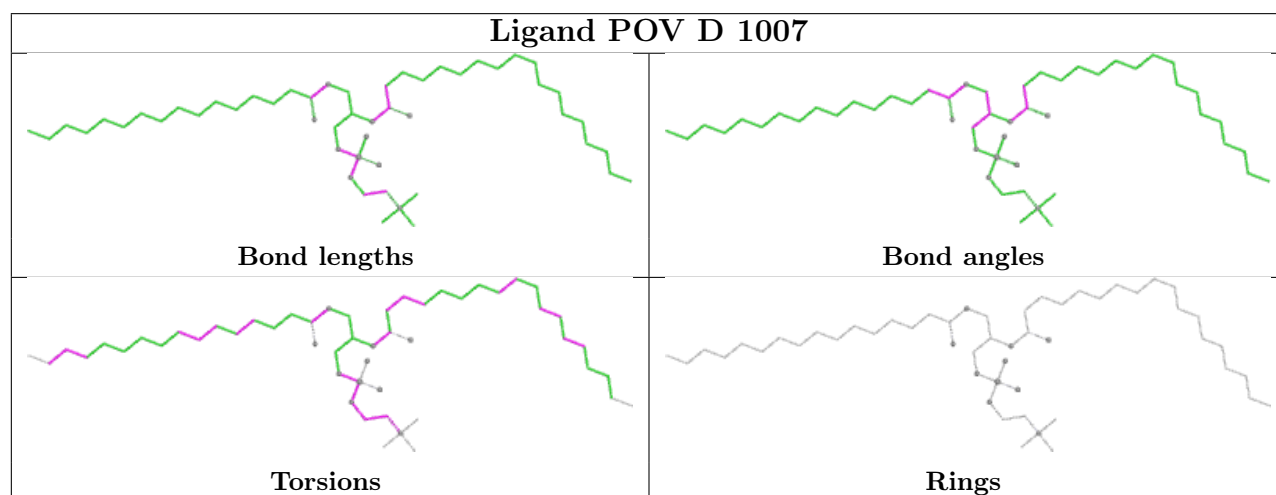
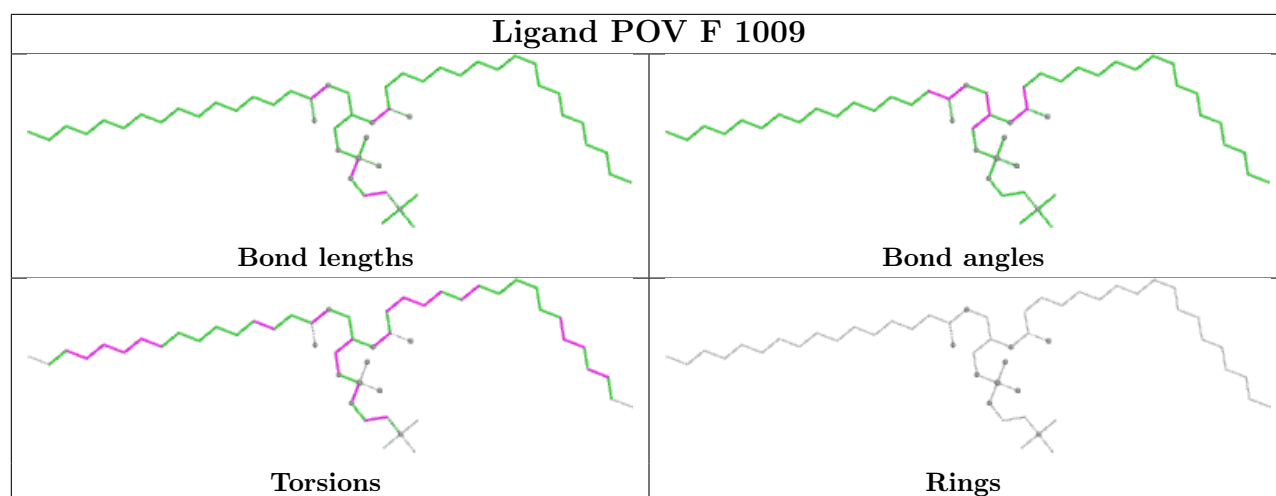


