



## wwPDB EM Validation Summary Report ⓘ

Jul 15, 2025 – 10:37 AM JST

PDB ID : 8IMY / pdb\_00008imy  
EMDB ID : EMD-35576  
Title : Cryo-EM structure of GPI-T (inactive mutant) with GPI and proULBP2, a  
proprotein substrate  
Authors : Li, T.; Xu, Y.; Qu, Q.; Li, D.  
Deposited on : 2023-03-07  
Resolution : 3.22 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](mailto: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 : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

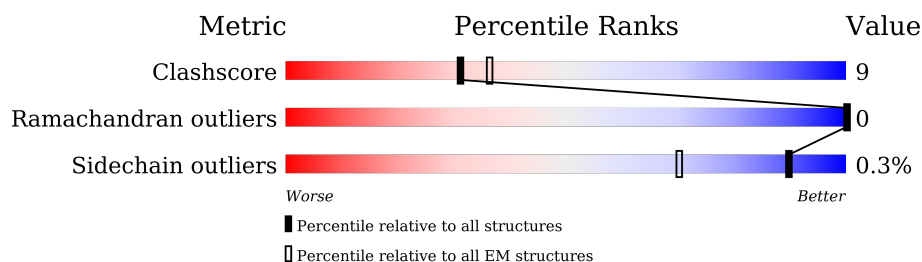
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.22 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	G	886	<div> <div style="width: 54%; background-color: green;"></div> <div style="width: 12%; background-color: yellow;"></div> <div style="width: 34%; background-color: grey;"></div> </div> <div>54% 12% 34%</div>
2	K	647	<div> <div style="width: 40%; background-color: green;"></div> <div style="width: 11%; background-color: yellow;"></div> <div style="width: 49%; background-color: grey;"></div> </div> <div>40% 11% 49%</div>
3	U	712	<div> <div style="width: 49%; background-color: green;"></div> <div style="width: 10%; background-color: yellow;"></div> <div style="width: 41%; background-color: grey;"></div> </div> <div>49% 10% 41%</div>
4	T	821	<div> <div style="width: 51%; background-color: green;"></div> <div style="width: 14%; background-color: yellow;"></div> <div style="width: 35%; background-color: grey;"></div> </div> <div>51% 14% 35%</div>
5	S	816	<div> <div style="width: 50%; background-color: green;"></div> <div style="width: 11%; background-color: yellow;"></div> <div style="width: 39%; background-color: grey;"></div> </div> <div>50% 11% 39%</div>
6	D	258	<div> <div style="width: 11%; background-color: green;"></div> <div style="width: 1%; background-color: yellow;"></div> <div style="width: 86%; background-color: grey;"></div> </div> <div>11% . 86%</div>
7	A	2	<div> <div style="width: 100%; background-color: green;"></div> </div> <div>100%</div>

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 19986 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 Glycosylphosphatidylinositol anchor attachment 1 protein, GFP-like fluorescent chromoprotein cFP484.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	581	Total	C	N	O	S	0	0
			4397	2879	748	751	19		

There are 95 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	MET	-	initiating methionine	UNP O43292
G	0	GLY	-	expression tag	UNP O43292
G	1	SER	-	expression tag	UNP O43292
G	622	GLY	-	linker	UNP O43292
G	623	THR	-	linker	UNP O43292
G	624	LEU	-	linker	UNP O43292
G	625	GLU	-	linker	UNP O43292
G	626	VAL	-	linker	UNP O43292
G	627	LEU	-	linker	UNP O43292
G	628	PHE	-	linker	UNP O43292
G	629	GLN	-	linker	UNP O43292
G	630	GLY	-	linker	UNP O43292
G	631	PRO	-	linker	UNP O43292
G	632	GLY	-	linker	UNP O43292
G	633	GLY	-	linker	UNP O43292
G	634	SER	-	linker	UNP O43292
G	635	GLY	-	linker	UNP O43292
G	636	GLY	-	linker	UNP O43292
G	637	SER	-	linker	UNP O43292
G	638	ALA	-	linker	UNP O43292
G	639	SER	-	linker	UNP O43292
G	644	GLU	ASP	conflict	UNP Q9U6Y3
G	650	ARG	LYS	conflict	UNP Q9U6Y3
G	654	ALA	ASN	conflict	UNP Q9U6Y3
G	659	LYS	ALA	conflict	UNP Q9U6Y3
G	667	ILE	GLU	conflict	UNP Q9U6Y3
G	672	GLU	ASP	conflict	UNP Q9U6Y3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	675	GLN	HIS	conflict	UNP Q9U6Y3
G	678	ASP	ASN	conflict	UNP Q9U6Y3
G	680	THR	GLU	conflict	UNP Q9U6Y3
G	682	GLU	LYS	conflict	UNP Q9U6Y3
G	695	THR	SER	conflict	UNP Q9U6Y3
G	696	PRO	ASN	conflict	UNP Q9U6Y3
G	705	PHE	LEU	conflict	UNP Q9U6Y3
G	710	GLU	ASP	conflict	UNP Q9U6Y3
G	713	PRO	ALA	conflict	UNP Q9U6Y3
G	719	ALA	SER	conflict	UNP Q9U6Y3
G	729	SER	THR	conflict	UNP Q9U6Y3
G	732	TYR	PHE	conflict	UNP Q9U6Y3
G	735	GLN	LYS	conflict	UNP Q9U6Y3
G	738	CYS	VAL	conflict	UNP Q9U6Y3
G	739	ILE	LYS	conflict	UNP Q9U6Y3
G	740	ALA	VAL	conflict	UNP Q9U6Y3
G	741	THR	LYS	conflict	UNP Q9U6Y3
G	745	THR	SER	conflict	UNP Q9U6Y3
G	748	GLY	GLU	conflict	UNP Q9U6Y3
G	750	CYS	SER	conflict	UNP Q9U6Y3
G	752	PHE	ILE	conflict	UNP Q9U6Y3
G	760	THR	MET	conflict	UNP Q9U6Y3
G	782	LYS	ILE	conflict	UNP Q9U6Y3
G	786	GLU	ARG	conflict	UNP Q9U6Y3
G	791	LYS	VAL	conflict	UNP Q9U6Y3
G	794	VAL	ILE	conflict	UNP Q9U6Y3
G	795	GLU	SER	conflict	UNP Q9U6Y3
G	796	MET	HIS	conflict	UNP Q9U6Y3
G	797	ALA	SER	conflict	UNP Q9U6Y3
G	812	THR	SER	conflict	UNP Q9U6Y3
G	813	THR	ILE	conflict	UNP Q9U6Y3
G	819	ASP	VAL	conflict	UNP Q9U6Y3
G	821	ARG	LYS	conflict	UNP Q9U6Y3
G	825	ALA	TYR	conflict	UNP Q9U6Y3
G	827	GLU	PHE	conflict	UNP Q9U6Y3
G	836	SER	ASN	conflict	UNP Q9U6Y3
G	845	ARG	THR	conflict	UNP Q9U6Y3
G	849	HIS	ASN	conflict	UNP Q9U6Y3
G	851	GLU	VAL	conflict	UNP Q9U6Y3
G	856	GLY	-	expression tag	UNP Q9U6Y3
G	857	GLY	-	expression tag	UNP Q9U6Y3
G	858	GLY	-	expression tag	UNP Q9U6Y3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	859	SER	-	expression tag	UNP Q9U6Y3
G	860	GLY	-	expression tag	UNP Q9U6Y3
G	861	GLY	-	expression tag	UNP Q9U6Y3
G	862	GLY	-	expression tag	UNP Q9U6Y3
G	863	GLY	-	expression tag	UNP Q9U6Y3
G	864	SER	-	expression tag	UNP Q9U6Y3
G	865	GLY	-	expression tag	UNP Q9U6Y3
G	866	GLY	-	expression tag	UNP Q9U6Y3
G	867	GLY	-	expression tag	UNP Q9U6Y3
G	868	GLY	-	expression tag	UNP Q9U6Y3
G	869	ASP	-	expression tag	UNP Q9U6Y3
G	870	TYR	-	expression tag	UNP Q9U6Y3
G	871	LYS	-	expression tag	UNP Q9U6Y3
G	872	ASP	-	expression tag	UNP Q9U6Y3
G	873	ASP	-	expression tag	UNP Q9U6Y3
G	874	ASP	-	expression tag	UNP Q9U6Y3
G	875	ASP	-	expression tag	UNP Q9U6Y3
G	876	ALA	-	expression tag	UNP Q9U6Y3
G	877	ASP	-	expression tag	UNP Q9U6Y3
G	878	TYR	-	expression tag	UNP Q9U6Y3
G	879	LYS	-	expression tag	UNP Q9U6Y3
G	880	ASP	-	expression tag	UNP Q9U6Y3
G	881	ASP	-	expression tag	UNP Q9U6Y3
G	882	ASP	-	expression tag	UNP Q9U6Y3
G	883	ASP	-	expression tag	UNP Q9U6Y3
G	884	ALA	-	expression tag	UNP Q9U6Y3

- Molecule 2 is a protein called GPI-anchor transamidase, GFP-like fluorescent chromoprotein cFP484.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	330	Total	C	N	O	S	0	0
			2633	1685	450	484	14		

There are 83 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	MET	-	initiating methionine	UNP Q92643
K	0	GLY	-	expression tag	UNP Q92643
K	1	SER	-	expression tag	UNP Q92643
K	206	SER	CYS	conflict	UNP Q92643
K	396	GLY	-	linker	UNP Q92643

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
K	397	THR	-	linker	UNP Q92643
K	398	LEU	-	linker	UNP Q92643
K	399	GLU	-	linker	UNP Q92643
K	400	VAL	-	linker	UNP Q92643
K	401	LEU	-	linker	UNP Q92643
K	402	PHE	-	linker	UNP Q92643
K	403	GLN	-	linker	UNP Q92643
K	404	GLY	-	linker	UNP Q92643
K	405	PRO	-	linker	UNP Q92643
K	406	GLY	-	linker	UNP Q92643
K	407	GLY	-	linker	UNP Q92643
K	408	SER	-	linker	UNP Q92643
K	409	GLY	-	linker	UNP Q92643
K	410	GLY	-	linker	UNP Q92643
K	411	SER	-	linker	UNP Q92643
K	412	ALA	-	linker	UNP Q92643
K	413	SER	-	linker	UNP Q92643
K	418	GLU	ASP	conflict	UNP Q9U6Y3
K	424	ARG	LYS	conflict	UNP Q9U6Y3
K	428	ALA	ASN	conflict	UNP Q9U6Y3
K	433	LYS	ALA	conflict	UNP Q9U6Y3
K	441	ILE	GLU	conflict	UNP Q9U6Y3
K	446	GLU	ASP	conflict	UNP Q9U6Y3
K	449	GLN	HIS	conflict	UNP Q9U6Y3
K	452	ASP	ASN	conflict	UNP Q9U6Y3
K	454	THR	GLU	conflict	UNP Q9U6Y3
K	456	GLU	LYS	conflict	UNP Q9U6Y3
K	469	THR	SER	conflict	UNP Q9U6Y3
K	470	PRO	ASN	conflict	UNP Q9U6Y3
K	479	PHE	LEU	conflict	UNP Q9U6Y3
K	484	GLU	ASP	conflict	UNP Q9U6Y3
K	487	PRO	ALA	conflict	UNP Q9U6Y3
K	493	ALA	SER	conflict	UNP Q9U6Y3
K	503	SER	THR	conflict	UNP Q9U6Y3
K	506	TYR	PHE	conflict	UNP Q9U6Y3
K	509	GLN	LYS	conflict	UNP Q9U6Y3
K	512	CYS	VAL	conflict	UNP Q9U6Y3
K	513	ILE	LYS	conflict	UNP Q9U6Y3
K	514	ALA	VAL	conflict	UNP Q9U6Y3
K	515	THR	LYS	conflict	UNP Q9U6Y3
K	519	THR	SER	conflict	UNP Q9U6Y3
K	522	GLY	GLU	conflict	UNP Q9U6Y3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
K	524	CYS	SER	conflict	UNP Q9U6Y3
K	526	PHE	ILE	conflict	UNP Q9U6Y3
K	534	THR	MET	conflict	UNP Q9U6Y3
K	556	LYS	ILE	conflict	UNP Q9U6Y3
K	560	GLU	ARG	conflict	UNP Q9U6Y3
K	565	LYS	VAL	conflict	UNP Q9U6Y3
K	568	VAL	ILE	conflict	UNP Q9U6Y3
K	569	GLU	SER	conflict	UNP Q9U6Y3
K	570	MET	HIS	conflict	UNP Q9U6Y3
K	571	ALA	SER	conflict	UNP Q9U6Y3
K	586	THR	SER	conflict	UNP Q9U6Y3
K	587	THR	ILE	conflict	UNP Q9U6Y3
K	593	ASP	VAL	conflict	UNP Q9U6Y3
K	595	ARG	LYS	conflict	UNP Q9U6Y3
K	599	ALA	TYR	conflict	UNP Q9U6Y3
K	601	GLU	PHE	conflict	UNP Q9U6Y3
K	610	SER	ASN	conflict	UNP Q9U6Y3
K	619	ARG	THR	conflict	UNP Q9U6Y3
K	623	HIS	ASN	conflict	UNP Q9U6Y3
K	625	GLU	VAL	conflict	UNP Q9U6Y3
K	630	GLY	-	expression tag	UNP Q9U6Y3
K	631	GLY	-	expression tag	UNP Q9U6Y3
K	632	GLY	-	expression tag	UNP Q9U6Y3
K	633	SER	-	expression tag	UNP Q9U6Y3
K	634	GLY	-	expression tag	UNP Q9U6Y3
K	635	GLY	-	expression tag	UNP Q9U6Y3
K	636	GLY	-	expression tag	UNP Q9U6Y3
K	637	TYR	-	expression tag	UNP Q9U6Y3
K	638	PRO	-	expression tag	UNP Q9U6Y3
K	639	TYR	-	expression tag	UNP Q9U6Y3
K	640	ASP	-	expression tag	UNP Q9U6Y3
K	641	VAL	-	expression tag	UNP Q9U6Y3
K	642	PRO	-	expression tag	UNP Q9U6Y3
K	643	ASP	-	expression tag	UNP Q9U6Y3
K	644	TYR	-	expression tag	UNP Q9U6Y3
K	645	ALA	-	expression tag	UNP Q9U6Y3

- Molecule 3 is a protein called Phosphatidylinositol glycan anchor biosynthesis class U protein, GFP-like fluorescent chromoprotein cFP484.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	419	Total	C	N	O	S	0	0
			3406	2332	507	553	14		



There are 107 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	-1	MET	-	initiating methionine	UNP Q9H490
U	0	GLY	-	expression tag	UNP Q9H490
U	1	SER	-	expression tag	UNP Q9H490
U	436	GLY	-	linker	UNP Q9H490
U	437	THR	-	linker	UNP Q9H490
U	438	LEU	-	linker	UNP Q9H490
U	439	GLU	-	linker	UNP Q9H490
U	440	VAL	-	linker	UNP Q9H490
U	441	LEU	-	linker	UNP Q9H490
U	442	PHE	-	linker	UNP Q9H490
U	443	GLN	-	linker	UNP Q9H490
U	444	GLY	-	linker	UNP Q9H490
U	445	PRO	-	linker	UNP Q9H490
U	446	GLY	-	linker	UNP Q9H490
U	447	GLY	-	linker	UNP Q9H490
U	448	SER	-	linker	UNP Q9H490
U	449	GLY	-	linker	UNP Q9H490
U	450	GLY	-	linker	UNP Q9H490
U	451	SER	-	linker	UNP Q9H490
U	452	ALA	-	linker	UNP Q9H490
U	453	SER	-	linker	UNP Q9H490
U	458	GLU	ASP	conflict	UNP Q9U6Y3
U	464	ARG	LYS	conflict	UNP Q9U6Y3
U	468	ALA	ASN	conflict	UNP Q9U6Y3
U	473	LYS	ALA	conflict	UNP Q9U6Y3
U	481	ILE	GLU	conflict	UNP Q9U6Y3
U	486	GLU	ASP	conflict	UNP Q9U6Y3
U	489	GLN	HIS	conflict	UNP Q9U6Y3
U	492	ASP	ASN	conflict	UNP Q9U6Y3
U	494	THR	GLU	conflict	UNP Q9U6Y3
U	496	GLU	LYS	conflict	UNP Q9U6Y3
U	509	THR	SER	conflict	UNP Q9U6Y3
U	510	PRO	ASN	conflict	UNP Q9U6Y3
U	519	PHE	LEU	conflict	UNP Q9U6Y3
U	524	GLU	ASP	conflict	UNP Q9U6Y3
U	527	PRO	ALA	conflict	UNP Q9U6Y3
U	533	ALA	SER	conflict	UNP Q9U6Y3
U	543	SER	THR	conflict	UNP Q9U6Y3
U	546	TYR	PHE	conflict	UNP Q9U6Y3
U	549	GLN	LYS	conflict	UNP Q9U6Y3
U	552	CYS	VAL	conflict	UNP Q9U6Y3
U	553	ILE	LYS	conflict	UNP Q9U6Y3

