



## Full wwPDB EM Validation Report ⓘ

Apr 27, 2025 – 03:48 AM JST

PDB ID : 9JLN / pdb\_00009jln  
EMDB ID : EMD-61591  
Title : Cryo-EM structure of human TauT in presence of taurine, observed only one sodium ion, determined in an inward-occluded conformation  
Authors : Qu, Q.; Chao, Y.; Zhou, Z.  
Deposited on : 2024-09-19  
Resolution : 2.84 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](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>.

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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 : 4.02b-467  
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) : 2.42

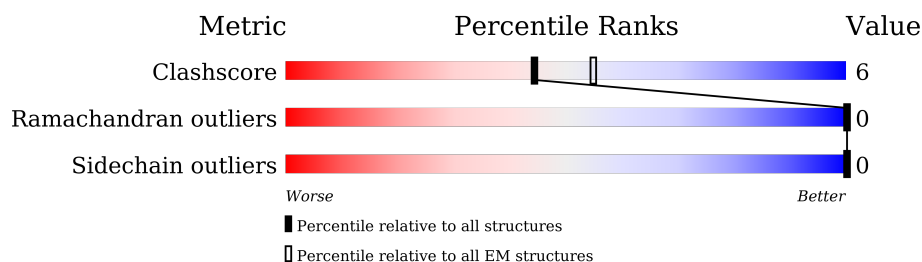
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.84 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	A	606	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4295 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 Sodium- and chloride-dependent taurine transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	521	4139	2779	625	703	32	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	583	SER	-	expression tag	UNP P31641
A	584	ARG	-	expression tag	UNP P31641
A	585	LEU	-	expression tag	UNP P31641
A	586	GLU	-	expression tag	UNP P31641
A	587	GLU	-	expression tag	UNP P31641
A	588	GLU	-	expression tag	UNP P31641
A	589	LEU	-	expression tag	UNP P31641
A	590	ARG	-	expression tag	UNP P31641
A	591	ARG	-	expression tag	UNP P31641
A	592	ARG	-	expression tag	UNP P31641
A	593	THR	-	expression tag	UNP P31641
A	594	GLU	-	expression tag	UNP P31641
A	595	PRO	-	expression tag	UNP P31641
A	596	GLY	-	expression tag	UNP P31641
A	597	LEU	-	expression tag	UNP P31641
A	598	ARG	-	expression tag	UNP P31641
A	599	SER	-	expression tag	UNP P31641
A	600	ARG	-	expression tag	UNP P31641
A	601	LEU	-	expression tag	UNP P31641
A	602	GLU	-	expression tag	UNP P31641
A	603	VAL	-	expression tag	UNP P31641
A	604	LEU	-	expression tag	UNP P31641
A	605	PHE	-	expression tag	UNP P31641
A	606	GLN	-	expression tag	UNP P31641

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

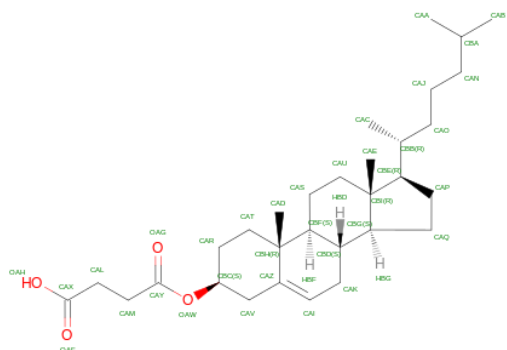
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Na	0
			1	1	

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

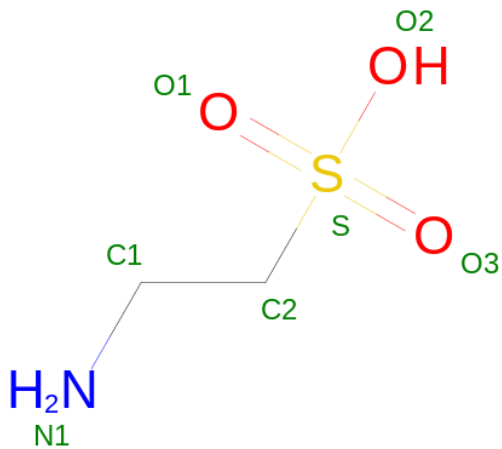
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Cl	0
			1	1	

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>).