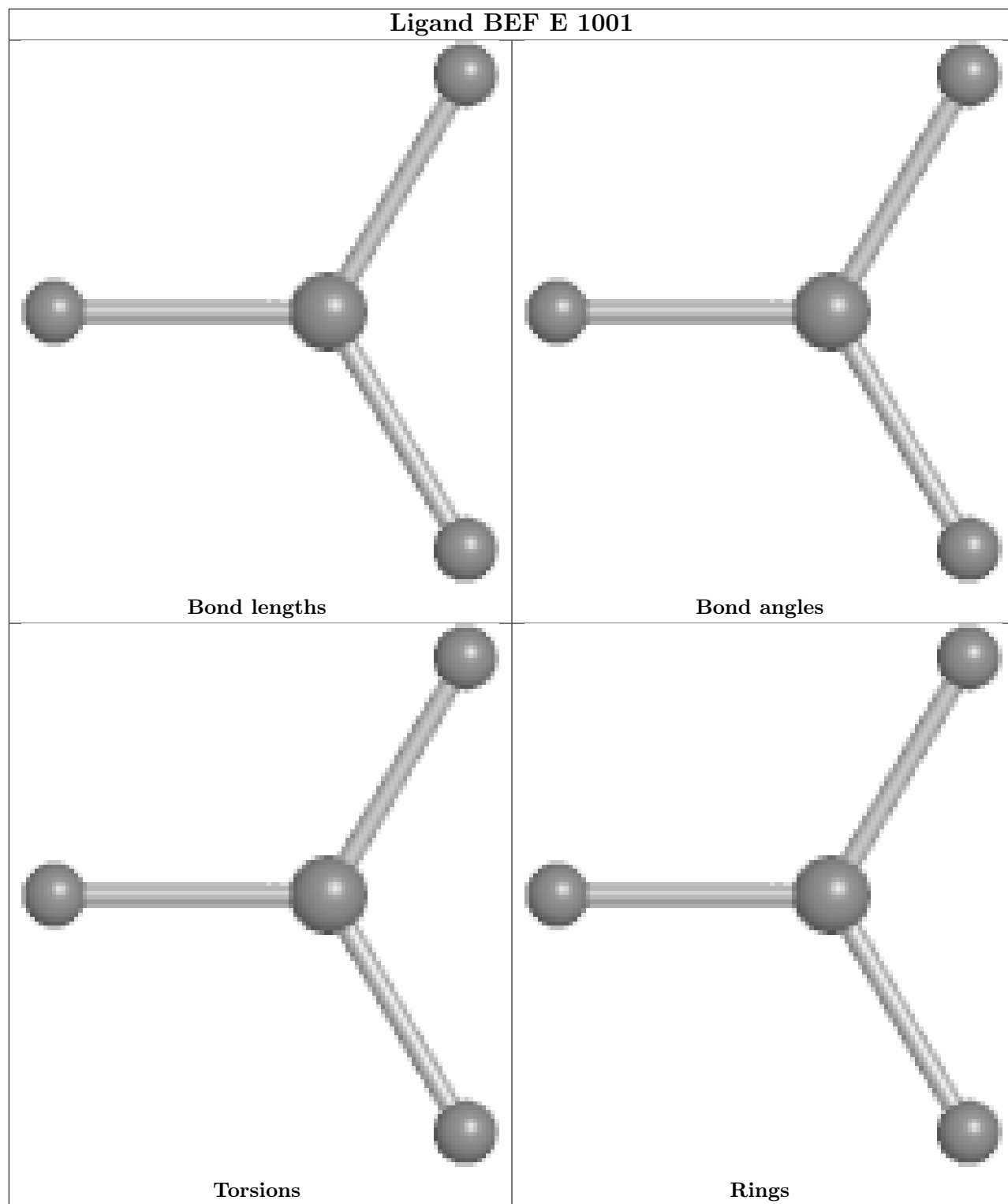


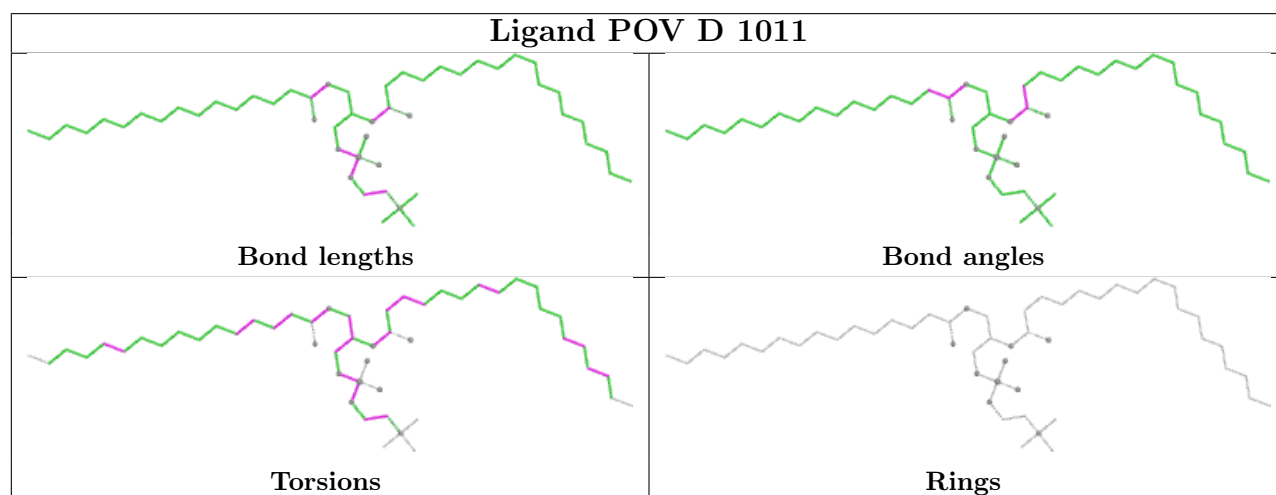
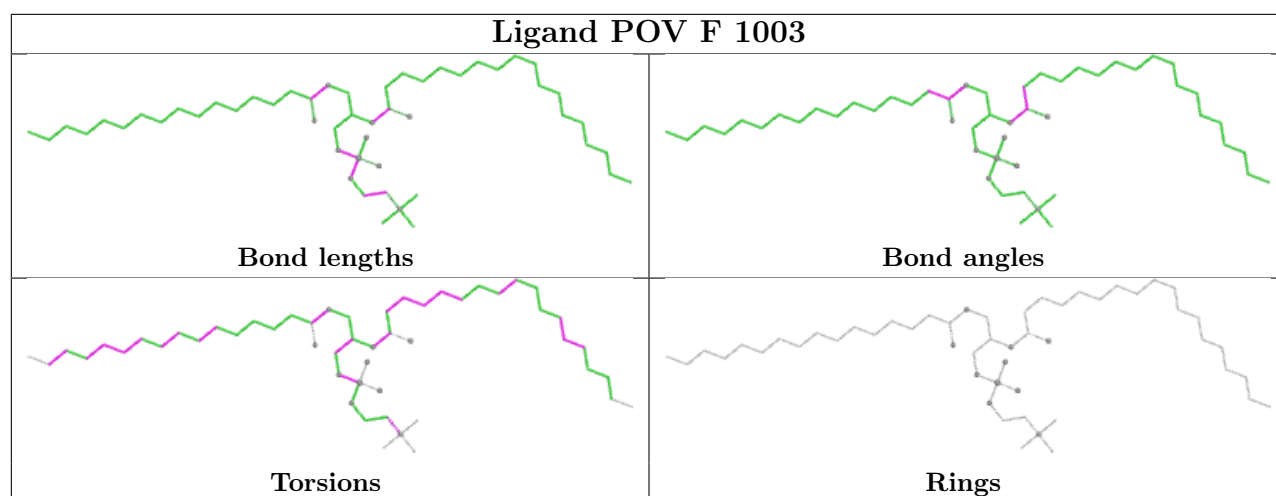