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
U	554	ALA	VAL	conflict	UNP Q9U6Y3
U	555	THR	LYS	conflict	UNP Q9U6Y3
U	559	THR	SER	conflict	UNP Q9U6Y3
U	562	GLY	GLU	conflict	UNP Q9U6Y3
U	564	CYS	SER	conflict	UNP Q9U6Y3
U	566	PHE	ILE	conflict	UNP Q9U6Y3
U	574	THR	MET	conflict	UNP Q9U6Y3
U	596	LYS	ILE	conflict	UNP Q9U6Y3
U	600	GLU	ARG	conflict	UNP Q9U6Y3
U	605	LYS	VAL	conflict	UNP Q9U6Y3
U	608	VAL	ILE	conflict	UNP Q9U6Y3
U	609	GLU	SER	conflict	UNP Q9U6Y3
U	610	MET	HIS	conflict	UNP Q9U6Y3
U	611	ALA	SER	conflict	UNP Q9U6Y3
U	626	THR	SER	conflict	UNP Q9U6Y3
U	627	THR	ILE	conflict	UNP Q9U6Y3
U	633	ASP	VAL	conflict	UNP Q9U6Y3
U	635	ARG	LYS	conflict	UNP Q9U6Y3
U	639	ALA	TYR	conflict	UNP Q9U6Y3
U	641	GLU	PHE	conflict	UNP Q9U6Y3
U	650	SER	ASN	conflict	UNP Q9U6Y3
U	659	ARG	THR	conflict	UNP Q9U6Y3
U	663	HIS	ASN	conflict	UNP Q9U6Y3
U	665	GLU	VAL	conflict	UNP Q9U6Y3
U	670	GLY	-	expression tag	UNP Q9U6Y3
U	671	GLY	-	expression tag	UNP Q9U6Y3
U	672	GLY	-	expression tag	UNP Q9U6Y3
U	673	SER	-	expression tag	UNP Q9U6Y3
U	674	GLY	-	expression tag	UNP Q9U6Y3
U	675	GLY	-	expression tag	UNP Q9U6Y3
U	676	GLY	-	expression tag	UNP Q9U6Y3
U	677	LYS	-	expression tag	UNP Q9U6Y3
U	678	LEU	-	expression tag	UNP Q9U6Y3
U	679	GLU	-	expression tag	UNP Q9U6Y3
U	680	PHE	-	expression tag	UNP Q9U6Y3
U	681	SER	-	expression tag	UNP Q9U6Y3
U	682	ALA	-	expression tag	UNP Q9U6Y3
U	683	TRP	-	expression tag	UNP Q9U6Y3
U	684	SER	-	expression tag	UNP Q9U6Y3
U	685	HIS	-	expression tag	UNP Q9U6Y3
U	686	PRO	-	expression tag	UNP Q9U6Y3
U	687	GLN	-	expression tag	UNP Q9U6Y3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
U	688	PHE	-	expression tag	UNP Q9U6Y3
U	689	GLU	-	expression tag	UNP Q9U6Y3
U	690	LYS	-	expression tag	UNP Q9U6Y3
U	691	GLY	-	expression tag	UNP Q9U6Y3
U	692	GLY	-	expression tag	UNP Q9U6Y3
U	693	GLY	-	expression tag	UNP Q9U6Y3
U	694	SER	-	expression tag	UNP Q9U6Y3
U	695	GLY	-	expression tag	UNP Q9U6Y3
U	696	GLY	-	expression tag	UNP Q9U6Y3
U	697	GLY	-	expression tag	UNP Q9U6Y3
U	698	SER	-	expression tag	UNP Q9U6Y3
U	699	GLY	-	expression tag	UNP Q9U6Y3
U	700	GLY	-	expression tag	UNP Q9U6Y3
U	701	SER	-	expression tag	UNP Q9U6Y3
U	702	ALA	-	expression tag	UNP Q9U6Y3
U	703	TRP	-	expression tag	UNP Q9U6Y3
U	704	SER	-	expression tag	UNP Q9U6Y3
U	705	HIS	-	expression tag	UNP Q9U6Y3
U	706	PRO	-	expression tag	UNP Q9U6Y3
U	707	GLN	-	expression tag	UNP Q9U6Y3
U	708	PHE	-	expression tag	UNP Q9U6Y3
U	709	GLU	-	expression tag	UNP Q9U6Y3
U	710	LYS	-	expression tag	UNP Q9U6Y3

- Molecule 4 is a protein called GPI transamidase component PIG-T, GFP-like fluorescent chromoprotein cFP484.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	530	Total	C	N	O	S	0	0
			4221	2745	710	752	14		

There are 73 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-1	MET	-	initiating methionine	UNP Q969N2
T	0	GLY	-	expression tag	UNP Q969N2
T	1	SER	-	expression tag	UNP Q969N2
T	579	GLY	-	linker	UNP Q969N2
T	580	THR	-	linker	UNP Q969N2
T	581	LEU	-	linker	UNP Q969N2
T	582	GLU	-	linker	UNP Q969N2
T	583	VAL	-	linker	UNP Q969N2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
T	584	LEU	-	linker	UNP Q969N2
T	585	PHE	-	linker	UNP Q969N2
T	586	GLN	-	linker	UNP Q969N2
T	587	GLY	-	linker	UNP Q969N2
T	588	PRO	-	linker	UNP Q969N2
T	589	GLY	-	linker	UNP Q969N2
T	590	GLY	-	linker	UNP Q969N2
T	591	SER	-	linker	UNP Q969N2
T	592	GLY	-	linker	UNP Q969N2
T	593	GLY	-	linker	UNP Q969N2
T	594	SER	-	linker	UNP Q969N2
T	595	ALA	-	linker	UNP Q969N2
T	596	SER	-	linker	UNP Q969N2
T	601	GLU	ASP	conflict	UNP Q9U6Y3
T	607	ARG	LYS	conflict	UNP Q9U6Y3
T	611	ALA	ASN	conflict	UNP Q9U6Y3
T	616	LYS	ALA	conflict	UNP Q9U6Y3
T	624	ILE	GLU	conflict	UNP Q9U6Y3
T	629	GLU	ASP	conflict	UNP Q9U6Y3
T	632	GLN	HIS	conflict	UNP Q9U6Y3
T	635	ASP	ASN	conflict	UNP Q9U6Y3
T	637	THR	GLU	conflict	UNP Q9U6Y3
T	639	GLU	LYS	conflict	UNP Q9U6Y3
T	652	THR	SER	conflict	UNP Q9U6Y3
T	653	PRO	ASN	conflict	UNP Q9U6Y3
T	662	PHE	LEU	conflict	UNP Q9U6Y3
T	667	GLU	ASP	conflict	UNP Q9U6Y3
T	670	PRO	ALA	conflict	UNP Q9U6Y3
T	676	ALA	SER	conflict	UNP Q9U6Y3
T	686	SER	THR	conflict	UNP Q9U6Y3
T	689	TYR	PHE	conflict	UNP Q9U6Y3
T	692	GLN	LYS	conflict	UNP Q9U6Y3
T	695	CYS	VAL	conflict	UNP Q9U6Y3
T	696	ILE	LYS	conflict	UNP Q9U6Y3
T	697	ALA	VAL	conflict	UNP Q9U6Y3
T	698	THR	LYS	conflict	UNP Q9U6Y3
T	702	THR	SER	conflict	UNP Q9U6Y3
T	705	GLY	GLU	conflict	UNP Q9U6Y3
T	707	CYS	SER	conflict	UNP Q9U6Y3
T	709	PHE	ILE	conflict	UNP Q9U6Y3
T	717	THR	MET	conflict	UNP Q9U6Y3
T	739	LYS	ILE	conflict	UNP Q9U6Y3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
T	743	GLU	ARG	conflict	UNP Q9U6Y3
T	748	LYS	VAL	conflict	UNP Q9U6Y3
T	751	VAL	ILE	conflict	UNP Q9U6Y3
T	752	GLU	SER	conflict	UNP Q9U6Y3
T	753	MET	HIS	conflict	UNP Q9U6Y3
T	754	ALA	SER	conflict	UNP Q9U6Y3
T	769	THR	SER	conflict	UNP Q9U6Y3
T	770	THR	ILE	conflict	UNP Q9U6Y3
T	776	ASP	VAL	conflict	UNP Q9U6Y3
T	778	ARG	LYS	conflict	UNP Q9U6Y3
T	782	ALA	TYR	conflict	UNP Q9U6Y3
T	784	GLU	PHE	conflict	UNP Q9U6Y3
T	793	SER	ASN	conflict	UNP Q9U6Y3
T	802	ARG	THR	conflict	UNP Q9U6Y3
T	806	HIS	ASN	conflict	UNP Q9U6Y3
T	808	GLU	VAL	conflict	UNP Q9U6Y3
T	813	GLY	-	expression tag	UNP Q9U6Y3
T	814	GLY	-	expression tag	UNP Q9U6Y3
T	815	GLY	-	expression tag	UNP Q9U6Y3
T	816	SER	-	expression tag	UNP Q9U6Y3
T	817	GLY	-	expression tag	UNP Q9U6Y3
T	818	GLY	-	expression tag	UNP Q9U6Y3
T	819	GLY	-	expression tag	UNP Q9U6Y3

- Molecule 5 is a protein called GPI transamidase component PIG-S, GFP-like fluorescent chromoprotein cFP484.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	498	Total	C	N	O	S	0	0
			3724	2422	621	669	12		

There are 91 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-1	MET	-	initiating methionine	UNP Q96S52
S	0	GLY	-	expression tag	UNP Q96S52
S	1	SER	-	expression tag	UNP Q96S52
S	556	GLY	-	linker	UNP Q96S52
S	557	THR	-	linker	UNP Q96S52
S	558	LEU	-	linker	UNP Q96S52
S	559	GLU	-	linker	UNP Q96S52
S	560	VAL	-	linker	UNP Q96S52

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
S	561	LEU	-	linker	UNP Q96S52
S	562	PHE	-	linker	UNP Q96S52
S	563	GLN	-	linker	UNP Q96S52
S	564	GLY	-	linker	UNP Q96S52
S	565	PRO	-	linker	UNP Q96S52
S	566	GLY	-	linker	UNP Q96S52
S	567	GLY	-	linker	UNP Q96S52
S	568	SER	-	linker	UNP Q96S52
S	569	GLY	-	linker	UNP Q96S52
S	570	GLY	-	linker	UNP Q96S52
S	571	SER	-	linker	UNP Q96S52
S	572	ALA	-	linker	UNP Q96S52
S	573	SER	-	linker	UNP Q96S52
S	578	GLU	ASP	conflict	UNP Q9U6Y3
S	584	ARG	LYS	conflict	UNP Q9U6Y3
S	588	ALA	ASN	conflict	UNP Q9U6Y3
S	593	LYS	ALA	conflict	UNP Q9U6Y3
S	601	ILE	GLU	conflict	UNP Q9U6Y3
S	606	GLU	ASP	conflict	UNP Q9U6Y3
S	609	GLN	HIS	conflict	UNP Q9U6Y3
S	612	ASP	ASN	conflict	UNP Q9U6Y3
S	614	THR	GLU	conflict	UNP Q9U6Y3
S	616	GLU	LYS	conflict	UNP Q9U6Y3
S	629	THR	SER	conflict	UNP Q9U6Y3
S	630	PRO	ASN	conflict	UNP Q9U6Y3
S	639	PHE	LEU	conflict	UNP Q9U6Y3
S	644	GLU	ASP	conflict	UNP Q9U6Y3
S	647	PRO	ALA	conflict	UNP Q9U6Y3
S	653	ALA	SER	conflict	UNP Q9U6Y3
S	663	SER	THR	conflict	UNP Q9U6Y3
S	666	TYR	PHE	conflict	UNP Q9U6Y3
S	669	GLN	LYS	conflict	UNP Q9U6Y3
S	672	CYS	VAL	conflict	UNP Q9U6Y3
S	673	ILE	LYS	conflict	UNP Q9U6Y3
S	674	ALA	VAL	conflict	UNP Q9U6Y3
S	675	THR	LYS	conflict	UNP Q9U6Y3
S	679	THR	SER	conflict	UNP Q9U6Y3
S	682	GLY	GLU	conflict	UNP Q9U6Y3
S	684	CYS	SER	conflict	UNP Q9U6Y3
S	686	PHE	ILE	conflict	UNP Q9U6Y3
S	694	THR	MET	conflict	UNP Q9U6Y3
S	716	LYS	ILE	conflict	UNP Q9U6Y3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
S	720	GLU	ARG	conflict	UNP Q9U6Y3
S	725	LYS	VAL	conflict	UNP Q9U6Y3
S	728	VAL	ILE	conflict	UNP Q9U6Y3
S	729	GLU	SER	conflict	UNP Q9U6Y3
S	730	MET	HIS	conflict	UNP Q9U6Y3
S	731	ALA	SER	conflict	UNP Q9U6Y3
S	746	THR	SER	conflict	UNP Q9U6Y3
S	747	THR	ILE	conflict	UNP Q9U6Y3
S	753	ASP	VAL	conflict	UNP Q9U6Y3
S	755	ARG	LYS	conflict	UNP Q9U6Y3
S	759	ALA	TYR	conflict	UNP Q9U6Y3
S	761	GLU	PHE	conflict	UNP Q9U6Y3
S	770	SER	ASN	conflict	UNP Q9U6Y3
S	779	ARG	THR	conflict	UNP Q9U6Y3
S	783	HIS	ASN	conflict	UNP Q9U6Y3
S	785	GLU	VAL	conflict	UNP Q9U6Y3
S	790	GLY	-	expression tag	UNP Q9U6Y3
S	791	GLY	-	expression tag	UNP Q9U6Y3
S	792	GLY	-	expression tag	UNP Q9U6Y3
S	793	SER	-	expression tag	UNP Q9U6Y3
S	794	GLY	-	expression tag	UNP Q9U6Y3
S	795	GLY	-	expression tag	UNP Q9U6Y3
S	796	GLY	-	expression tag	UNP Q9U6Y3
S	797	GLY	-	expression tag	UNP Q9U6Y3
S	798	GLY	-	expression tag	UNP Q9U6Y3
S	799	GLY	-	expression tag	UNP Q9U6Y3
S	800	GLY	-	expression tag	UNP Q9U6Y3
S	801	GLY	-	expression tag	UNP Q9U6Y3
S	802	GLY	-	expression tag	UNP Q9U6Y3
S	803	GLY	-	expression tag	UNP Q9U6Y3
S	804	GLY	-	expression tag	UNP Q9U6Y3
S	805	GLU	-	expression tag	UNP Q9U6Y3
S	806	GLN	-	expression tag	UNP Q9U6Y3
S	807	LYS	-	expression tag	UNP Q9U6Y3
S	808	LEU	-	expression tag	UNP Q9U6Y3
S	809	ILE	-	expression tag	UNP Q9U6Y3
S	810	SER	-	expression tag	UNP Q9U6Y3
S	811	GLU	-	expression tag	UNP Q9U6Y3
S	812	GLU	-	expression tag	UNP Q9U6Y3
S	813	ASP	-	expression tag	UNP Q9U6Y3
S	814	LEU	-	expression tag	UNP Q9U6Y3

- Molecule 6 is a protein called UL16-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	35	Total	C	N	O	S	0	0
			253	166	39	44	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	15	GLY	-	insertion	UNP Q9BZM5
D	16	SER	-	insertion	UNP Q9BZM5
D	17	HIS	-	insertion	UNP Q9BZM5
D	18	HIS	-	insertion	UNP Q9BZM5
D	19	HIS	-	insertion	UNP Q9BZM5
D	20	HIS	-	insertion	UNP Q9BZM5
D	21	HIS	-	insertion	UNP Q9BZM5
D	22	HIS	-	insertion	UNP Q9BZM5
D	23	HIS	-	insertion	UNP Q9BZM5
D	24	HIS	-	insertion	UNP Q9BZM5
D	25	GLY	-	insertion	UNP Q9BZM5
D	26	SER	-	insertion	UNP Q9BZM5

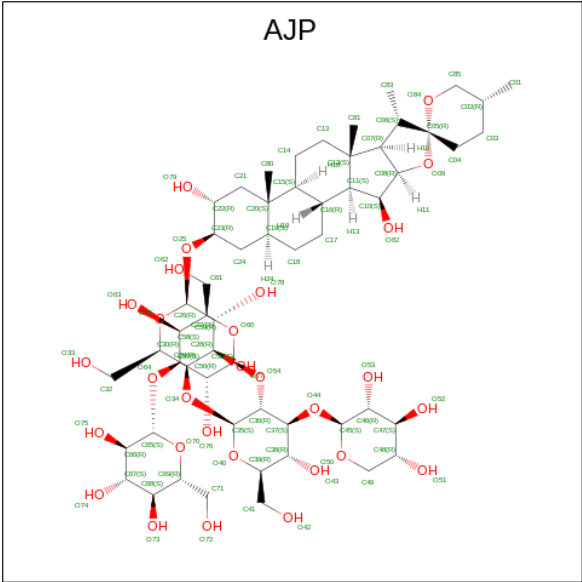
- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	A	2	Total	C	N	O	0	0
			28	16	2	10		

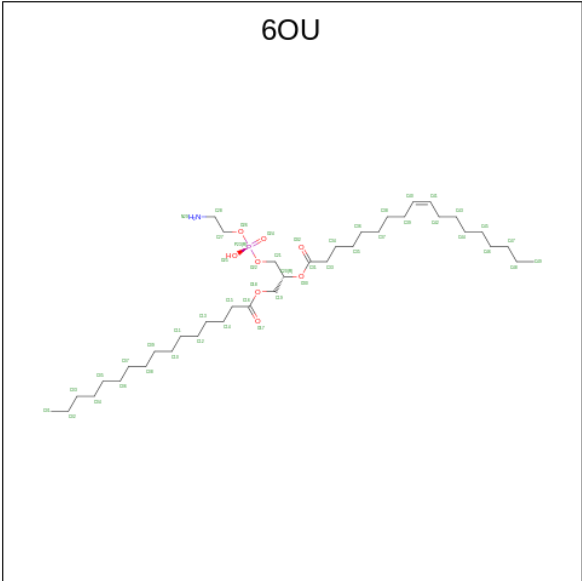
- Molecule 8 is Digitonin (CCD ID: AJP) (formula: C<sub>56</sub>H<sub>92</sub>O<sub>29</sub>).





Mol	Chain	Residues	Atoms			AltConf
8	G	1	Total	C	O	0
			85	56	29	

- Molecule 9 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ( {Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C<sub>39</sub>H<sub>76</sub>NO<sub>8</sub>P).



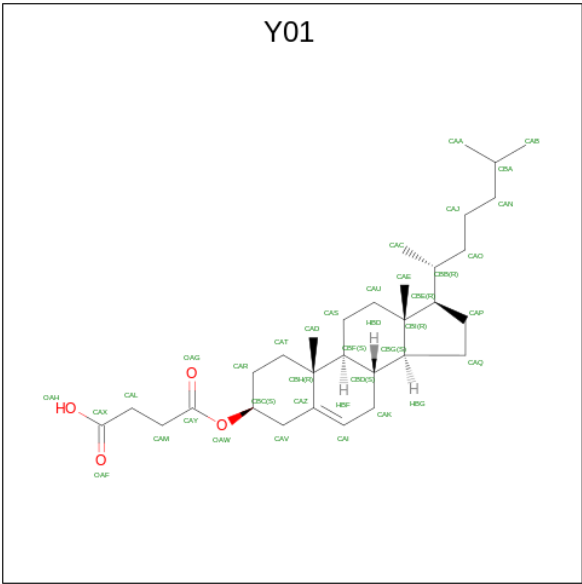
Mol	Chain	Residues	Atoms					AltConf
9	G	1	Total	C	N	O	P	0
			45	35	1	8	1	
9	G	1	Total	C	N	O	P	0
			49	39	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
9	G	1	Total	C	N	O	P	0
			39	29	1	8	1	
9	U	1	Total	C	N	O	P	0
			40	30	1	8	1	
9	U	1	Total	C	N	O	P	0
			49	39	1	8	1	
9	S	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 10 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
10	G	1	Total	C	O	0
			35	31	4	
10	G	1	Total	C	O	0
			35	31	4	
10	G	1	Total	C	O	0
			35	31	4	
10	G	1	Total	C	O	0
			35	31	4	
10	G	1	Total	C	O	0
			35	31	4	
10	G	1	Total	C	O	0
			35	31	4	
10	G	1	Total	C	O	0
			35	31	4	
10	G	1	Total	C	O	0
			35	31	4	

Continued on next page...

