



Full wwPDB EM Validation Report ⓘ

Jul 16, 2025 – 10:53 AM JST

PDB ID : 8IMX / pdb_00008imx
EMDB ID : EMD-35575
Title : Cryo-EM structure of GPI-T with a chimeric GPI-anchored protein
Authors : Xu, Y.; Li, T.; Qu, Q.; Li, D.
Deposited on : 2023-03-07
Resolution : 2.85 Å(reported)

This is a Full wwPDB EM Validation 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 : **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

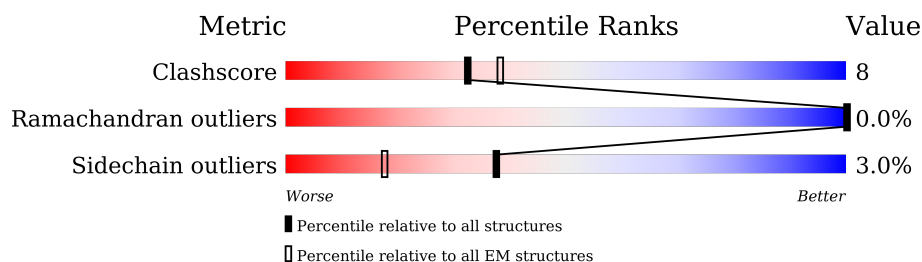
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 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 ≥ 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	D	327	5% 92%
2	G	886	53% 12% 35%
3	K	647	39% 11% 49%
4	S	816	53% 9% 37%
5	T	831	51% 12% 36%
6	U	678	47% 14% 38%
7	P	3	33% 67%
8	R	2	100%

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 19779 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 UL16-binding protein 2,GFP-like fluorescent chromoprotein cFP484.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	27	Total	C	N	O	S	0	0
			200	133	31	33	3		

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-80	MET	-	initiating methionine	UNP Q9BZM5
D	-55	GLY	-	linker	UNP Q9BZM5
D	-54	GLY	-	linker	UNP Q9BZM5
D	-53	SER	-	linker	UNP Q9BZM5
D	-52	GLY	-	linker	UNP Q9BZM5
D	-51	GLY	-	linker	UNP Q9BZM5
D	-50	SER	-	linker	UNP Q9BZM5
D	-49	ALA	-	linker	UNP Q9BZM5
D	-48	SER	-	linker	UNP Q9BZM5
D	-43	GLU	ASP	conflict	UNP Q9U6Y3
D	-37	ARG	LYS	conflict	UNP Q9U6Y3
D	-33	ALA	ASN	conflict	UNP Q9U6Y3
D	-28	LYS	ALA	conflict	UNP Q9U6Y3
D	-20	ILE	GLU	conflict	UNP Q9U6Y3
D	-15	GLU	ASP	conflict	UNP Q9U6Y3
D	-12	GLN	HIS	conflict	UNP Q9U6Y3
D	-9	ASP	ASN	conflict	UNP Q9U6Y3
D	-7	THR	GLU	conflict	UNP Q9U6Y3
D	-5	GLU	LYS	conflict	UNP Q9U6Y3
D	8	THR	SER	conflict	UNP Q9U6Y3
D	9	PRO	ASN	conflict	UNP Q9U6Y3
D	18	PHE	LEU	conflict	UNP Q9U6Y3
D	23	GLU	ASP	conflict	UNP Q9U6Y3
D	26	PRO	ALA	conflict	UNP Q9U6Y3
D	32	ALA	SER	conflict	UNP Q9U6Y3
D	42	SER	THR	conflict	UNP Q9U6Y3
D	45	TYR	PHE	conflict	UNP Q9U6Y3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	48	GLN	LYS	conflict	UNP Q9U6Y3
D	51	CYS	VAL	conflict	UNP Q9U6Y3
D	52	ILE	LYS	conflict	UNP Q9U6Y3
D	53	ALA	VAL	conflict	UNP Q9U6Y3
D	54	THR	LYS	conflict	UNP Q9U6Y3
D	58	THR	SER	conflict	UNP Q9U6Y3
D	61	GLY	GLU	conflict	UNP Q9U6Y3
D	63	CYS	SER	conflict	UNP Q9U6Y3
D	65	PHE	ILE	conflict	UNP Q9U6Y3
D	73	THR	MET	conflict	UNP Q9U6Y3
D	95	LYS	ILE	conflict	UNP Q9U6Y3
D	99	GLU	ARG	conflict	UNP Q9U6Y3
D	104	LYS	VAL	conflict	UNP Q9U6Y3
D	107	VAL	ILE	conflict	UNP Q9U6Y3
D	108	GLU	SER	conflict	UNP Q9U6Y3
D	109	MET	HIS	conflict	UNP Q9U6Y3
D	110	ALA	SER	conflict	UNP Q9U6Y3
D	125	THR	SER	conflict	UNP Q9U6Y3
D	126	THR	ILE	conflict	UNP Q9U6Y3
D	132	ASP	VAL	conflict	UNP Q9U6Y3
D	134	ARG	LYS	conflict	UNP Q9U6Y3
D	138	ALA	TYR	conflict	UNP Q9U6Y3
D	140	GLU	PHE	conflict	UNP Q9U6Y3
D	149	SER	ASN	conflict	UNP Q9U6Y3
D	158	ARG	THR	conflict	UNP Q9U6Y3
D	162	HIS	ASN	conflict	UNP Q9U6Y3
D	164	GLU	VAL	conflict	UNP Q9U6Y3
D	169	GLY	-	linker	UNP Q9U6Y3
D	170	GLY	-	linker	UNP Q9U6Y3
D	171	GLY	-	linker	UNP Q9U6Y3
D	172	SER	-	linker	UNP Q9U6Y3
D	173	GLY	-	linker	UNP Q9U6Y3
D	174	GLY	-	linker	UNP Q9U6Y3
D	175	GLY	-	linker	UNP Q9U6Y3
D	176	SER	-	linker	UNP Q9U6Y3
D	177	ALA	-	linker	UNP Q9U6Y3
D	178	TRP	-	linker	UNP Q9U6Y3
D	179	SER	-	linker	UNP Q9U6Y3
D	180	HIS	-	linker	UNP Q9U6Y3
D	181	PRO	-	linker	UNP Q9U6Y3
D	182	GLN	-	linker	UNP Q9U6Y3
D	183	PHE	-	linker	UNP Q9U6Y3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	184	GLU	-	linker	UNP Q9U6Y3
D	185	LYS	-	linker	UNP Q9U6Y3
D	186	GLY	-	linker	UNP Q9U6Y3
D	187	GLY	-	linker	UNP Q9U6Y3
D	188	GLY	-	linker	UNP Q9U6Y3
D	189	SER	-	linker	UNP Q9U6Y3
D	190	GLY	-	linker	UNP Q9U6Y3
D	191	GLY	-	linker	UNP Q9U6Y3
D	192	GLY	-	linker	UNP Q9U6Y3
D	193	SER	-	linker	UNP Q9U6Y3
D	194	GLY	-	linker	UNP Q9U6Y3
D	195	GLY	-	linker	UNP Q9U6Y3
D	196	SER	-	linker	UNP Q9U6Y3
D	197	ALA	-	linker	UNP Q9U6Y3
D	198	TRP	-	linker	UNP Q9U6Y3
D	199	SER	-	linker	UNP Q9U6Y3
D	200	HIS	-	linker	UNP Q9U6Y3
D	201	PRO	-	linker	UNP Q9U6Y3
D	202	GLN	-	linker	UNP Q9U6Y3
D	203	PHE	-	linker	UNP Q9U6Y3
D	204	GLU	-	linker	UNP Q9U6Y3
D	205	LYS	-	linker	UNP Q9U6Y3
D	206	GLY	-	linker	UNP Q9U6Y3
D	207	SER	-	linker	UNP Q9U6Y3

- Molecule 2 is a protein called Glycosylphosphatidylinositol anchor attachment 1 protein, GFP-like fluorescent chromoprotein cFP484.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	579	Total	C	N	O	S	0	0
			4398	2881	744	754	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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 3 is a protein called GPI-anchor transamidase,GFP-like fluorescent chromoprotein cFP484.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	330	Total	C	N	O	S	0	0
			2634	1685	451	483	15		

There are 82 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	396	GLY	-	linker	UNP Q92643
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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 4 is a protein called GPI transamidase component PIG-S, GFP-like fluorescent chromoprotein cFP484.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	513	Total	C	N	O	S	0	0
			3820	2482	639	686	13		

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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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 5 is a protein called GPI transamidase component PIG-T,GFP-like fluorescent chromoprotein cFP484.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	530	Total	C	N	O	S	0	0
			4223	2747	708	754	14		

There are 83 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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
T	820	HIS	-	expression tag	UNP Q9U6Y3
T	821	HIS	-	expression tag	UNP Q9U6Y3
T	822	HIS	-	expression tag	UNP Q9U6Y3
T	823	HIS	-	expression tag	UNP Q9U6Y3
T	824	HIS	-	expression tag	UNP Q9U6Y3
T	825	HIS	-	expression tag	UNP Q9U6Y3
T	826	HIS	-	expression tag	UNP Q9U6Y3
T	827	HIS	-	expression tag	UNP Q9U6Y3
T	828	HIS	-	expression tag	UNP Q9U6Y3
T	829	HIS	-	expression tag	UNP Q9U6Y3

- Molecule 6 is a protein called Phosphatidylinositol glycan anchor biosynthesis class U protein, GFP-like fluorescent chromoprotein cFP484.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	420	Total	C	N	O	S	0	0
			3422	2345	508	555	14		

There are 73 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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 7 is a protein called Met-Ser-Ser peptide.

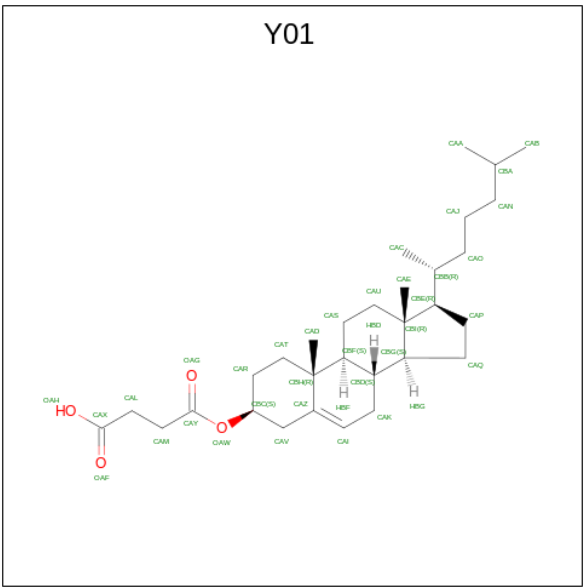
Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	3	Total	C	N	O	S	0	0
			20	11	3	5	1		

- Molecule 8 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
8	R	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



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

Continued on next page...

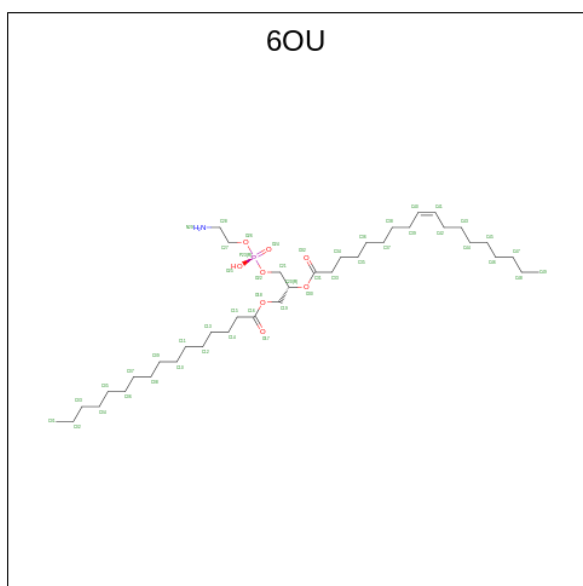
Continued from previous page...

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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 11 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propyl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C₃₉H₇₆NO₈P).



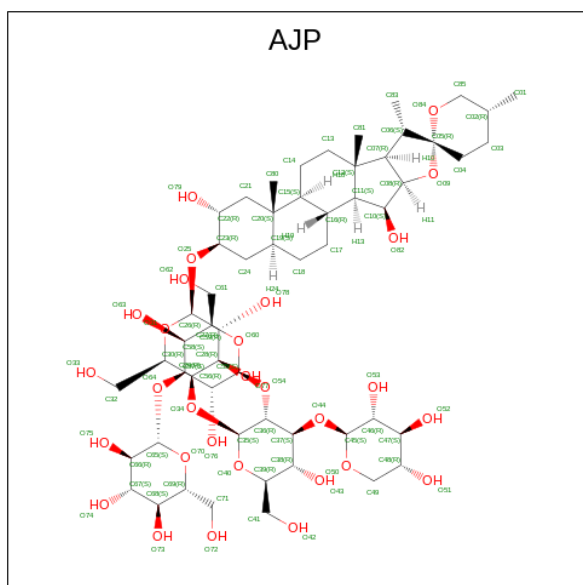
Mol	Chain	Residues	Atoms					AltConf
11	G	1	Total	C	N	O	P	0
			45	35	1	8	1	
11	G	1	Total	C	N	O	P	0
			49	39	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
11	G	1	Total	C	N	O	P	0
			39	29	1	8	1	
11	U	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 12 is Digitonin (CCD ID: AJP) (formula: $C_{56}H_{92}O_{29}$).



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

- Molecule 13 is CALCIUM ION (CCD ID: CA) (formula: Ca).

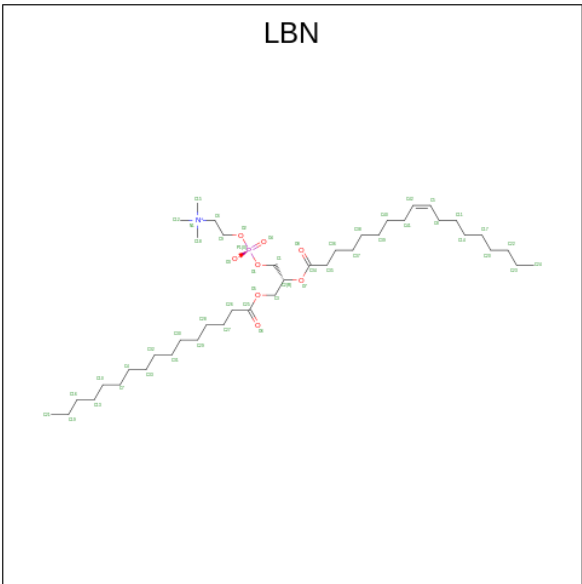
Mol	Chain	Residues	Atoms		AltConf
13	K	1	Total	Ca	0
			1	1	

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

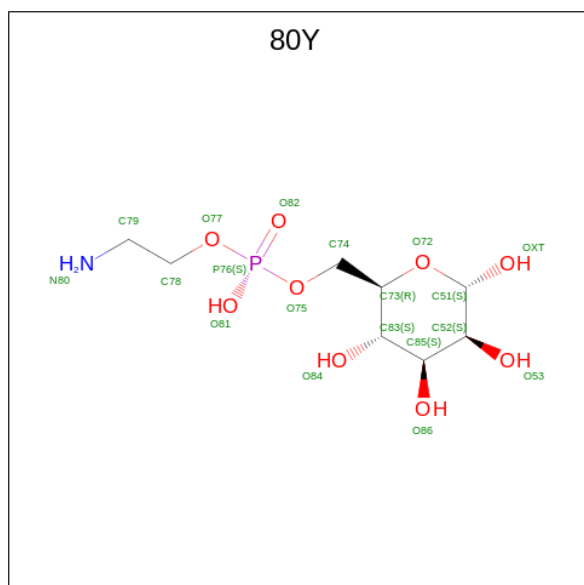
- Molecule 15 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: $C_{42}H_{82}NO_8P$).



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

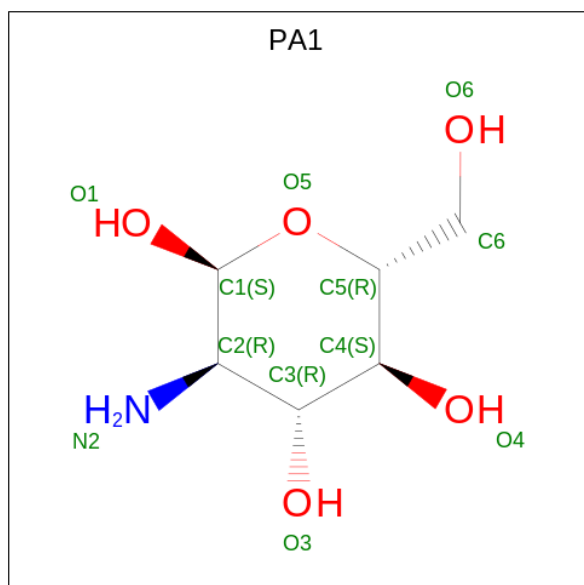
- 80T
-
- Chemical structure of 80T, a complex organophosphorus compound. The structure features a central phosphorus atom bonded to two hydroxyl groups and two diethylphosphoryl groups. The diethylphosphoryl groups are further substituted with long, branched alkyl chains. The structure is highly symmetrical and complex, with multiple ester and ether linkages.

- Molecule 17 is 2-azanylethyl [(2R,3S,4S,5S,6S)-3,4,5,6-tetrakis(oxidanyl)oxan-2-yl]methyl hydrogen phosphate (CCD ID: 80Y) (formula: $\text{C}_8\text{H}_{18}\text{NO}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



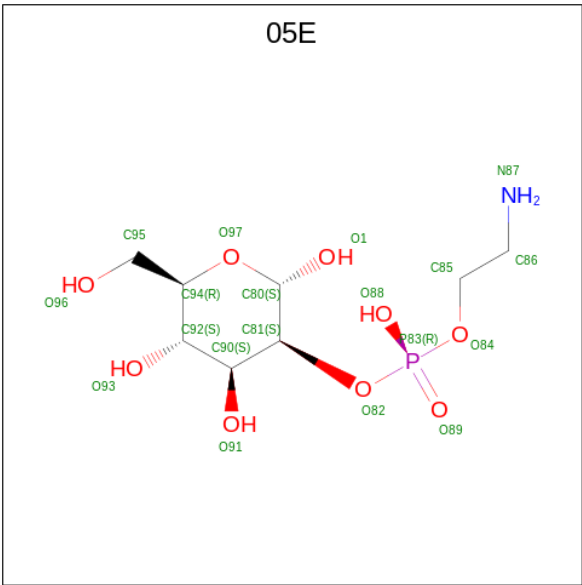
Mol	Chain	Residues	Atoms					AltConf
17	P	1	Total	C	N	O	P	0
			18	8	1	8	1	
17	P	1	Total	C	N	O	P	0
			18	8	1	8	1	

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



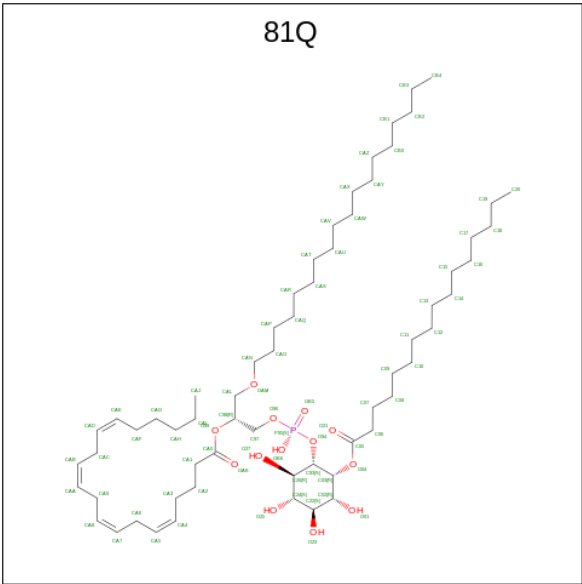
Mol	Chain	Residues	Atoms				AltConf
18	P	1	Total	C	N	O	0
			11	6	1	4	

- Molecule 19 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: $C_8H_{18}NO_9P$) (labeled as "Ligand of Interest" by depositor).