Id	Chain	Residues	Atoms			AltConf
5	A	1	Total 35	C 31	O 4	0
5	A	1	Total 35	C 31	O 4	0
5	A	1	Total 35	C 31	O 4	0

- Molecule 6 is 2-AMINOETHANESULFONIC ACID (CCD ID: TAU) (formula:  $\text{C}_2\text{H}_7\text{NO}_3\text{S}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
6	A	1	7	2	1	3	1	0



- Molecule 1: Sodium- and chloride-dependent taurine transporter

V557	P558	L559	Q567	THR	GLU	GLY	GLU	PRO	PHE	LEU	LEU	VAL	ARG	VAL	TYR	LEU	LEU	THR	PRO	SER	ARG	LEU	GLU	GLU	LEU	ARG	ARG	THR	PRO	GLU	PRO	GLY	LEU	ARG	SER	SER	GLY	THR	ARG	THR	ARG	THR	GLY	LEU	GLY	LEU	VAL	LEU	PHE	GLN																																																																																																																																																																																																																																																																																																																																																																																																																								
T347	M351	E354	P367	Y374	G399	L400	D401	S402	Q403	F404	E408	G409	P410	T411	T412	V415	L422	R427	T430	L442	F458	D459	A462	A463	S464	G465	V471	I479	E493	I496	G497	Y498	R499	T512	P513	L551	S552	L555	G556	Y69	L97	I123	L134	M135	V136	Y137	Y138	I139	L142	W166	W167	T168	W183	I184	E197	W202	P213	D219	L220	L224	C231	V246	Y247	F248	T251	A270	I274	T296	Y320	N333	S337	F338	V339	S340	G341	F342	A343	I344	Y69	L97	I123	L134	M135	V136	Y137	Y138	I139	L142	W166	W167	T168	W183	I184	E197	W202	P213	D219	L220	L224	C231	V246	Y247	F248	T251	A270	I274	T296	Y320	N333	S337	F338	V339	S340	G341	F342	A343	I344	Y69	L97	I123	L134	M135	V136	Y137	Y138	I139	L142	W166	W167	T168	W183	I184	E197	W202	P213	D219	L220	L224	C231	V246	Y247	F248	T251	A270	I274	T296	Y320	N333	S337	F338	V339	S340	G341	F342	A343	I344	Y69	L97	I123	L134	M135	V136	Y137	Y138	I139	L142	W166	W167	T168	W183	I184	E197	W202	P213	D219	L220	L224	C231	V246	Y247	F248	T251	A270	I274	T296	Y320	N333	S337	F338	V339	S340	G341	F342	A343	I344	Y69	L97	I123	L134	M135	V136	Y137	Y138	I139	L142	W166	W167	T168	W183	I184	E197	W202	P213	D219	L220	L224	C231	V246	Y247	F248	T251	A270	I274	T296	Y320	N333	S337	F338	V339	S340	G341	F342	A343	I344	Y69	L97	I123	L134	M135	V136	Y137	Y138	I139	L142	W166	W167	T168	W183	I184	E197	W202	P213	D219	L220	L224	C231	V246	Y247	F248	T251	A270	I274	T296	Y320	N333	S337	F338	V339	S340	G341	F342	A343	I344	Y69	L97	I123	L134	M135	V136	Y137	Y138	I139	L142	W166	W167	T168	W183	I184	E197	W202	P213	D219	L220	L224	C231	V246	Y247	F248	T251	A270	I274	T296	Y320	N333	S337	F338	V339	S340	G341	F342	A343	I344	Y69	L97	I123	L134	M135	V136	Y137	Y138	I139	L142	W166	W167	T168	W183	I184	E197	W202	P213	D219	L220	L224	C231	V246	Y247	F248	T251	A270	I274	T296	Y320	N333	S337	F338	V339	S340	G341	F342	A343	I344	Y69	L97	I123	L134	M135	V136	Y137	Y138	I139	L142	W166	W167	T168	W183	I184	E197	W202	P213	D219	L220	L224	C231	V246	Y247	F248	T251	A270	I274	T296	Y320	N333	S337	F338	V339	S340	G341	F342	A343	I344	Y69	L97	I123	L134	M135	V136	Y137	Y138	I139	L142	W166	W167	T168	W183	I184	E197	W202	P213	D219	L220	L224	C231	V246	Y247	F248	T251	A270	I274	T296	Y320	N333	S337	F338	V339	S340	G341	F342	A343	I344	Y69	L97	I123	L134	M135	V136	Y137	Y138	I139	L142	W166	W167	T168	W183	I184	E197	W202	P213	D219	L220	L224	C231	V246	Y247	F248	T251	A270	I274	T296