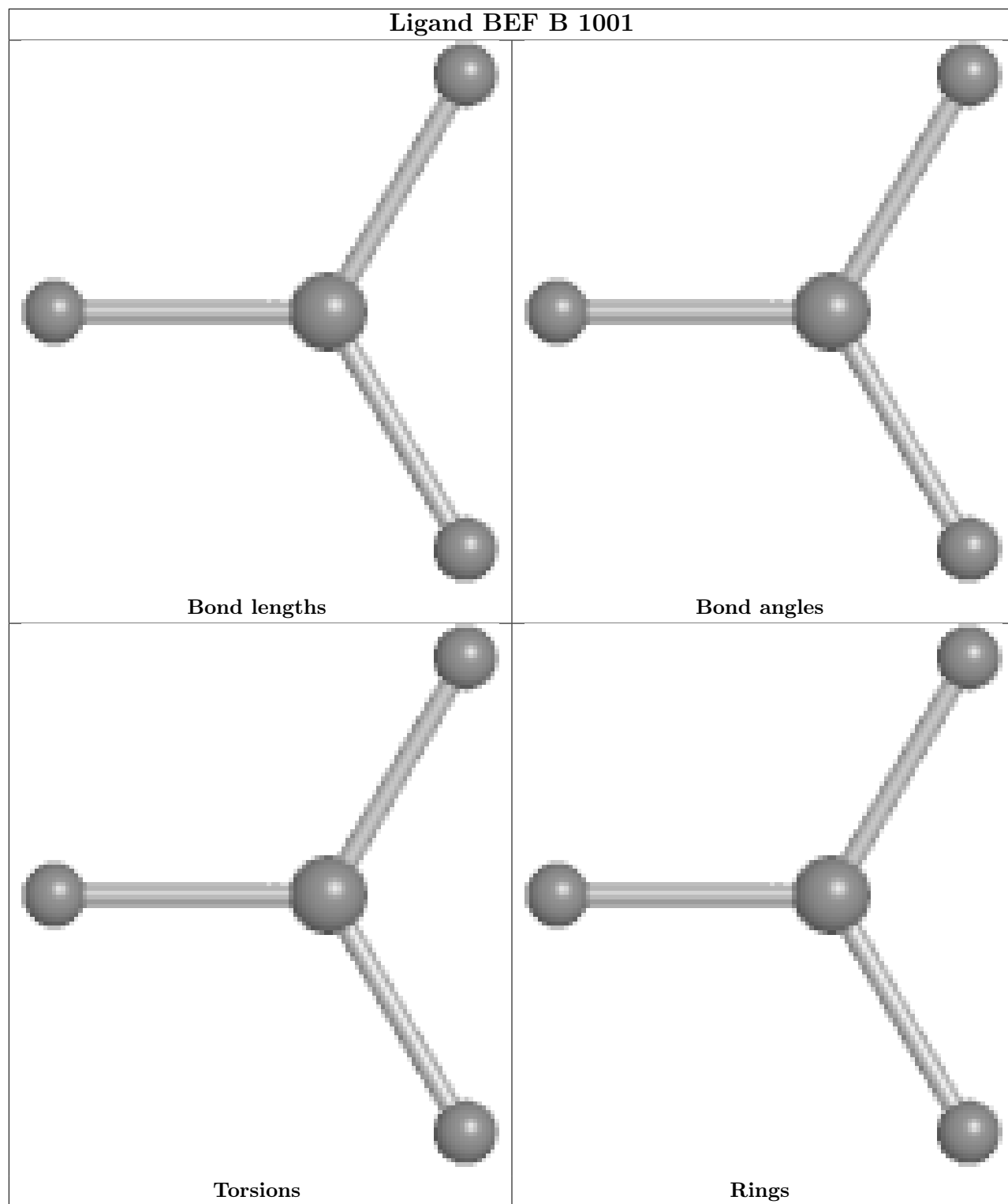


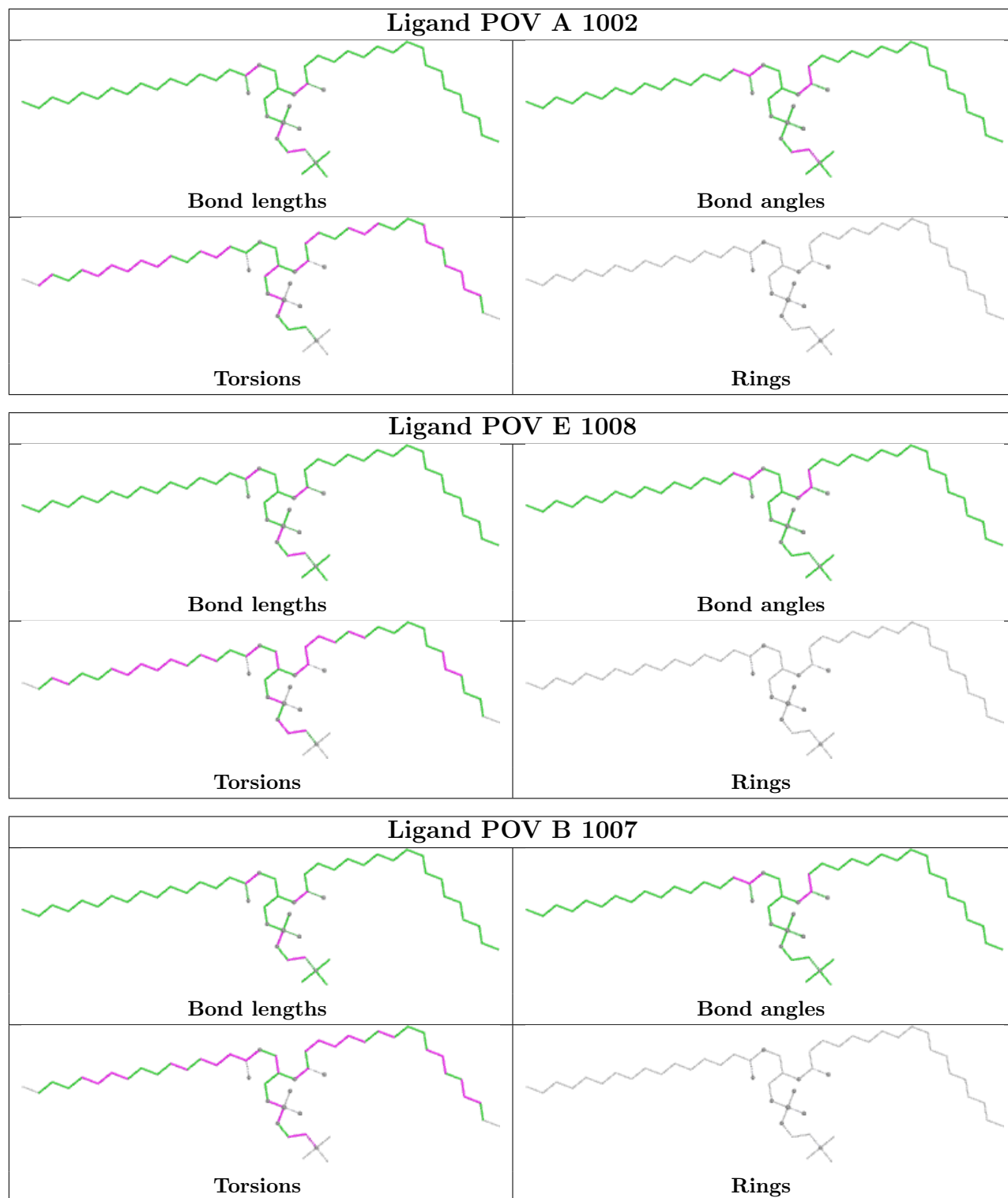


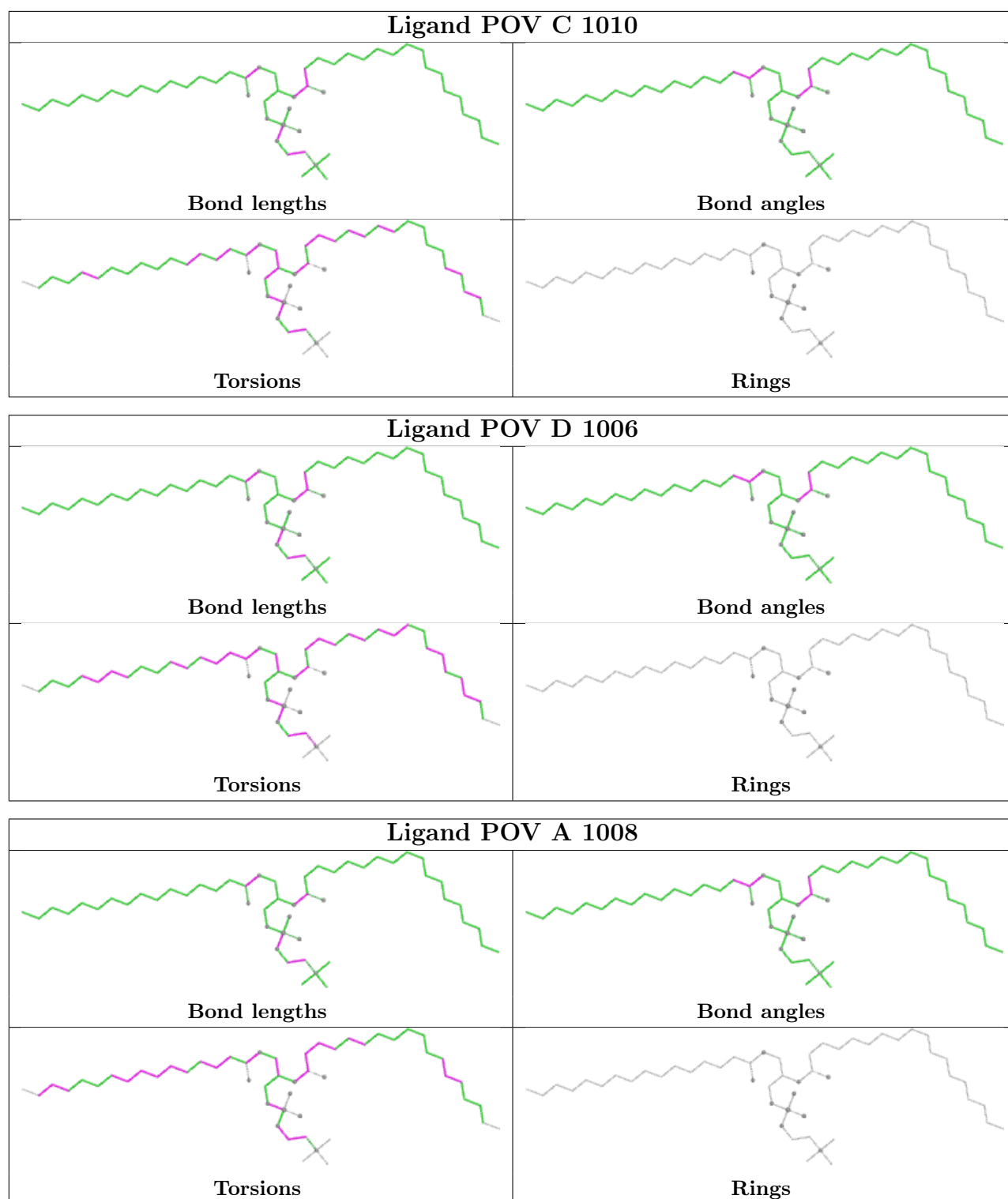


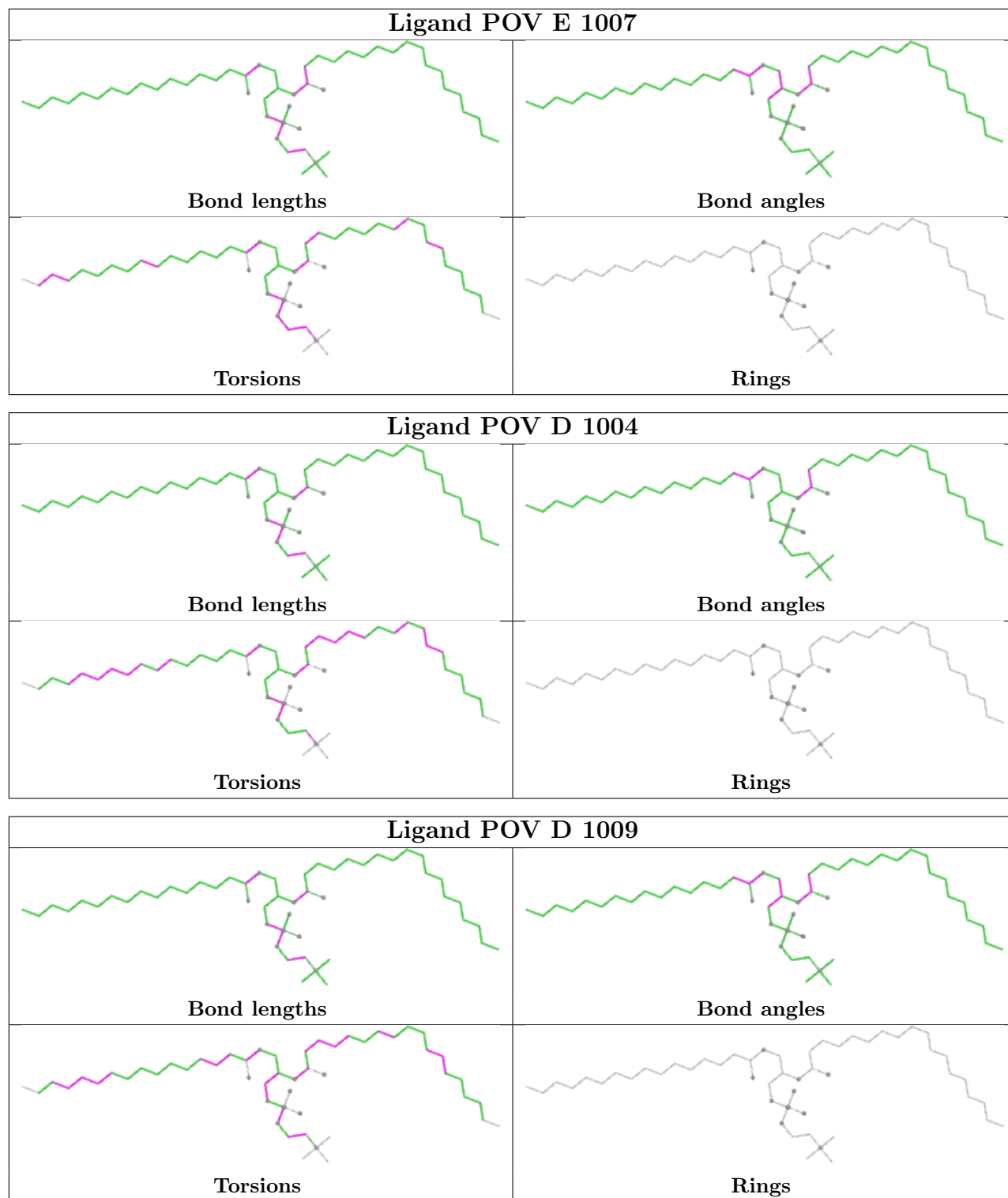