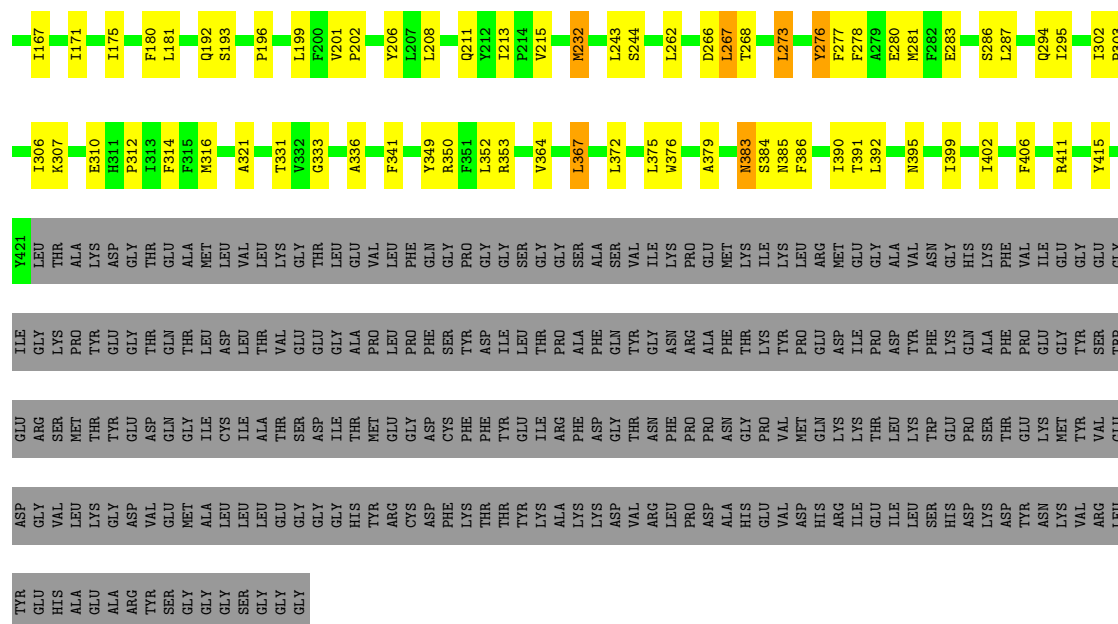


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
19	P	1	18	8	1	8	1	0

- Molecule 20 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: C₆₃H₁₁₅O₁₃P) (labeled as "Ligand of Interest" by depositor).



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



- Molecule 7: Met-Ser-Ser peptide



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34261	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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: MG, 80T, CA, 80Y, NAG, 81Q, PA1, LBN, 05E, AJP, 6OU, Y01

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	D	0.37	0/202	0.76	0/277
2	G	0.18	0/4503	0.36	0/6141
3	K	0.14	0/2702	0.33	0/3674
4	S	0.17	0/3909	0.33	0/5350
5	T	0.16	0/4356	0.31	0/5969
6	U	0.23	0/3535	0.40	0/4831
7	P	0.50	0/19	1.13	0/23
All	All	0.18	0/19226	0.36	0/26265

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	D	200	0	227	12	0
2	G	4398	0	4469	68	0
3	K	2634	0	2549	58	0
4	S	3820	0	3754	51	0
5	T	4223	0	4146	65	0
6	U	3422	0	3487	82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	20	0	21	6	0
8	R	28	0	25	0	0
9	D	35	0	49	5	0
9	G	245	0	343	10	0
9	U	175	0	245	20	0
10	G	1	0	0	0	0
11	G	133	0	0	0	0
11	U	49	0	0	0	0
12	G	85	0	0	0	0
13	K	1	0	0	0	0
14	S	14	0	13	0	0
14	T	14	0	13	0	0
15	S	52	0	0	0	0
16	U	88	0	0	0	0
17	P	36	0	0	1	0
18	P	11	0	10	1	0
19	P	18	0	0	0	0
20	P	77	0	0	6	0
All	All	19779	0	19351	326	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 8.

All (326) 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)
9:U:704:Y01:HAR1	9:U:704:Y01:HAL1	1.54	0.89
5:T:32:GLU:HG3	5:T:201:LEU:HD12	1.66	0.78
6:U:372:LEU:HD13	6:U:386:PHE:HB3	1.66	0.77
3:K:87:ALA:HB1	3:K:173:GLN:HE21	1.51	0.76
1:D:228:THR:HG21	9:D:301:Y01:HAL1	1.71	0.73
4:S:202:ALA:HB1	4:S:220:PRO:HG2	1.70	0.71
5:T:113:TRP:HB3	5:T:173:TYR:HD1	1.57	0.70
4:S:85:THR:HG22	4:S:85:THR:O	1.92	0.69
2:G:249:LEU:HB3	2:G:356:SER:OG	1.93	0.69
9:U:703:Y01:HAT2	9:U:704:Y01:HAV1	1.77	0.67
5:T:359:SER:HB2	5:T:367:GLU:HB2	1.76	0.67
2:G:528:MET:HE1	2:G:607:LEU:HD12	1.76	0.66
2:G:142:GLU:OE1	2:G:178:LYS:NZ	2.27	0.66
2:G:288:GLN:HE21	9:G:907:Y01:HAT1	1.60	0.66
3:K:104:SER:OG	3:K:246:MET:SD	2.52	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:294:GLN:HB2	9:U:704:Y01:HAU2	1.78	0.65
2:G:240:GLU:OE2	2:G:269:GLN:NE2	2.30	0.65
5:T:417:GLN:HG2	5:T:427:LEU:HB3	1.79	0.64
5:T:383:VAL:HG23	5:T:473:ALA:HB2	1.78	0.64
2:G:204:VAL:HG23	2:G:205:THR:HG23	1.80	0.63
4:S:182:ILE:O	4:S:186:ILE:HD12	1.99	0.63
3:K:212:TYR:HE2	3:K:224:ALA:HB2	1.64	0.62
3:K:67:SER:HB2	3:K:254:LEU:HD12	1.82	0.61
2:G:110:ARG:NH1	2:G:205:THR:O	2.32	0.61
6:U:262:LEU:HD22	9:U:704:Y01:HAE2	1.82	0.61
2:G:574:LEU:HD22	9:G:909:Y01:HAU2	1.82	0.60
3:K:170:LEU:HD13	3:K:203:ILE:HD11	1.82	0.60
4:S:404:LEU:HD11	4:S:410:LEU:HB2	1.83	0.60
5:T:38:PRO:HD2	5:T:283:ASP:HB3	1.82	0.60
4:S:525:LEU:HB2	5:T:533:CYS:HB3	1.82	0.60
2:G:39:LEU:HD22	2:G:369:VAL:HG11	1.81	0.60
4:S:60:ARG:NH2	4:S:89:GLU:OE2	2.35	0.59
2:G:325:PHE:O	2:G:325:PHE:HD1	1.85	0.59
4:S:204:LEU:HD12	4:S:207:HIS:HB2	1.84	0.59
4:S:287:ASP:HB2	4:S:294:TYR:HE1	1.67	0.59
6:U:314:PHE:HE2	6:U:406:PHE:HD1	1.50	0.59
3:K:45:ASN:ND2	3:K:305:GLY:O	2.36	0.59
5:T:466:VAL:HB	5:T:513:LEU:HB2	1.85	0.59
3:K:54:ARG:HA	3:K:88:ASP:HB2	1.84	0.58
3:K:203:ILE:HD13	3:K:211:MET:HG3	1.84	0.58
2:G:296:ARG:HG2	2:G:303:HIS:CE1	2.38	0.58
2:G:291:LEU:HD11	9:G:907:Y01:HAC2	1.86	0.58
2:G:49:TYR:O	2:G:253:ASN:ND2	2.36	0.58
5:T:524:MET:HE3	5:T:527:ASN:HB2	1.85	0.57
2:G:115:PRO:HG3	2:G:122:TYR:HD2	1.69	0.57
2:G:311:ARG:NH2	2:G:595:TYR:O	2.37	0.57
5:T:294:LEU:HD23	5:T:336:LEU:HD11	1.86	0.57
5:T:524:MET:N	5:T:525:PRO:HD3	2.19	0.57
6:U:211:GLN:HB3	6:U:213:ILE:HD12	1.86	0.57
2:G:313:ARG:O	2:G:352:ARG:NH1	2.37	0.57
4:S:69:PHE:HA	4:S:146:VAL:HB	1.86	0.57
4:S:402:PRO:HB3	4:S:421:TRP:HH2	1.69	0.57
5:T:395:LEU:HD23	5:T:446:PHE:HB3	1.87	0.57
6:U:283:GLU:CD	6:U:283:GLU:H	2.11	0.57
6:U:294:GLN:CB	9:U:704:Y01:HAU2	2.34	0.57
9:D:301:Y01:HAB3	20:P:105:81Q:CAG	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:227:GLN:HG2	3:K:283:THR:HG23	1.86	0.56
2:G:93:GLU:HA	2:G:103:VAL:HG21	1.86	0.56
1:D:229:LEU:HD21	20:P:105:81Q:C08	2.35	0.56
6:U:142:LEU:HG	6:U:146:LEU:HD12	1.87	0.56
2:G:250:ASP:OD1	2:G:356:SER:HB2	2.06	0.56
5:T:535:VAL:HG21	6:U:392:LEU:HD22	1.87	0.56
5:T:40:PRO:HB3	5:T:347:PRO:HD2	1.88	0.56
9:D:301:Y01:HAN2	20:P:105:81Q:CAF	2.35	0.55
1:D:226:ALA:HA	1:D:230:ILE:HD12	1.90	0.55
3:K:234:SER:CB	7:P:2:SER:HA	2.36	0.55
6:U:267:LEU:HD11	6:U:278:PHE:HB2	1.88	0.55
3:K:233:LEU:HA	7:P:2:SER:O	2.06	0.54
5:T:67:ARG:O	5:T:69:PHE:N	2.40	0.54
6:U:128:ARG:NH2	6:U:133:MET:SD	2.81	0.54
2:G:170:PHE:HE1	2:G:340:GLU:HG3	1.72	0.54
3:K:161:MET:HE3	3:K:170:LEU:HD22	1.90	0.54
5:T:385:LEU:HD23	5:T:430:MET:HE3	1.90	0.54
18:P:102:PA1:O5	20:P:105:81Q:O25	2.26	0.54
5:T:535:VAL:HG11	6:U:273:LEU:HD21	1.90	0.54
2:G:239:VAL:HG12	2:G:317:LEU:HD11	1.90	0.53
2:G:149:PRO:O	2:G:156:ASN:ND2	2.41	0.53
6:U:262:LEU:HD22	9:U:704:Y01:CAE	2.37	0.53
5:T:393:LEU:HD21	5:T:515:VAL:HG21	1.90	0.53
3:K:128:VAL:HG23	3:K:176:GLU:HG3	1.90	0.53
3:K:289:ASP:OD1	3:K:289:ASP:N	2.36	0.53
6:U:98:ALA:HB1	6:U:175:ILE:HD12	1.91	0.53
5:T:286:THR:OG1	5:T:292:GLU:O	2.27	0.53
4:S:154:LEU:O	4:S:171:ARG:NH2	2.42	0.52
5:T:422:ARG:NE	5:T:455:GLU:OE1	2.41	0.52
3:K:232:SER:O	7:P:3:SER:HB3	2.09	0.52
3:K:185:ASP:O	3:K:189:GLN:HG3	2.09	0.52
4:S:259:LEU:HD13	4:S:268:PHE:HB3	1.91	0.52
4:S:527:LEU:O	4:S:531:VAL:HG23	2.10	0.52
2:G:28:SER:OG	2:G:380:PHE:O	2.28	0.52
3:K:160:TYR:OH	3:K:250:THR:OG1	2.28	0.52
6:U:295:ILE:CG1	9:U:704:Y01:HAC1	2.40	0.51
1:D:237:ILE:HD11	5:T:534:THR:HG23	1.93	0.51
5:T:224:PRO:HB2	5:T:234:ILE:HD12	1.93	0.51
5:T:51:ARG:NE	5:T:237:GLU:OE2	2.43	0.51
2:G:140:SER:O	2:G:140:SER:OG	2.27	0.51
5:T:135:SER:HB2	5:T:142:LEU:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:319:LEU:HD13	4:S:254:TYR:CG	2.46	0.51
2:G:476:LEU:HD22	9:G:911:Y01:HAB3	1.92	0.51
5:T:85:LEU:HD11	5:T:134:LEU:HD11	1.92	0.51
3:K:212:TYR:O	3:K:287:ARG:NH1	2.33	0.50
4:S:460:ASP:OD1	4:S:460:ASP:N	2.44	0.50
9:G:909:Y01:HAD3	9:G:910:Y01:HAD1	1.93	0.50
6:U:349:TYR:HA	6:U:352:LEU:HD12	1.93	0.50
9:U:704:Y01:CAE	9:U:704:Y01:HAO2	2.42	0.50
4:S:221:LEU:HD11	4:S:322:LEU:HD21	1.94	0.50
4:S:236:PRO:HB2	4:S:330:GLU:HG2	1.94	0.50
1:D:233:CYS:HB3	5:T:534:THR:OG1	2.12	0.50
6:U:302:ILE:O	6:U:306:ILE:HG13	2.12	0.50
2:G:392:LEU:HD22	2:G:496:MET:HG2	1.94	0.50
2:G:523:LEU:HD22	9:G:906:Y01:HAA2	1.95	0.49
4:S:248:GLU:HG3	5:T:65:HIS:CD2	2.48	0.49
3:K:313:THR:HG21	4:S:392:GLN:HE21	1.77	0.49
5:T:252:GLY:HA2	5:T:262:ARG:NH2	2.28	0.49
5:T:547:LEU:HD13	6:U:303:PRO:HB2	1.95	0.49
1:D:229:LEU:HD21	20:P:105:81Q:C09	2.43	0.49
6:U:193:SER:O	6:U:196:PRO:HD2	2.13	0.49
4:S:479:LEU:HG	4:S:487:ALA:HB1	1.95	0.48
9:U:703:Y01:CAT	9:U:704:Y01:HAV1	2.43	0.48
4:S:203:ALA:HB2	4:S:429:ALA:HB1	1.95	0.48
6:U:99:ILE:HG13	6:U:140:VAL:HG21	1.95	0.48
2:G:492:ASP:OD1	2:G:493:ARG:N	2.46	0.48
5:T:94:TRP:CE2	5:T:102:PRO:HB3	2.48	0.48
2:G:71:ARG:O	2:G:75:ARG:HG2	2.13	0.48
1:D:243:LEU:HB2	1:D:244:PRO:HD3	1.96	0.48
2:G:508:LEU:HD21	6:U:364:VAL:HA	1.96	0.48
3:K:55:PHE:O	3:K:90:MET:HE1	2.13	0.48
3:K:293:ARG:HE	3:K:298:VAL:HG22	1.79	0.48
2:G:241:GLY:HA3	2:G:310:LEU:HD12	1.96	0.48
2:G:429:ALA:HB3	2:G:430:PRO:HD3	1.96	0.48
6:U:276:TYR:O	6:U:277:PHE:C	2.57	0.48
4:S:281:GLY:HA3	4:S:306:PRO:HG2	1.95	0.47
2:G:68:ASP:OD1	2:G:68:ASP:N	2.35	0.47
2:G:359:LEU:HD13	2:G:371:ILE:HD12	1.96	0.47
2:G:608:TYR:HB3	2:G:609:PRO:HD3	1.96	0.47
3:K:64:ASN:ND2	3:K:247:ASP:OD2	2.47	0.47
5:T:396:TYR:O	5:T:399:THR:OG1	2.30	0.47
2:G:492:ASP:HA	2:G:495:TRP:CD1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:280:LEU:HD22	4:S:303:VAL:HG13	1.97	0.47
4:S:60:ARG:HH22	4:S:101:LYS:HD3	1.79	0.47
6:U:9:LEU:HD23	6:U:145:LEU:HD11	1.95	0.47
4:S:22:PHE:CE1	6:U:303:PRO:HD3	2.49	0.47
3:K:234:SER:HB3	7:P:2:SER:HA	1.96	0.47
6:U:321:ALA:HB1	6:U:402:ILE:HG13	1.97	0.47
4:S:30:LEU:HD21	6:U:295:ILE:HD13	1.96	0.47
4:S:192:ALA:O	4:S:425:ARG:NH1	2.48	0.47
6:U:391:THR:O	6:U:395:ASN:ND2	2.34	0.47
2:G:233:THR:OG1	2:G:326:ARG:HB2	2.15	0.46
5:T:81:SER:HB3	5:T:117:GLN:HB2	1.98	0.46
6:U:277:PHE:O	6:U:281:MET:HB2	2.16	0.46
2:G:598:LEU:O	2:G:602:LEU:HB3	2.16	0.46
4:S:287:ASP:HB2	4:S:294:TYR:CE1	2.47	0.46
6:U:171:ILE:HG12	6:U:316:MET:SD	2.55	0.46
3:K:256:PHE:HZ	3:K:266:THR:HG21	1.80	0.46
5:T:520:PRO:HB2	6:U:280:GLU:OE2	2.16	0.46
6:U:281:MET:HE3	6:U:286:SER:HA	1.96	0.46
5:T:55:ASP:HB3	5:T:227:ARG:NH1	2.31	0.46
4:S:532:PRO:HB2	5:T:544:TYR:CE2	2.51	0.46
5:T:162:LEU:HD12	5:T:234:ILE:HD13	1.97	0.46
6:U:82:LEU:HA	6:U:85:MET:HE2	1.97	0.46
9:U:705:Y01:HAP1	9:U:705:Y01:HAO2	1.46	0.46
3:K:87:ALA:CB	3:K:173:GLN:HE21	2.25	0.46
6:U:267:LEU:HD12	6:U:267:LEU:HA	1.77	0.46
2:G:162:LEU:HD23	2:G:225:LEU:HD21	1.98	0.46
5:T:404:SER:HB3	5:T:440:THR:HG23	1.98	0.46
3:K:90:MET:O	3:K:96:ASN:ND2	2.49	0.45
6:U:180:PHE:HD1	6:U:232:MET:SD	2.40	0.45
9:U:703:Y01:CAR	9:U:704:Y01:HAV1	2.46	0.45
9:D:301:Y01:HAU2	20:P:105:81Q:C15	2.47	0.45
6:U:295:ILE:HG13	9:U:704:Y01:HAC1	1.97	0.45
4:S:85:THR:HA	4:S:106:LYS:O	2.17	0.45
5:T:459:ASP:OD1	5:T:459:ASP:N	2.44	0.45
3:K:79:ASP:OD1	3:K:79:ASP:C	2.59	0.45
3:K:267:ASN:N	3:K:267:ASN:HD22	2.13	0.45
6:U:63:PHE:HZ	6:U:70:ILE:HG22	1.81	0.45
6:U:331:THR:HG22	6:U:333:GLY:H	1.81	0.45
6:U:175:ILE:HA	6:U:206:TYR:CE1	2.52	0.45
4:S:219:ARG:O	4:S:220:PRO:C	2.59	0.45
2:G:49:TYR:CE2	2:G:51:SER:HB2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:163:ASN:O	6:U:167:ILE:HG13	2.17	0.45
6:U:411:ARG:NH2	6:U:415:TYR:OH	2.50	0.45
3:K:207:GLN:HA	3:K:227:GLN:O	2.17	0.44
3:K:210:SER:HB3	3:K:228:VAL:HG13	1.99	0.44
4:S:239:LYS:HE2	4:S:239:LYS:HB3	1.89	0.44
4:S:322:LEU:HD22	4:S:396:LEU:HD13	1.99	0.44
6:U:199:LEU:C	6:U:202:PRO:HD2	2.42	0.44
6:U:283:GLU:OE1	6:U:283:GLU:N	2.44	0.44
2:G:179:ASP:HB2	2:G:216:ALA:HB1	1.98	0.44
4:S:541:PHE:HA	4:S:544:THR:HG22	1.99	0.44
3:K:122:ARG:O	3:K:125:GLU:HG2	2.17	0.44
2:G:232:VAL:O	2:G:330:TYR:N	2.50	0.44
3:K:54:ARG:HG3	3:K:173:GLN:NE2	2.32	0.44
2:G:62:GLU:OE1	2:G:261:LYS:NZ	2.50	0.44
2:G:601:PRO:O	2:G:605:LEU:HB2	2.18	0.44
3:K:252:TYR:HD2	3:K:275:CYS:SG	2.40	0.44
3:K:268:MET:HE2	3:K:268:MET:HB2	1.77	0.44
3:K:361:LEU:HD23	3:K:361:LEU:HA	1.86	0.44
4:S:37:LYS:HB3	4:S:37:LYS:HE3	1.70	0.44
9:D:301:Y01:HAA1	9:D:301:Y01:HAJ2	1.49	0.44
9:G:907:Y01:HAC3	9:G:907:Y01:HAJ2	1.84	0.44
2:G:106:GLN:HE21	2:G:209:SER:HB2	1.82	0.44
2:G:342:MET:HE2	2:G:342:MET:HB3	1.84	0.44
2:G:445:PRO:HG2	2:G:468:LEU:HD13	1.99	0.44
3:K:102:VAL:HB	3:K:113:TYR:HB2	1.99	0.44
6:U:294:GLN:HB2	9:U:704:Y01:CAU	2.43	0.44
1:D:219:THR:OG1	1:D:220:THR:N	2.51	0.43
3:K:256:PHE:CZ	3:K:266:THR:HG21	2.53	0.43
6:U:104:LYS:O	6:U:108:LYS:HG2	2.18	0.43
6:U:310:GLU:H	6:U:310:GLU:HG2	1.65	0.43
4:S:311:LEU:HD11	4:S:325:LEU:HD21	1.99	0.43
9:G:906:Y01:HAP1	9:G:906:Y01:HAO2	1.70	0.43
2:G:424:LEU:HD22	9:U:706:Y01:HAI	1.99	0.43
2:G:513:ILE:HD11	2:G:602:LEU:HD11	2.01	0.43
4:S:264:ALA:HB1	4:S:427:LEU:HD11	2.01	0.43
4:S:527:LEU:HB3	4:S:528:PRO:HD3	2.00	0.43
6:U:108:LYS:HA	6:U:108:LYS:HD3	1.89	0.43
6:U:120:ALA:HB3	6:U:123:VAL:HG13	2.00	0.43
1:D:218:GLY:HA3	17:P:101:80Y:O81	2.18	0.43
2:G:111:LYS:HE3	2:G:111:LYS:HB3	1.90	0.43
3:K:103:PHE:CZ	3:K:108:MET:HG2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:370:PHE:HE1	6:U:244:SER:HA	1.84	0.43
4:S:86:VAL:HG13	4:S:106:LYS:HE3	2.00	0.43
4:S:222:LYS:HD2	4:S:222:LYS:HA	1.66	0.43
6:U:109:LYS:O	6:U:113:LEU:HD12	2.19	0.43
6:U:232:MET:HE2	6:U:232:MET:HB2	1.71	0.43
2:G:33:ILE:HD11	2:G:526:THR:HG23	2.00	0.43
6:U:149:TYR:HB2	6:U:336:ALA:HB2	2.01	0.43
3:K:209:ALA:HA	3:K:212:TYR:CE2	2.54	0.43
5:T:521:ASP:OD2	6:U:385:ASN:ND2	2.52	0.43
5:T:545:ASN:O	5:T:549:ARG:HG3	2.18	0.43
6:U:16:ARG:HG2	6:U:154:CYS:SG	2.59	0.43
5:T:208:ASP:N	5:T:208:ASP:OD1	2.51	0.43
5:T:402:ILE:HG22	5:T:409:ASN:HB3	2.00	0.43
6:U:163:ASN:OD1	6:U:192:GLN:NE2	2.47	0.43
1:D:235:LEU:O	1:D:239:PRO:HD2	2.19	0.43
2:G:174:ILE:HD12	5:T:250:ILE:HD13	2.01	0.43
4:S:62:MET:HB3	4:S:62:MET:HE3	1.76	0.43
5:T:34:LEU:HD11	5:T:46:ALA:HB1	2.00	0.43
6:U:171:ILE:HD13	6:U:341:PHE:HZ	1.83	0.42
2:G:197:GLU:OE2	2:G:205:THR:OG1	2.31	0.42
2:G:325:PHE:O	2:G:325:PHE:CD1	2.68	0.42
6:U:41:TRP:O	6:U:45:VAL:HG23	2.19	0.42
2:G:248:ASN:OD1	2:G:356:SER:HB3	2.18	0.42
5:T:68:LEU:HD21	5:T:274:LEU:HB3	2.01	0.42
6:U:76:LEU:HD21	9:U:707:Y01:HBD	2.01	0.42
6:U:375:LEU:HA	6:U:379:ALA:HB3	2.01	0.42
4:S:61:LEU:HD22	4:S:479:LEU:HD22	2.01	0.42
6:U:31:ARG:NH2	6:U:33:GLU:OE2	2.48	0.42
2:G:317:LEU:HD12	2:G:317:LEU:HA	1.83	0.42
5:T:529:ILE:HG12	6:U:277:PHE:CE1	2.54	0.42
4:S:216:GLU:O	4:S:218:ARG:N	2.47	0.42
6:U:287:LEU:HD13	9:U:704:Y01:HBC	2.00	0.42
3:K:381:VAL:HG13	6:U:180:PHE:HE2	1.85	0.42
5:T:405:LYS:HG3	5:T:438:SER:HB2	2.02	0.42
6:U:208:LEU:HD13	6:U:215:VAL:HG22	2.02	0.42
6:U:273:LEU:HD11	6:U:392:LEU:HD23	2.02	0.42
7:P:1:MET:H3	7:P:1:MET:HG2	1.49	0.42
5:T:113:TRP:HB3	5:T:173:TYR:CD1	2.46	0.42
5:T:160:LEU:HD23	5:T:160:LEU:HA	1.90	0.42
6:U:372:LEU:HD12	6:U:390:ILE:CG1	2.50	0.42
3:K:171:LYS:HD3	3:K:174:ASP:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:234:SER:HB2	7:P:2:SER:HA	2.01	0.42
5:T:337:LYS:HB3	5:T:337:LYS:HE3	1.77	0.42
5:T:524:MET:SD	6:U:385:ASN:ND2	2.93	0.42
6:U:402:ILE:HD13	6:U:402:ILE:HA	1.79	0.42
9:G:909:Y01:HAE1	9:G:910:Y01:HAD3	2.02	0.41
3:K:46:TRP:HB2	3:K:157:ILE:HG12	2.01	0.41
3:K:267:ASN:N	3:K:267:ASN:ND2	2.67	0.41
6:U:206:TYR:HD2	6:U:312:PRO:HG2	1.85	0.41
2:G:240:GLU:H	2:G:240:GLU:CD	2.28	0.41
2:G:440:ALA:O	2:G:444:LEU:HB2	2.20	0.41
3:K:267:ASN:HD22	3:K:267:ASN:C	2.27	0.41
3:K:312:ILE:HD12	4:S:346:VAL:HG21	2.03	0.41
5:T:396:TYR:HE1	5:T:447:GLU:HG3	1.86	0.41
6:U:383:ASN:ND2	6:U:383:ASN:N	2.68	0.41
2:G:315:GLU:H	2:G:315:GLU:HG2	1.70	0.41
3:K:106:LYS:HB2	3:K:106:LYS:HE3	1.91	0.41
4:S:200:LEU:O	4:S:204:LEU:HD23	2.21	0.41
5:T:266:ARG:NH1	5:T:267:THR:O	2.54	0.41
5:T:279:ARG:HE	5:T:317:ILE:HG21	1.85	0.41
6:U:262:LEU:HB3	9:U:704:Y01:HAD2	2.02	0.41
9:U:707:Y01:HAE2	9:U:707:Y01:HBB	1.96	0.41
1:D:238:LEU:HD21	4:S:531:VAL:HG21	2.01	0.41
2:G:565:ARG:HG3	2:G:572:LEU:HD22	2.01	0.41
3:K:377:LEU:HD12	6:U:243:LEU:HD22	2.03	0.41
4:S:65:VAL:O	4:S:106:LYS:HA	2.20	0.41
3:K:64:ASN:HD21	3:K:247:ASP:CG	2.28	0.41
4:S:85:THR:O	4:S:85:THR:CG2	2.63	0.41
5:T:71:LYS:O	5:T:75:GLN:HG2	2.21	0.41
6:U:83:VAL:HG22	9:U:707:Y01:HAQ1	2.02	0.41
2:G:193:GLU:HB2	2:G:308:LEU:HD13	2.02	0.41
3:K:267:ASN:ND2	3:K:267:ASN:H	2.19	0.41
5:T:37:THR:HG22	5:T:283:ASP:HB2	2.03	0.41
3:K:200:LEU:HD11	3:K:223:LEU:HD13	2.03	0.41
4:S:243:VAL:HG11	4:S:328:VAL:HG21	2.03	0.41
5:T:453:TRP:NE1	6:U:281:MET:O	2.47	0.41
5:T:521:ASP:CG	5:T:524:MET:HG3	2.46	0.41
6:U:201:VAL:HB	6:U:202:PRO:HD3	2.03	0.41
6:U:273:LEU:HD12	6:U:273:LEU:HA	1.84	0.41
6:U:367:LEU:HD13	6:U:367:LEU:O	2.20	0.41
2:G:251:LEU:HG	2:G:317:LEU:HD22	2.02	0.41
3:K:257:LEU:HA	3:K:260:ILE:HG12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:171:ARG:O	4:S:185:ARG:NH1	2.52	0.41
3:K:142:SER:OG	5:T:128:LYS:NZ	2.54	0.40
5:T:300:PRO:HB3	5:T:316:ALA:HB1	2.03	0.40
5:T:539:CYS:HB2	6:U:399:ILE:HD13	2.03	0.40
6:U:353:ARG:H	6:U:353:ARG:HG3	1.65	0.40
1:D:222:LEU:O	1:D:223:ARG:NH1	2.54	0.40
2:G:95:THR:HG21	2:G:164:LEU:HD13	2.03	0.40
2:G:202:VAL:HG13	5:T:360:GLY:HA2	2.03	0.40
3:K:344:LYS:HE2	3:K:344:LYS:HB2	1.90	0.40
2:G:146:LEU:HB2	2:G:343:PHE:CZ	2.57	0.40
2:G:293:MET:HE2	2:G:361:LEU:HA	2.04	0.40
3:K:161:MET:HE3	3:K:161:MET:HB3	1.90	0.40
4:S:147:ILE:HD12	4:S:147:ILE:HA	1.85	0.40
6:U:71:TYR:CD1	6:U:71:TYR:C	2.99	0.40
2:G:498:LEU:HD11	2:G:613:LEU:HD22	2.03	0.40
3:K:79:ASP:OD1	3:K:80:SER:N	2.54	0.40
5:T:325:MET:HG3	5:T:326:ILE:HG22	2.04	0.40
5:T:471:LEU:HD12	5:T:471:LEU:HA	1.91	0.40
2:G:171:ARG:NH1	5:T:247:ASP:OD2	2.46	0.40
2:G:515:LEU:HD13	6:U:372:LEU:HD21	2.02	0.40
9:G:902:Y01:HAS1	9:G:902:Y01:HAT1	1.95	0.40
6:U:181:LEU:HD23	6:U:181:LEU:HA	1.93	0.40
6:U:376:TRP:CZ2	6:U:384:SER:HB3	2.56	0.40
9:U:704:Y01:HAE2	9:U:704:Y01:CAO	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	25/327 (8%)	23 (92%)	2 (8%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	573/886 (65%)	558 (97%)	15 (3%)	0	100	100
3	K	326/647 (50%)	315 (97%)	11 (3%)	0	100	100
4	S	503/816 (62%)	495 (98%)	8 (2%)	0	100	100
5	T	528/831 (64%)	520 (98%)	8 (2%)	0	100	100
6	U	418/678 (62%)	410 (98%)	8 (2%)	0	100	100
7	P	1/3 (33%)	0	0	1 (100%)	0	0
All	All	2374/4188 (57%)	2321 (98%)	52 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	P	2	SER