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96380	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	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: Y01, TAU, CL, NA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/4275	0.44	0/5832

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	A	4139	0	4121	48	0
2	A	42	0	39	0	0
3	A	1	0	0	0	0
4	A	1	0	0	1	0
5	A	105	0	147	8	0
6	A	7	0	7	0	0
All	All	4295	0	4314	53	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 6.

All (53) 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:A:427:ARG:HE	1:A:430:ILE:HD11	1.50	0.74
1:A:63:ASN:ND2	1:A:333:ASN:OD1	2.22	0.72
1:A:68:PRO:HB3	1:A:344:ILE:HG21	1.76	0.68
1:A:65:TRP:NE1	1:A:367:PRO:O	2.30	0.60
1:A:52:LEU:HD23	1:A:246:VAL:HG21	1.82	0.59
1:A:415:VAL:HG23	1:A:422:LEU:HB3	1.83	0.59
1:A:142:LEU:HD21	1:A:399:GLY:HA3	1.87	0.56
1:A:401:ASP:OD1	1:A:402:SER:N	2.37	0.56
1:A:97:LEU:HD21	1:A:479:ILE:HG13	1.88	0.55
1:A:123:ILE:HG23	1:A:471:VAL:HG13	1.88	0.54
1:A:135:ASN:ND2	1:A:410:GLN:OE1	2.40	0.54
1:A:552:SER:HB2	5:A:708:Y01:HAC2	1.90	0.53
1:A:442:LEU:HD21	5:A:706:Y01:HAB3	1.89	0.52
1:A:69:TYR:OH	1:A:459:ASP:OD2	2.26	0.51
1:A:219:ASP:OD1	1:A:220:LEU:N	2.43	0.51
1:A:139:ILE:HG23	1:A:224:LEU:HD11	1.92	0.50
5:A:707:Y01:OAH	5:A:708:Y01:OAH	2.28	0.50
1:A:139:ILE:HG13	1:A:142:LEU:HD12	1.95	0.49
1:A:496:ILE:HG13	1:A:498:TYR:H	1.77	0.49
1:A:458:PHE:O	1:A:462:ALA:HB3	2.14	0.48
1:A:351:MET:HA	1:A:354:GLU:HG2	1.96	0.48
1:A:47:LYS:HG2	1:A:320:TYR:HE1	1.79	0.47
1:A:248:PHE:HA	1:A:251:THR:HG22	1.96	0.47
1:A:464:SER:OG	1:A:465:GLY:N	2.47	0.47
1:A:63:ASN:ND2	1:A:337:SER:OG	2.48	0.46
5:A:707:Y01:HAO2	5:A:707:Y01:HAU2	1.98	0.46
1:A:54:VAL:HG22	1:A:58:PHE:HE2	1.80	0.46
5:A:706:Y01:OAW	5:A:706:Y01:HAD1	2.16	0.46
1:A:213:PRO:HG3	5:A:706:Y01:HAV2	1.98	0.46
1:A:183:TRP:CG	1:A:184:ILE:N	2.83	0.46
1:A:347:ILE:O	1:A:351:MET:HG3	2.16	0.46
1:A:296:THR:HG21	1:A:465:GLY:H	1.81	0.45
1:A:344:ILE:HD11	1:A:374:TYR:CZ	2.52	0.44
1:A:412:THR:HA	1:A:415:VAL:HG12	1.99	0.44
1:A:493:GLU:OE2	1:A:499:ARG:HB2	2.17	0.44
1:A:512:THR:HB	1:A:513:PRO:HD3	1.99	0.44
5:A:706:Y01:HAP1	5:A:706:Y01:HAO2	1.51	0.44
1:A:551:LEU:HD21	1:A:555:LEU:HD13	2.00	0.43
1:A:67:PHE:CD1	4:A:705:CL:CL	3.08	0.43