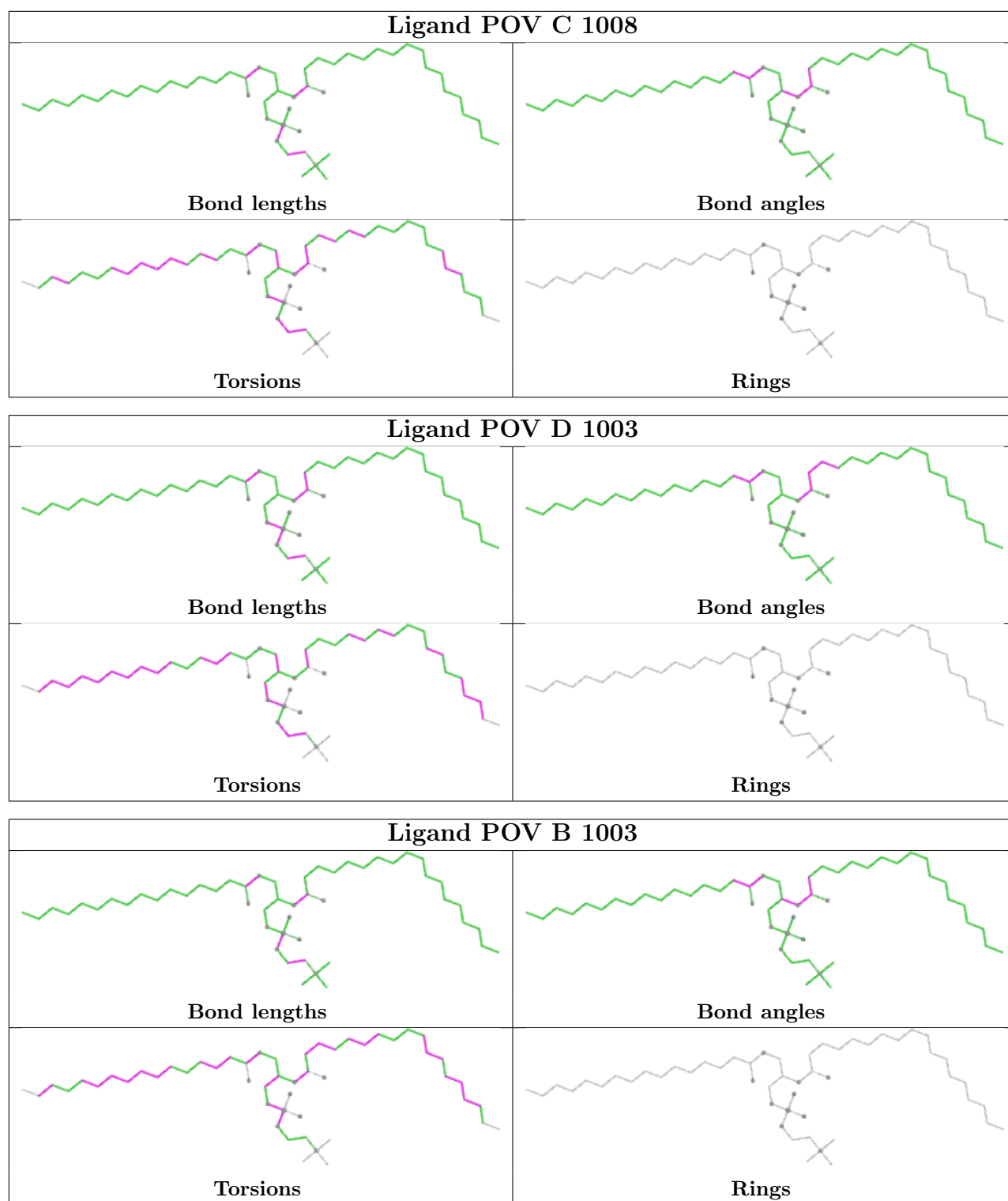


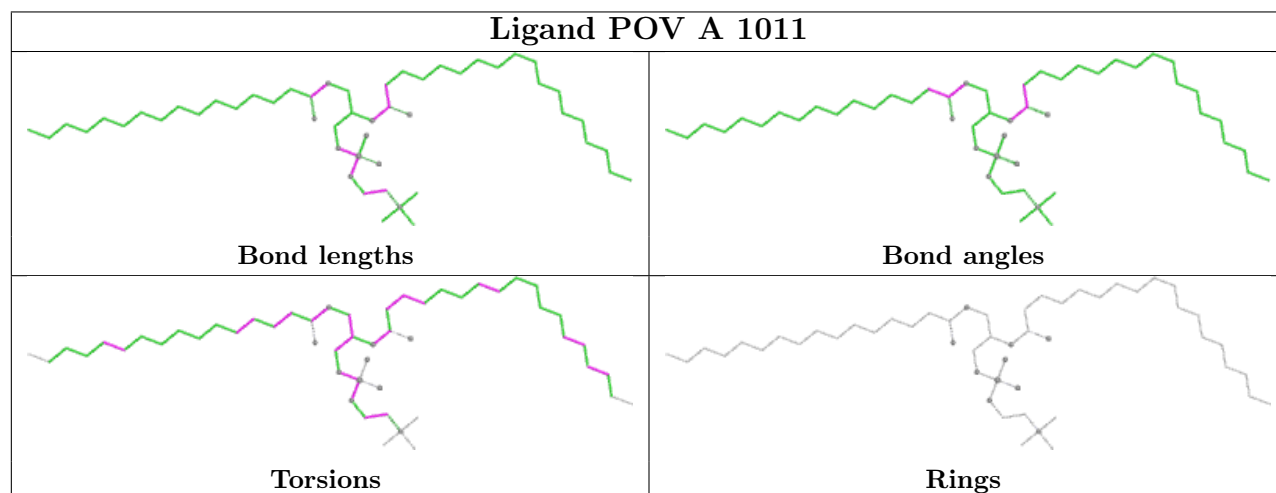
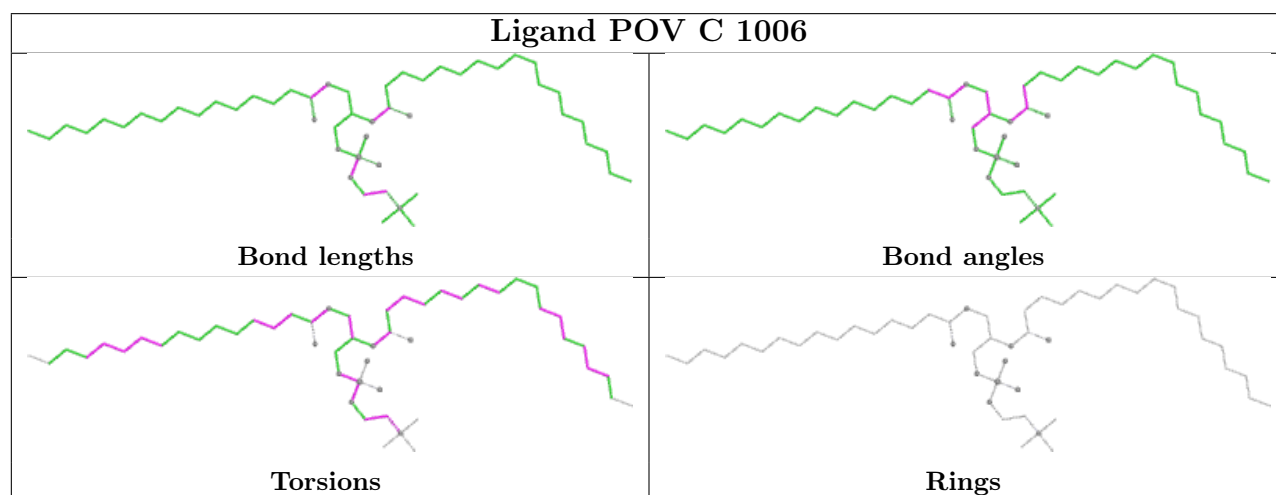
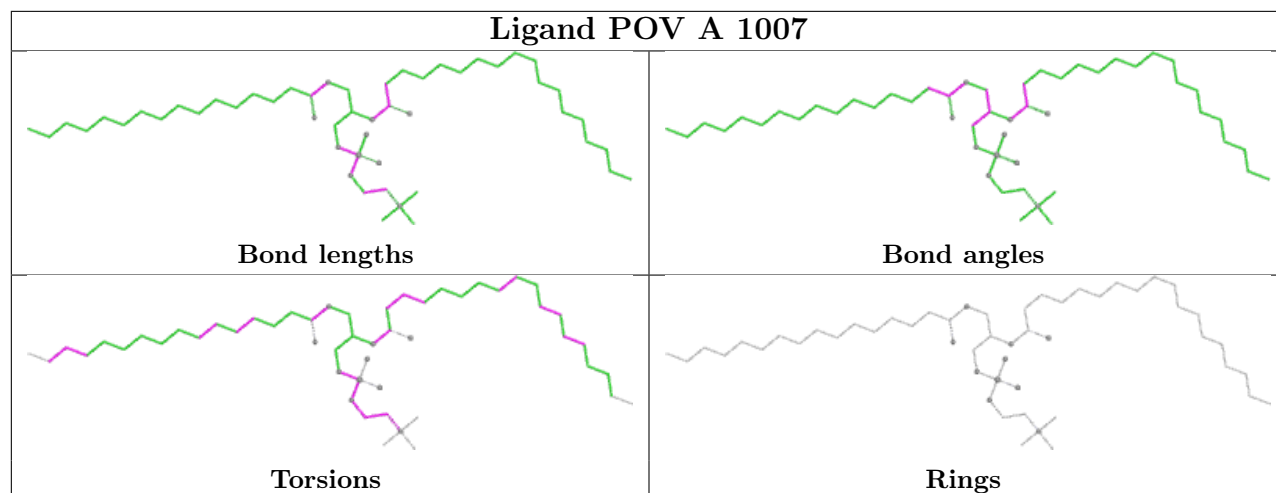