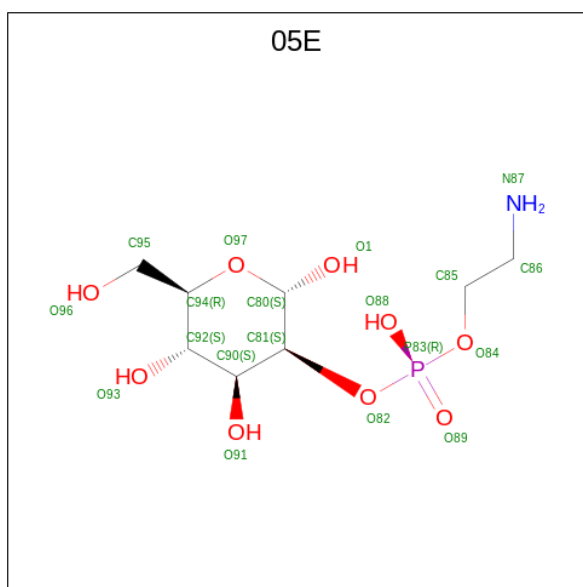
*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
10	G	1	Total	C	O	0
			35	31	4	
10	U	1	Total	C	O	0
			35	31	4	
10	U	1	Total	C	O	0
			35	31	4	
10	U	1	Total	C	O	0
			35	31	4	
10	U	1	Total	C	O	0
			35	31	4	
10	U	1	Total	C	O	0
			35	31	4	
10	U	1	Total	C	O	0
			35	31	4	
10	U	1	Total	C	O	0
			35	31	4	
10	S	1	Total	C	O	0
			35	31	4	
10	S	1	Total	C	O	0
			35	31	4	
10	D	1	Total	C	O	0
			35	31	4	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

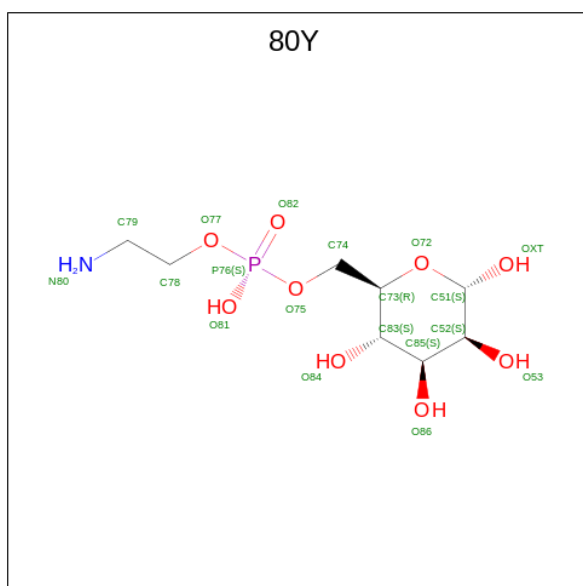
Mol	Chain	Residues	Atoms		AltConf
11	G	1	Total	Mg	0
			1	1	

- Molecule 12 is 2-azanylethyl [(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-2,4,5-tris(oxidanyl)oxan-3-yl] hydrogen phosphate (CCD ID: 05E) (formula: C<sub>8</sub>H<sub>18</sub>NO<sub>9</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	G	1	Total	C	N	O	P	0
			18	8	1	8	1	

- Molecule 13 is 2-azanylethyl [(2R,3S,4S,5S,6S)-3,4,5,6-tetrakis(oxidanyl)oxan-2-yl]methyl hydrogen phosphate (CCD ID: 80Y) (formula:  $C_8H_{18}NO_9P$ ) (labeled as "Ligand of Interest" by depositor).

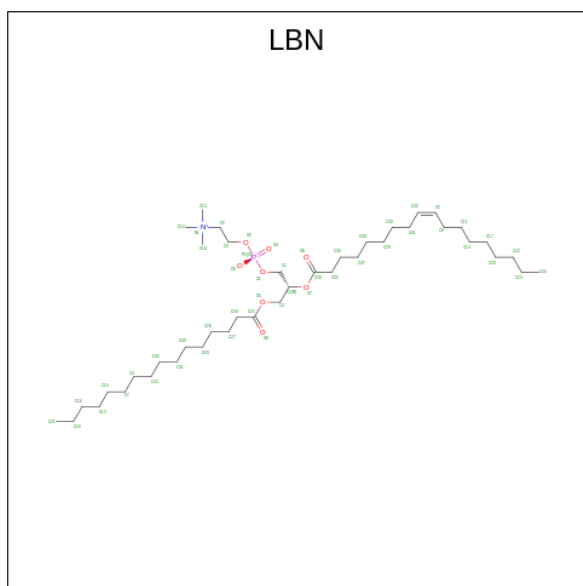


Mol	Chain	Residues	Atoms					AltConf
13	G	1	Total	C	N	O	P	0
			18	8	1	8	1	
13	D	1	Total	C	N	O	P	0
			18	8	1	8	1	

- Molecule 14 is CALCIUM ION (CCD ID: CA) (formula: Ca).

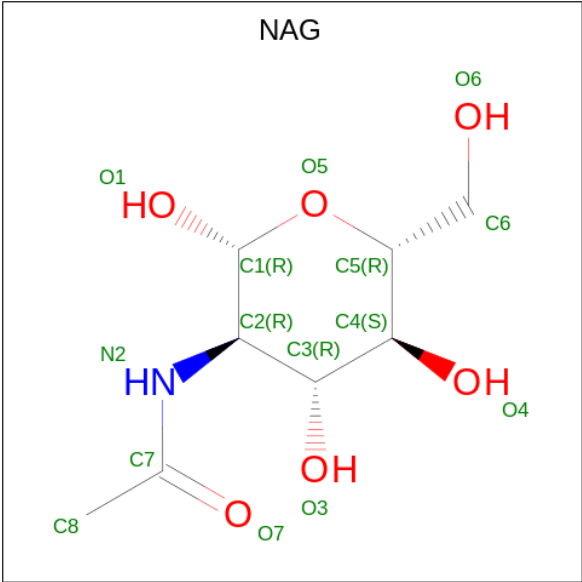
Mol	Chain	Residues	Atoms		AltConf
14	K	1	Total	Ca	0
			1	1	

- Molecule 15 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



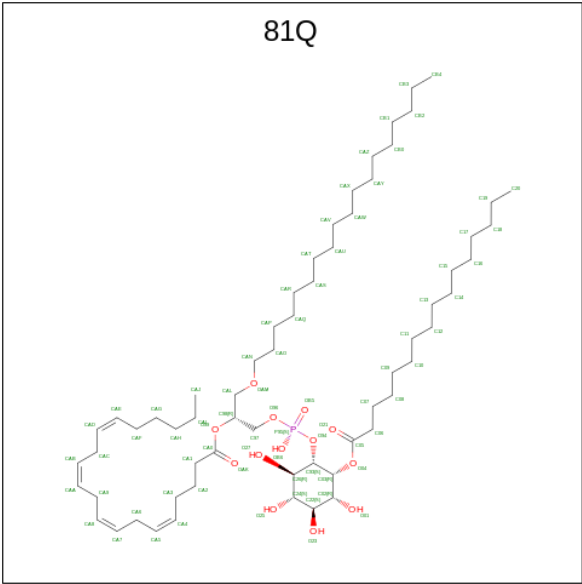
Mol	Chain	Residues	Atoms					AltConf
15	U	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



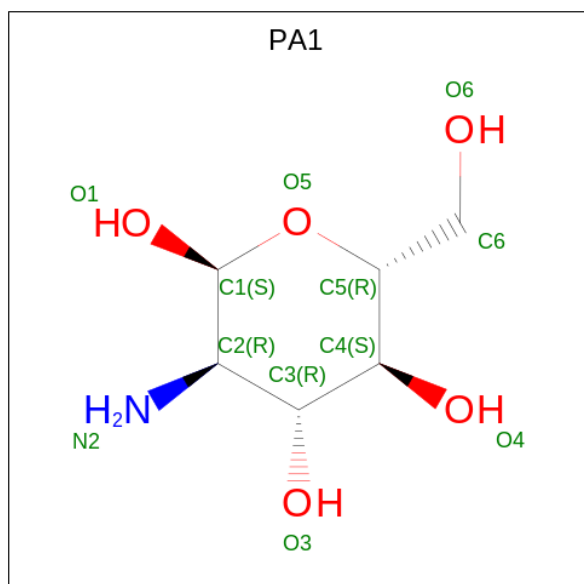
Mol	Chain	Residues	Atoms				AltConf
16	T	1	Total	C	N	O	0
			14	8	1	5	
16	S	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 17 is [(2R)-1-[(1S,2R,3R,4S,5S,6R)-2-hexadecanoyloxy-3,4,5,6-tetrakis(oxidanyl)cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-3-octadecoxy-propan-2-yl] (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoate (CCD ID: 81Q) (formula: C<sub>63</sub>H<sub>115</sub>O<sub>13</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
17	T	1	Total	C	O	P	0
			77	63	13	1	

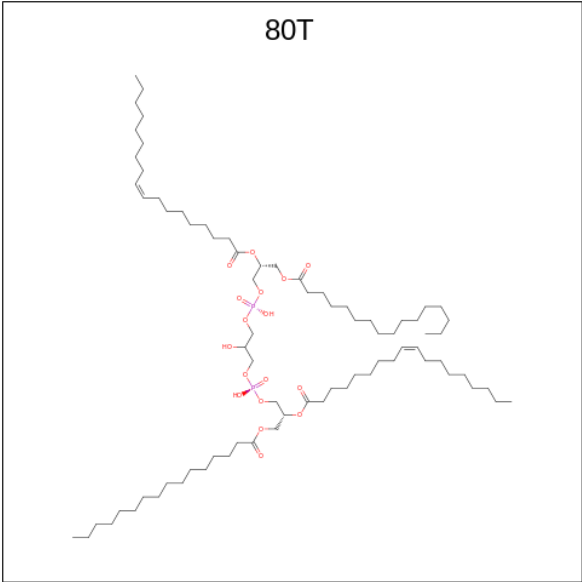
- Molecule 18 is 2-amino-2-deoxy-alpha-D-glucopyranose (CCD ID: PA1) (formula:  $C_6H_{13}NO_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
18	T	1	Total	C	N	O	0
			11	6	1	4	

- Molecule 19 is [(2R)-1-hexadecanoyloxy-3-[[3-[(2R)-3-hexadecanoyloxy-2-[(Z)-octadec-9-enoyl]oxy-propoxy]-oxidanyl-phosphoryl]oxy-2-oxidanyl-propoxy]-oxidanyl-phosphoryl]oxy-propan-2-yl] (Z)-octadec-9-enoate (CCD ID: 80T) (formula:  $C_{77}H_{146}O_{17}P_2$ ).





Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	S	1	88	69	17	2	0

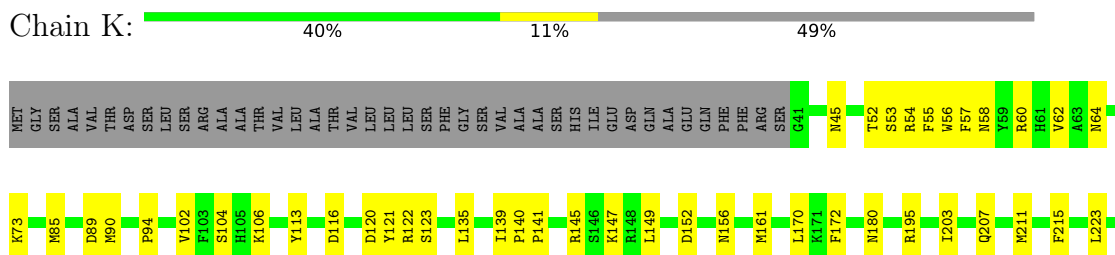
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Glycosylphosphatidylinositol anchor attachment 1 protein,GFP-like fluorescent chromoprotein cFP484



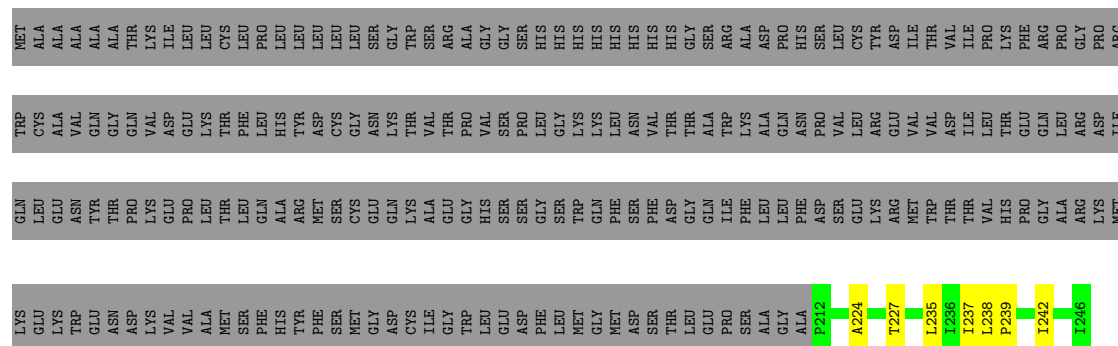
- Molecule 2: GPI-anchor transamidase,GFP-like fluorescent chromoprotein cFP484







Chain D:  11% . 86%



Chain A:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	176889	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	53648	Depositor
Image detector	GATAN K3 (6k x 4k)	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: PA1, NAG, Y01, 80Y, 6OU, AJP, LBN, CA, 05E, MG, 81Q, 80T

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	G	0.31	0/4501	0.48	0/6138
2	K	0.24	0/2701	0.38	0/3674
3	U	0.12	0/3518	0.28	0/4808
4	T	0.19	0/4354	0.35	0/5967
5	S	0.25	0/3809	0.42	0/5207
6	D	0.19	0/256	0.52	0/348
All	All	0.23	0/19139	0.40	0/26142

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	G	4397	0	4466	72	0
2	K	2633	0	2547	64	0
3	U	3406	0	3467	60	0
4	T	4221	0	4142	84	0
5	S	3724	0	3690	60	0
6	D	253	0	284	6	0
7	A	28	0	25	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	85	0	0	0	0
9	G	133	0	0	1	0
9	S	40	0	0	0	0
9	U	89	0	0	0	0
10	D	35	0	49	3	0
10	G	280	0	392	26	0
10	S	70	0	98	5	0
10	U	280	0	392	35	0
11	G	1	0	0	0	0
12	G	18	0	0	0	0
13	D	18	0	0	0	0
13	G	18	0	0	0	0
14	K	1	0	0	0	0
15	U	52	0	0	0	0
16	S	14	0	13	0	0
16	T	14	0	13	0	0
17	T	77	0	0	2	0
18	T	11	0	10	1	0
19	S	88	0	0	0	0
All	All	19986	0	19588	340	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 340 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:G:55:MET:SD	1:G:349:LEU:HD21	1.77	1.23
5:S:418:LEU:HD13	5:S:423:LEU:HD21	1.33	1.11
3:U:259:GLY:CA	10:U:802:Y01:HAD3	1.91	1.00
1:G:55:MET:SD	1:G:349:LEU:CD2	2.59	0.90
3:U:259:GLY:HA3	10:U:802:Y01:HAD3	1.52	0.90

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	G	573/886 (65%)	561 (98%)	12 (2%)	0	100	100
2	K	326/647 (50%)	317 (97%)	9 (3%)	0	100	100
3	U	417/712 (59%)	408 (98%)	9 (2%)	0	100	100
4	T	528/821 (64%)	519 (98%)	9 (2%)	0	100	100
5	S	486/816 (60%)	480 (99%)	6 (1%)	0	100	100
6	D	33/258 (13%)	30 (91%)	3 (9%)	0	100	100
All	All	2363/4140 (57%)	2315 (98%)	48 (2%)	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	G	443/714 (62%)	439 (99%)	4 (1%)	75	87
2	K	288/563 (51%)	288 (100%)	0	100	100
3	U	366/609 (60%)	366 (100%)	0	100	100
4	T	464/718 (65%)	464 (100%)	0	100	100
5	S	380/681 (56%)	378 (100%)	2 (0%)	86	92
6	D	30/221 (14%)	30 (100%)	0	100	100
All	All	1971/3506 (56%)	1965 (100%)	6 (0%)	90	95

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	356	SER
5	S	425	ARG
5	S	529	MET
1	G	347	ASN
1	G	76	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
3	U	64	HIS
5	S	50	GLN
3	U	319	GLN
5	S	447	GLN
4	T	376	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

2 monosaccharides 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	$\# Z  > 2$
7	NAG	A	1	1,7	14,14,15	0.23	0	17,19,21	0.45	0
7	NAG	A	2	7	14,14,15	0.21	0	17,19,21	0.42	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	NAG	A	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