1:A:338:PHE:CE2	1:A:342:PHE:HE2	2.35	0.43
1:A:231:CYS:HA	1:A:404:PHE:HE1	1.83	0.43
5:A:707:Y01:HAC1	5:A:707:Y01:HAP1	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LEU:HD23	1:A:555:LEU:O	2.18	0.43
1:A:66:ARG:HG3	1:A:69:TYR:HE1	1.84	0.42
1:A:408:GLU:O	1:A:412:THR:HG23	2.19	0.42
1:A:557:VAL:HB	1:A:558:PRO:HD3	2.00	0.42
1:A:555:LEU:HD23	1:A:559:LEU:HG	2.03	0.41
1:A:168:THR:OG1	1:A:197:GLU:OE2	2.36	0.41
1:A:270:ALA:O	1:A:274:ILE:HG12	2.20	0.41
1:A:183:TRP:CE2	1:A:184:ILE:HG13	2.55	0.41
1:A:166:TRP:CD1	1:A:202:ASN:HB2	2.56	0.41
1:A:134:LEU:HA	1:A:137:TYR:CE1	2.55	0.40
1:A:340:SER:O	1:A:344:ILE:HG12	2.21	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	A	519/606 (86%)	503 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/523 (85%)	445 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z  > 2$
2	NAG	A	703	1	14,14,15	0.82	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	A	702	1	14,14,15	0.23	0	17,19,21	0.43	0
5	Y01	A	706	-	38,38,38	0.67	2 (5%)	57,57,57	0.79	2 (3%)
5	Y01	A	707	-	38,38,38	0.19	0	57,57,57	0.40	0
6	TAU	A	709	-	6,6,6	1.84	3 (50%)	6,8,8	2.91	4 (66%)
5	Y01	A	708	-	38,38,38	0.64	2 (5%)	57,57,57	0.62	2 (3%)
2	NAG	A	701	1	14,14,15	0.21	0	17,19,21	0.44	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
2	NAG	A	703	1	-	1/6/23/26	0/1/1/1
2	NAG	A	702	1	-	2/6/23/26	0/1/1/1
5	Y01	A	706	-	-	8/19/77/77	0/4/4/4
5	Y01	A	707	-	-	10/19/77/77	0/4/4/4
6	TAU	A	709	-	-	0/4/4/4	-
5	Y01	A	708	-	-	3/19/77/77	0/4/4/4
2	NAG	A	701	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	709	TAU	C2-S	3.16	1.82	1.77
5	A	706	Y01	OAF-CAX	2.76	1.31	1.22
5	A	708	Y01	OAF-CAX	2.72	1.31	1.22
2	A	703	NAG	O5-C1	2.68	1.48	1.43
5	A	708	Y01	OAH-CAX	-2.65	1.21	1.30
5	A	706	Y01	OAH-CAX	-2.63	1.21	1.30
6	A	709	TAU	O3-S	2.13	1.51	1.45
6	A	709	TAU	O1-S	2.11	1.51	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	709	TAU	O2-S-O1	-4.20	101.02	111.27
2	A	703	NAG	C1-O5-C5	3.77	117.30	112.19
6	A	709	TAU	O1-S-C2	3.54	111.17	106.92
6	A	709	TAU	O2-S-C2	3.50	111.42	105.77
5	A	708	Y01	OAF-CAX-CAL	-3.04	113.32	123.08
5	A	706	Y01	OAF-CAX-CAL	-3.02	113.39	123.08
5	A	708	Y01	OAH-CAX-CAL	2.84	123.15	114.03
6	A	709	TAU	O3-S-C2	2.83	110.32	106.92
5	A	706	Y01	OAH-CAX-CAL	2.82	123.11	114.03