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	D	24/261 (9%)	24 (100%)	0	100	100
2	G	445/714 (62%)	435 (98%)	10 (2%)	47	71
3	K	288/563 (51%)	280 (97%)	8 (3%)	38	64
4	S	385/681 (56%)	366 (95%)	19 (5%)	21	41
5	T	465/728 (64%)	455 (98%)	10 (2%)	47	71
6	U	367/585 (63%)	355 (97%)	12 (3%)	33	59
7	P	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1977/3535 (56%)	1917 (97%)	60 (3%)	37	62

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	76	ASP
2	G	140	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	260	GLN
2	G	293	MET
2	G	317	LEU
2	G	355	GLN
2	G	375	MET
2	G	434	SER
2	G	439	LEU
2	G	446	VAL
3	K	52	THR
3	K	116	ASP
3	K	152	ASP
3	K	220	ILE
3	K	228	VAL
3	K	267	ASN
3	K	283	THR
3	K	289	ASP
4	S	29	VAL
4	S	30	LEU
4	S	58	GLN
4	S	62	MET
4	S	65	VAL
4	S	66	THR
4	S	89	GLU
4	S	100	ILE
4	S	144	VAL
4	S	147	ILE
4	S	219	ARG
4	S	221	LEU
4	S	222	LYS
4	S	232	SER
4	S	313	SER
4	S	328	VAL
4	S	460	ASP
4	S	473	GLN
4	S	495	VAL
5	T	59	GLN
5	T	71	LYS
5	T	78	SER
5	T	91	GLN
5	T	208	ASP
5	T	274	LEU
5	T	302	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	T	388	THR
5	T	401	THR
5	T	439	VAL
6	U	62	VAL
6	U	70	ILE
6	U	232	MET
6	U	266	ASP
6	U	267	LEU
6	U	268	THR
6	U	273	LEU
6	U	276	TYR
6	U	307	LYS
6	U	350	ARG
6	U	367	LEU
6	U	383	ASN
7	P	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	80	HIS
2	G	200	HIS
2	G	260	GLN
2	G	288	GLN
2	G	435	GLN
2	G	568	GLN
2	G	593	HIS
3	K	81	HIS
3	K	173	GLN
3	K	197	ASN
3	K	235	HIS
3	K	244	HIS
3	K	267	ASN
3	K	348	GLN
4	S	188	GLN
4	S	207	HIS
4	S	302	HIS
5	T	149	ASN
5	T	415	HIS
6	U	383	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
8	NAG	R	1	2,8	14,14,15	0.23	0	17,19,21	0.40	0
8	NAG	R	2	8	14,14,15	0.21	0	17,19,21	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	R	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	R	2	8	-	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.

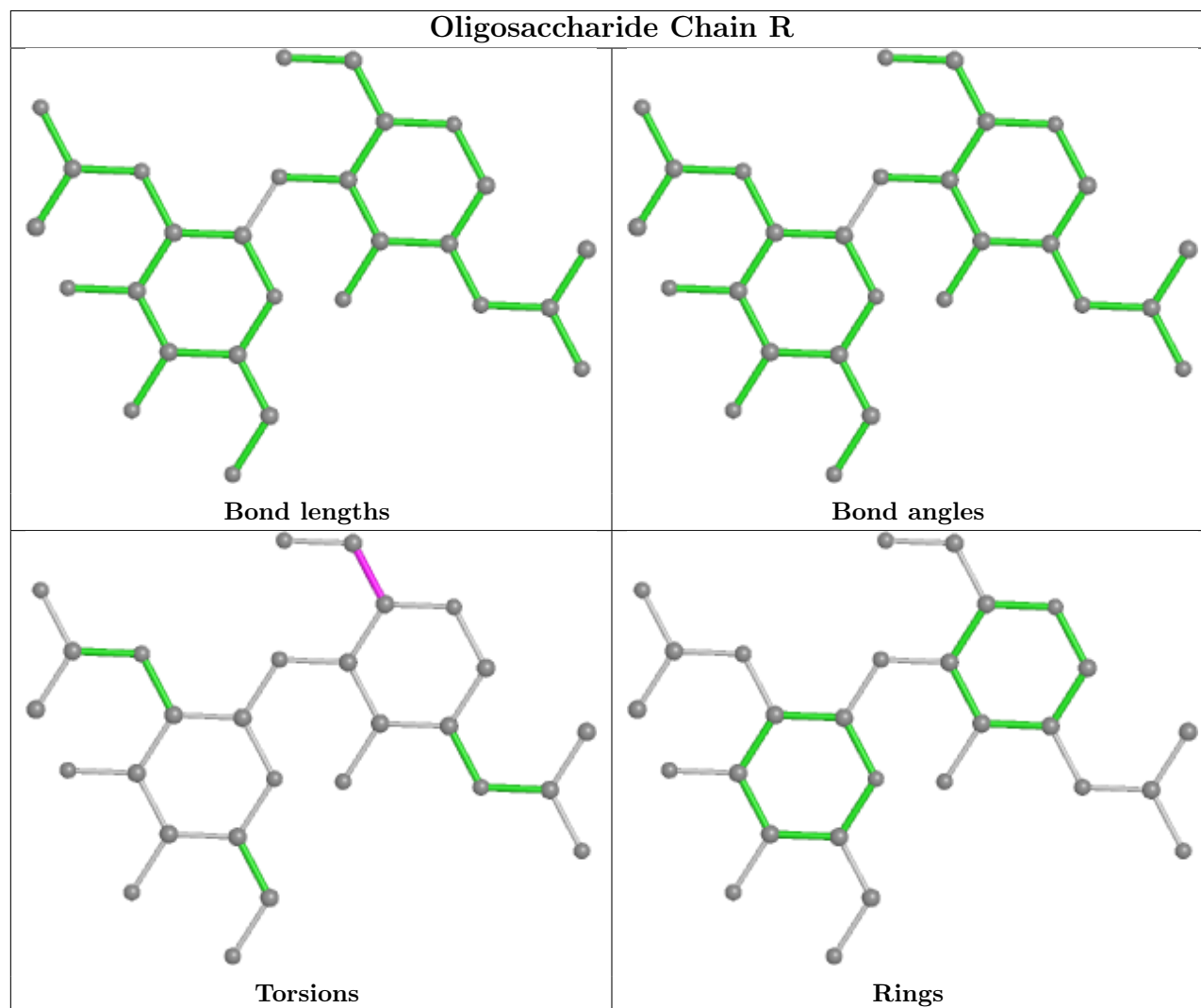
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	R	1	NAG	O5-C5-C6-O6
8	R	1	NAG	C4-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 ⓘ

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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
20	81Q	P	105	18	77,77,77	0.34	0	87,89,89	0.82	3 (3%)
11	6OU	U	701	-	48,48,48	0.88	4 (8%)	51,53,53	0.89	2 (3%)
15	LBN	S	902	-	51,51,51	1.04	3 (5%)	57,59,59	0.87	2 (3%)
14	NAG	T	901	5	14,14,15	0.26	0	17,19,21	0.40	0
9	Y01	U	705	-	38,38,38	0.64	2 (5%)	57,57,57	0.60	2 (3%)
9	Y01	G	910	-	38,38,38	0.64	2 (5%)	57,57,57	0.60	2 (3%)
17	80Y	P	103	19,17	18,18,19	0.56	0	24,25,27	0.76	1 (4%)
9	Y01	U	704	-	38,38,38	0.64	2 (5%)	57,57,57	0.60	2 (3%)
14	NAG	S	901	4	14,14,15	0.24	0	17,19,21	0.46	0
12	AJP	G	912	-	95,95,95	0.13	0	143,149,149	0.43	0
11	6OU	G	905	-	38,38,48	0.99	4 (10%)	41,43,53	0.98	2 (4%)
9	Y01	G	902	-	38,38,38	0.66	2 (5%)	57,57,57	0.68	2 (3%)
9	Y01	U	707	-	38,38,38	0.64	2 (5%)	57,57,57	0.62	2 (3%)
9	Y01	U	703	-	38,38,38	0.64	2 (5%)	57,57,57	0.61	2 (3%)
9	Y01	G	911	-	38,38,38	0.64	2 (5%)	57,57,57	0.60	2 (3%)
9	Y01	G	907	-	38,38,38	0.64	2 (5%)	57,57,57	0.60	2 (3%)
18	PA1	P	102	19,20	11,11,12	1.12	1 (9%)	12,15,17	1.41	2 (16%)
16	80T	U	702	-	87,87,95	1.48	14 (16%)	93,99,107	0.95	4 (4%)
11	6OU	G	903	-	44,44,48	0.92	4 (9%)	47,49,53	0.86	2 (4%)
9	Y01	G	906	-	38,38,38	0.64	2 (5%)	57,57,57	0.59	2 (3%)
17	80Y	P	101	17,7	18,18,19	0.50	0	24,25,27	0.70	0
9	Y01	G	909	-	38,38,38	0.64	2 (5%)	57,57,57	0.62	2 (3%)
11	6OU	G	904	-	48,48,48	0.89	3 (6%)	51,53,53	0.90	2 (3%)
9	Y01	U	706	-	38,38,38	0.64	2 (5%)	57,57,57	0.60	2 (3%)
19	05E	P	104	10,18,17	18,18,19	0.65	0	22,25,27	0.64	0
9	Y01	G	908	-	38,38,38	0.64	2 (5%)	57,57,57	0.58	2 (3%)
9	Y01	D	301	-	38,38,38	0.65	2 (5%)	57,57,57	0.59	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
20	81Q	P	105	18	-	41/73/97/97	0/1/1/1
11	6OU	U	701	-	-	34/52/52/52	-
15	LBN	S	902	-	-	32/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	T	901	5	-	2/6/23/26	0/1/1/1
9	Y01	U	705	-	-	12/19/77/77	0/4/4/4
9	Y01	G	910	-	-	9/19/77/77	0/4/4/4
17	80Y	P	103	19,17	-	4/11/28/31	0/1/1/1
9	Y01	U	704	-	-	12/19/77/77	0/4/4/4
14	NAG	S	901	4	-	2/6/23/26	0/1/1/1
12	AJP	G	912	-	-	6/28/220/220	0/11/11/11
11	6OU	G	905	-	-	22/42/42/52	-
9	Y01	G	902	-	-	6/19/77/77	0/4/4/4
9	Y01	U	707	-	-	11/19/77/77	0/4/4/4
9	Y01	U	703	-	-	3/19/77/77	0/4/4/4
9	Y01	G	911	-	-	10/19/77/77	0/4/4/4
9	Y01	G	907	-	-	4/19/77/77	0/4/4/4
18	PA1	P	102	19,20	-	1/2/19/22	0/1/1/1
16	80T	U	702	-	-	49/98/98/106	-
11	6OU	G	903	-	-	21/48/48/52	-
9	Y01	G	906	-	-	10/19/77/77	0/4/4/4
17	80Y	P	101	17,7	-	10/11/28/31	1/1/1/1
9	Y01	G	909	-	-	8/19/77/77	0/4/4/4
11	6OU	G	904	-	-	22/52/52/52	-
9	Y01	U	706	-	-	13/19/77/77	0/4/4/4
19	05E	P	104	10,18,17	-	6/12/29/32	0/1/1/1
9	Y01	G	908	-	-	8/19/77/77	0/4/4/4
9	Y01	D	301	-	-	7/19/77/77	0/4/4/4