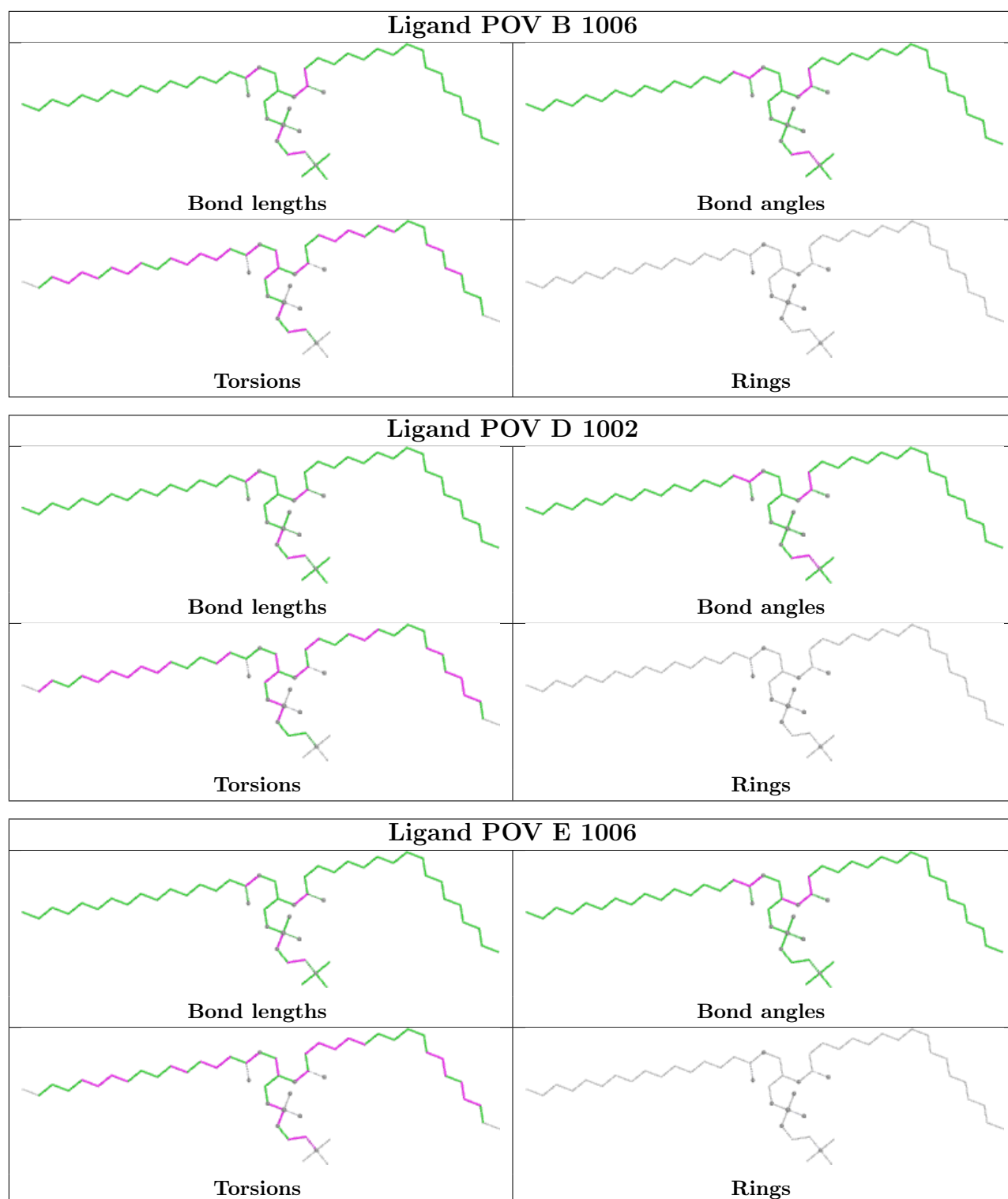


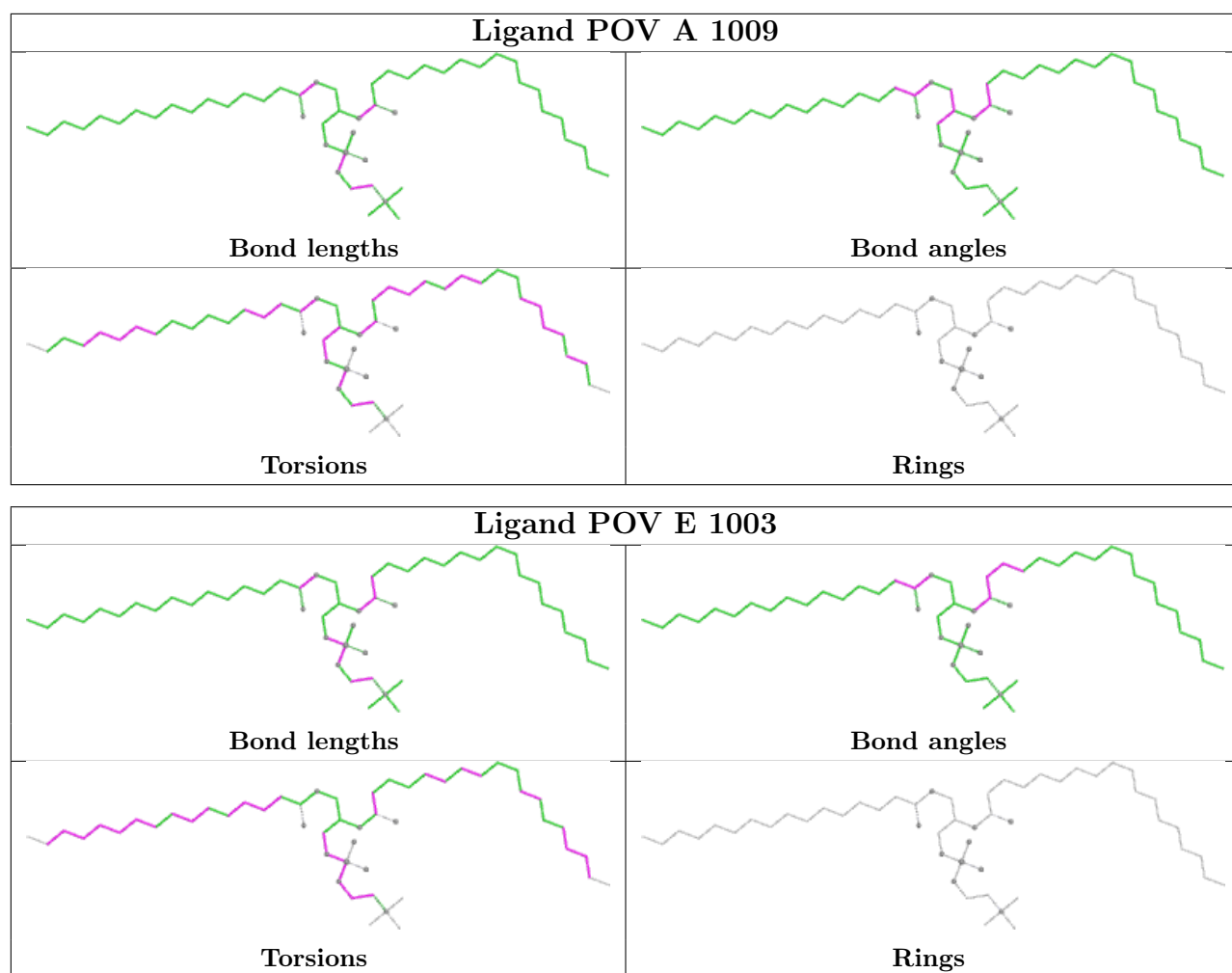


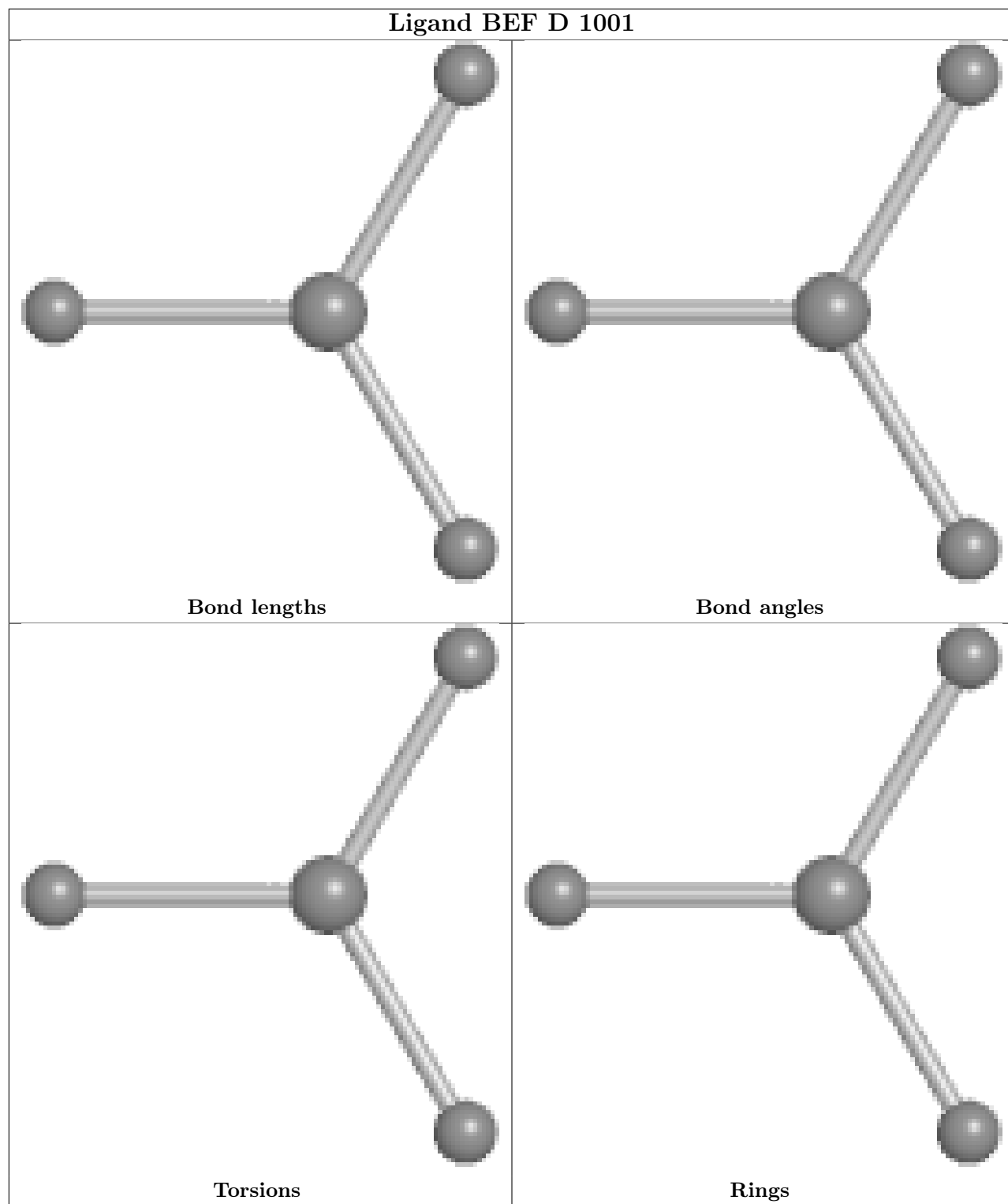


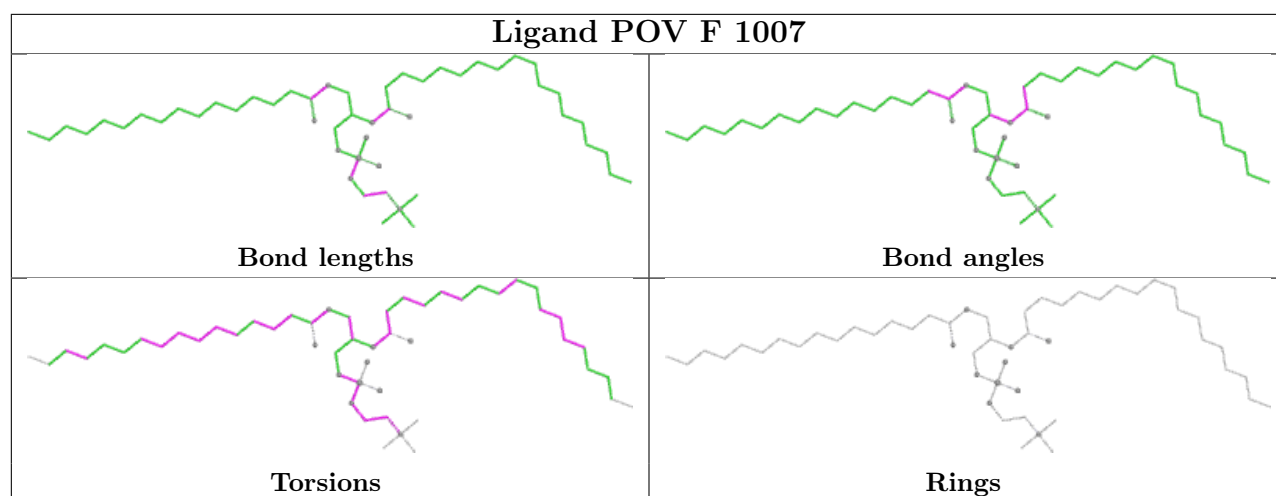












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

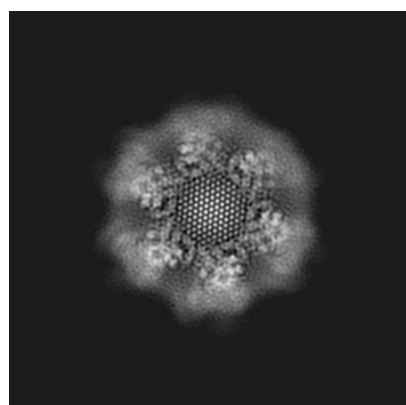
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31988. These allow visual inspection of the internal detail of the map and identification of artifacts.

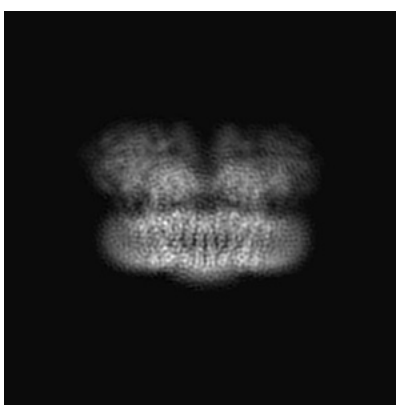
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

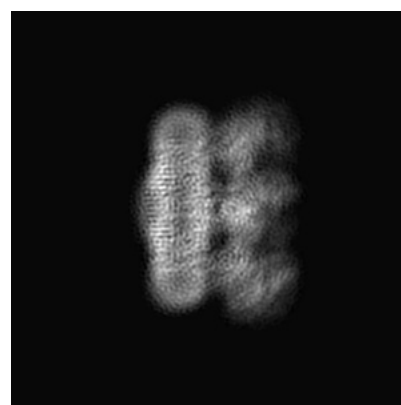