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	706	Y01	OAG-CAY-OAW-CBC
5	A	707	Y01	CAO-CBB-CBE-CBI
5	A	707	Y01	CAM-CAY-OAW-CBC
5	A	707	Y01	OAG-CAY-OAW-CBC
5	A	706	Y01	CAM-CAY-OAW-CBC
5	A	706	Y01	CAJ-CAO-CBB-CAC
5	A	707	Y01	CAO-CBB-CBE-CAP
5	A	706	Y01	CAJ-CAO-CBB-CBE
5	A	707	Y01	CAJ-CAO-CBB-CAC
2	A	702	NAG	C4-C5-C6-O6
5	A	707	Y01	CAC-CBB-CBE-CAP
5	A	706	Y01	CAC-CBB-CBE-CAP
5	A	706	Y01	CAO-CBB-CBE-CBI
5	A	706	Y01	CAC-CBB-CBE-CBI
5	A	707	Y01	CAC-CBB-CBE-CBI
2	A	701	NAG	O5-C5-C6-O6
2	A	702	NAG	O5-C5-C6-O6
5	A	706	Y01	CAO-CBB-CBE-CAP
2	A	703	NAG	O5-C5-C6-O6
5	A	708	Y01	CAM-CAL-CAX-OAH
5	A	708	Y01	CAM-CAL-CAX-OAF
2	A	701	NAG	C4-C5-C6-O6
5	A	708	Y01	CAL-CAM-CAY-OAW
5	A	707	Y01	CAM-CAL-CAX-OAH
5	A	707	Y01	CAM-CAL-CAX-OAF
5	A	707	Y01	CAN-CAJ-CAO-CBB

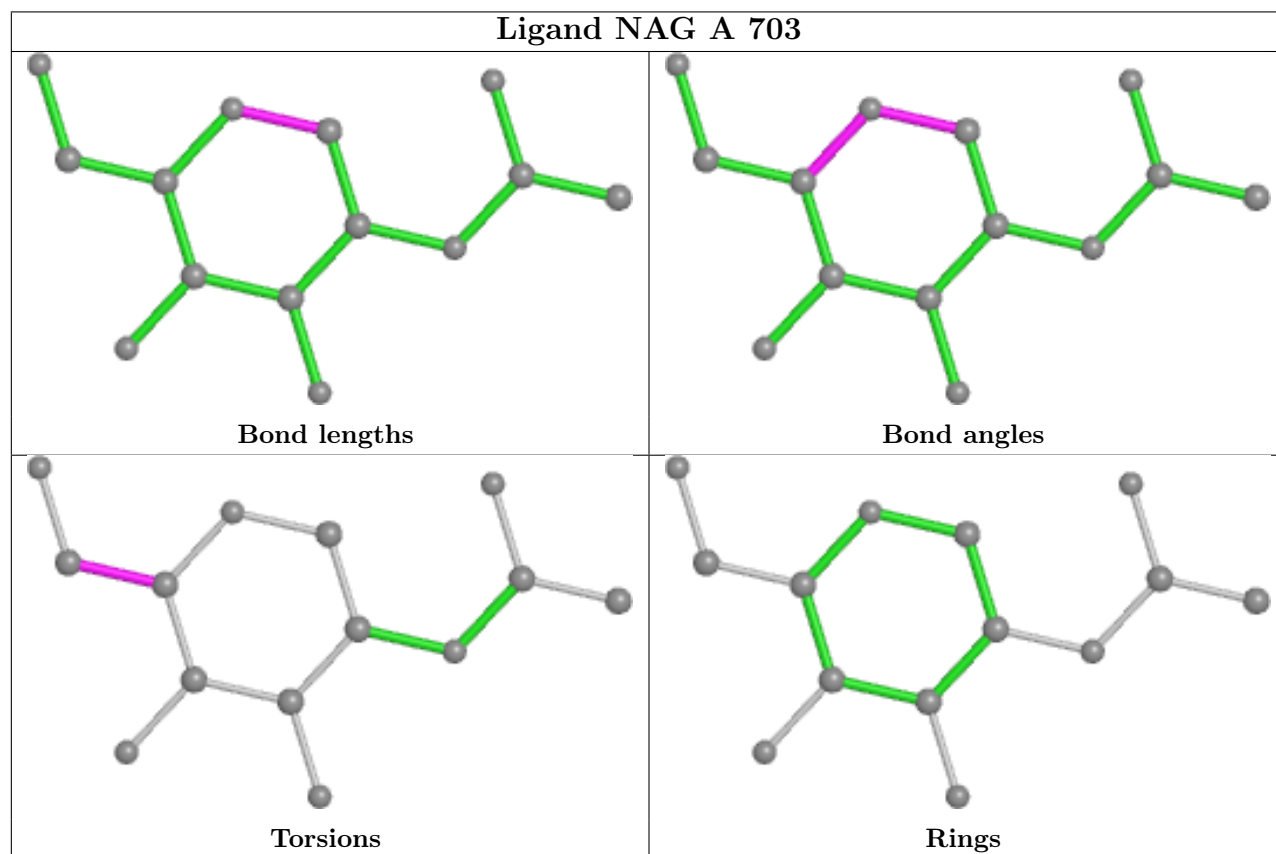
There are no ring outliers.