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	U	702	80T	O23-C24	4.68	1.47	1.33
16	U	702	80T	O54-C55	3.83	1.44	1.33
16	U	702	80T	O20-C02	3.74	1.44	1.34
16	U	702	80T	O72-C52	-3.58	1.37	1.46
18	P	102	PA1	C1-C2	-3.24	1.48	1.52
16	U	702	80T	P43-O42	2.99	1.71	1.59
11	G	904	6OU	O30-C20	-2.92	1.39	1.46
15	S	902	LBN	O5-C25	2.83	1.41	1.33
9	D	301	Y01	OAH-CAX	-2.77	1.21	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	902	Y01	OAF-CAX	2.77	1.31	1.22
9	G	907	Y01	OAF-CAX	2.76	1.31	1.22
16	U	702	80T	O20-C21	-2.76	1.39	1.46
9	U	703	Y01	OAF-CAX	2.75	1.31	1.22
9	G	910	Y01	OAF-CAX	2.75	1.31	1.22
9	G	908	Y01	OAF-CAX	2.75	1.31	1.22
9	U	707	Y01	OAF-CAX	2.74	1.31	1.22
9	U	706	Y01	OAF-CAX	2.74	1.31	1.22
9	G	906	Y01	OAF-CAX	2.74	1.31	1.22
9	G	909	Y01	OAF-CAX	2.74	1.31	1.22
9	U	705	Y01	OAF-CAX	2.73	1.31	1.22
9	G	911	Y01	OAF-CAX	2.73	1.31	1.22
15	S	902	LBN	O7-C2	-2.70	1.39	1.46
16	U	702	80T	P43-O44	2.69	1.70	1.59
9	G	906	Y01	OAH-CAX	-2.67	1.21	1.30
9	U	706	Y01	OAH-CAX	-2.67	1.21	1.30
9	U	704	Y01	OAH-CAX	-2.66	1.21	1.30
9	U	705	Y01	OAH-CAX	-2.66	1.21	1.30
9	G	902	Y01	OAH-CAX	-2.65	1.21	1.30
9	U	704	Y01	OAF-CAX	2.65	1.30	1.22
9	G	907	Y01	OAH-CAX	-2.65	1.21	1.30
9	G	908	Y01	OAH-CAX	-2.65	1.21	1.30
9	U	703	Y01	OAH-CAX	-2.64	1.21	1.30
9	G	910	Y01	OAH-CAX	-2.64	1.21	1.30
9	U	707	Y01	OAH-CAX	-2.64	1.21	1.30
9	D	301	Y01	OAF-CAX	2.63	1.30	1.22
9	G	909	Y01	OAH-CAX	-2.63	1.21	1.30
9	G	911	Y01	OAH-CAX	-2.62	1.21	1.30
16	U	702	80T	C25-C24	2.61	1.58	1.50
16	U	702	80T	O72-C73	2.58	1.41	1.34
11	U	701	6OU	O30-C20	-2.58	1.40	1.46
11	G	905	6OU	O30-C20	-2.57	1.40	1.46
11	G	903	6OU	O30-C20	-2.53	1.40	1.46
16	U	702	80T	C03-C02	2.41	1.57	1.50
11	G	903	6OU	O18-C16	2.41	1.40	1.33
16	U	702	80T	P49-O50	2.38	1.68	1.59
11	G	904	6OU	O18-C19	-2.37	1.39	1.45
16	U	702	80T	P49-O48	2.35	1.68	1.59
11	G	905	6OU	O18-C16	2.35	1.40	1.33
11	U	701	6OU	O18-C16	2.33	1.40	1.33
16	U	702	80T	C56-C55	2.27	1.57	1.50
11	G	904	6OU	O18-C16	2.26	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	903	6OU	O18-C19	-2.25	1.40	1.45
15	S	902	LBN	O7-C34	2.23	1.40	1.34
11	G	905	6OU	O18-C19	-2.22	1.40	1.45
11	U	701	6OU	O18-C19	-2.21	1.40	1.45
11	G	903	6OU	O30-C31	2.15	1.40	1.34
11	G	905	6OU	O30-C31	2.10	1.40	1.34
16	U	702	80T	C47-C46	2.09	1.58	1.51
11	U	701	6OU	O30-C31	2.08	1.40	1.34

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	U	702	80T	O20-C02-C03	4.27	120.71	111.50
11	G	904	6OU	O30-C31-C33	4.13	120.40	111.50
11	G	905	6OU	O30-C31-C33	4.10	120.34	111.50
16	U	702	80T	O72-C73-C74	4.07	120.28	111.50
11	U	701	6OU	O30-C31-C33	3.98	120.08	111.50
15	S	902	LBN	O7-C34-C35	3.97	120.06	111.50
18	P	102	PA1	C1-O5-C5	3.58	117.04	112.19
11	G	903	6OU	O30-C31-C33	3.57	119.20	111.50
20	P	105	81Q	O04-C03-C93	3.27	114.79	108.25
9	G	909	Y01	OAF-CAX-CAL	-3.07	113.22	123.08
9	U	706	Y01	OAF-CAX-CAL	-3.06	113.24	123.08
9	G	902	Y01	OAF-CAX-CAL	-3.04	113.33	123.08
9	U	703	Y01	OAF-CAX-CAL	-3.03	113.33	123.08
9	U	705	Y01	OAF-CAX-CAL	-3.03	113.33	123.08
9	U	707	Y01	OAF-CAX-CAL	-3.02	113.36	123.08
9	G	906	Y01	OAF-CAX-CAL	-3.02	113.37	123.08
9	G	908	Y01	OAF-CAX-CAL	-3.02	113.37	123.08
9	G	911	Y01	OAF-CAX-CAL	-3.00	113.43	123.08
9	G	910	Y01	OAF-CAX-CAL	-2.98	113.51	123.08
9	U	704	Y01	OAF-CAX-CAL	-2.95	113.59	123.08
16	U	702	80T	O23-C24-C25	2.93	121.10	111.91
9	G	907	Y01	OAF-CAX-CAL	-2.93	113.67	123.08
9	G	909	Y01	OAH-CAX-CAL	2.91	123.39	114.03
9	U	706	Y01	OAH-CAX-CAL	2.88	123.27	114.03
9	U	703	Y01	OAH-CAX-CAL	2.87	123.24	114.03
9	G	902	Y01	OAH-CAX-CAL	2.86	123.21	114.03
9	U	707	Y01	OAH-CAX-CAL	2.85	123.20	114.03
9	G	906	Y01	OAH-CAX-CAL	2.85	123.18	114.03
9	D	301	Y01	OAF-CAX-CAL	-2.84	113.95	123.08
9	U	705	Y01	OAH-CAX-CAL	2.84	123.16	114.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	908	Y01	OAH-CAX-CAL	2.84	123.14	114.03
9	G	911	Y01	OAH-CAX-CAL	2.82	123.09	114.03
9	G	910	Y01	OAH-CAX-CAL	2.80	123.03	114.03
9	U	704	Y01	OAH-CAX-CAL	2.79	123.00	114.03
9	G	907	Y01	OAH-CAX-CAL	2.78	122.97	114.03
9	D	301	Y01	OAH-CAX-CAL	2.75	122.88	114.03
16	U	702	80T	O54-C55-C56	2.70	120.39	111.91
11	G	903	6OU	O18-C16-C15	2.59	120.02	111.91
11	U	701	6OU	O18-C16-C15	2.57	119.98	111.91
11	G	905	6OU	O18-C16-C15	2.52	119.81	111.91
15	S	902	LBN	O5-C25-C26	2.51	119.77	111.91
20	P	105	81Q	C26-C93-C03	-2.48	106.00	111.66
18	P	102	PA1	O4-C4-C3	-2.32	104.98	110.35
17	P	103	80Y	C51-C52-C85	2.25	112.43	109.67
11	G	904	6OU	O18-C16-C15	2.24	118.94	111.91
20	P	105	81Q	P95-O94-C93	-2.23	111.28	119.41

There are no chirality outliers.

All (365) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	301	Y01	CAM-CAY-OAW-CBC
9	G	902	Y01	CAM-CAY-OAW-CBC
9	G	907	Y01	CAM-CAY-OAW-CBC
9	G	909	Y01	OAG-CAY-OAW-CBC
9	G	909	Y01	CAM-CAY-OAW-CBC
9	G	910	Y01	CAO-CBB-CBE-CBI
9	G	910	Y01	CAC-CBB-CBE-CAP
9	G	910	Y01	CAC-CBB-CBE-CBI
9	U	703	Y01	CAM-CAY-OAW-CBC
9	U	704	Y01	CAM-CAY-OAW-CBC
9	U	705	Y01	CAM-CAY-OAW-CBC
9	U	706	Y01	CAC-CBB-CBE-CAP
9	U	706	Y01	CAC-CBB-CBE-CBI
9	U	706	Y01	CAV-CBC-OAW-CAY
9	U	706	Y01	OAG-CAY-OAW-CBC
9	U	707	Y01	CAV-CBC-OAW-CAY
11	G	904	6OU	C21-O22-P23-O24
11	G	904	6OU	C21-O22-P23-O25
11	G	904	6OU	C21-O22-P23-O26
11	G	904	6OU	C27-O26-P23-O24
11	G	904	6OU	C27-O26-P23-O25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	G	904	6OU	O26-C27-C28-N29
11	G	905	6OU	C21-O22-P23-O24
11	G	905	6OU	C21-O22-P23-O25
11	G	905	6OU	C27-O26-P23-O22
11	G	905	6OU	C27-O26-P23-O24
11	G	905	6OU	O26-C27-C28-N29
11	G	905	6OU	C33-C31-O30-C20
11	U	701	6OU	C21-O22-P23-O24
11	U	701	6OU	C21-O22-P23-O25
11	U	701	6OU	C21-O22-P23-O26
11	U	701	6OU	O26-C27-C28-N29
15	S	902	LBN	C9-O2-P1-O3
15	S	902	LBN	C9-O2-P1-O4
15	S	902	LBN	N1-C6-C9-O2
16	U	702	80T	C45-O44-P43-O95
16	U	702	80T	C45-O44-P43-O96
16	U	702	80T	C47-O48-P49-O50
16	U	702	80T	C47-O48-P49-O92
16	U	702	80T	C47-O48-P49-O93
16	U	702	80T	C51-O50-P49-O92
16	U	702	80T	C51-O50-P49-O93
16	U	702	80T	O91-C73-O72-C52
17	P	101	80Y	O72-C73-C74-O75
17	P	101	80Y	C83-C73-C74-O75
17	P	101	80Y	C74-O75-P76-O81
17	P	101	80Y	C74-O75-P76-O82
17	P	101	80Y	C78-O77-P76-O75
17	P	101	80Y	C78-O77-P76-O82
17	P	101	80Y	O77-C78-C79-N80
17	P	103	80Y	C78-O77-P76-O81
17	P	103	80Y	C78-O77-P76-O82
19	P	104	05E	C90-C81-O82-P83
19	P	104	05E	C81-O82-P83-O88
20	P	105	81Q	C97-O96-P95-O94
20	P	105	81Q	C97-O96-P95-OB6
20	P	105	81Q	CA1-CA0-O99-C98
20	P	105	81Q	OAK-CA0-O99-C98
12	G	912	AJP	O50-C45-O44-C37
12	G	912	AJP	C46-C45-O44-C37
9	G	910	Y01	CAO-CBB-CBE-CAP
9	U	706	Y01	CAO-CBB-CBE-CBI
9	U	707	Y01	CAO-CBB-CBE-CBI