6.1.1 Primary map



X



Y

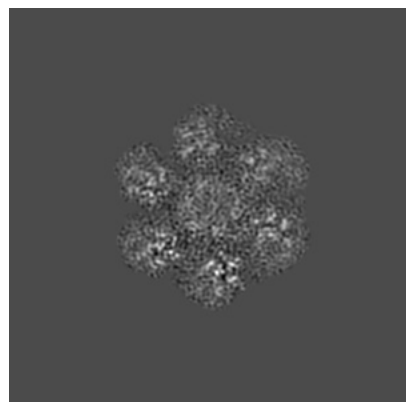


Z

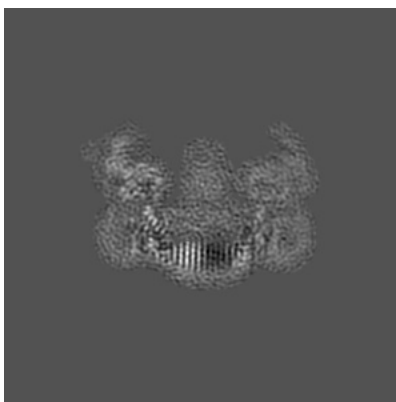
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150



Y Index: 150

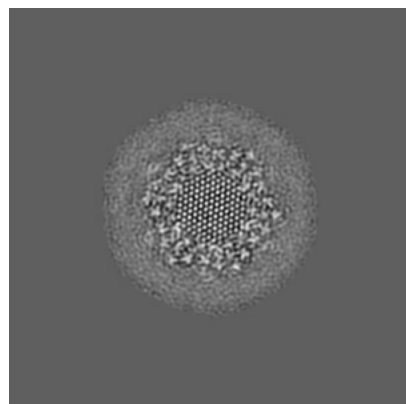


Z Index: 150

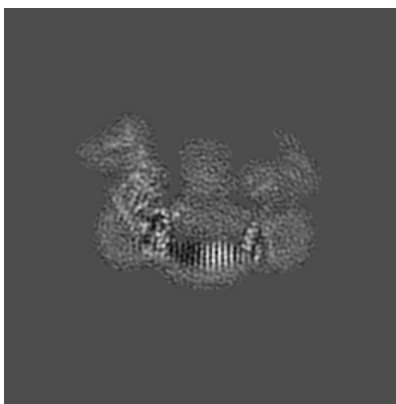
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 116



Y Index: 156

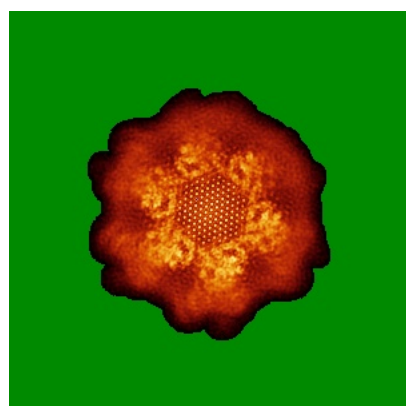


Z Index: 121

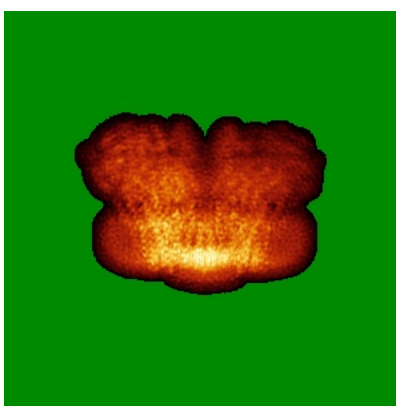
The images above show the largest variance slices of the map in three orthogonal directions.