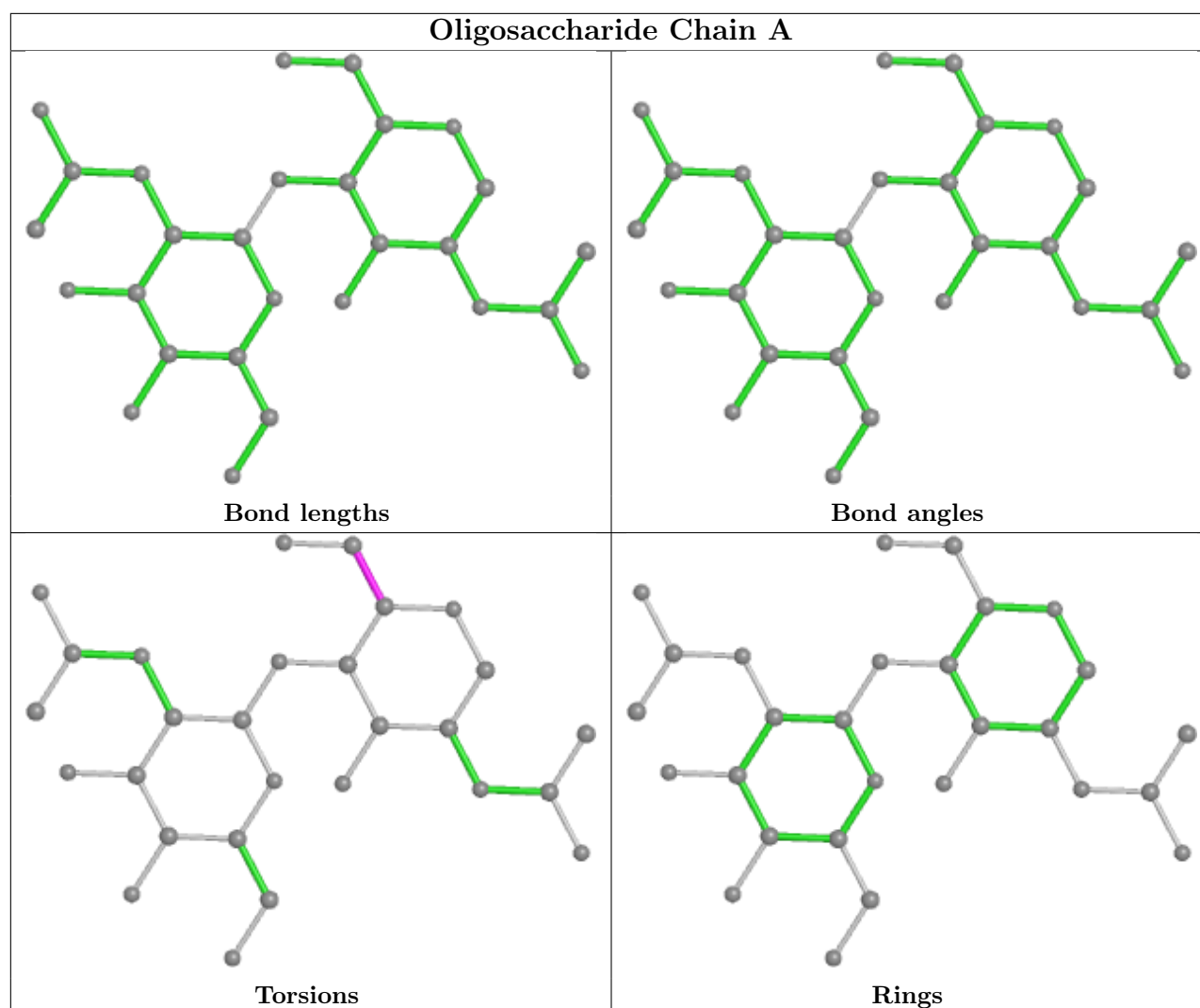
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1	NAG	C4-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 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	$\# Z  > 2$
18	PA1	T	903	17,12	11,11,12	1.61	4 (36%)	12,15,17	1.21	0
10	Y01	G	1807	-	38,38,38	0.70	2 (5%)	57,57,57	0.80	2 (3%)
10	Y01	U	805	-	38,38,38	0.65	2 (5%)	57,57,57	0.62	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	Y01	G	1805	-	38,38,38	0.68	2 (5%)	57,57,57	0.71	2 (3%)
9	6OU	S	903	-	39,39,48	0.96	4 (10%)	42,44,53	1.01	2 (4%)
12	05E	G	1814	13,18,11	18,18,19	1.35	3 (16%)	22,25,27	1.04	2 (9%)
10	Y01	G	1811	-	38,38,38	0.69	2 (5%)	57,57,57	0.83	3 (5%)
9	6OU	U	801	-	39,39,48	0.95	3 (7%)	42,44,53	1.14	2 (4%)
10	Y01	G	1806	-	38,38,38	0.68	2 (5%)	57,57,57	0.72	2 (3%)
16	NAG	T	901	4	14,14,15	0.24	0	17,19,21	0.51	0
9	6OU	U	810	-	48,48,48	0.89	2 (4%)	51,53,53	0.98	4 (7%)
13	80Y	D	302	13	18,18,19	1.31	1 (5%)	24,25,27	0.82	1 (4%)
9	6OU	G	1802	-	44,44,48	0.89	3 (6%)	47,49,53	1.31	5 (10%)
10	Y01	U	809	-	38,38,38	0.65	2 (5%)	57,57,57	0.82	2 (3%)
13	80Y	G	1815	13,12	18,18,19	1.64	2 (11%)	24,25,27	1.14	2 (8%)
8	AJP	G	1801	-	95,95,95	0.13	0	143,149,149	0.35	0
10	Y01	D	301	-	38,38,38	0.67	2 (5%)	57,57,57	0.95	4 (7%)
19	80T	S	901	-	87,87,95	1.41	12 (13%)	93,99,107	1.02	4 (4%)
16	NAG	S	902	5	14,14,15	0.24	0	17,19,21	0.47	0
10	Y01	U	803	-	38,38,38	0.65	2 (5%)	57,57,57	0.70	2 (3%)
10	Y01	U	802	-	38,38,38	0.67	2 (5%)	57,57,57	0.72	2 (3%)
10	Y01	U	806	-	38,38,38	0.67	2 (5%)	57,57,57	0.81	2 (3%)
10	Y01	G	1809	-	38,38,38	0.66	2 (5%)	57,57,57	0.78	2 (3%)
9	6OU	G	1804	-	38,38,48	0.99	4 (10%)	41,43,53	1.06	2 (4%)
9	6OU	G	1803	-	48,48,48	0.93	2 (4%)	51,53,53	1.04	3 (5%)
15	LBN	U	811	-	51,51,51	1.09	7 (13%)	57,59,59	0.95	3 (5%)
10	Y01	G	1810	-	38,38,38	0.69	2 (5%)	57,57,57	0.83	3 (5%)
10	Y01	S	904	-	38,38,38	0.66	2 (5%)	57,57,57	0.62	2 (3%)
10	Y01	G	1808	-	38,38,38	0.68	2 (5%)	57,57,57	0.69	2 (3%)
10	Y01	S	905	-	38,38,38	0.67	2 (5%)	57,57,57	0.79	2 (3%)
10	Y01	G	1812	-	38,38,38	0.68	2 (5%)	57,57,57	0.66	2 (3%)
10	Y01	U	808	-	38,38,38	0.75	2 (5%)	57,57,57	0.99	4 (7%)
10	Y01	U	807	-	38,38,38	0.66	2 (5%)	57,57,57	0.68	2 (3%)
17	81Q	T	902	18	77,77,77	1.17	7 (9%)	87,89,89	1.40	6 (6%)
10	Y01	U	804	-	38,38,38	0.67	2 (5%)	57,57,57	0.66	2 (3%)

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
18	PA1	T	903	17,12	-	2/2/19/22	0/1/1/1
10	Y01	G	1807	-	-	11/19/77/77	0/4/4/4
10	Y01	U	805	-	-	17/19/77/77	0/4/4/4
10	Y01	G	1805	-	-	11/19/77/77	0/4/4/4
9	6OU	S	903	-	-	25/43/43/52	-
12	05E	G	1814	13,18,11	-	9/12/29/32	0/1/1/1
10	Y01	G	1811	-	-	8/19/77/77	0/4/4/4
9	6OU	U	801	-	-	26/43/43/52	-
10	Y01	G	1806	-	-	10/19/77/77	0/4/4/4
16	NAG	T	901	4	-	1/6/23/26	0/1/1/1
9	6OU	U	810	-	-	22/52/52/52	-
13	80Y	D	302	13	-	8/11/28/31	0/1/1/1
9	6OU	G	1802	-	-	29/48/48/52	-
10	Y01	U	809	-	-	12/19/77/77	0/4/4/4
13	80Y	G	1815	13,12	-	8/11/28/31	0/1/1/1
8	AJP	G	1801	-	-	8/28/220/220	0/11/11/11
10	Y01	D	301	-	-	15/19/77/77	0/4/4/4
19	80T	S	901	-	-	53/98/98/106	-
16	NAG	S	902	5	-	2/6/23/26	0/1/1/1
10	Y01	U	803	-	-	10/19/77/77	0/4/4/4
10	Y01	U	802	-	-	11/19/77/77	0/4/4/4
10	Y01	U	806	-	-	12/19/77/77	0/4/4/4
10	Y01	G	1809	-	-	14/19/77/77	0/4/4/4
9	6OU	G	1804	-	-	24/42/42/52	-
9	6OU	G	1803	-	-	34/52/52/52	-
15	LBN	U	811	-	-	27/55/55/55	-
10	Y01	G	1810	-	-	12/19/77/77	0/4/4/4
10	Y01	S	904	-	-	14/19/77/77	0/4/4/4
10	Y01	G	1808	-	-	17/19/77/77	0/4/4/4
10	Y01	S	905	-	-	9/19/77/77	0/4/4/4
10	Y01	G	1812	-	-	14/19/77/77	0/4/4/4
10	Y01	U	808	-	-	9/19/77/77	0/4/4/4
10	Y01	U	807	-	-	13/19/77/77	0/4/4/4
17	81Q	T	902	18	-	34/73/97/97	0/1/1/1

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	Y01	U	804	-	-	16/19/77/77	0/4/4/4

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1815	80Y	C52-C85	-4.61	1.45	1.52
17	T	902	81Q	P95-O94	4.24	1.71	1.60
19	S	901	80T	O23-C24	3.99	1.45	1.33
17	T	902	81Q	O04-C05	3.71	1.44	1.34
19	S	901	80T	O72-C52	-3.67	1.37	1.46

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	902	81Q	C03-O04-C05	-5.85	107.78	117.53
17	T	902	81Q	O04-C05-C06	5.45	123.24	111.50
9	G	1802	6OU	O30-C31-C33	4.76	121.76	111.50
9	U	801	6OU	O30-C31-C33	4.68	121.60	111.50
9	G	1804	6OU	O30-C31-C33	4.34	120.85	111.50

There are no chirality outliers.

5 of 547 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	G	1802	6OU	C21-O22-P23-O24
9	G	1802	6OU	C21-O22-P23-O25
9	G	1802	6OU	C21-O22-P23-O26
9	G	1802	6OU	C27-O26-P23-O24
9	G	1802	6OU	O32-C31-O30-C20

There are no ring outliers.

22 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	T	903	PA1	1	0
10	G	1807	Y01	2	0
10	U	805	Y01	1	0
10	G	1805	Y01	3	0
10	G	1811	Y01	2	0
10	G	1806	Y01	1	0
9	G	1802	6OU	1	0

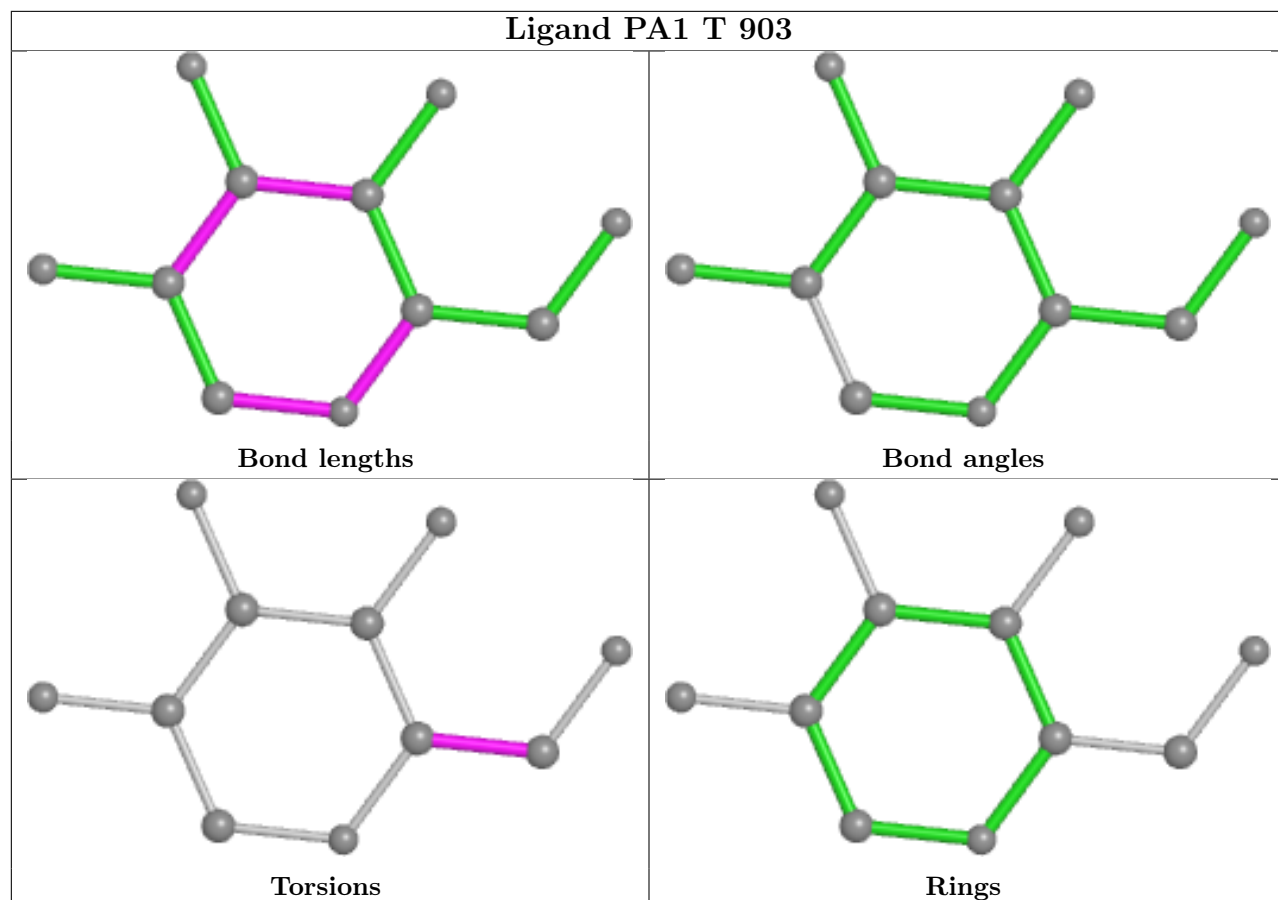
*Continued on next page...*

*Continued from previous page...*

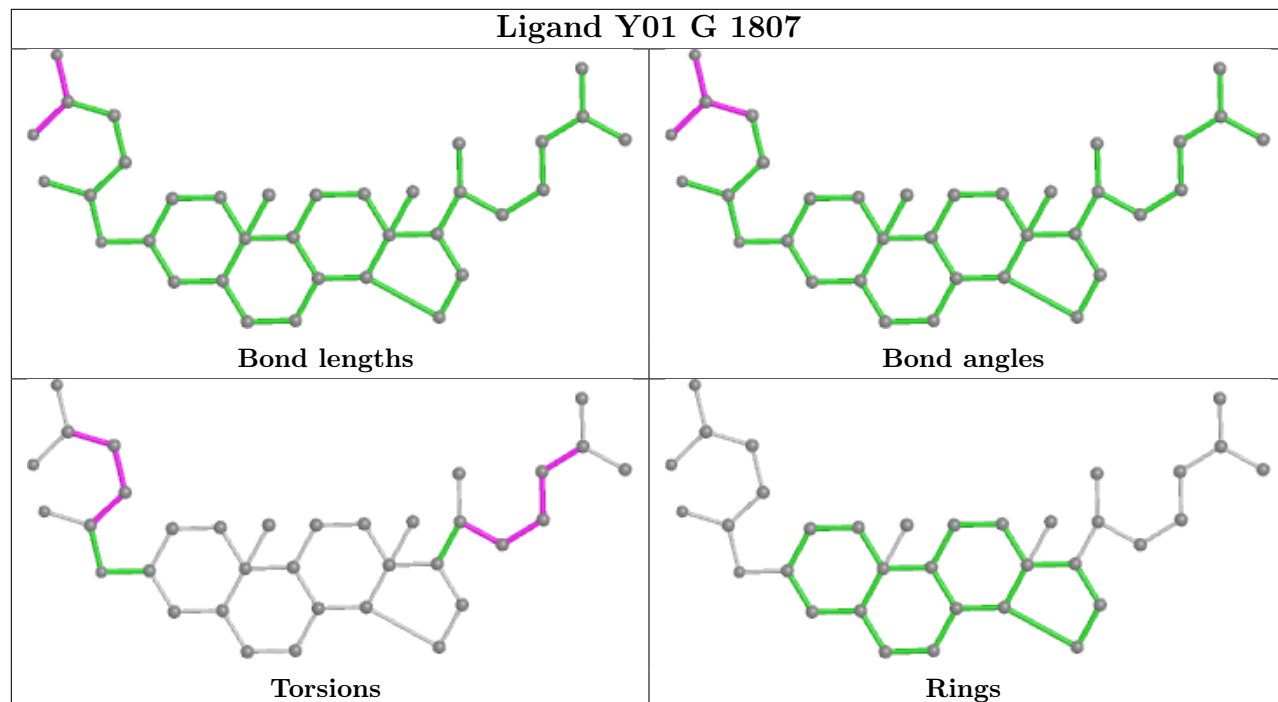
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	U	809	Y01	5	0
10	D	301	Y01	3	0
10	U	803	Y01	5	0
10	U	802	Y01	8	0
10	U	806	Y01	4	0
10	G	1809	Y01	6	0
10	G	1810	Y01	11	0
10	S	904	Y01	1	0
10	G	1808	Y01	6	0
10	S	905	Y01	4	0
10	G	1812	Y01	1	0
10	U	808	Y01	9	0
10	U	807	Y01	1	0
17	T	902	81Q	2	0
10	U	804	Y01	2	0