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	D	301	Y01	OAG-CAY-OAW-CBC
9	G	902	Y01	OAG-CAY-OAW-CBC
9	U	703	Y01	OAG-CAY-OAW-CBC
9	U	704	Y01	OAG-CAY-OAW-CBC
9	U	705	Y01	OAG-CAY-OAW-CBC
11	G	905	6OU	O32-C31-O30-C20
9	U	706	Y01	CAM-CAY-OAW-CBC
16	U	702	80T	C74-C73-O72-C52
9	G	907	Y01	CAJ-CAO-CBB-CAC
9	U	704	Y01	CAJ-CAO-CBB-CAC
9	U	705	Y01	CAJ-CAO-CBB-CAC
9	U	706	Y01	CAJ-CAO-CBB-CAC
15	S	902	LBN	O6-C25-O5-C3
9	U	705	Y01	CAC-CBB-CBE-CAP
9	U	707	Y01	CAC-CBB-CBE-CAP
9	U	705	Y01	CAC-CBB-CBE-CBI
9	U	707	Y01	CAC-CBB-CBE-CBI
9	U	706	Y01	CAO-CBB-CBE-CAP
9	G	906	Y01	CAO-CBB-CBE-CBI
9	G	911	Y01	CAX-CAL-CAM-CAY
15	S	902	LBN	C26-C27-C28-C29
9	G	907	Y01	OAG-CAY-OAW-CBC
9	G	909	Y01	CAJ-CAO-CBB-CAC
15	S	902	LBN	C10-C13-C16-C19
9	G	906	Y01	CAC-CBB-CBE-CAP
9	G	906	Y01	CAC-CBB-CBE-CBI
9	U	705	Y01	CAO-CBB-CBE-CAP
9	U	707	Y01	CAO-CBB-CBE-CAP
9	U	705	Y01	CAO-CBB-CBE-CBI
15	S	902	LBN	C26-C25-O5-C3
16	U	702	80T	C56-C55-O54-C53
11	G	903	6OU	C33-C34-C35-C36
11	U	701	6OU	C11-C12-C13-C14
15	S	902	LBN	C35-C36-C37-C38
11	G	904	6OU	C07-C08-C09-C10
11	G	904	6OU	C44-C45-C46-C47
9	G	907	Y01	CAJ-CAO-CBB-CBE
16	U	702	80T	O71-C55-O54-C53
9	G	908	Y01	CAJ-CAO-CBB-CAC
16	U	702	80T	C76-C77-C78-C79
20	P	105	81Q	CAP-CAQ-CAR-CAS
9	U	704	Y01	CAC-CBB-CBE-CAP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	G	906	Y01	CAO-CBB-CBE-CAP
9	G	906	Y01	CAJ-CAO-CBB-CBE
9	G	908	Y01	CAJ-CAO-CBB-CBE
9	G	909	Y01	CAJ-CAO-CBB-CBE
9	U	704	Y01	CAJ-CAO-CBB-CBE
11	G	905	6OU	C15-C16-O18-C19
9	U	704	Y01	CAO-CBB-CBE-CBI
16	U	702	80T	C74-C75-C76-C77
20	P	105	81Q	C11-C12-C13-C14
20	P	105	81Q	C13-C14-C15-C16
9	G	906	Y01	CAJ-CAO-CBB-CAC
11	G	904	6OU	C05-C06-C07-C08
9	D	301	Y01	CAO-CAJ-CAN-CBA
16	U	702	80T	C02-C03-C04-C05
16	U	702	80T	C73-C74-C75-C76
20	P	105	81Q	CA0-CA1-CA2-CA3
11	G	905	6OU	O17-C16-O18-C19
9	U	707	Y01	CAJ-CAO-CBB-CBE
19	P	104	05E	O97-C94-C95-O96
9	G	910	Y01	CAJ-CAO-CBB-CAC
11	G	904	6OU	C31-C33-C34-C35
11	G	905	6OU	C13-C14-C15-C16
15	S	902	LBN	C25-C26-C27-C28
9	U	705	Y01	CAJ-CAO-CBB-CBE
9	U	706	Y01	CAJ-CAO-CBB-CBE
9	U	707	Y01	CAJ-CAO-CBB-CAC
9	D	301	Y01	CAN-CAJ-CAO-CBB
9	U	704	Y01	CAC-CBB-CBE-CBI
9	U	703	Y01	CAN-CAJ-CAO-CBB
9	G	908	Y01	CAO-CAJ-CAN-CBA
11	G	904	6OU	C27-O26-P23-O22
11	G	905	6OU	C21-O22-P23-O26
15	S	902	LBN	C1-O1-P1-O2
15	S	902	LBN	C9-O2-P1-O1
16	U	702	80T	C45-O44-P43-O42
16	U	702	80T	C51-O50-P49-O48
17	P	101	80Y	C74-O75-P76-O77
17	P	103	80Y	C78-O77-P76-O75
11	U	701	6OU	C13-C14-C15-C16
9	G	910	Y01	CAR-CBC-OAW-CAY
11	G	905	6OU	C44-C45-C46-C47
11	G	903	6OU	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	G	911	Y01	CAM-CAY-OAW-CBC
11	G	903	6OU	C36-C37-C38-C39
20	P	105	81Q	C07-C08-C09-C10
11	U	701	6OU	C43-C44-C45-C46
16	U	702	80T	C32-C33-C34-C35
9	G	911	Y01	OAG-CAY-OAW-CBC
11	G	903	6OU	C45-C46-C47-C48
11	U	701	6OU	C07-C08-C09-C10
16	U	702	80T	C34-C35-C36-C37
20	P	105	81Q	C15-C16-C17-C18
11	G	903	6OU	C12-C13-C14-C15
11	G	904	6OU	C03-C04-C05-C06
20	P	105	81Q	CAU-CAV-CAW-CAX
9	U	704	Y01	CAJ-CAN-CBA-CAB
20	P	105	81Q	C14-C15-C16-C17
11	G	903	6OU	C07-C08-C09-C10
16	U	702	80T	C13-C14-C15-C16
15	S	902	LBN	C13-C10-C7-C4
15	S	902	LBN	C7-C10-C13-C16
16	U	702	80T	C86-C87-C88-C89
9	U	707	Y01	CAN-CAJ-CAO-CBB
9	G	908	Y01	CAM-CAY-OAW-CBC
16	U	702	80T	C06-C07-C08-C09
20	P	105	81Q	CAZ-CB0-CB1-CB2
11	G	905	6OU	C37-C38-C39-C40
11	U	701	6OU	C37-C38-C39-C40
16	U	702	80T	C78-C79-C80-C81
20	P	105	81Q	C05-C06-C07-C08
11	G	904	6OU	C35-C36-C37-C38
20	P	105	81Q	CAF-CAG-CAH-CAI
20	P	105	81Q	CAW-CAX-CAY-CAZ
11	G	905	6OU	C34-C35-C36-C37
9	G	911	Y01	CAO-CBB-CBE-CBI
15	S	902	LBN	C32-C33-C4-C7
11	U	701	6OU	O18-C19-C20-C21
12	G	912	AJP	O31-C26-O25-C23
11	U	701	6OU	C12-C13-C14-C15
15	S	902	LBN	C28-C29-C30-C31
20	P	105	81Q	C09-C10-C11-C12
11	G	905	6OU	C31-C33-C34-C35
20	P	105	81Q	C12-C13-C14-C15
11	G	905	6OU	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	U	702	80T	C83-C84-C85-C86
11	G	904	6OU	C37-C38-C39-C40
9	U	704	Y01	CAJ-CAN-CBA-CAA
11	U	701	6OU	C31-C33-C34-C35
16	U	702	80T	C24-C25-C26-C27
20	P	105	81Q	CAO-CAP-CAQ-CAR
9	G	908	Y01	OAG-CAY-OAW-CBC
11	G	904	6OU	C46-C47-C48-C49
16	U	702	80T	C25-C24-O23-C22
9	G	910	Y01	CAV-CBC-OAW-CAY
20	P	105	81Q	C06-C07-C08-C09
11	G	903	6OU	C31-C33-C34-C35
20	P	105	81Q	OAM-CAN-CAO-CAP
11	U	701	6OU	C46-C47-C48-C49
11	U	701	6OU	C10-C11-C12-C13
15	S	902	LBN	C29-C30-C31-C32
11	U	701	6OU	C42-C43-C44-C45
9	G	910	Y01	CAM-CAY-OAW-CBC
9	U	707	Y01	CAM-CAY-OAW-CBC
15	S	902	LBN	O1-C1-C2-O7
20	P	105	81Q	C16-C17-C18-C19
9	U	707	Y01	OAG-CAY-OAW-CBC
16	U	702	80T	C75-C76-C77-C78
20	P	105	81Q	CAV-CAW-CAX-CAY
16	U	702	80T	C82-C83-C84-C85
12	G	912	AJP	O31-C30-C32-O33
11	G	904	6OU	C34-C35-C36-C37
16	U	702	80T	O40-C24-O23-C22
9	G	910	Y01	OAG-CAY-OAW-CBC
20	P	105	81Q	CAN-CAO-CAP-CAQ
15	S	902	LBN	C8-C11-C14-C17
16	U	702	80T	C77-C78-C79-C80
11	U	701	6OU	C06-C07-C08-C09
20	P	105	81Q	CA1-CA2-CA3-CA4
14	T	901	NAG	C1-C2-N2-C7
16	U	702	80T	C45-C46-C47-O48
11	G	904	6OU	C36-C37-C38-C39
11	G	904	6OU	C08-C09-C10-C11
11	U	701	6OU	C01-C02-C03-C04
19	P	104	05E	C92-C94-C95-O96
16	U	702	80T	O94-C46-C47-O48
9	G	911	Y01	CAO-CBB-CBE-CAP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	G	912	AJP	C36-C37-O44-C45
16	U	702	80T	C87-C88-C89-C90
11	G	903	6OU	C42-C43-C44-C45
19	P	104	05E	C81-O82-P83-O84
20	P	105	81Q	C93-O94-P95-O96
11	U	701	6OU	C02-C03-C04-C05
9	G	911	Y01	CAO-CAJ-CAN-CBA
9	G	911	Y01	CAC-CBB-CBE-CAP
9	U	707	Y01	CAR-CBC-OAW-CAY
11	G	905	6OU	C42-C43-C44-C45
11	G	903	6OU	O30-C31-C33-C34
9	G	911	Y01	CAC-CBB-CBE-CBI
20	P	105	81Q	CAE-CAF-CAG-CAH
20	P	105	81Q	O99-C98-CAL-OAM
11	G	903	6OU	C10-C11-C12-C13
11	G	903	6OU	C33-C31-O30-C20
11	G	903	6OU	C43-C44-C45-C46
12	G	912	AJP	C38-C37-O44-C45
15	S	902	LBN	O1-C1-C2-C3
11	G	903	6OU	C35-C36-C37-C38
15	S	902	LBN	C36-C37-C38-C39
15	S	902	LBN	C30-C31-C32-C33
11	U	701	6OU	C35-C36-C37-C38
11	G	903	6OU	O18-C19-C20-C21
11	G	905	6OU	O18-C19-C20-C21
16	U	702	80T	C41-C21-C22-O23
20	P	105	81Q	C97-C98-CAL-OAM
19	P	104	05E	C81-O82-P83-O89
20	P	105	81Q	CAQ-CAR-CAS-CAT
11	G	903	6OU	C08-C09-C10-C11
16	U	702	80T	C85-C86-C87-C88
15	S	902	LBN	C20-C22-C23-C24
9	D	301	Y01	CAJ-CAN-CBA-CAA
11	G	903	6OU	O18-C19-C20-O30
11	G	905	6OU	O18-C19-C20-O30
11	G	903	6OU	O32-C31-O30-C20
9	G	902	Y01	CAO-CAJ-CAN-CBA
15	S	902	LBN	C31-C32-C33-C4
9	D	301	Y01	CAJ-CAN-CBA-CAB
18	P	102	PA1	C4-C5-C6-O6
11	G	905	6OU	C35-C36-C37-C38
11	G	903	6OU	C05-C06-C07-C08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	U	701	6OU	C33-C31-O30-C20
20	P	105	81Q	CAY-CAZ-CB0-CB1
16	U	702	80T	C57-C58-C59-C60
15	S	902	LBN	C39-C40-C41-C42
11	U	701	6OU	O32-C31-O30-C20
11	U	701	6OU	C41-C42-C43-C44
9	G	909	Y01	CAN-CAJ-CAO-CBB
16	U	702	80T	C27-C28-C29-C30
11	G	904	6OU	C01-C02-C03-C04
20	P	105	81Q	C98-CAL-OAM-CAN
17	P	101	80Y	C73-C74-O75-P76
15	S	902	LBN	C1-O1-P1-O4
20	P	105	81Q	C97-O96-P95-OB5
20	P	105	81Q	O96-C97-C98-CAL
16	U	702	80T	C26-C27-C28-C29
17	P	101	80Y	C79-C78-O77-P76
11	G	905	6OU	C43-C44-C45-C46
11	U	701	6OU	O18-C19-C20-O30
16	U	702	80T	O20-C21-C22-O23
16	U	702	80T	C30-C31-C32-C33
16	U	702	80T	C25-C26-C27-C28
20	P	105	81Q	O96-C97-C98-O99
20	P	105	81Q	C10-C11-C12-C13
11	G	905	6OU	C33-C34-C35-C36
11	G	903	6OU	C27-O26-P23-O22
11	U	701	6OU	C27-O26-P23-O22
15	S	902	LBN	C14-C17-C20-C22
11	U	701	6OU	C09-C10-C11-C12
14	S	901	NAG	C4-C5-C6-O6
11	U	701	6OU	C15-C16-O18-C19
11	U	701	6OU	C45-C46-C47-C48
11	U	701	6OU	O17-C16-O18-C19
11	G	904	6OU	C14-C15-C16-O18
11	G	904	6OU	C41-C42-C43-C44
9	G	911	Y01	CAM-CAL-CAX-OAF
15	S	902	LBN	O7-C2-C3-O5
9	U	705	Y01	CAM-CAL-CAX-OAH
9	U	706	Y01	CAM-CAL-CAX-OAF
9	G	911	Y01	CAM-CAL-CAX-OAH
9	U	705	Y01	CAM-CAL-CAX-OAF
20	P	105	81Q	CA7-CA8-CA9-CAA
9	U	706	Y01	CAM-CAL-CAX-OAH

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	G	903	6OU	O32-C31-C33-C34
11	U	701	6OU	C19-C20-C21-O22
20	P	105	81Q	CAT-CAU-CAV-CAW
14	S	901	NAG	O5-C5-C6-O6
20	P	105	81Q	CAG-CAH-CAI-CAJ
9	G	906	Y01	CAM-CAL-CAX-OAH
9	G	906	Y01	CAM-CAL-CAX-OAF
16	U	702	80T	C84-C85-C86-C87
11	U	701	6OU	C05-C06-C07-C08
11	U	701	6OU	O30-C20-C21-O22
11	G	904	6OU	C42-C43-C44-C45
9	G	902	Y01	CAJ-CAO-CBB-CBE
9	G	908	Y01	CAM-CAL-CAX-OAF
9	G	909	Y01	CAO-CBB-CBE-CAP
9	G	908	Y01	CAM-CAL-CAX-OAH
20	P	105	81Q	CA2-CA3-CA4-CA5
9	G	902	Y01	CAM-CAL-CAX-OAF
16	U	702	80T	O72-C73-C74-C75
9	G	906	Y01	CAL-CAM-CAY-OAW
15	S	902	LBN	C1-C2-C3-O5
9	U	704	Y01	CAL-CAM-CAY-OAW
11	U	701	6OU	C14-C15-C16-O18
15	S	902	LBN	C42-C5-C8-C11
9	U	705	Y01	CAL-CAM-CAY-OAW
9	U	706	Y01	CAL-CAM-CAY-OAW
15	S	902	LBN	C40-C41-C42-C5
9	G	902	Y01	CAM-CAL-CAX-OAH
9	U	704	Y01	CAL-CAM-CAY-OAG
14	T	901	NAG	C3-C2-N2-C7
20	P	105	81Q	C02-C03-O04-C05
9	G	909	Y01	CAC-CBB-CBE-CBI
16	U	702	80T	O91-C73-C74-C75
9	G	906	Y01	CAL-CAM-CAY-OAG
16	U	702	80T	O23-C24-C25-C26
16	U	702	80T	C08-C09-C10-C11
11	G	903	6OU	C27-O26-P23-O24
17	P	103	80Y	O77-C78-C79-N80
9	D	301	Y01	CAL-CAM-CAY-OAW
11	U	701	6OU	C14-C15-C16-O17
9	U	706	Y01	CAL-CAM-CAY-OAG
11	U	701	6OU	C40-C41-C42-C43
16	U	702	80T	O20-C02-C03-C04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	U	704	Y01	CAO-CAJ-CAN-CBA
9	U	705	Y01	CAL-CAM-CAY-OAG
16	U	702	80T	O40-C24-C25-C26
9	G	909	Y01	CAM-CAL-CAX-OAH
15	S	902	LBN	C37-C38-C39-C40
9	G	908	Y01	CAN-CAJ-CAO-CBB
16	U	702	80T	O01-C02-C03-C04
15	S	902	LBN	O7-C34-C35-C36

All (1) ring outliers are listed below:

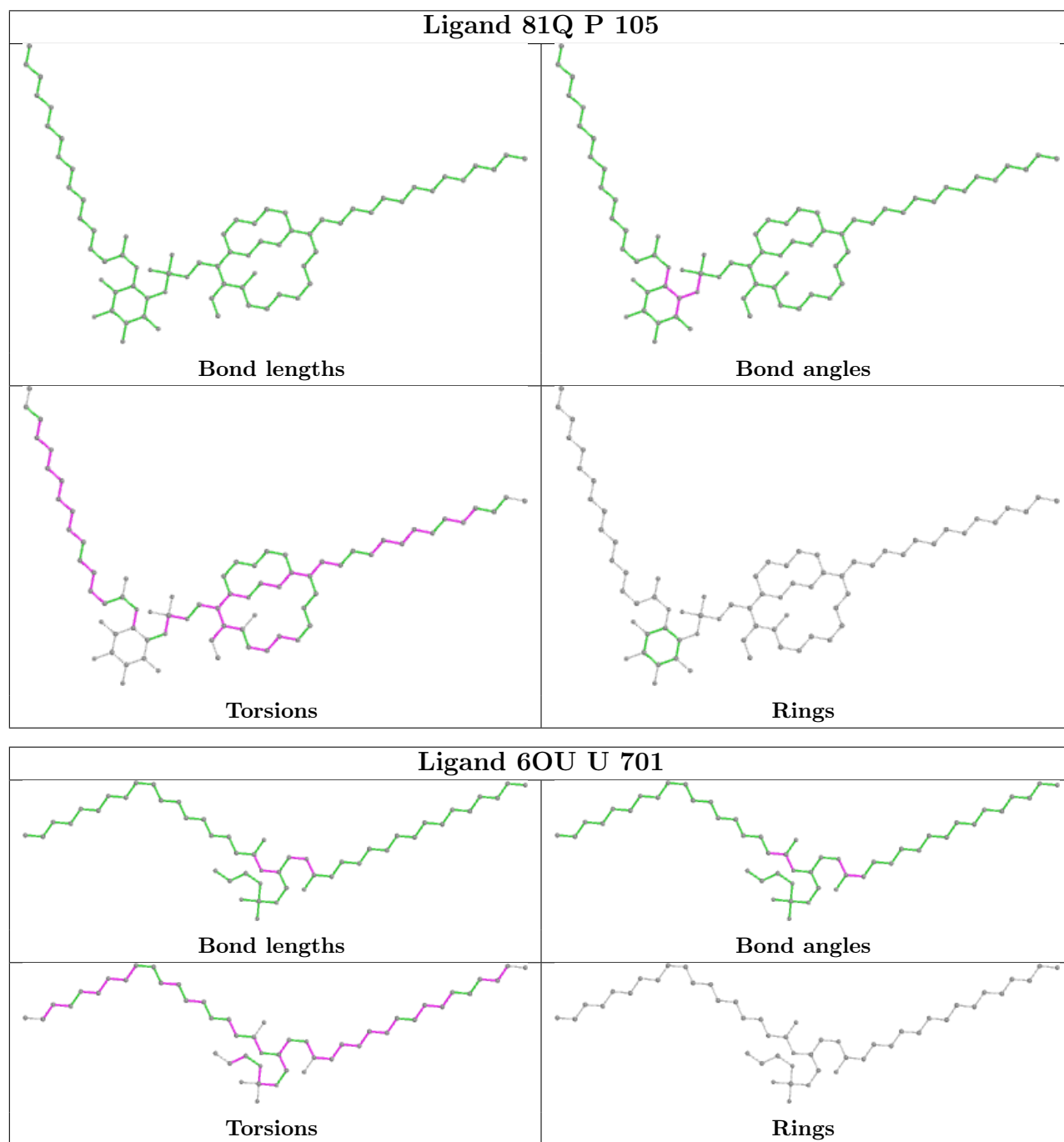
Mol	Chain	Res	Type	Atoms
17	P	101	80Y	C51-C52-C73-C83-C85-O72

15 monomers are involved in 39 short contacts:

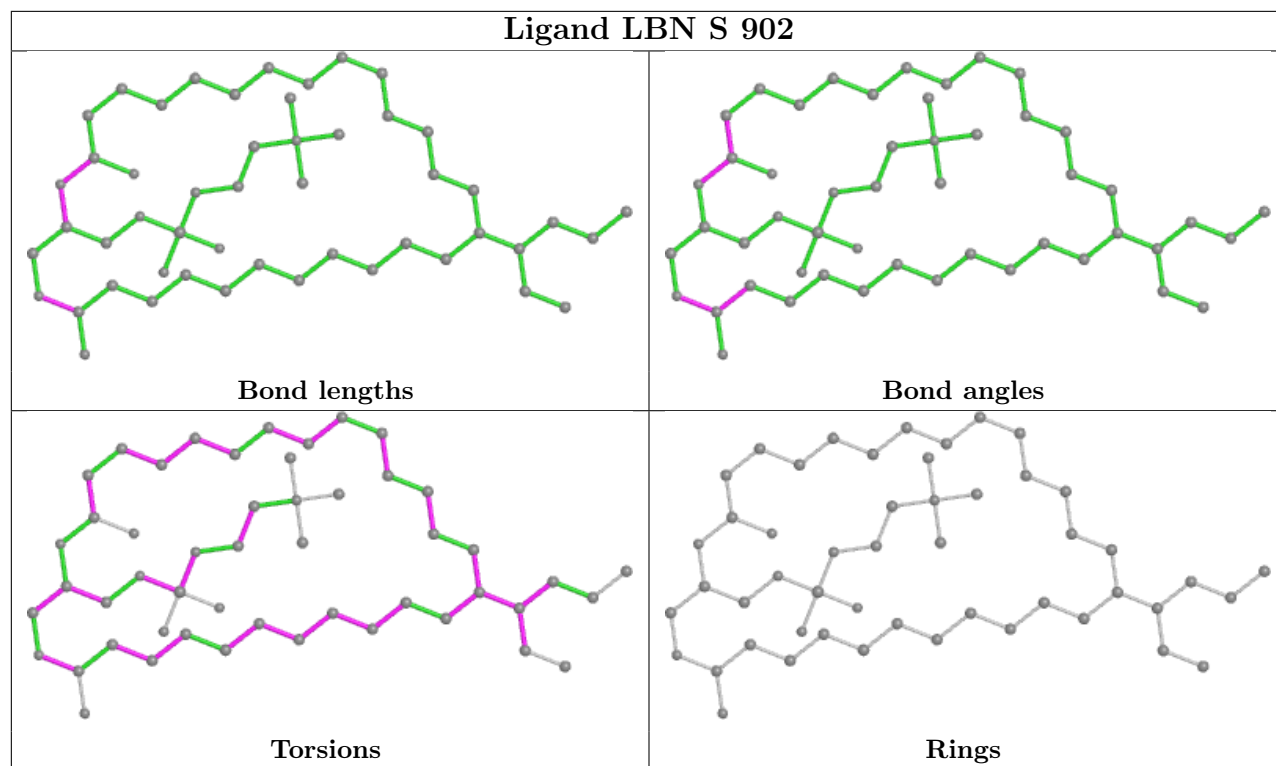
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	P	105	81Q	6	0
9	U	705	Y01	1	0
9	G	910	Y01	2	0
9	U	704	Y01	15	0
9	G	902	Y01	1	0
9	U	707	Y01	3	0
9	U	703	Y01	3	0
9	G	911	Y01	1	0
9	G	907	Y01	3	0
18	P	102	PA1	1	0
9	G	906	Y01	2	0
17	P	101	80Y	1	0
9	G	909	Y01	3	0
9	U	706	Y01	1	0
9	D	301	Y01	5	0

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.