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

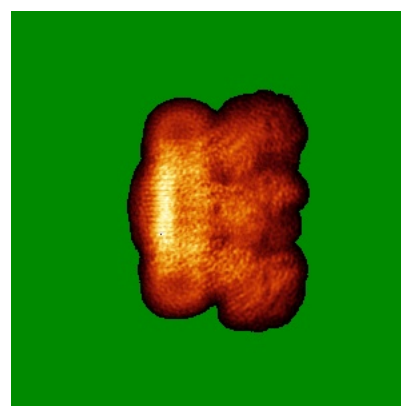
6.4.1 Primary map



X



Y

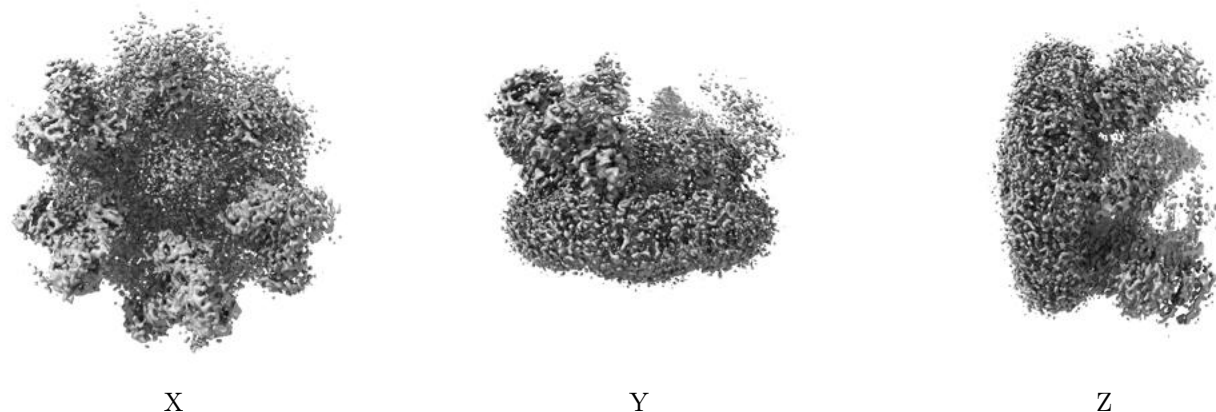


Z

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

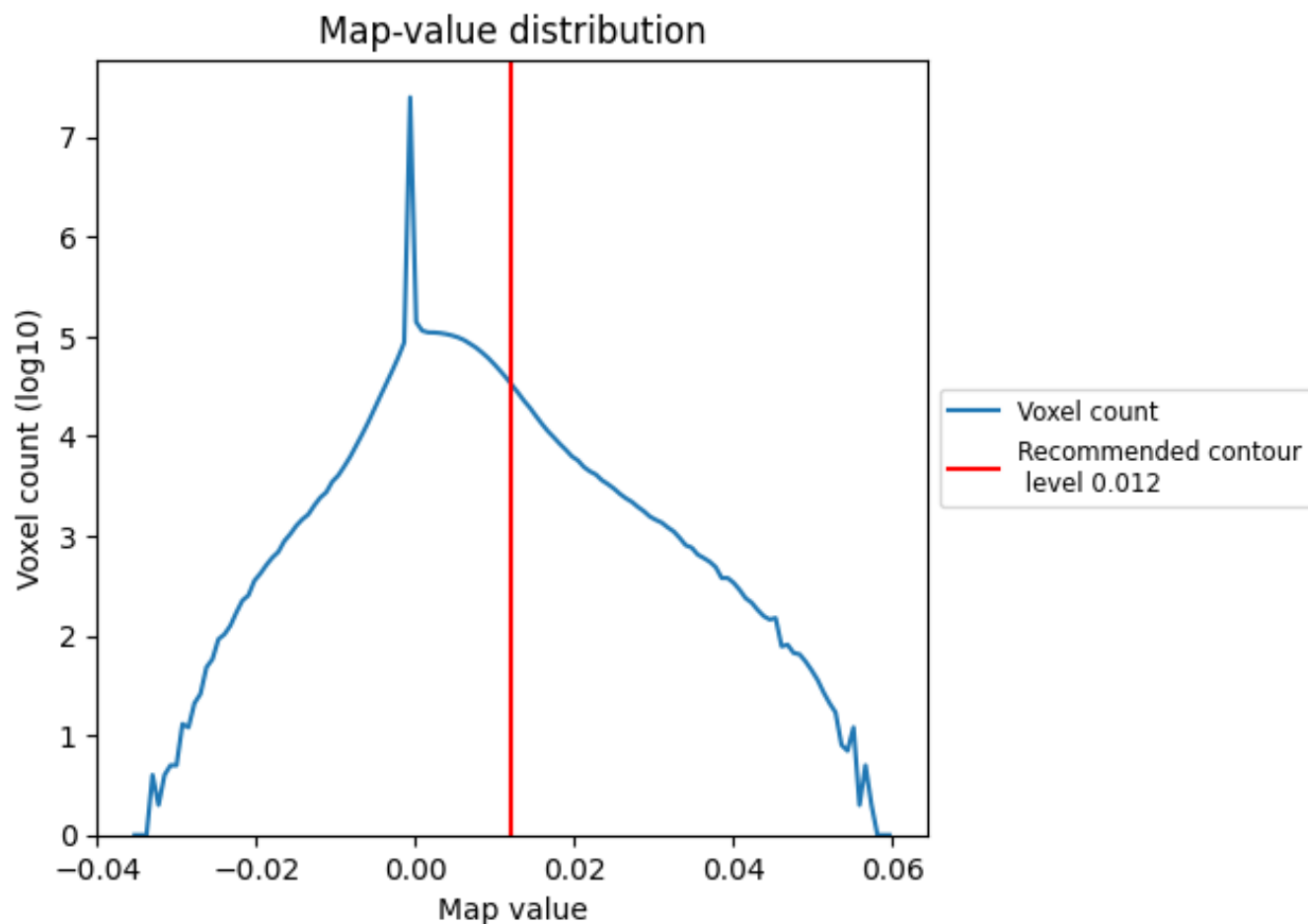
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

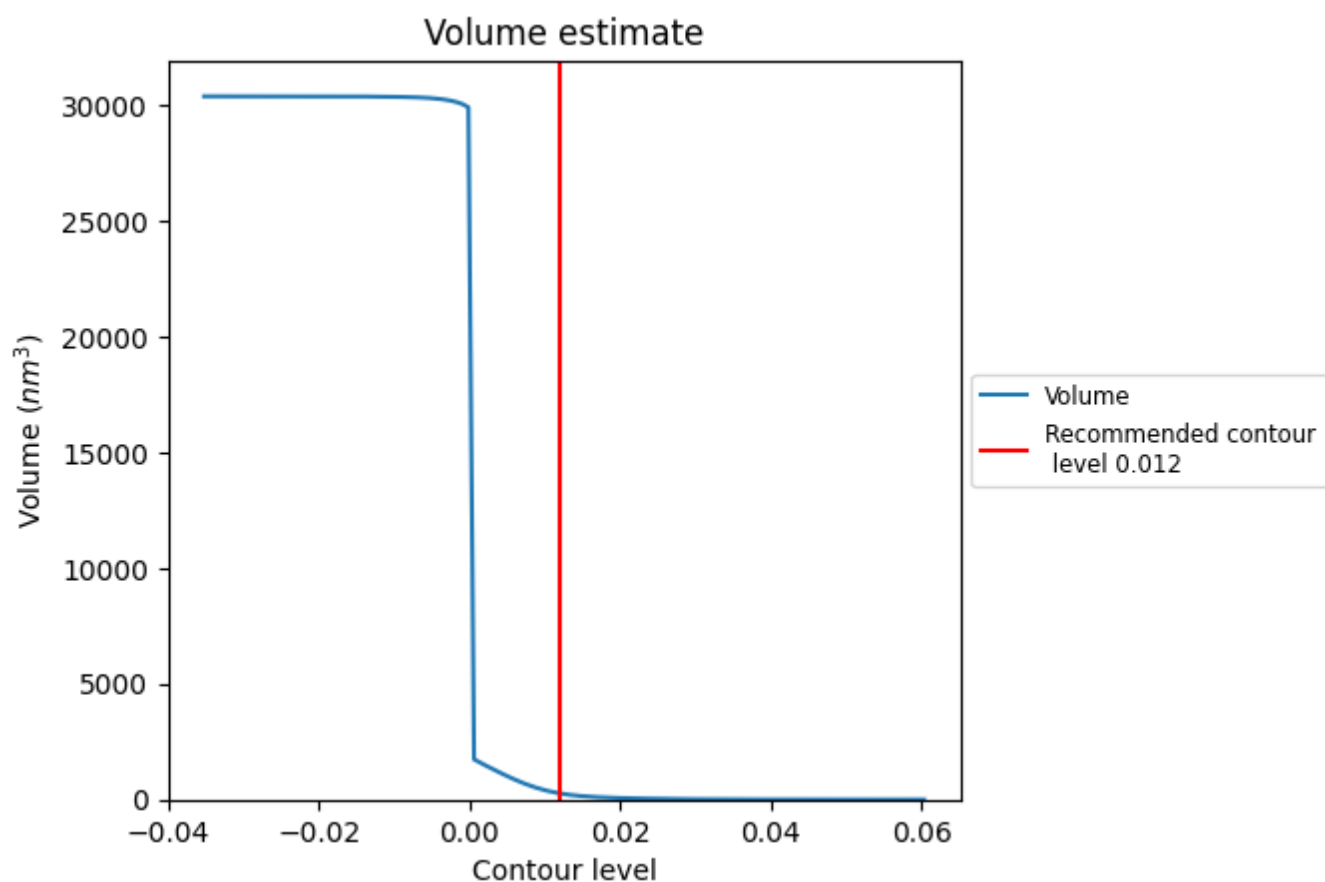
This section contains the results of statistical analysis of the map.

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.