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

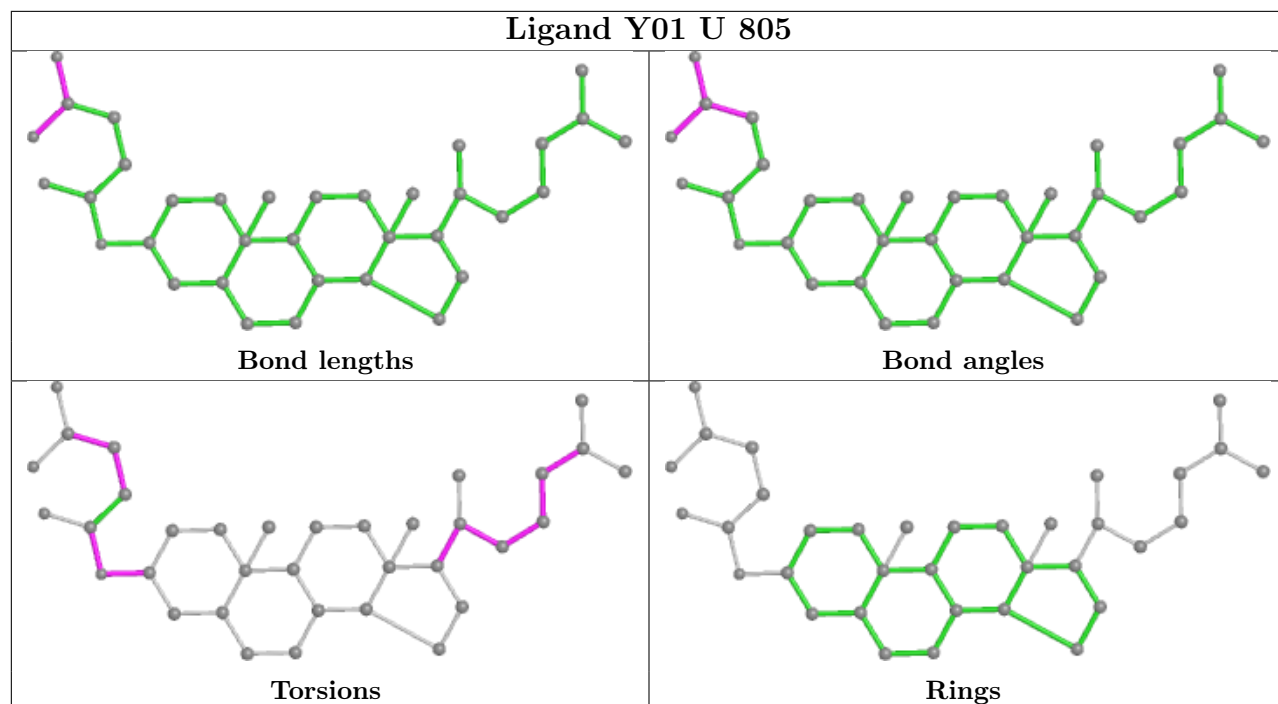
## Ligand PA1 T 903



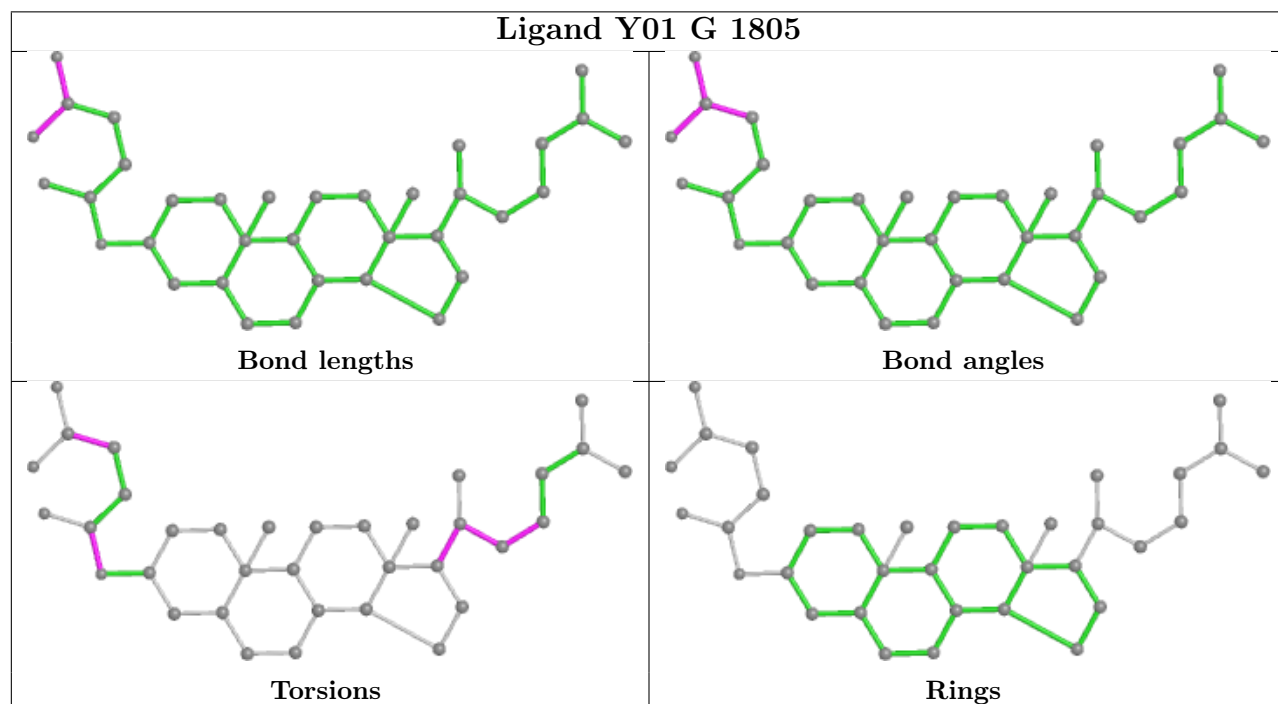
## Ligand Y01 G 1807

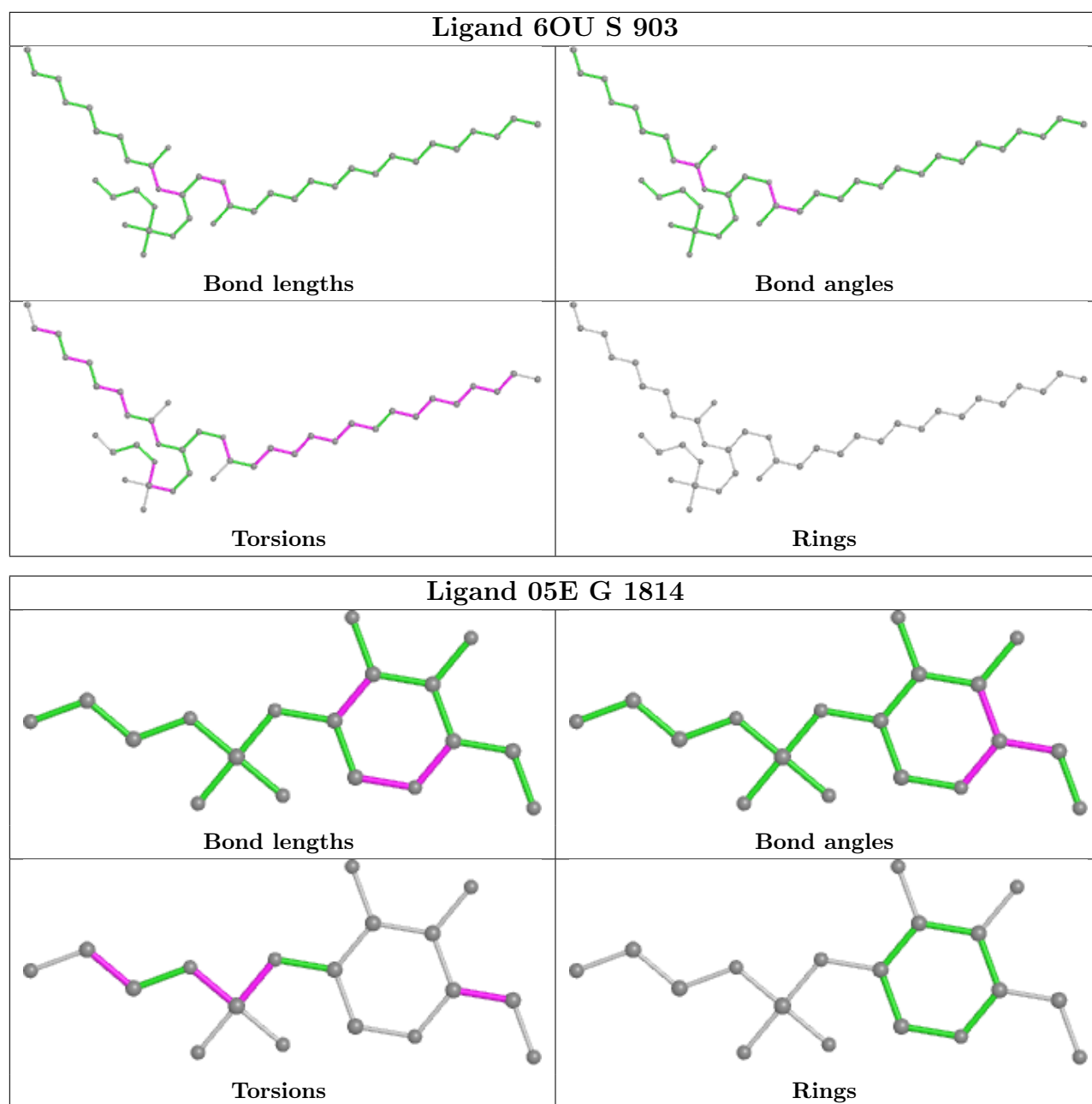


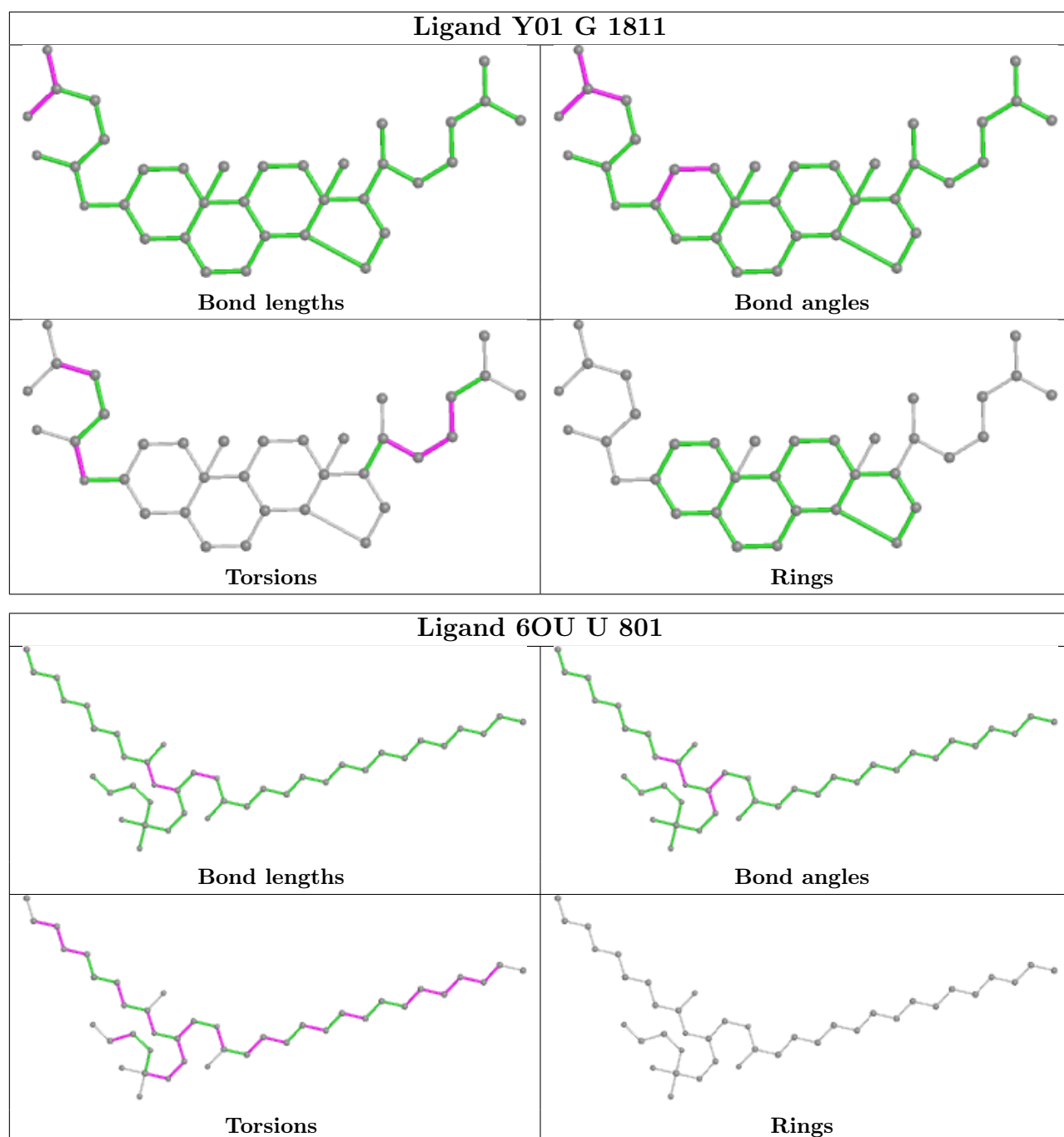
## Ligand Y01 U 805

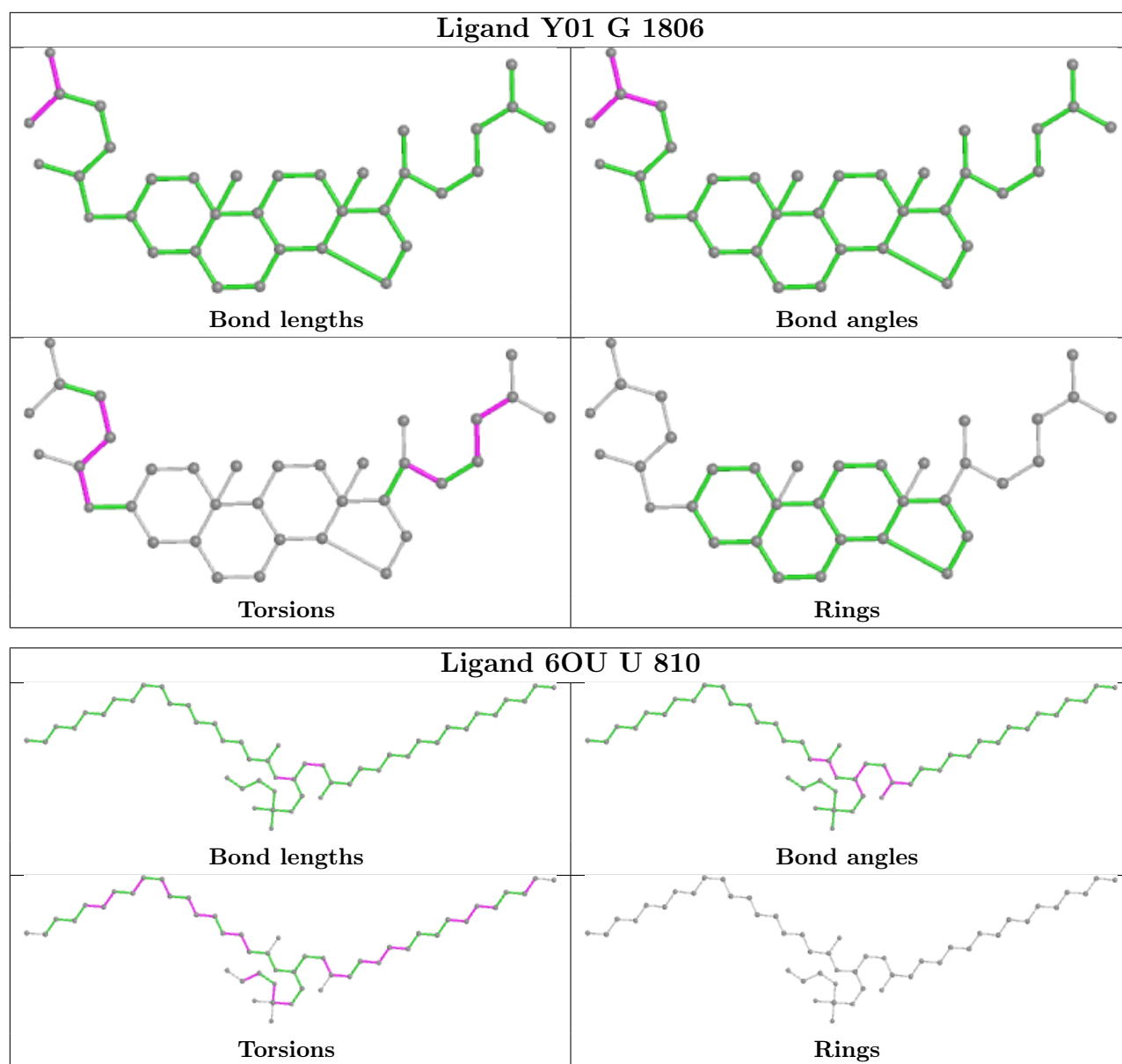


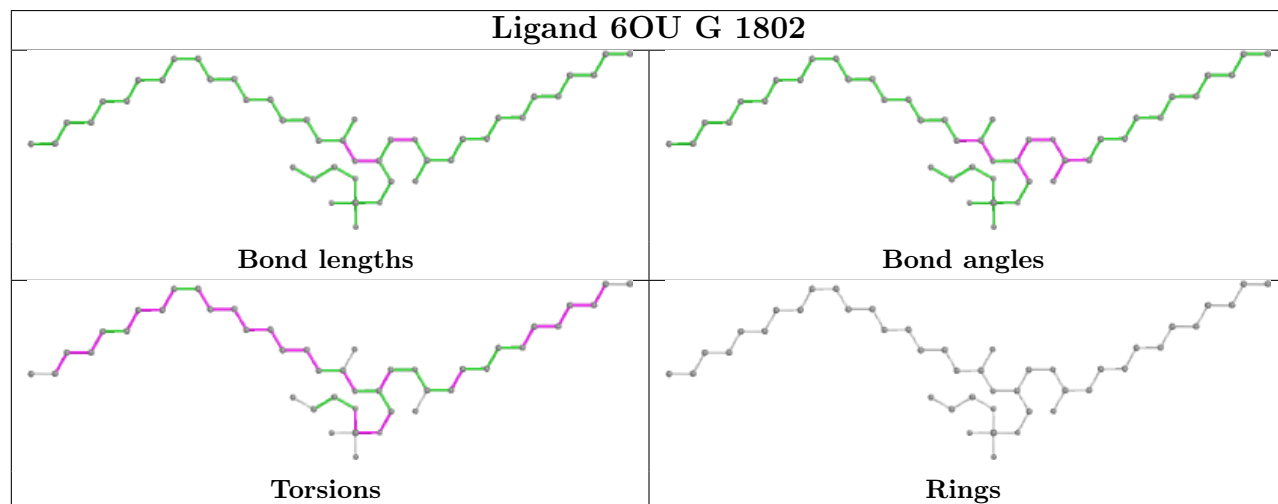
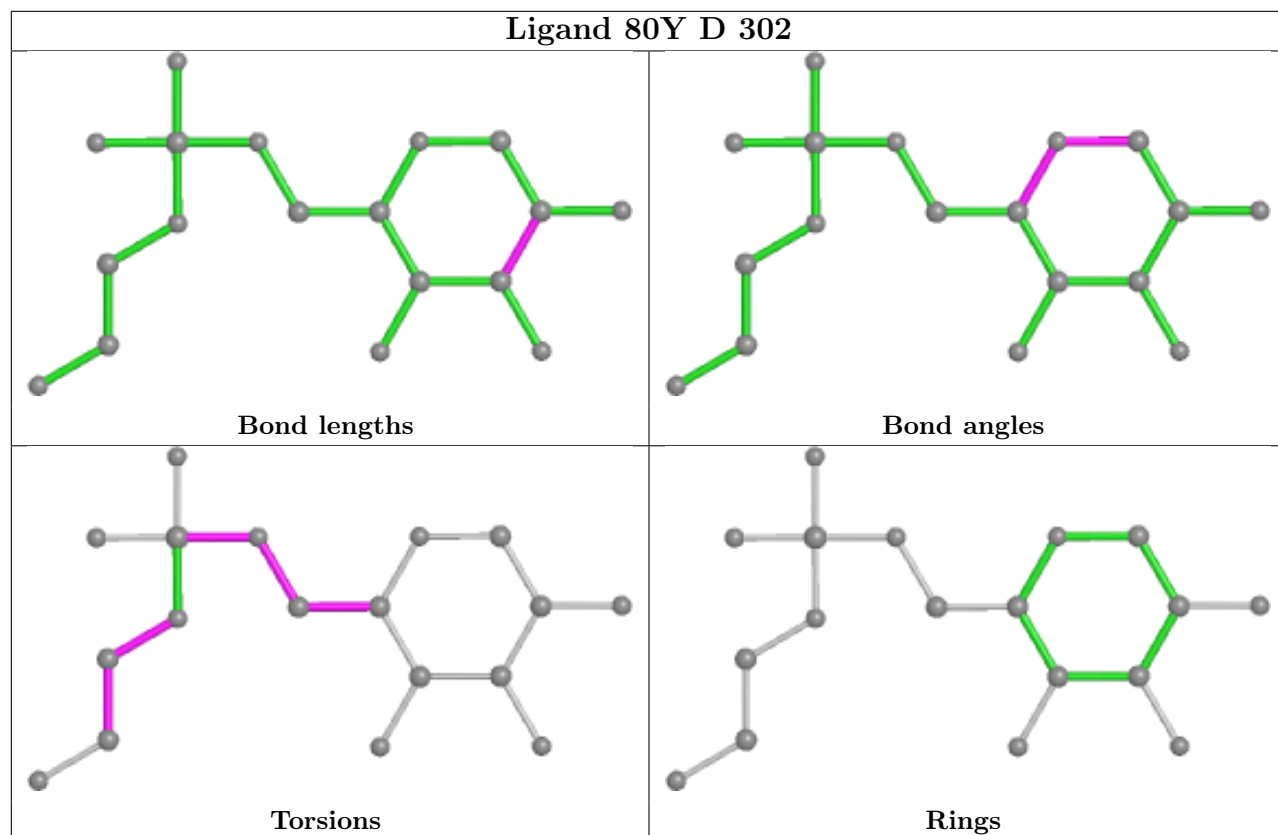
## Ligand Y01 G 1805