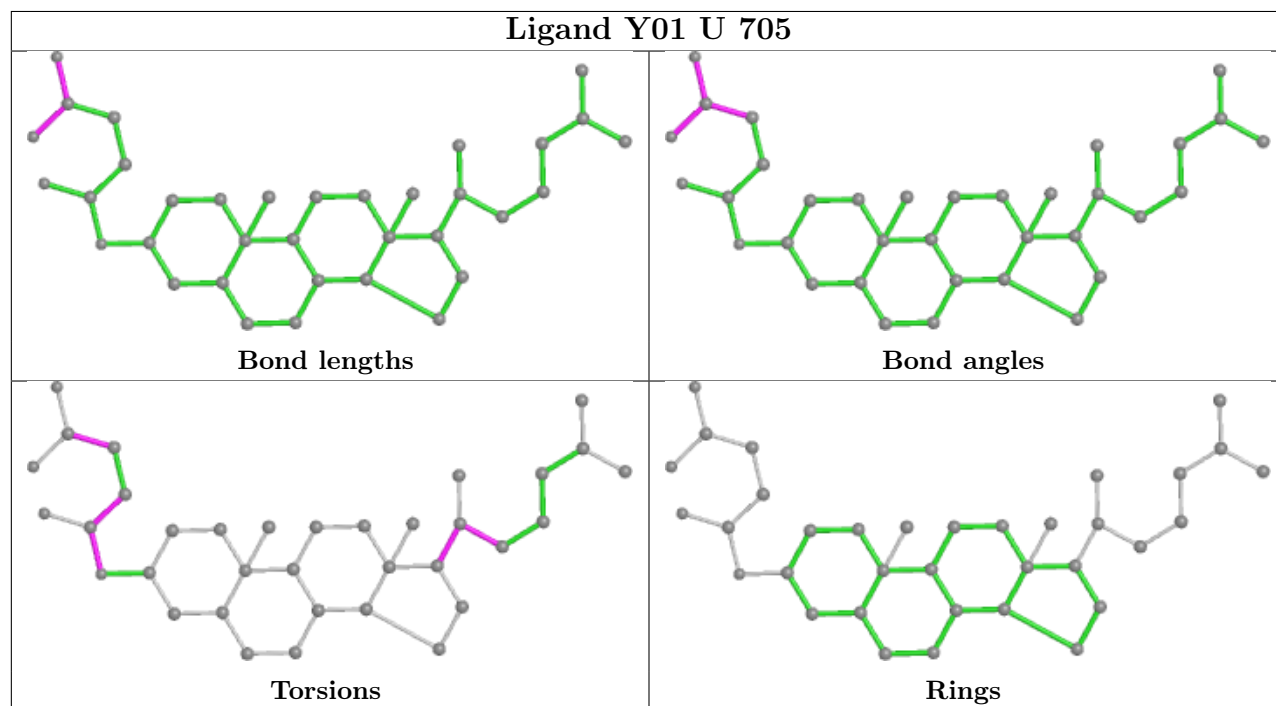
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



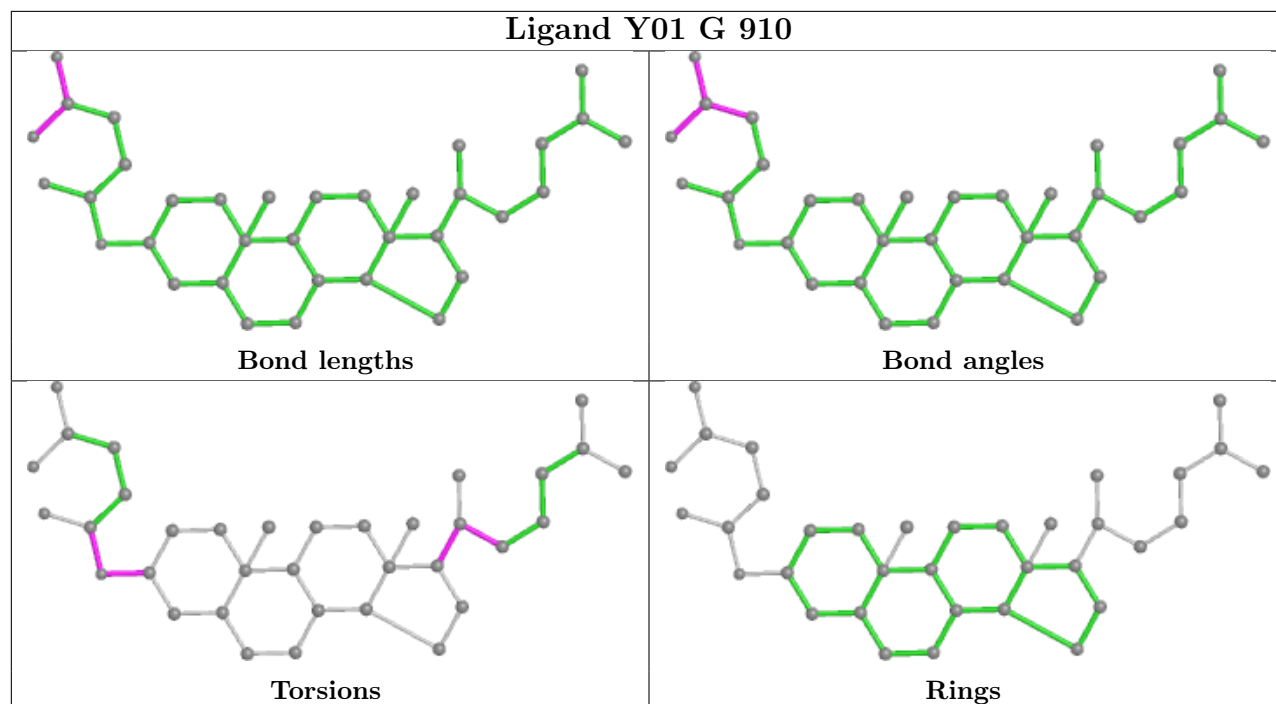
Ligand LBN S 902



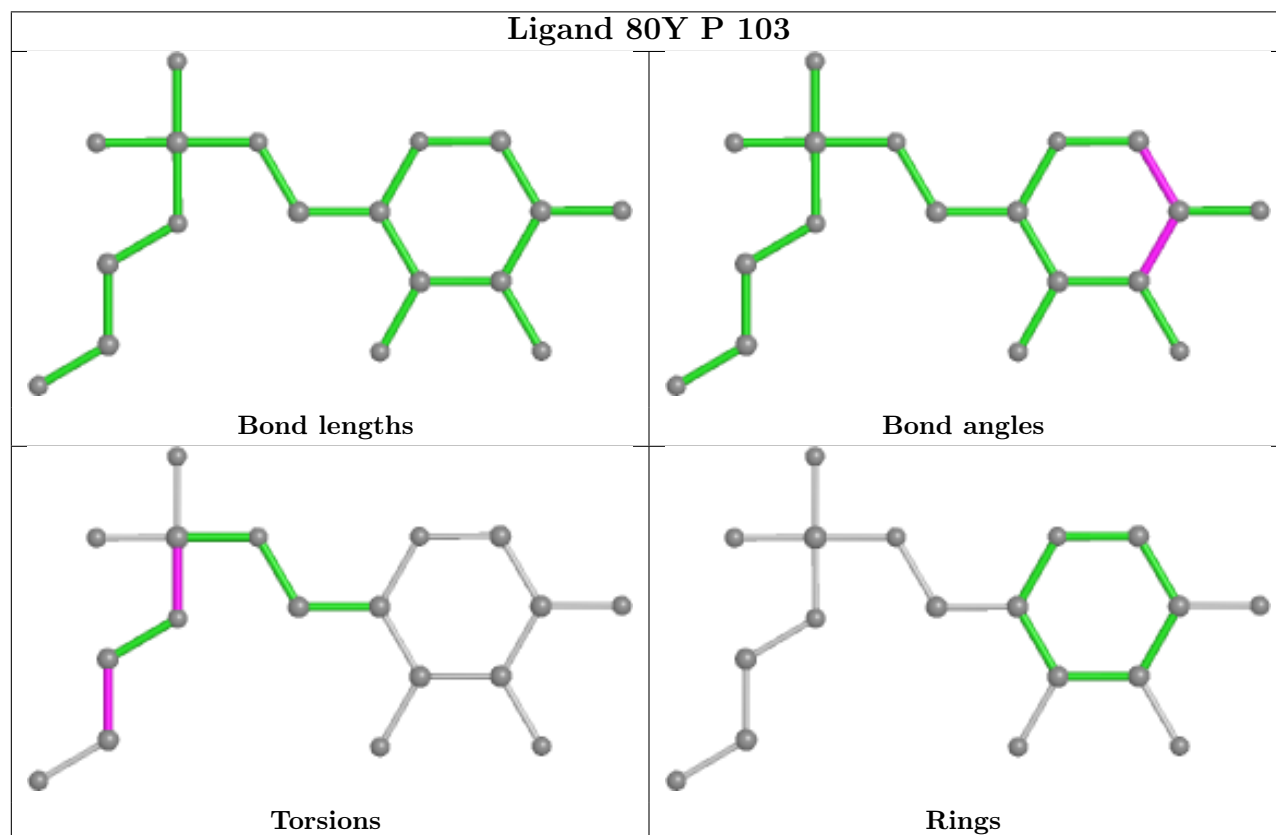
Ligand Y01 U 705



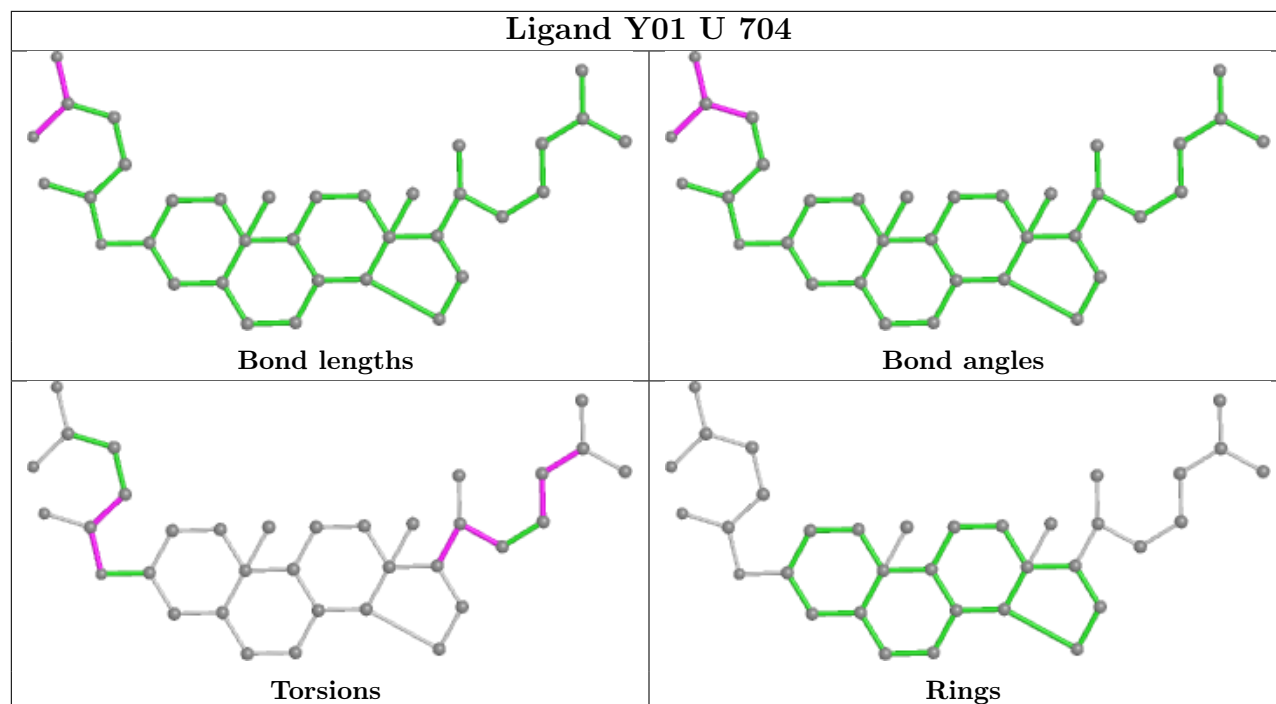
Ligand Y01 G 910



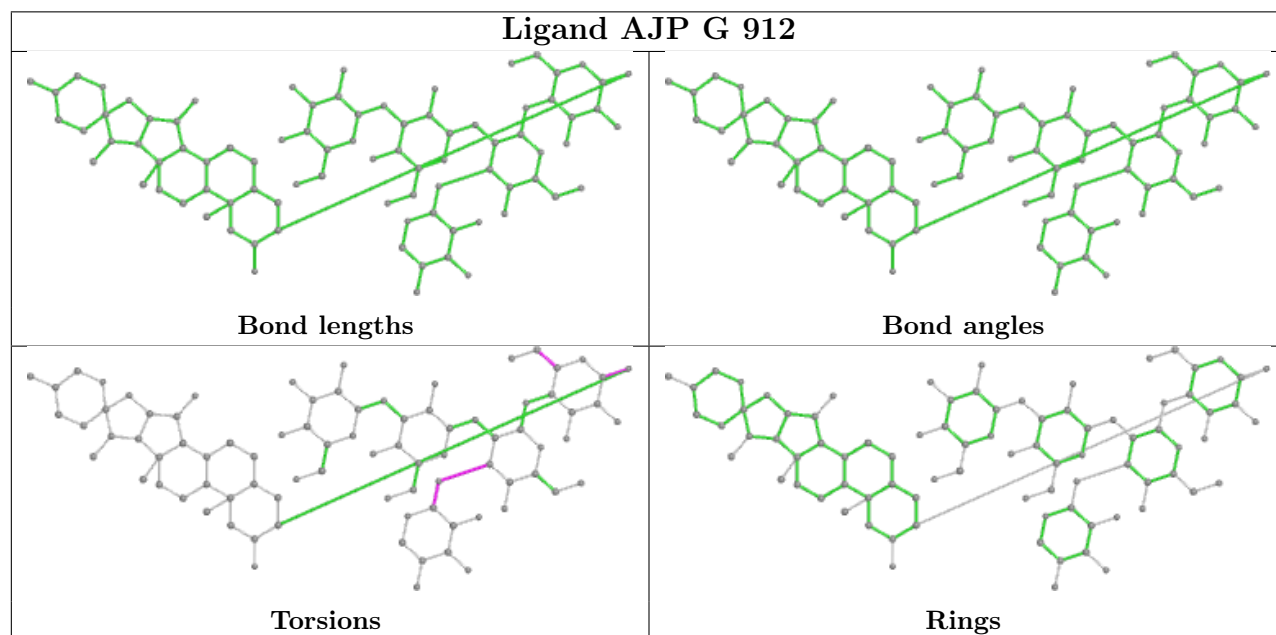
Ligand 80Y P 103

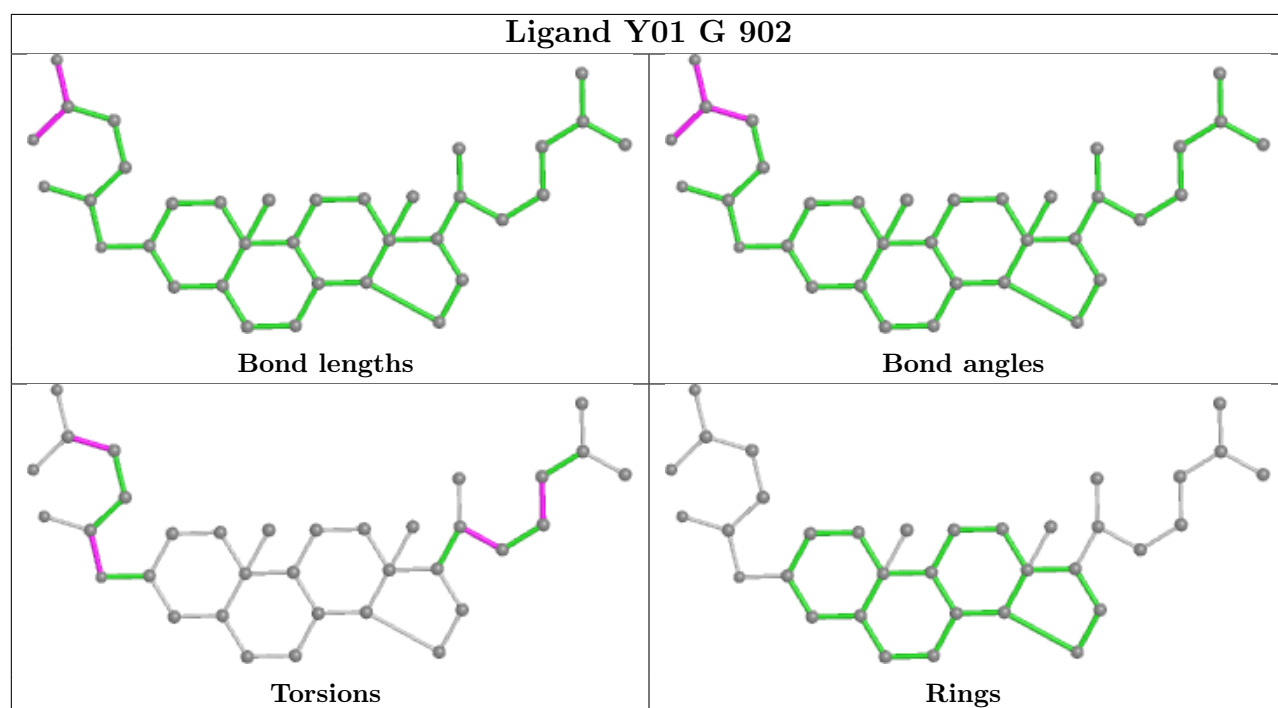
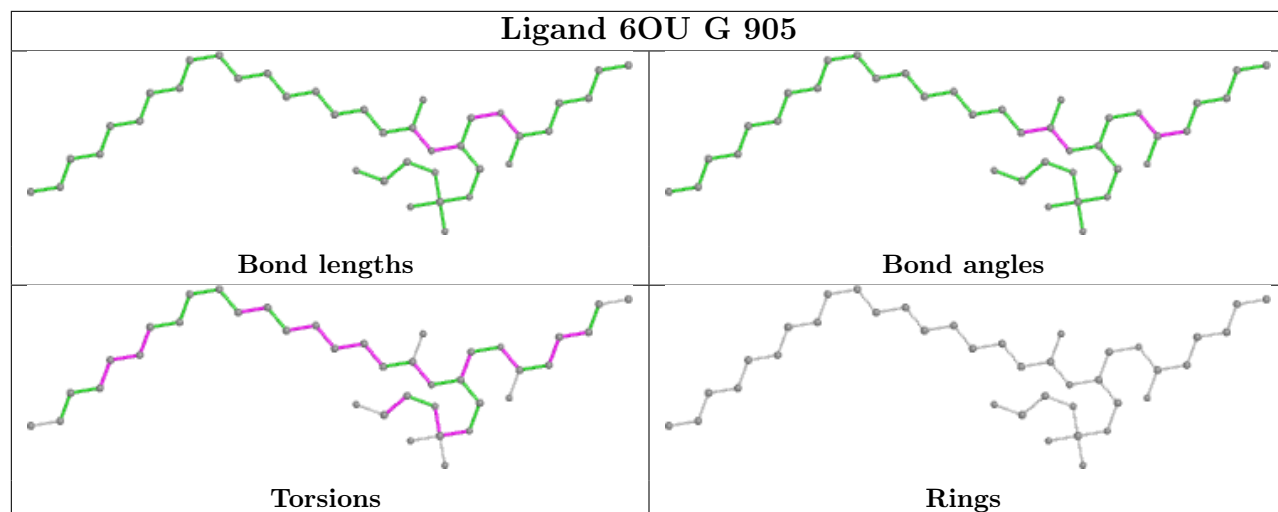