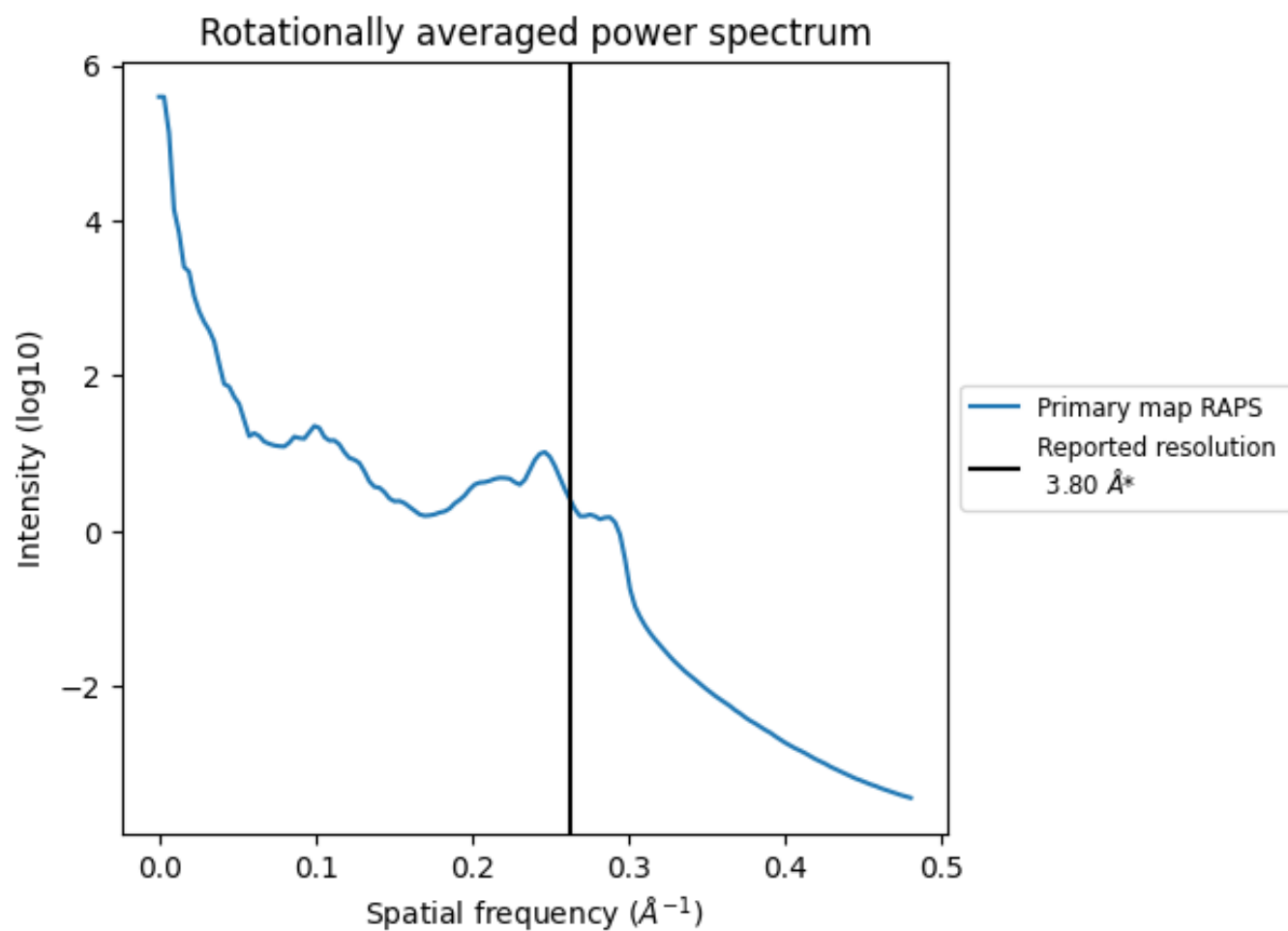
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 267 nm³; this corresponds to an approximate mass of 241 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 0.263 Å⁻¹

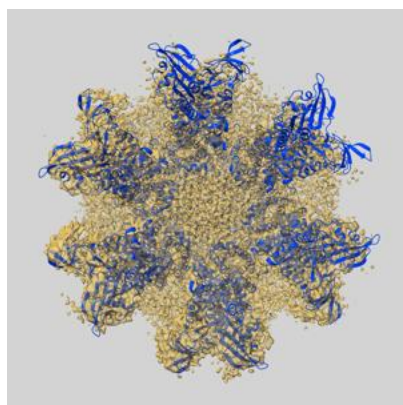
8 Fourier-Shell correlation

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

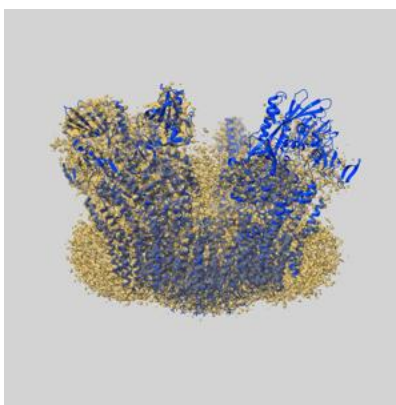
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31988 and PDB model 7VH6. Per-residue inclusion information can be found in section [3](#) on page [9](#).

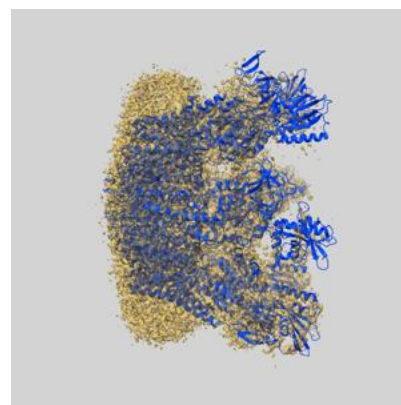
9.1 Map-model overlay [i](#)



X



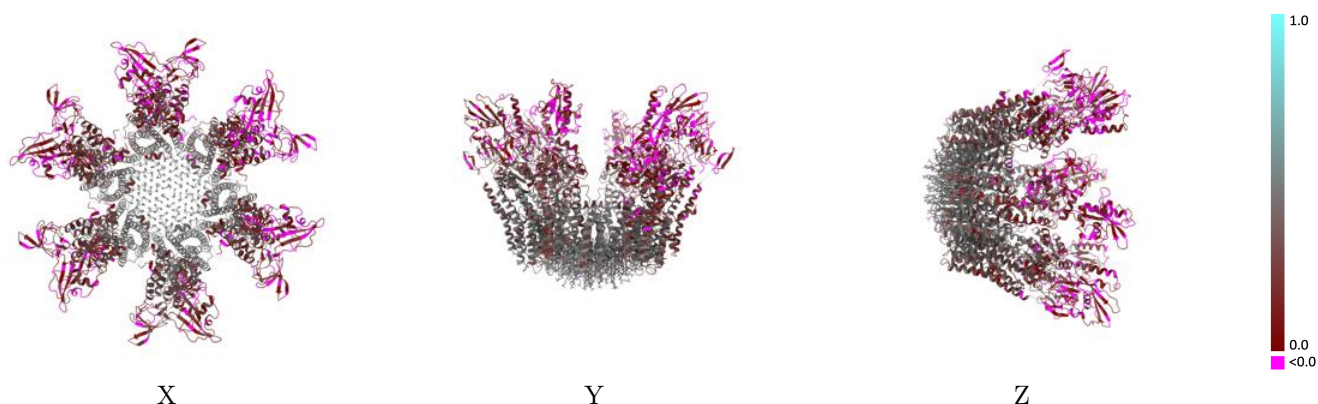
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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](#)

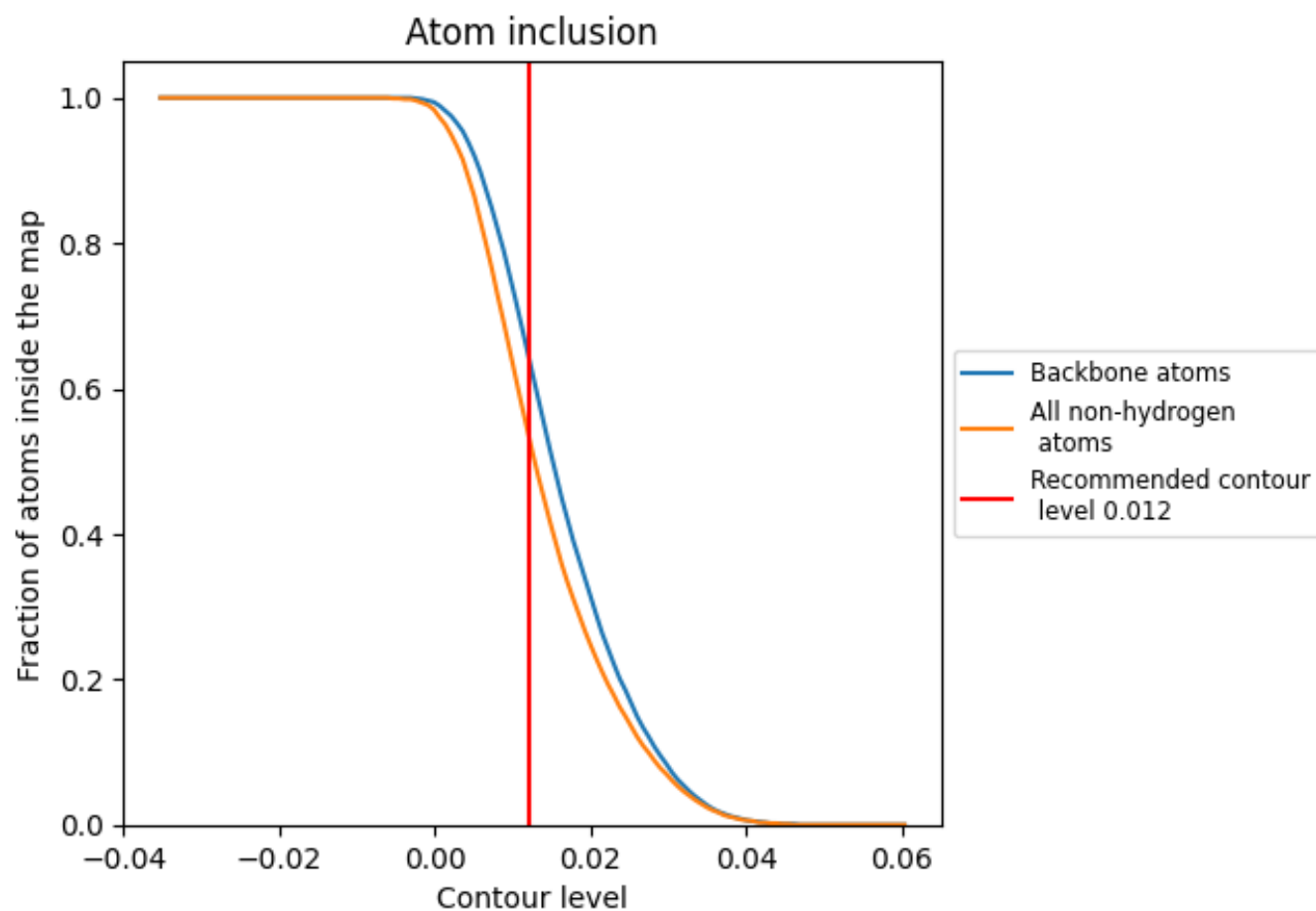


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 54% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5380	0.2890
A	0.6940	0.3680
B	0.6390	0.3170
C	0.5320	0.2870
D	0.4090	0.2460
E	0.3860	0.2290
F	0.5650	0.2870