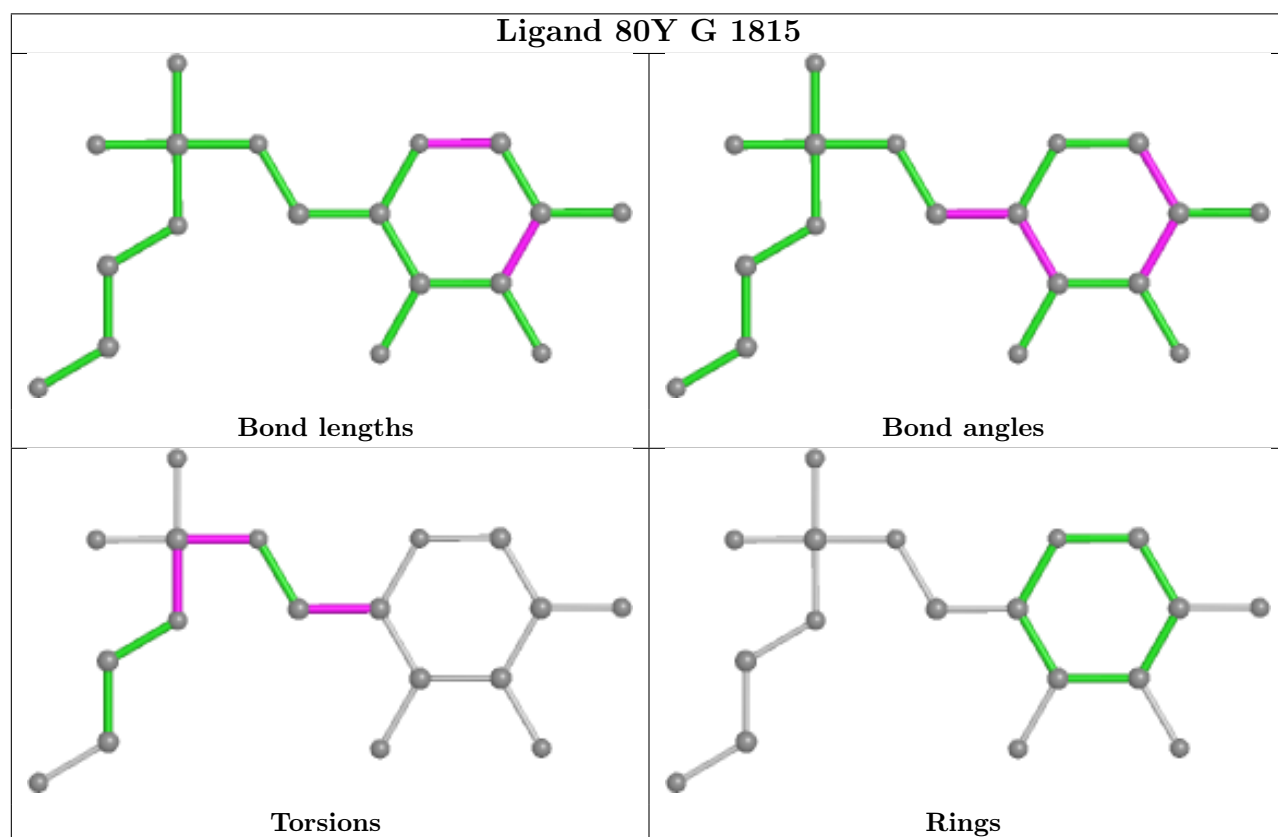
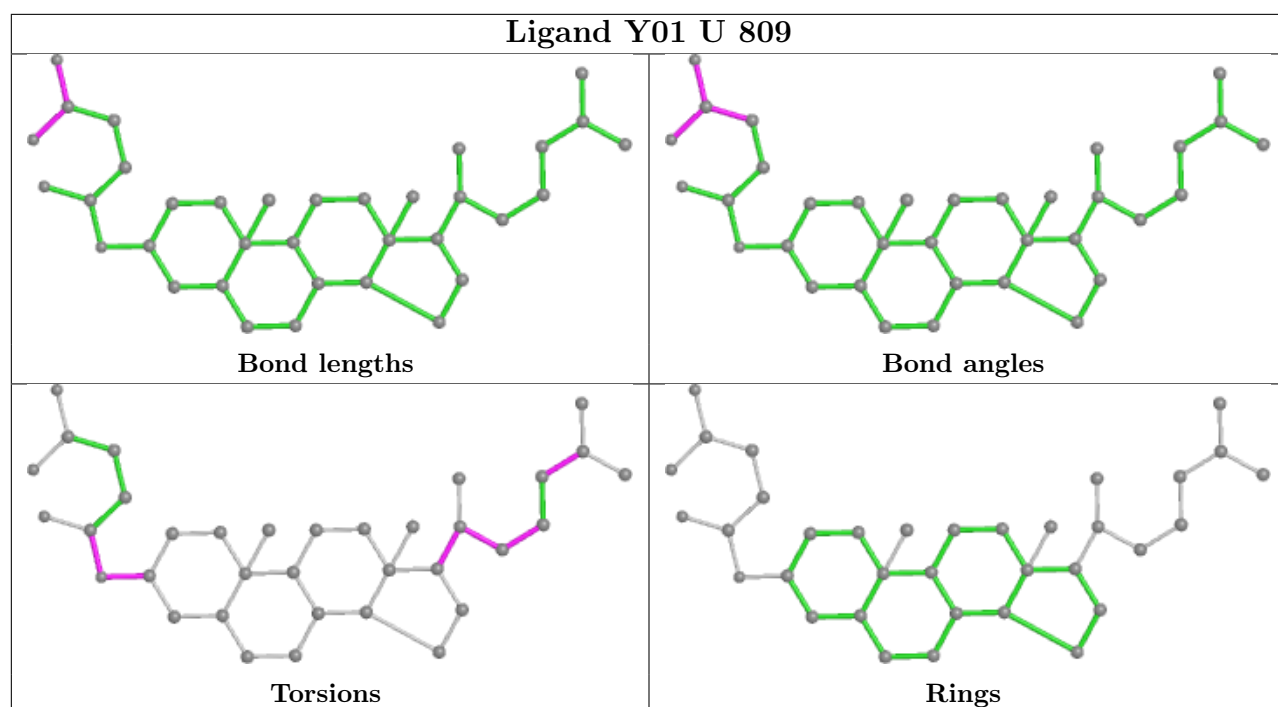


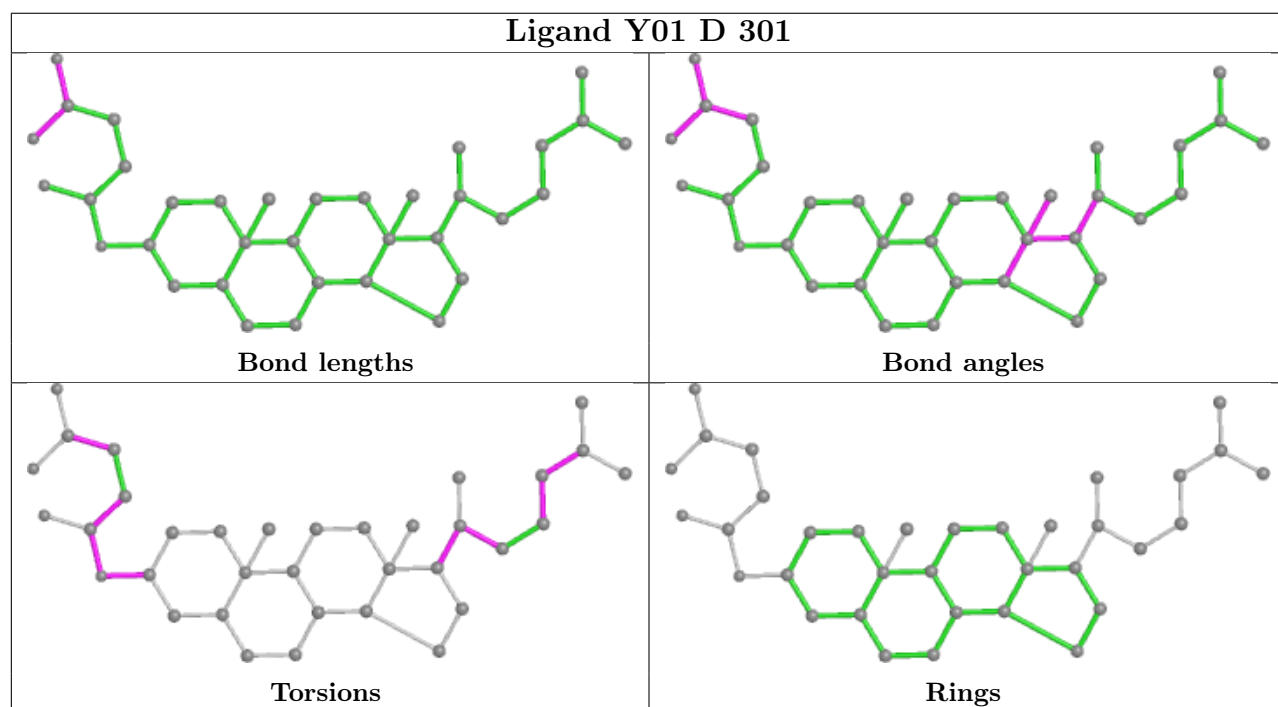
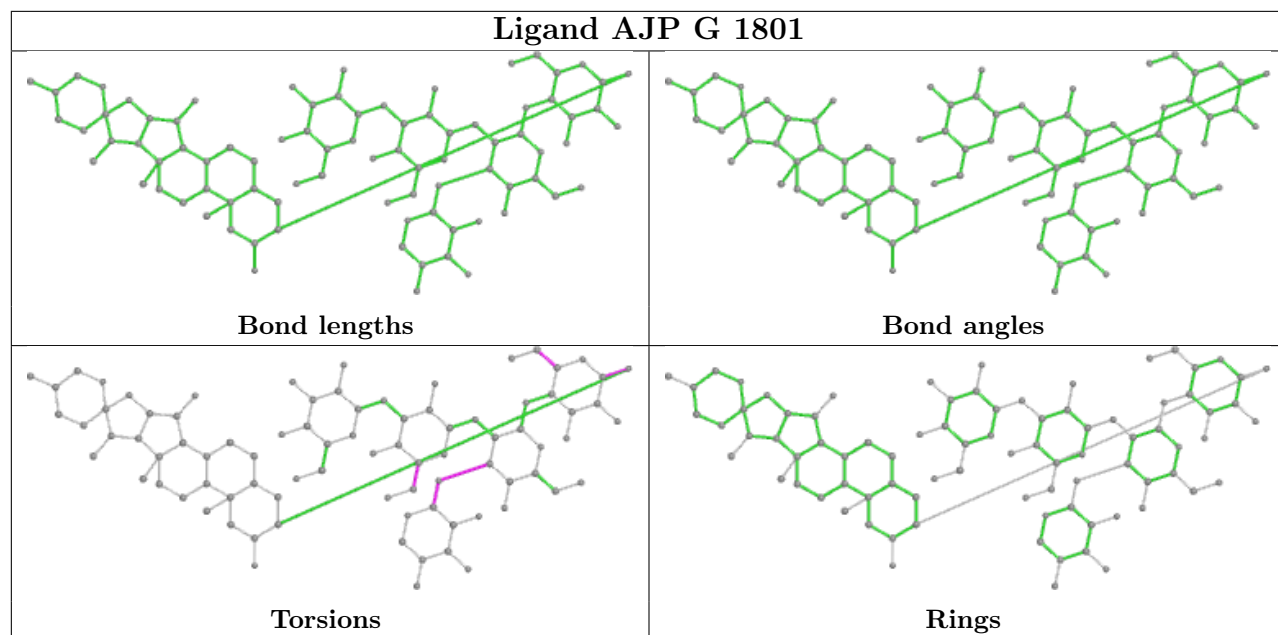


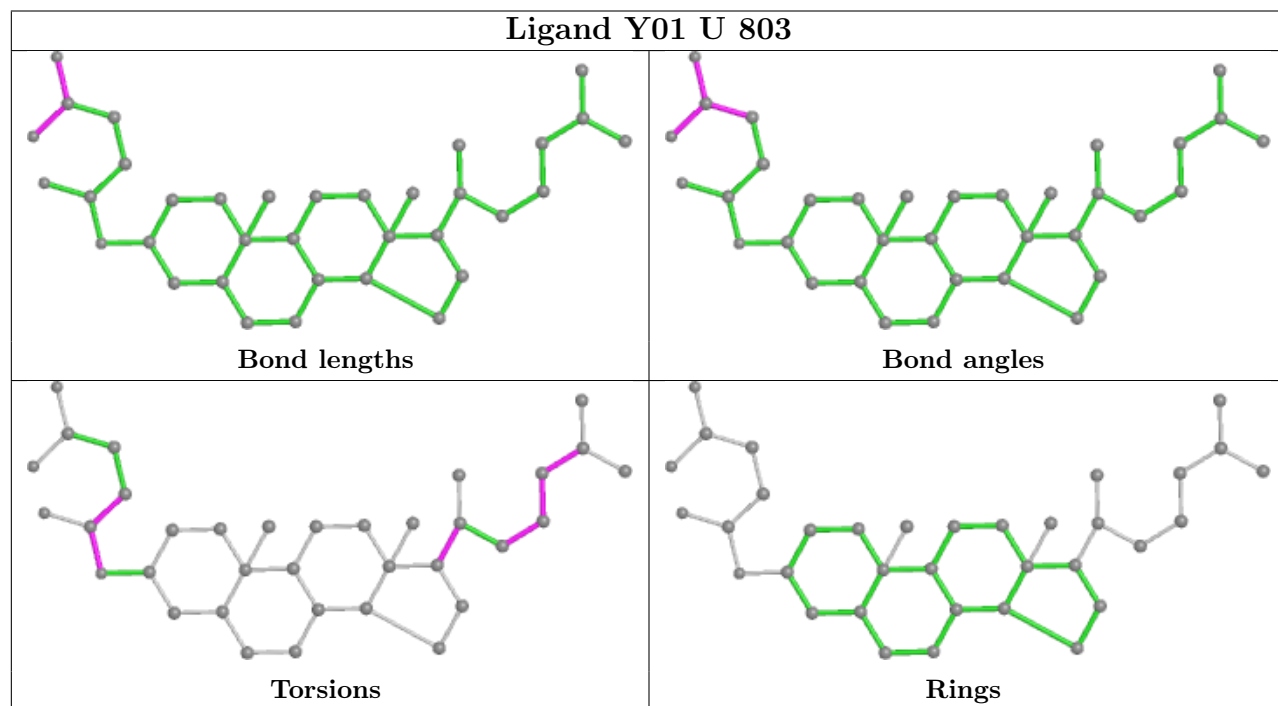
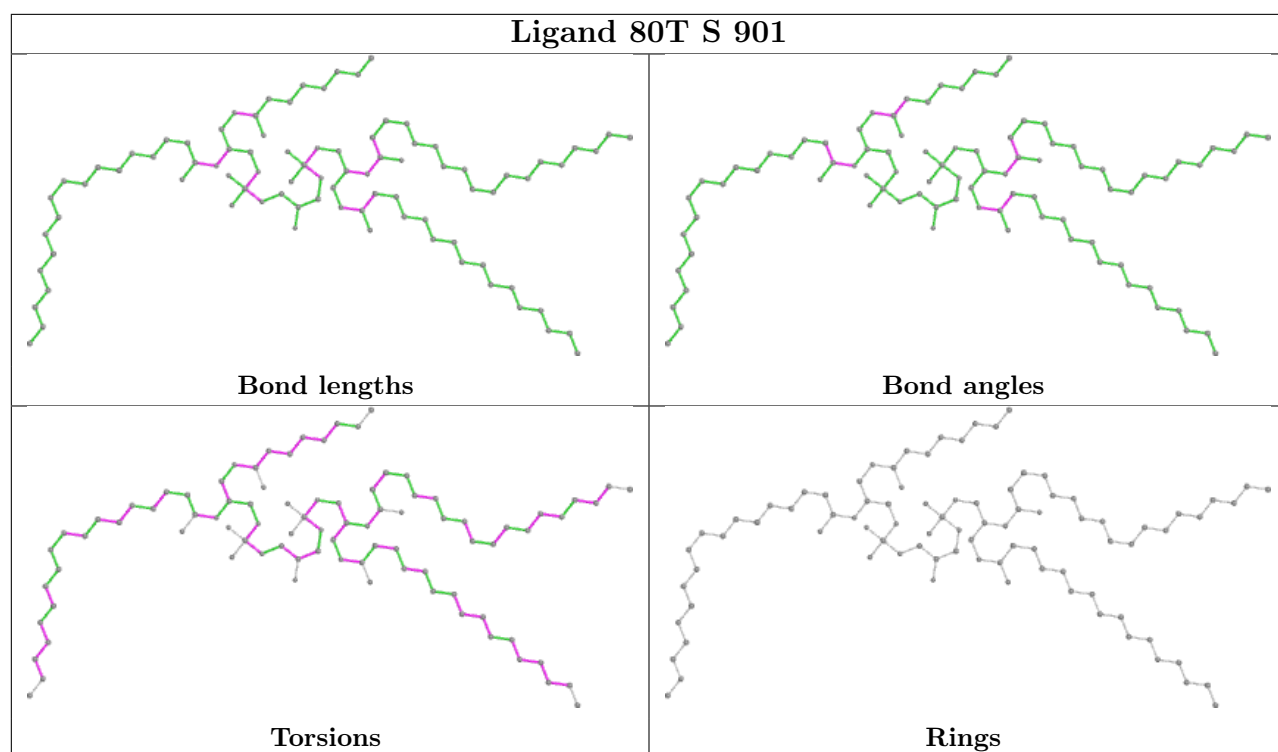