Ligand Y01 U 704

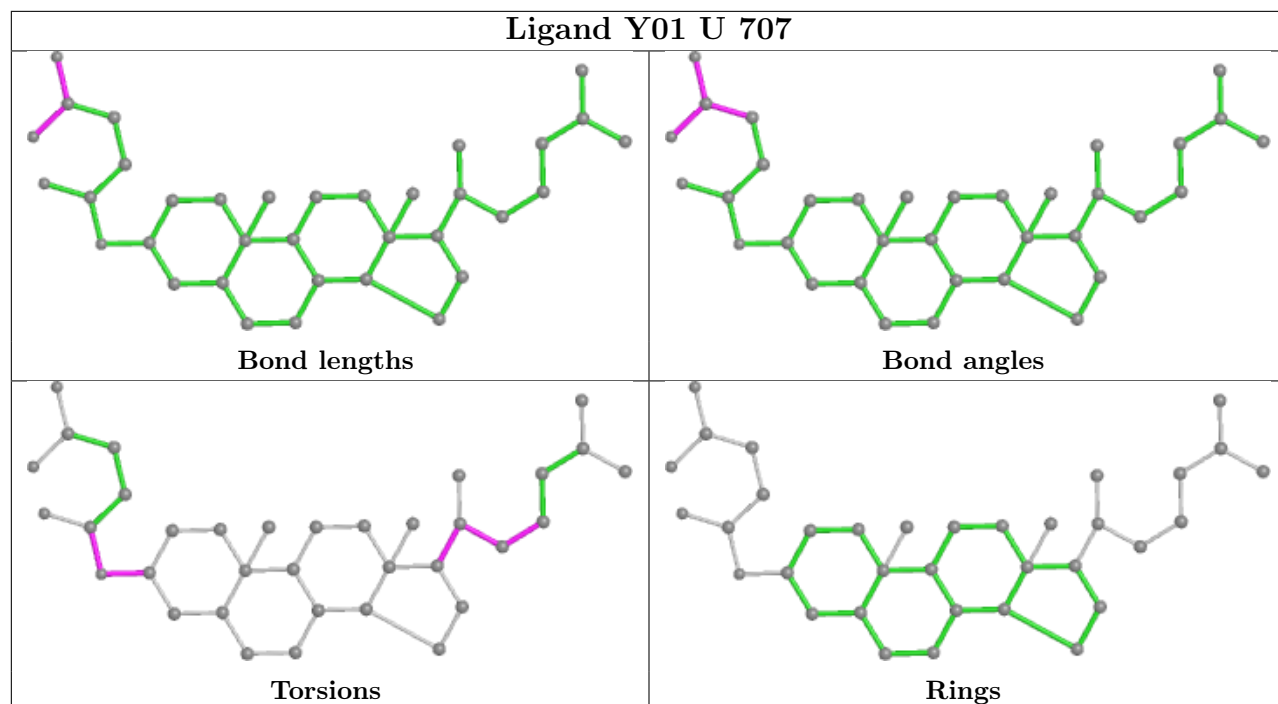


Ligand AJP G 912

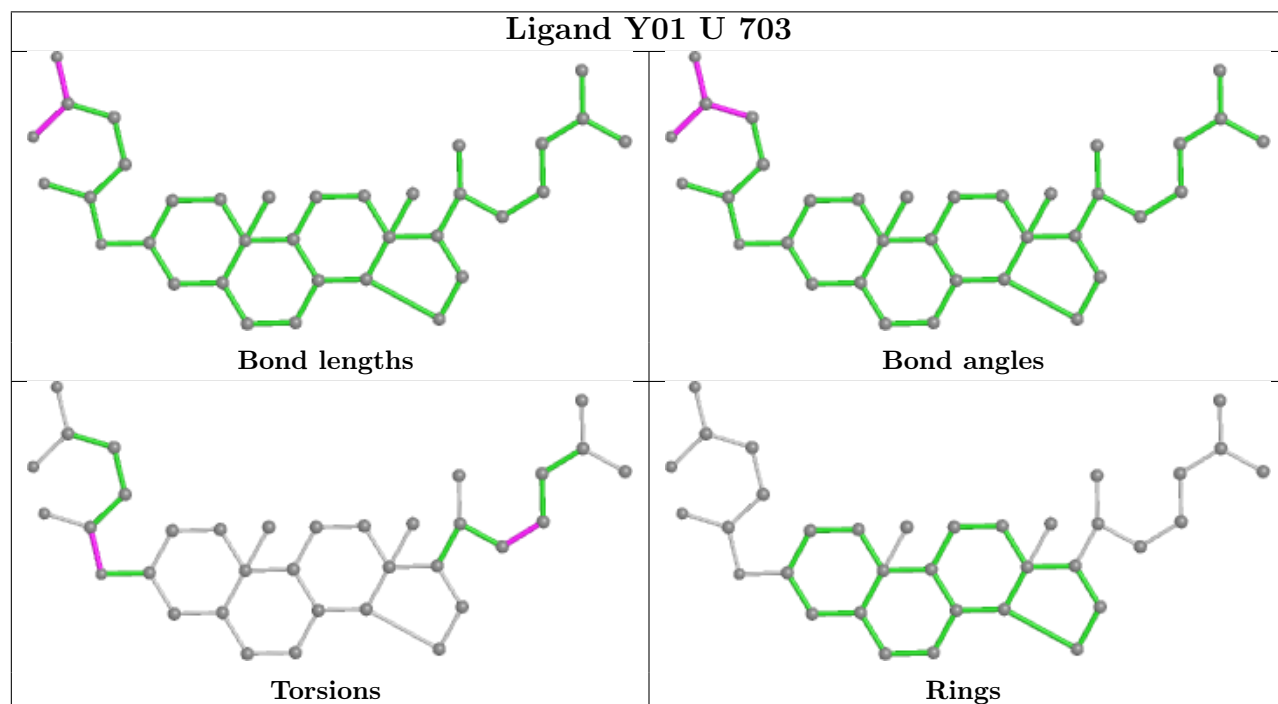




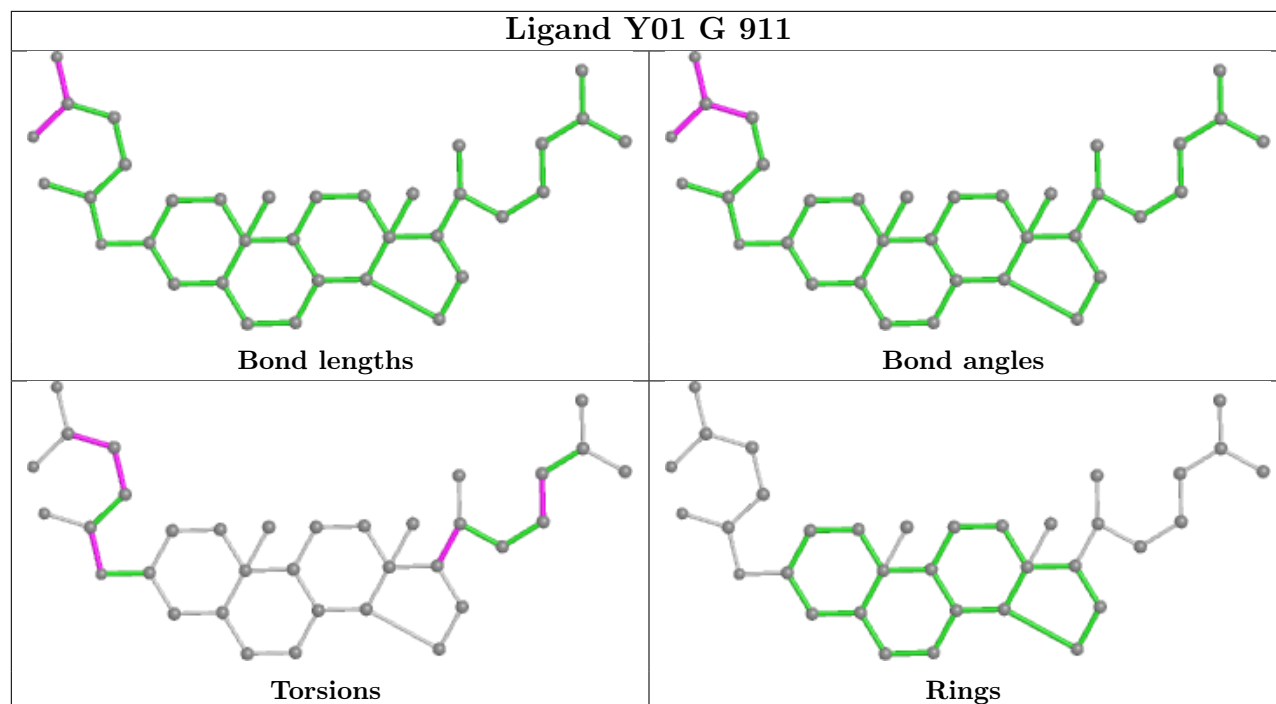
Ligand Y01 U 707



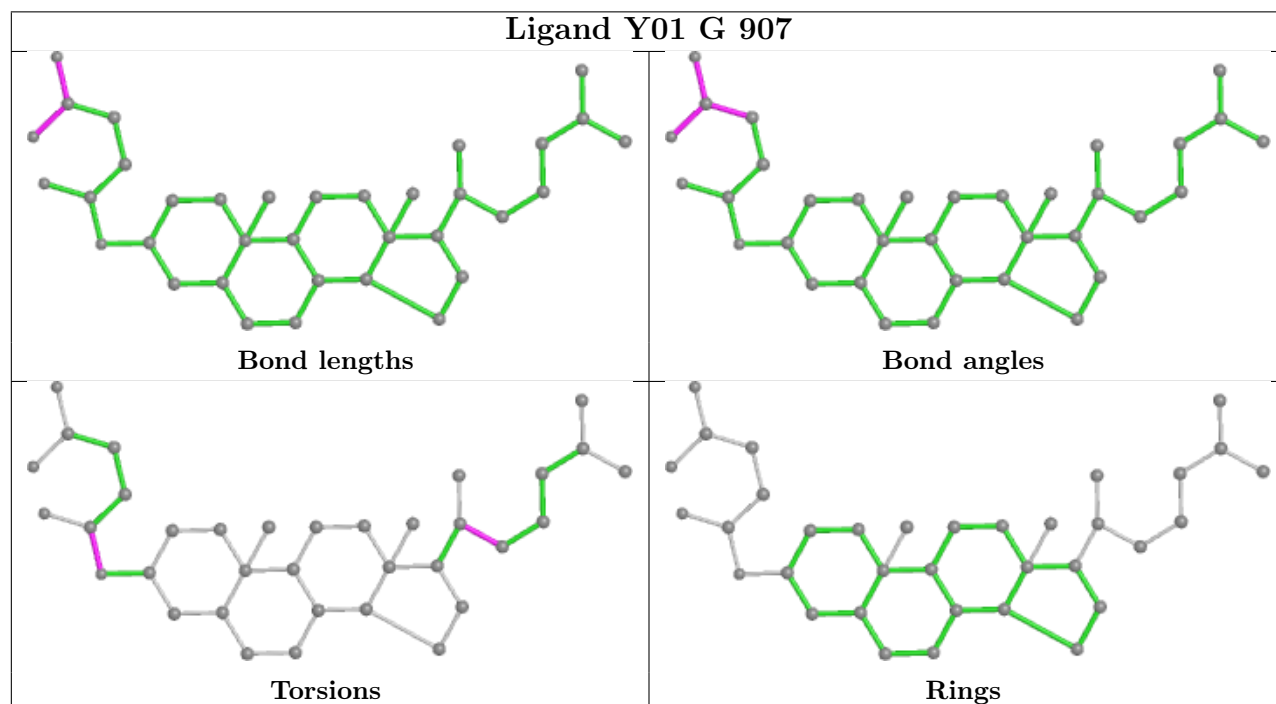
Ligand Y01 U 703



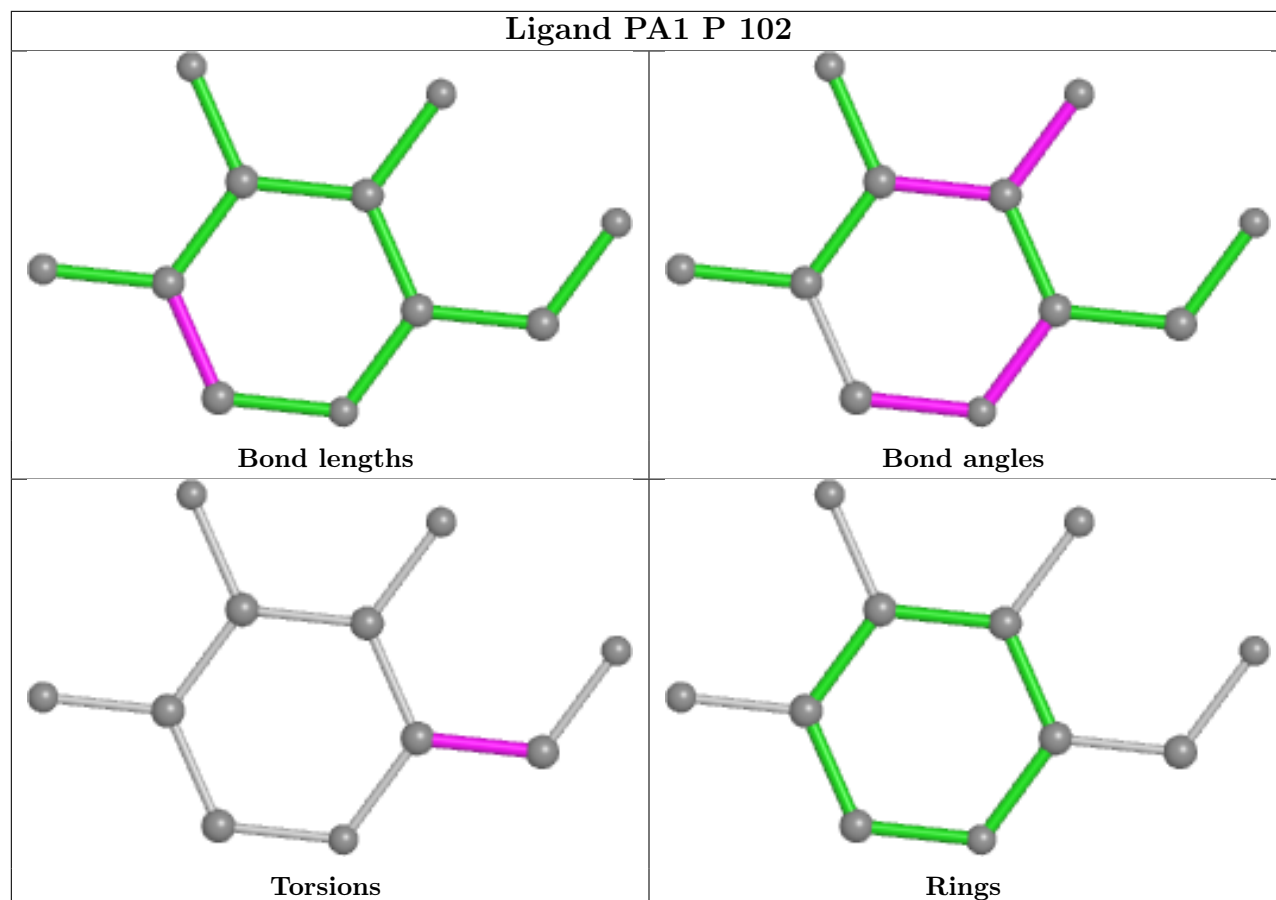
Ligand Y01 G 911



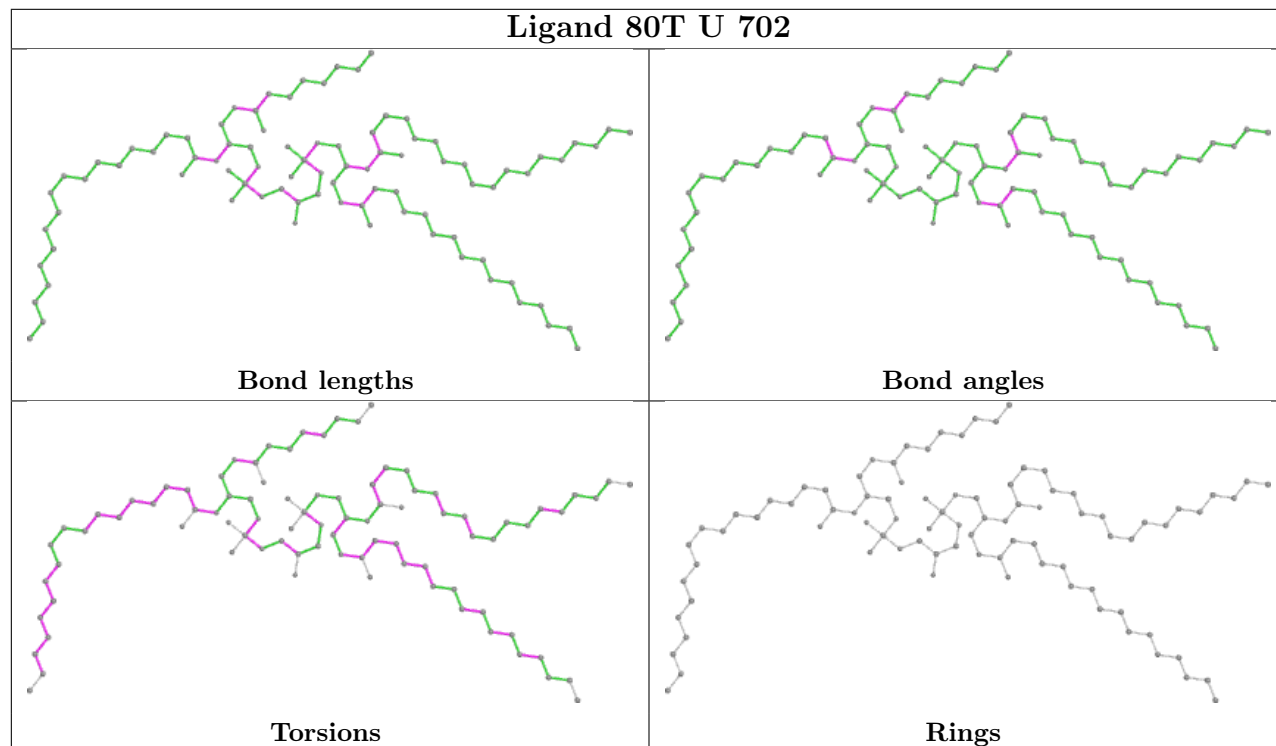
Ligand Y01 G 907

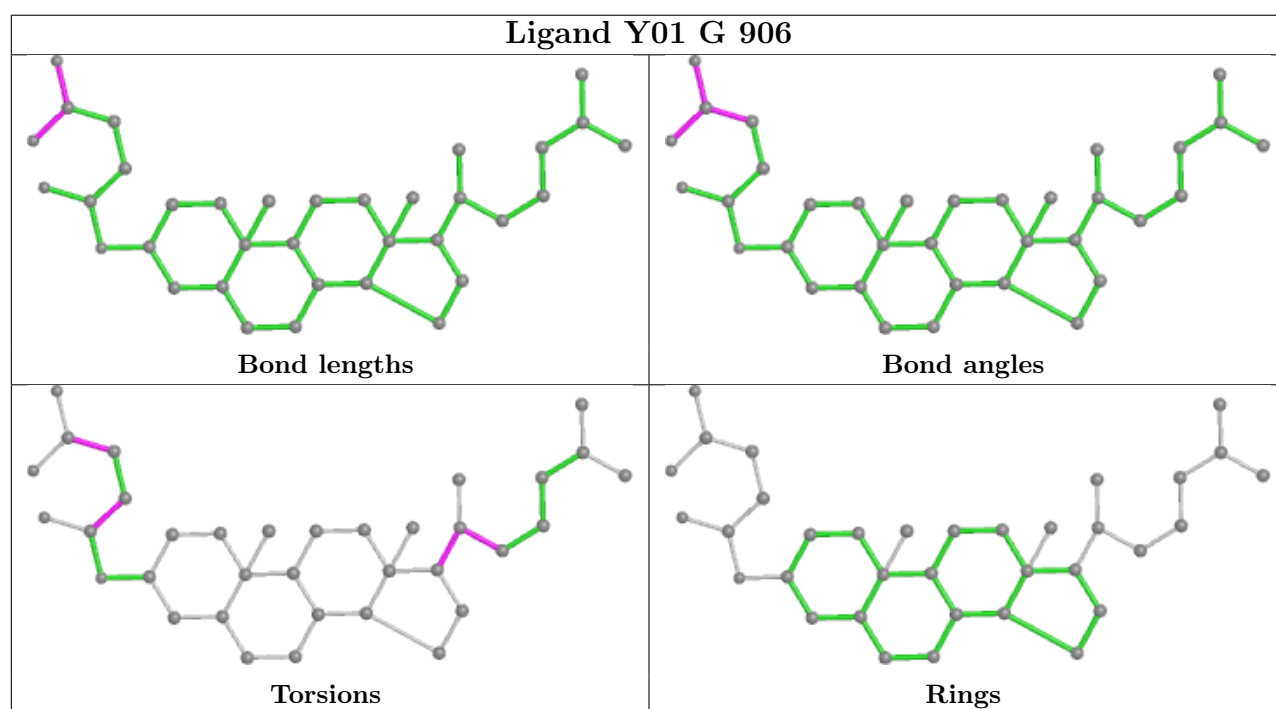
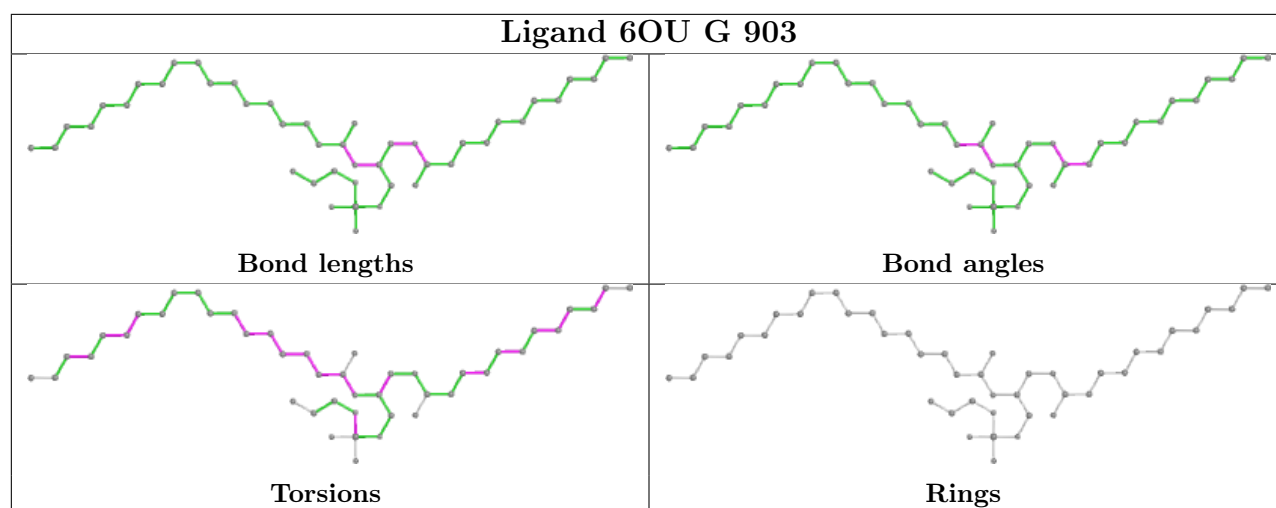


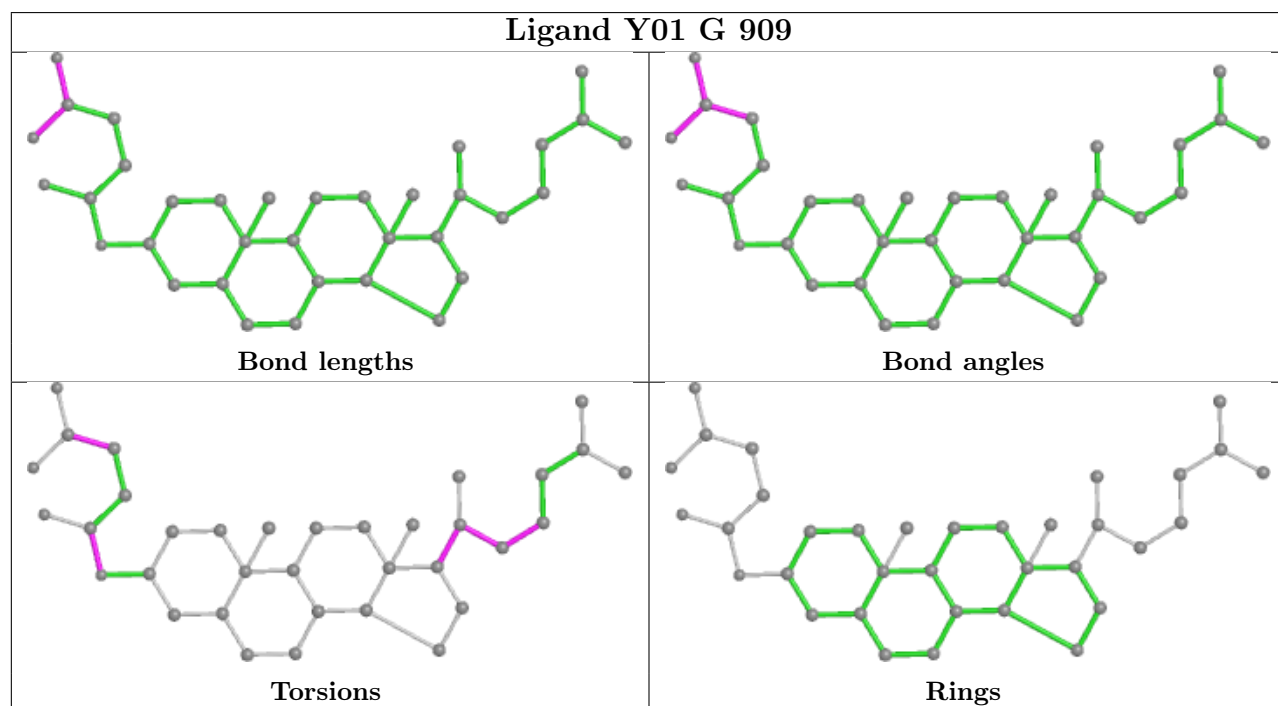
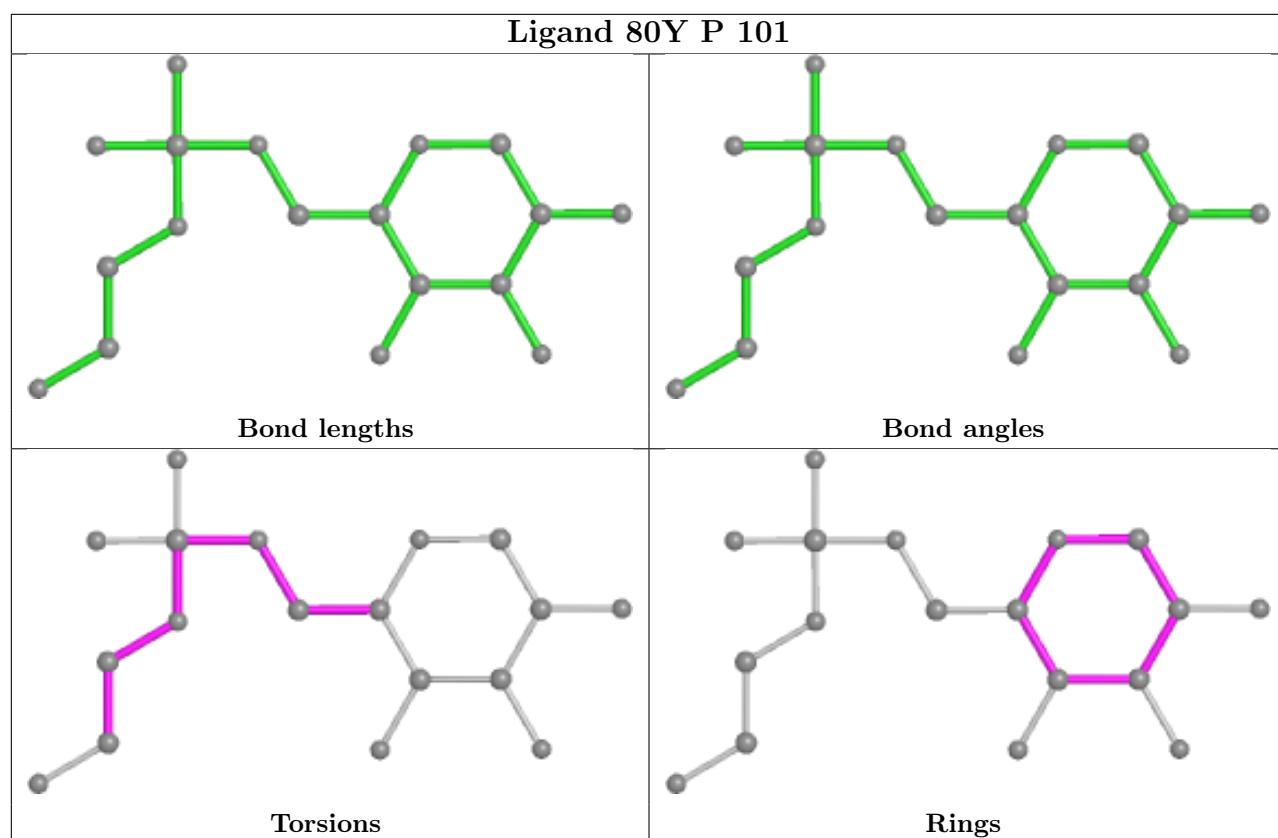
Ligand PA1 P 102

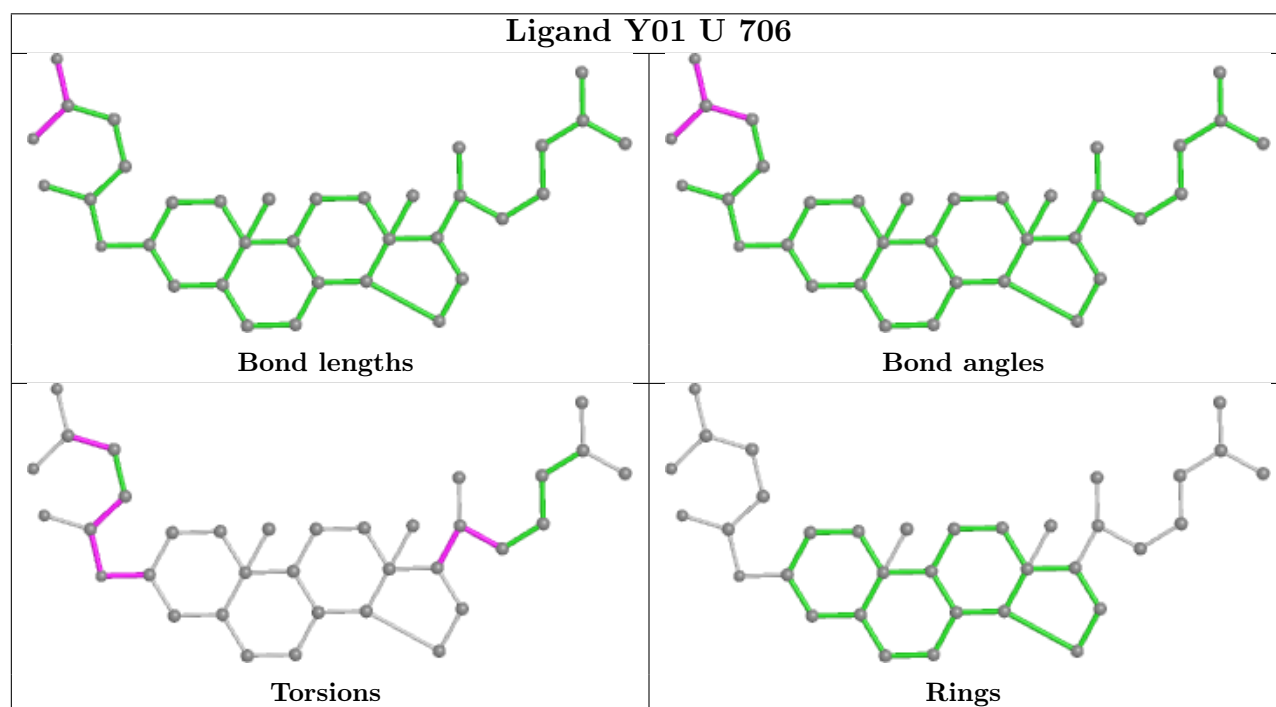
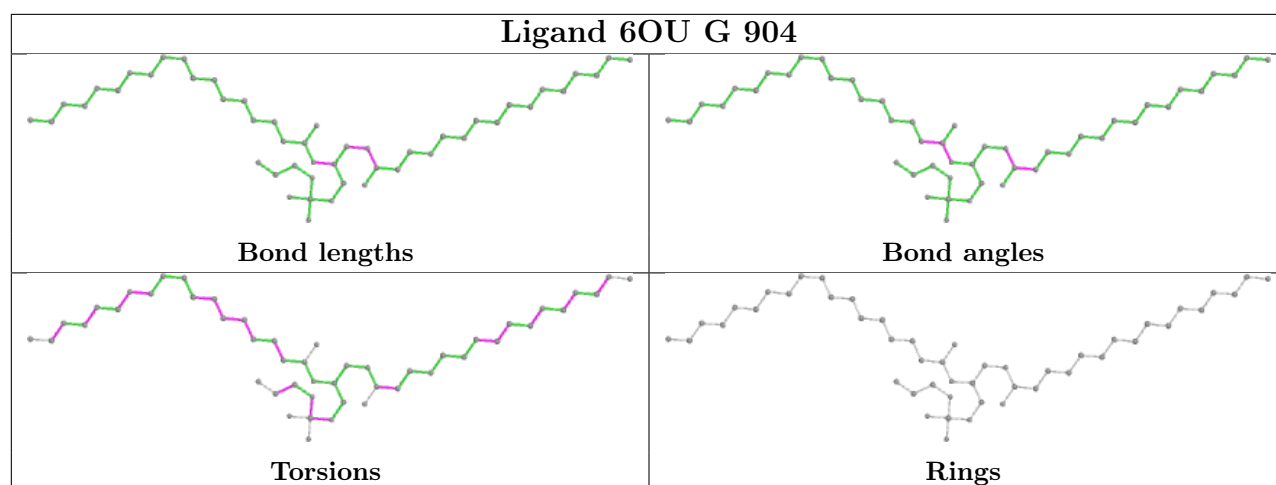


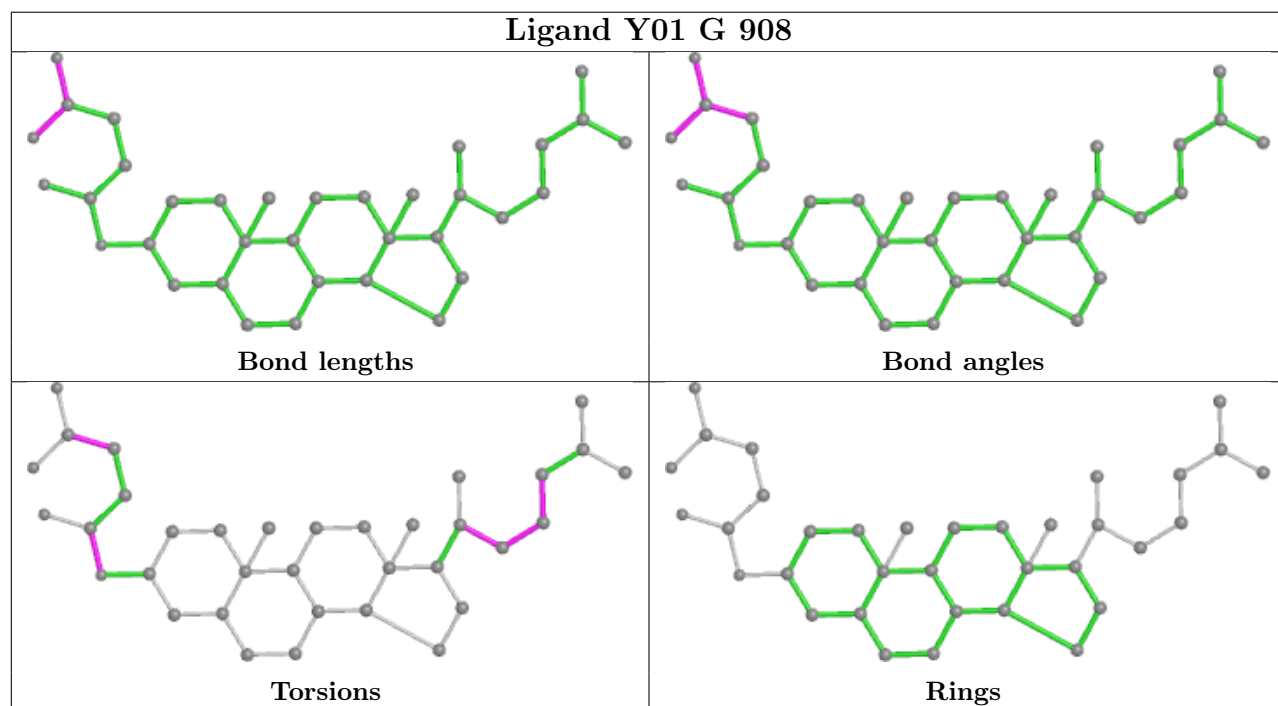
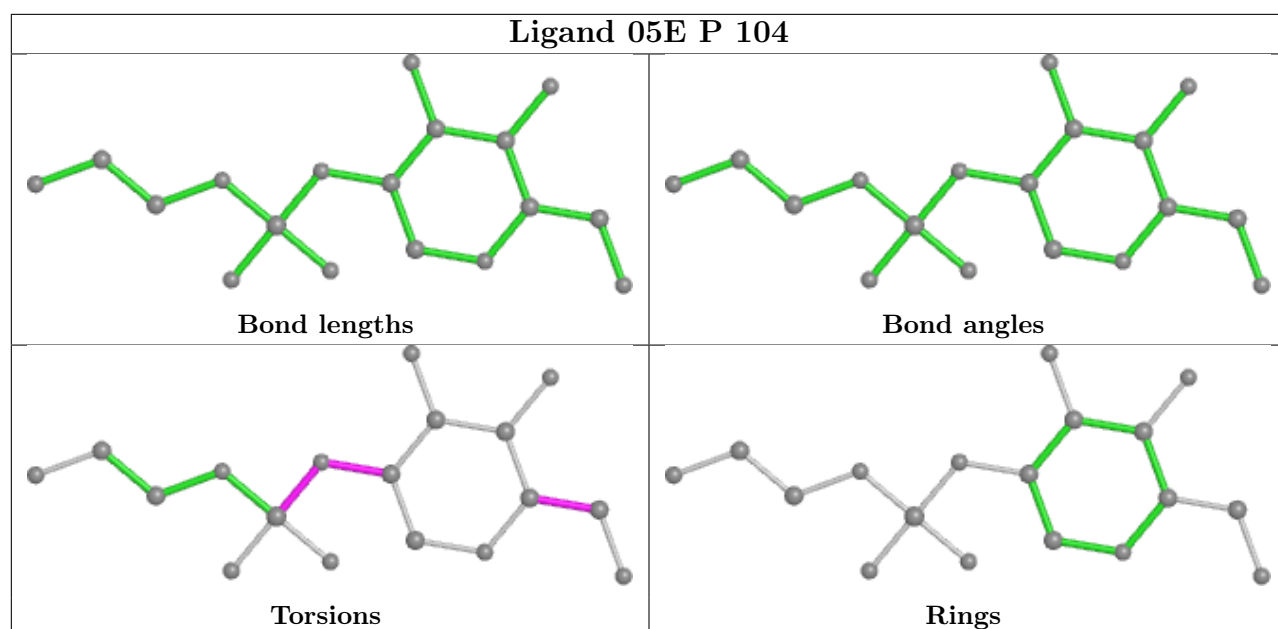
Ligand 80T U 702

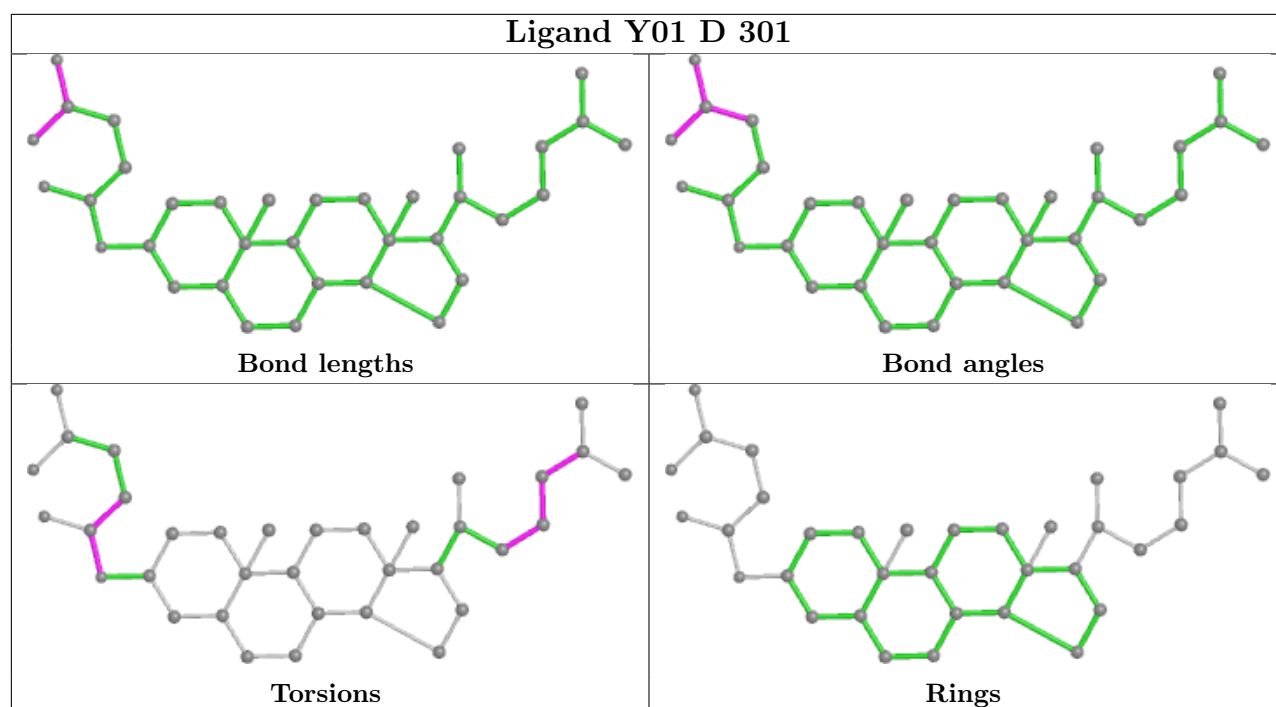












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.