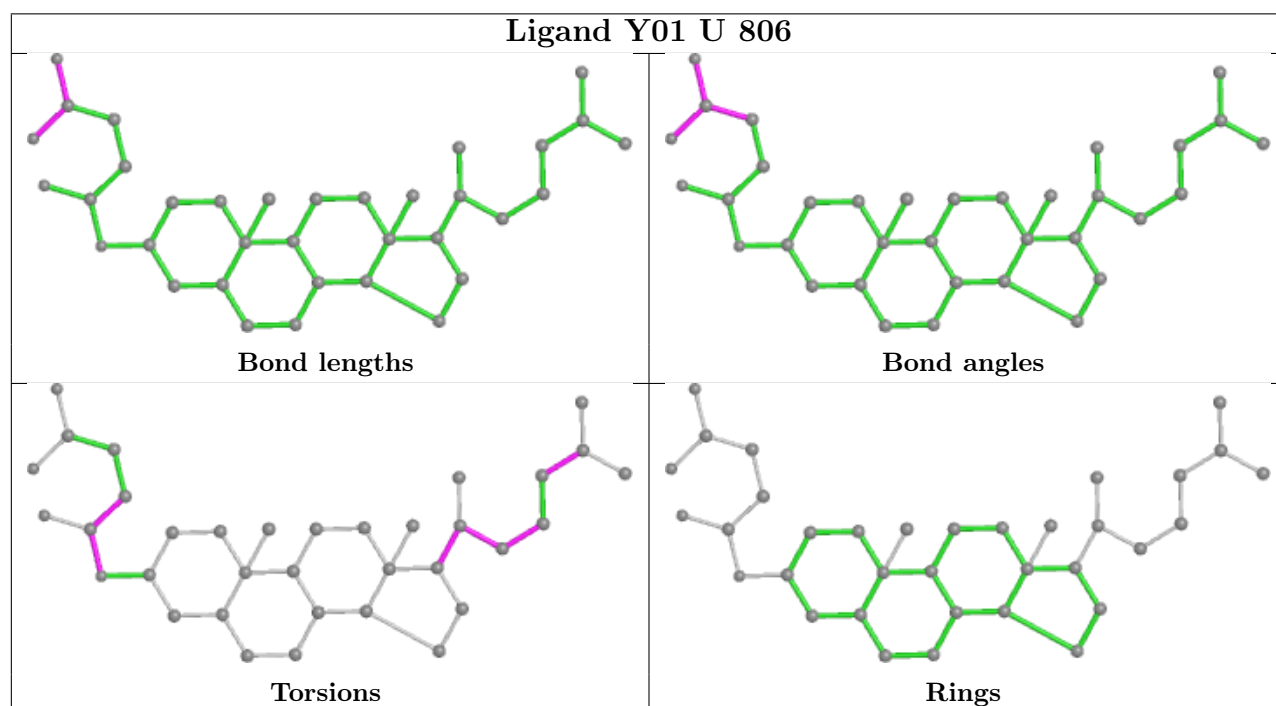
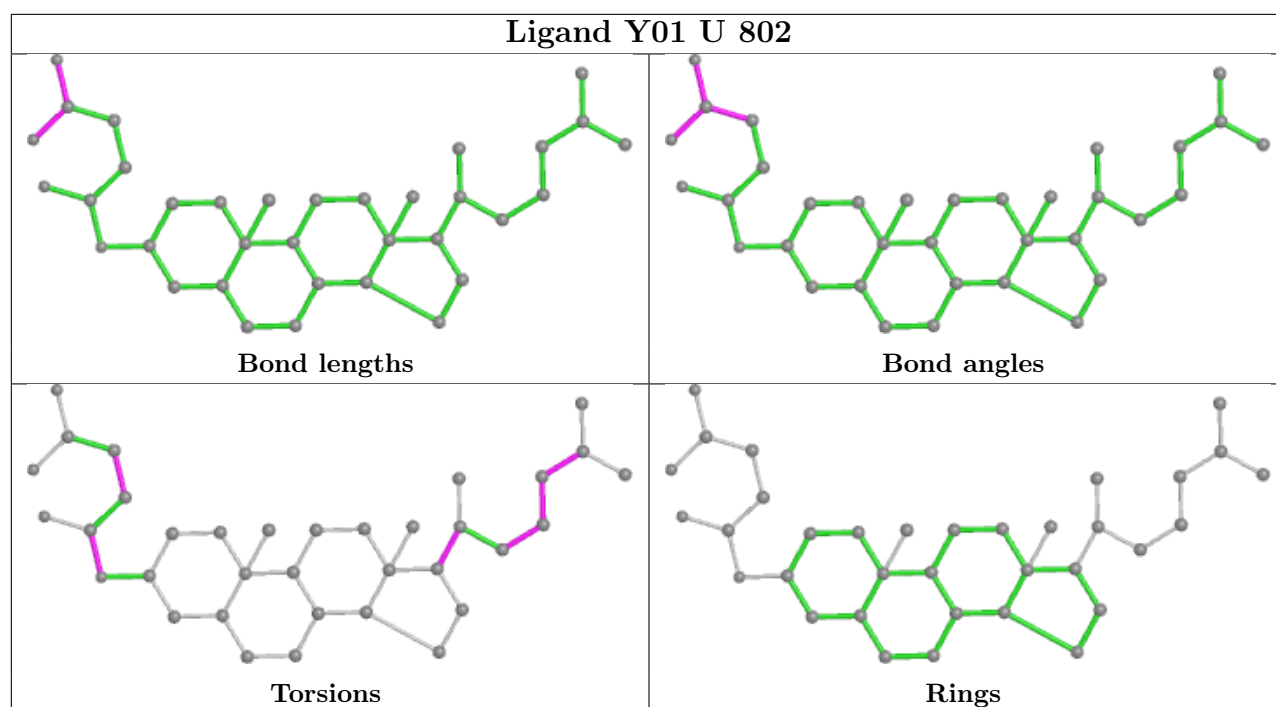


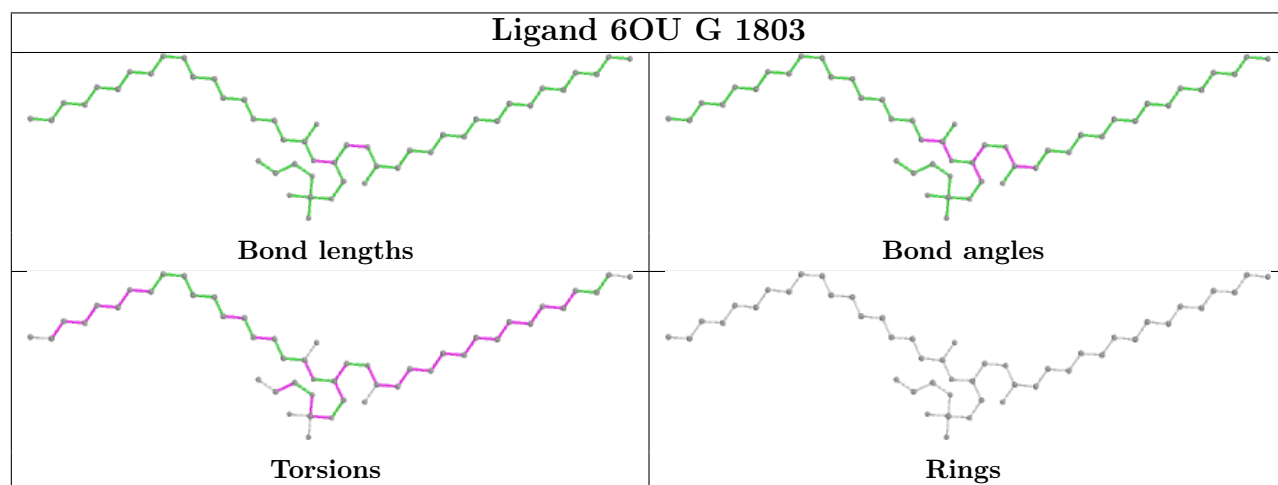
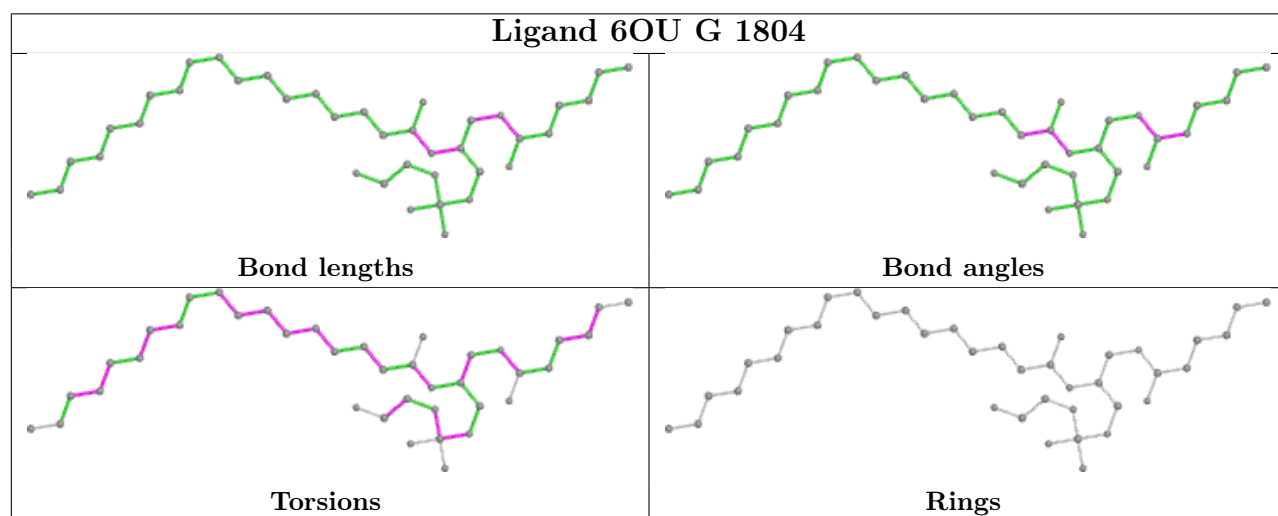
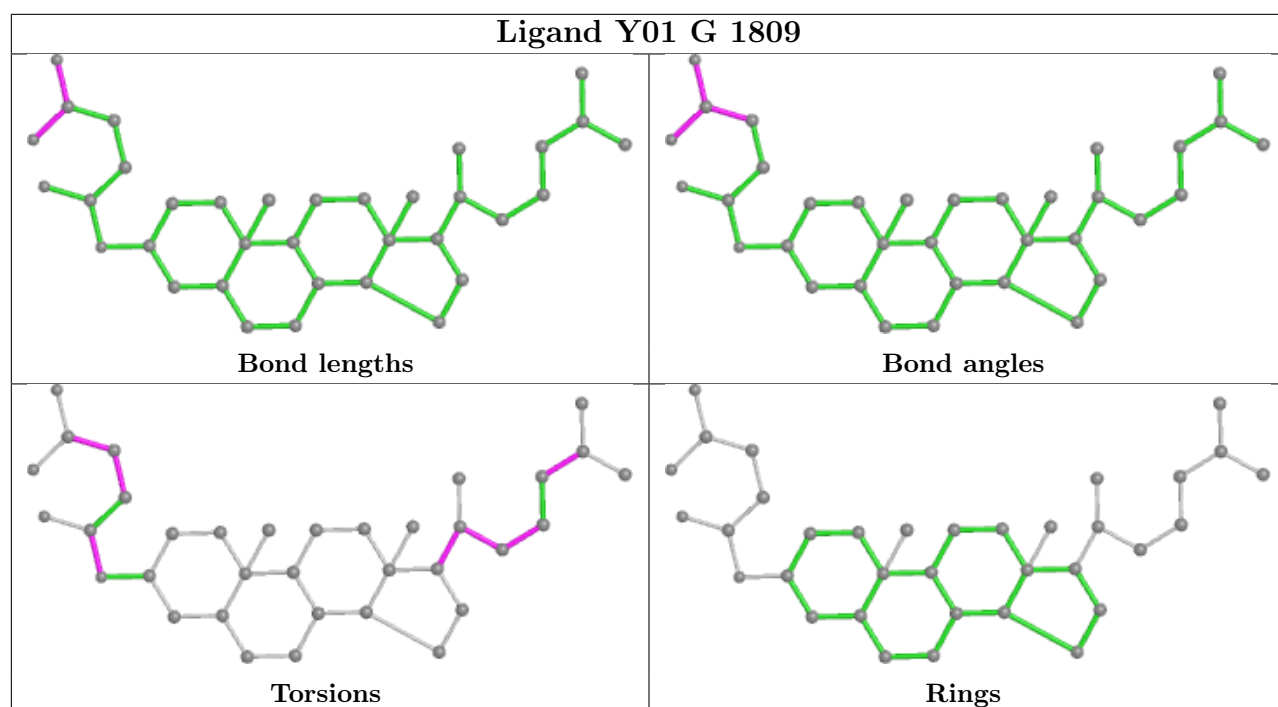


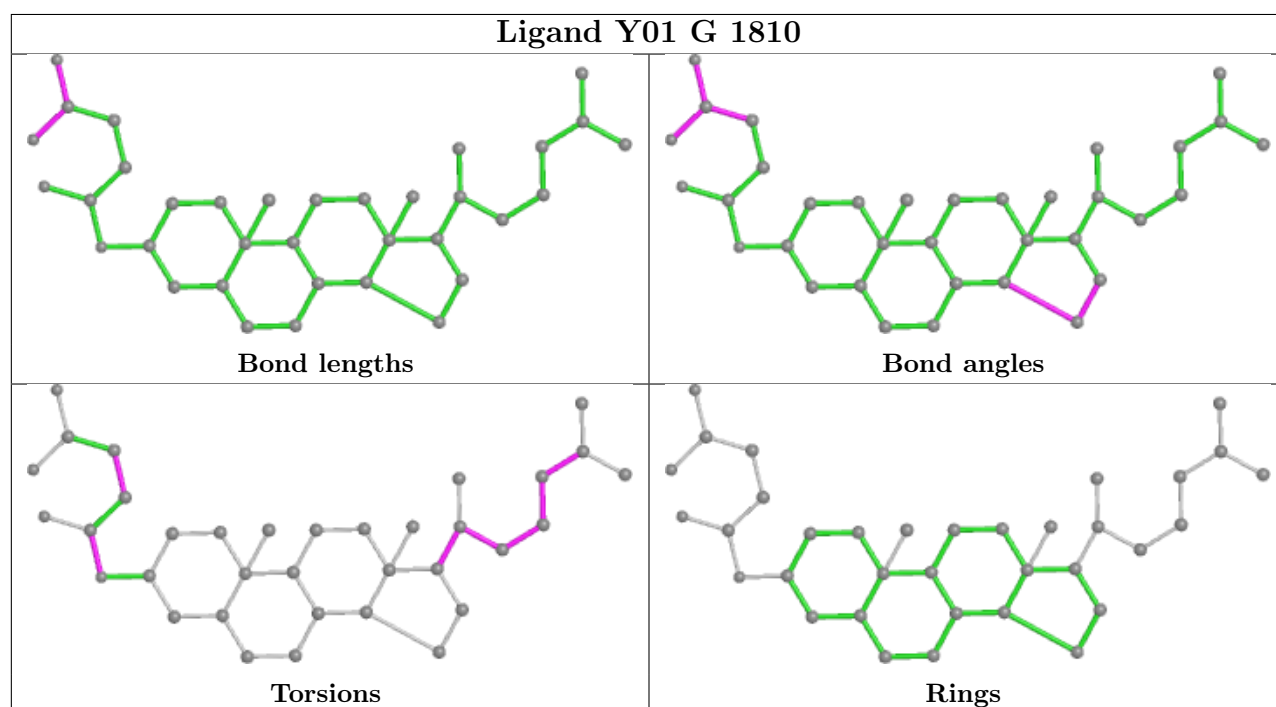
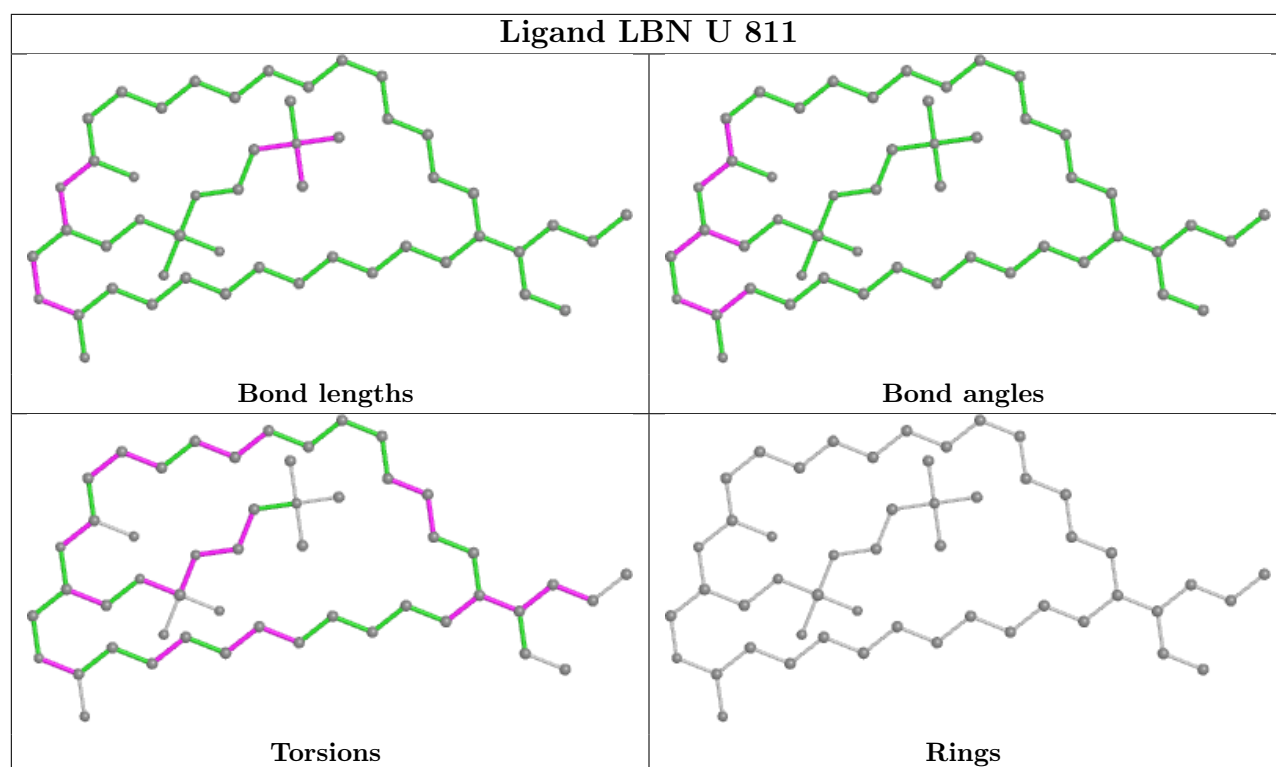


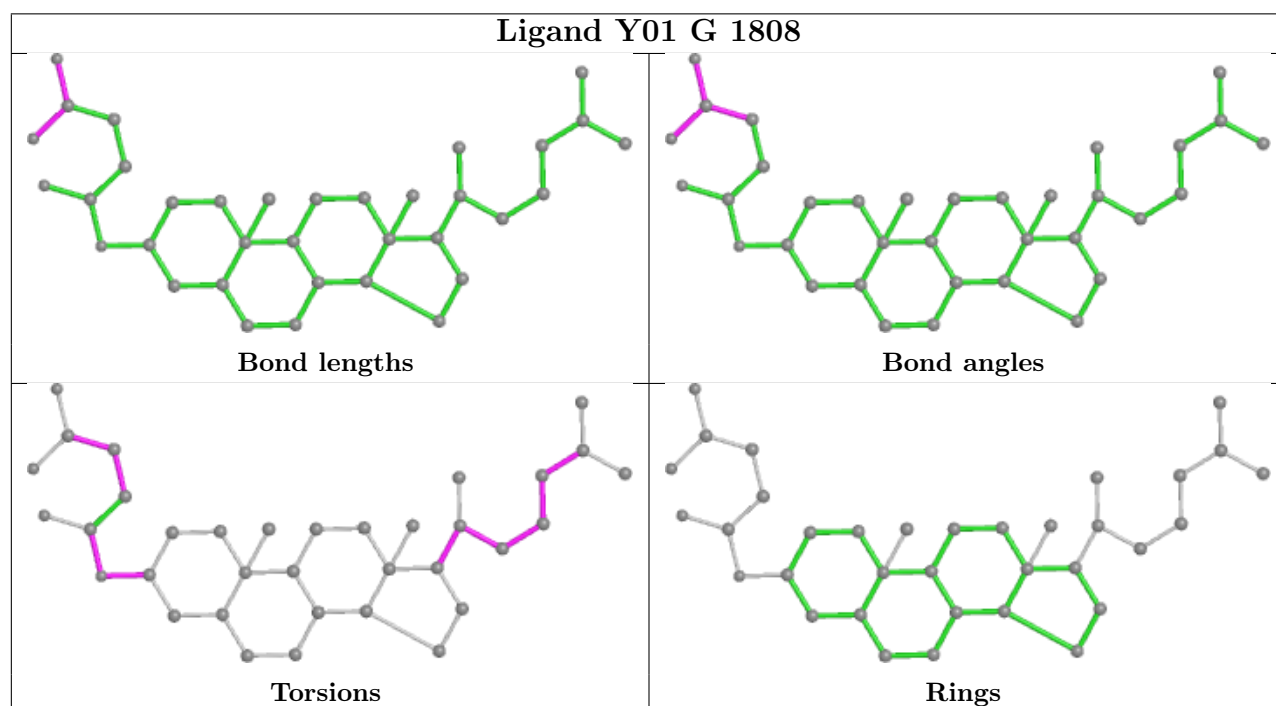
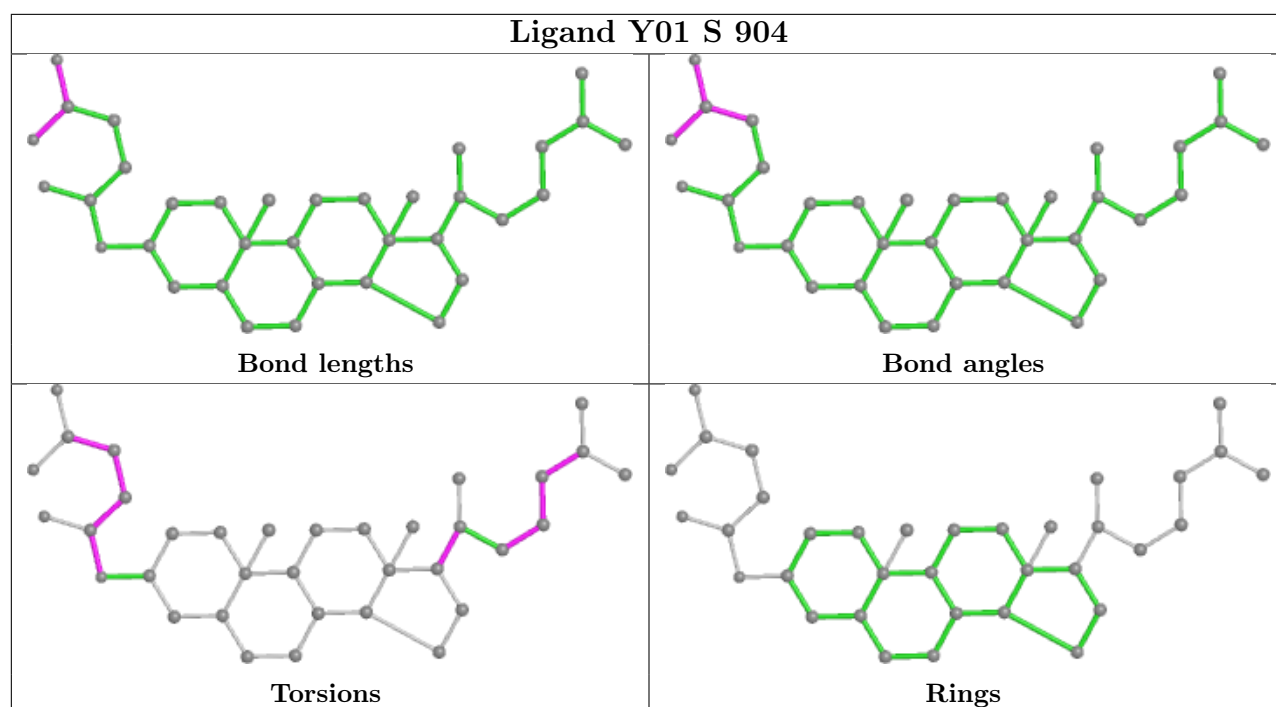




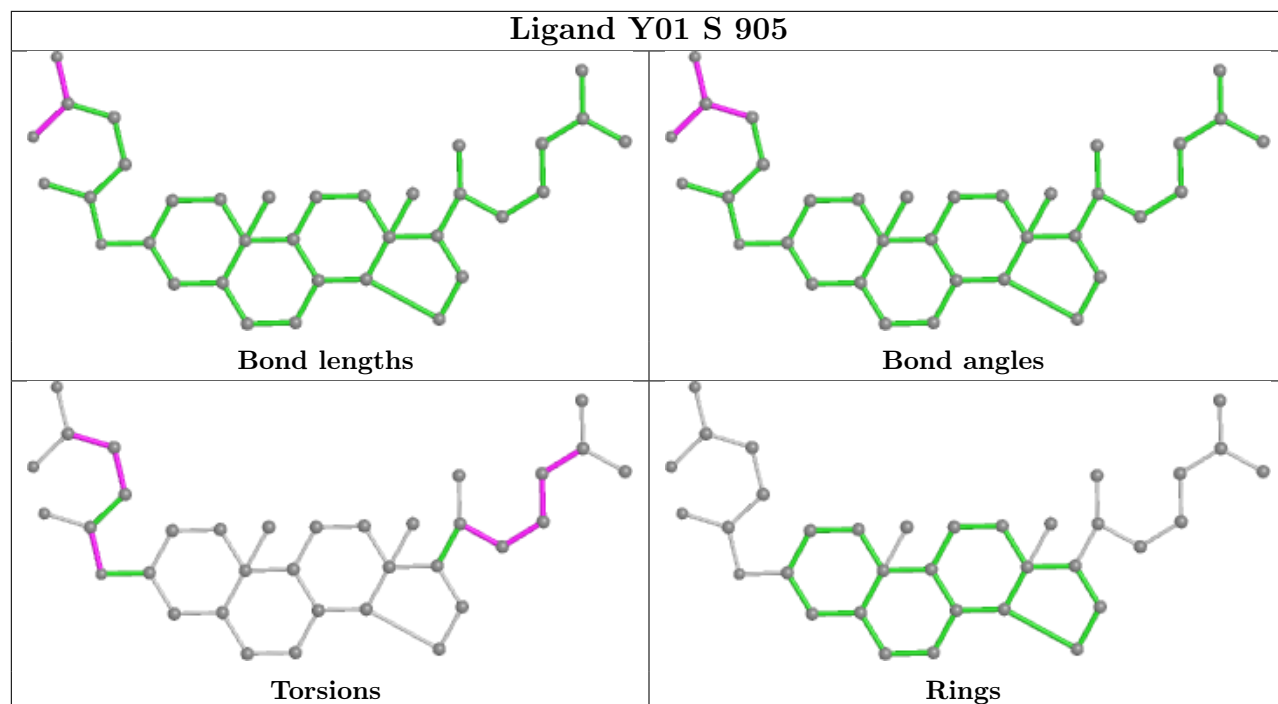




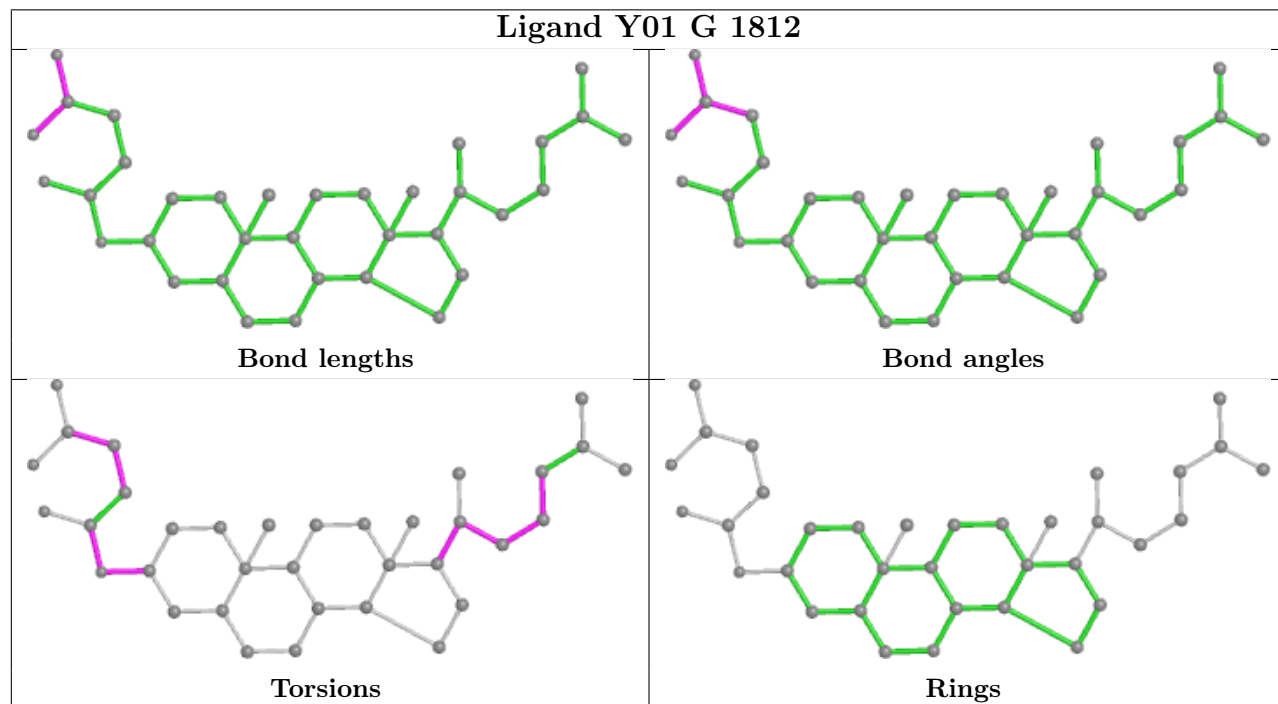




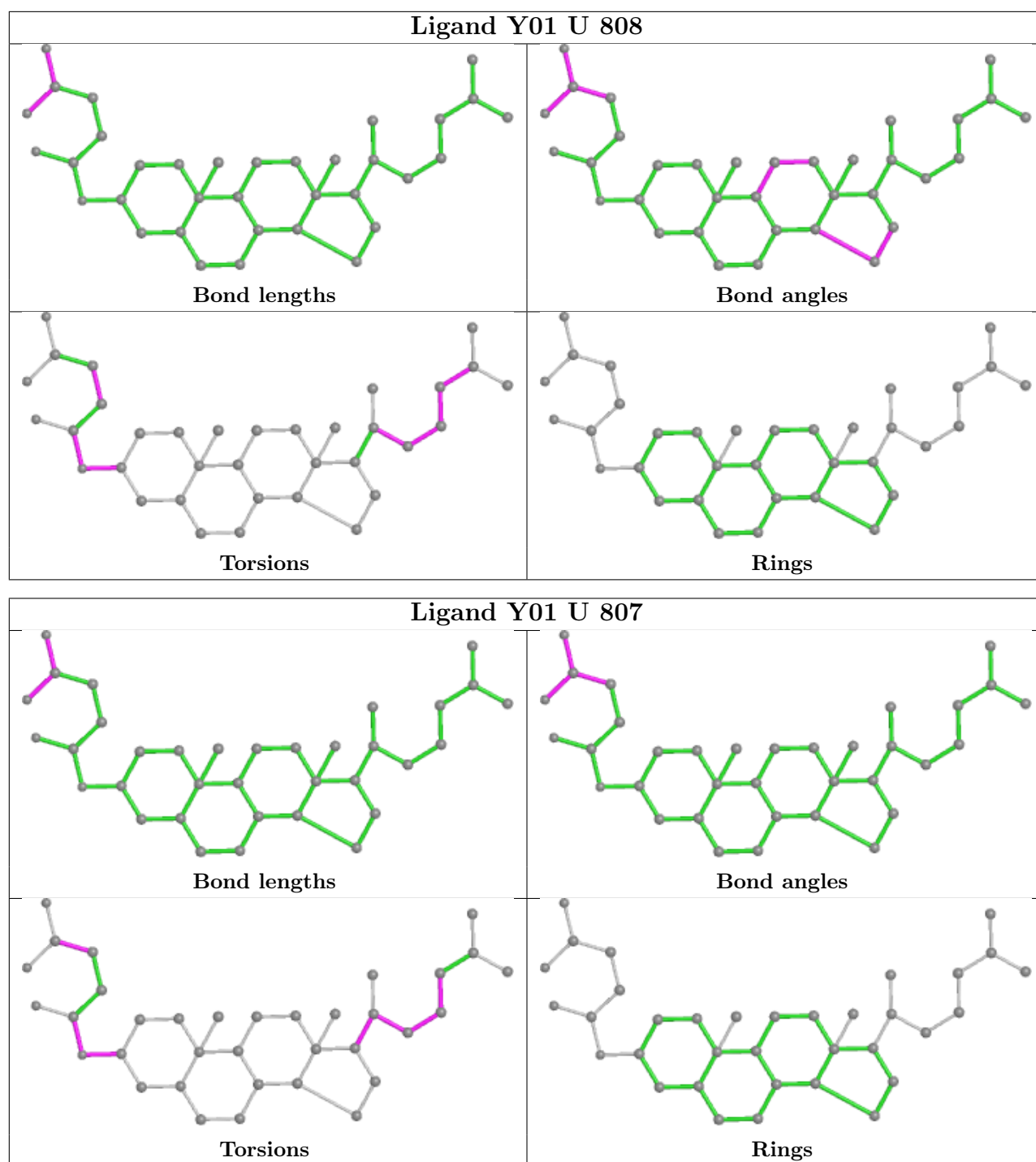
## Ligand Y01 S 905

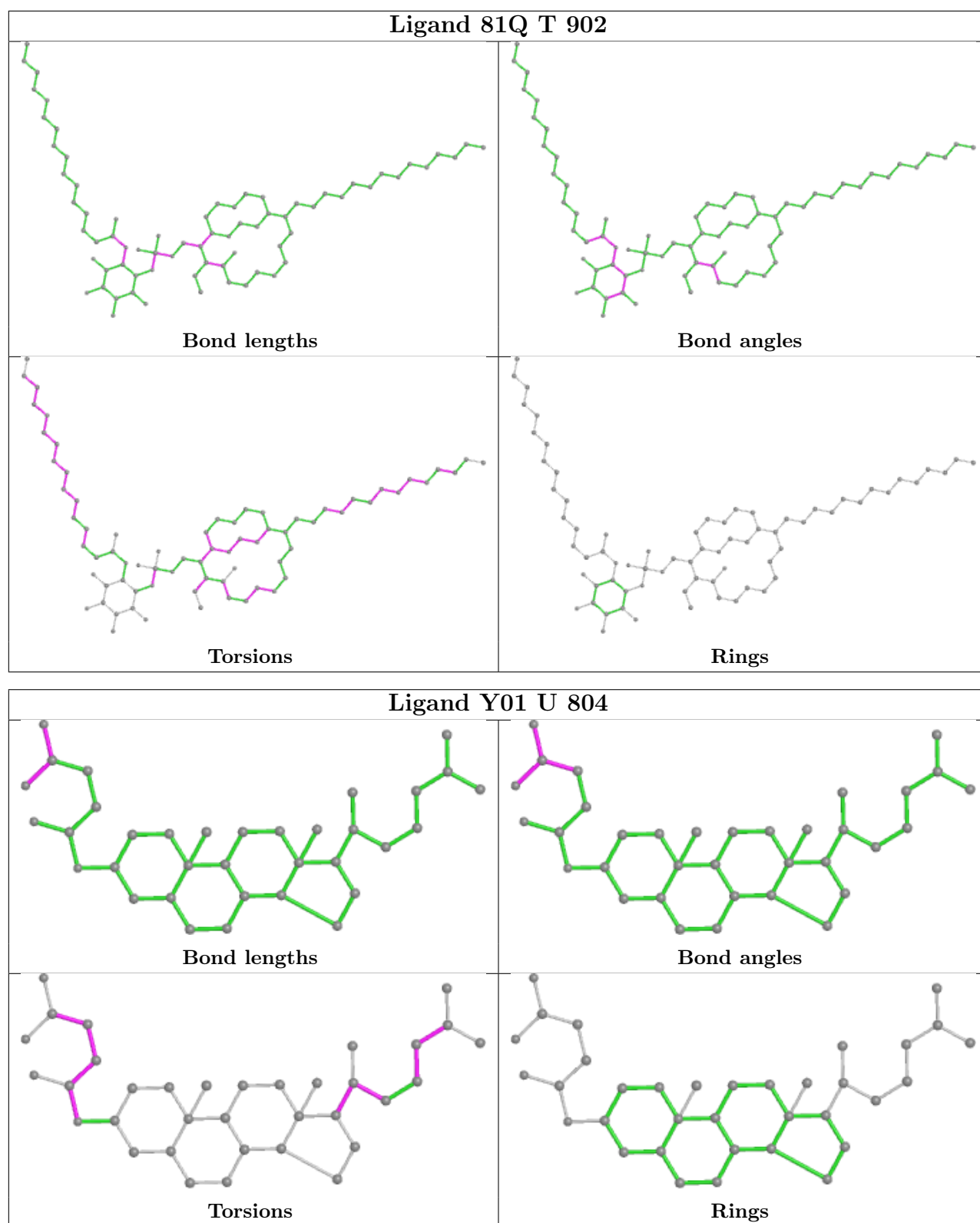


## Ligand Y01 G 1812









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.