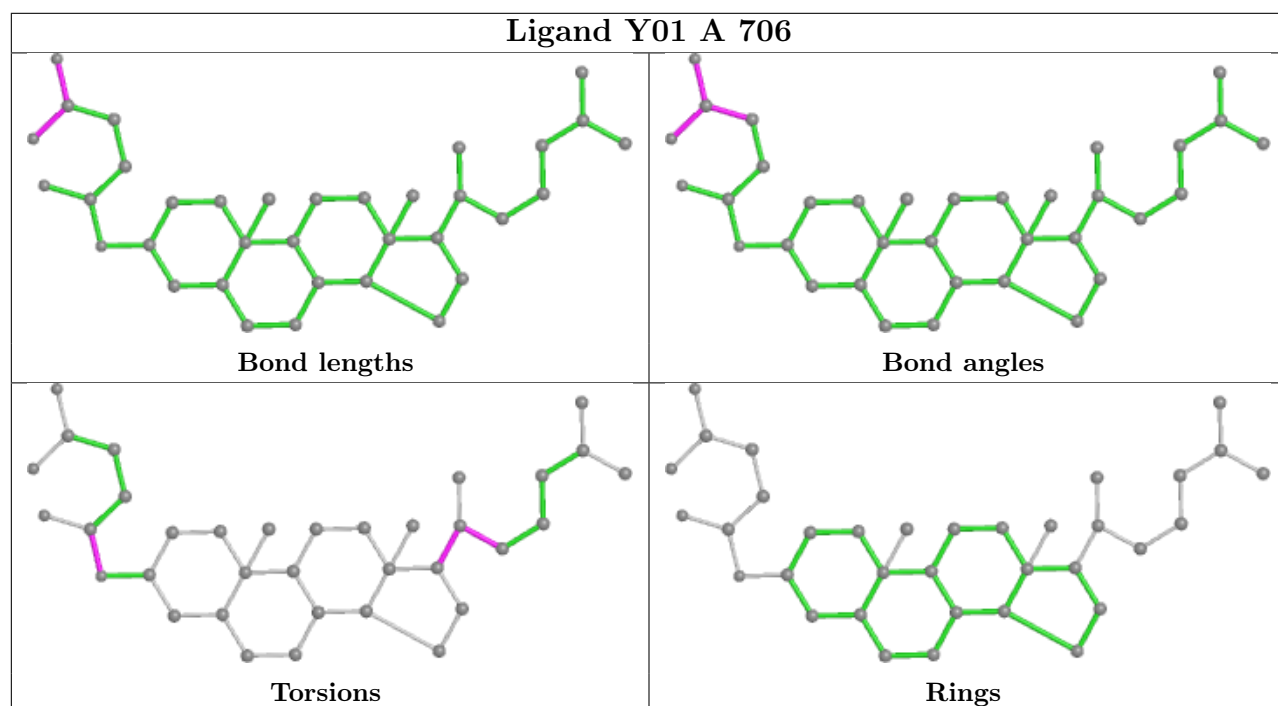
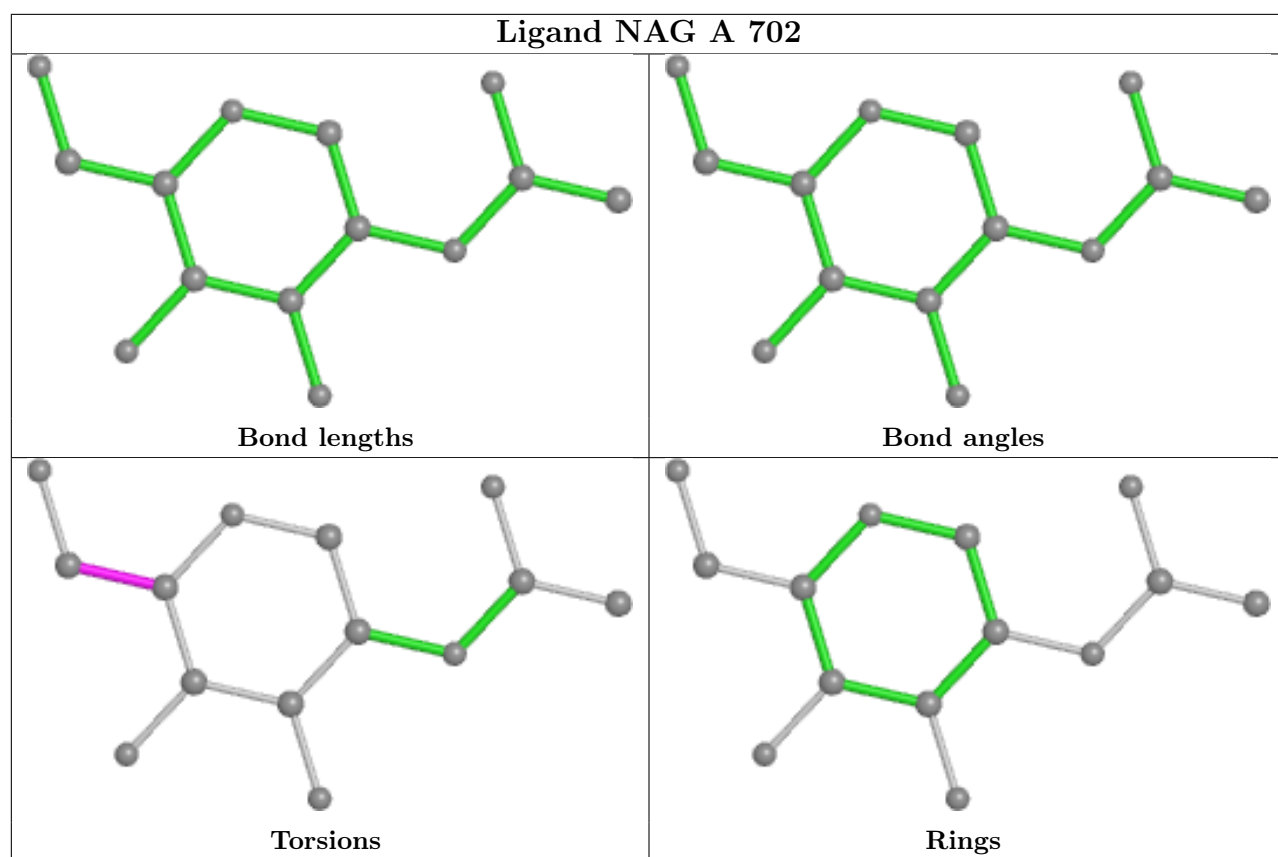
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	706	Y01	4	0
5	A	707	Y01	3	0
5	A	708	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

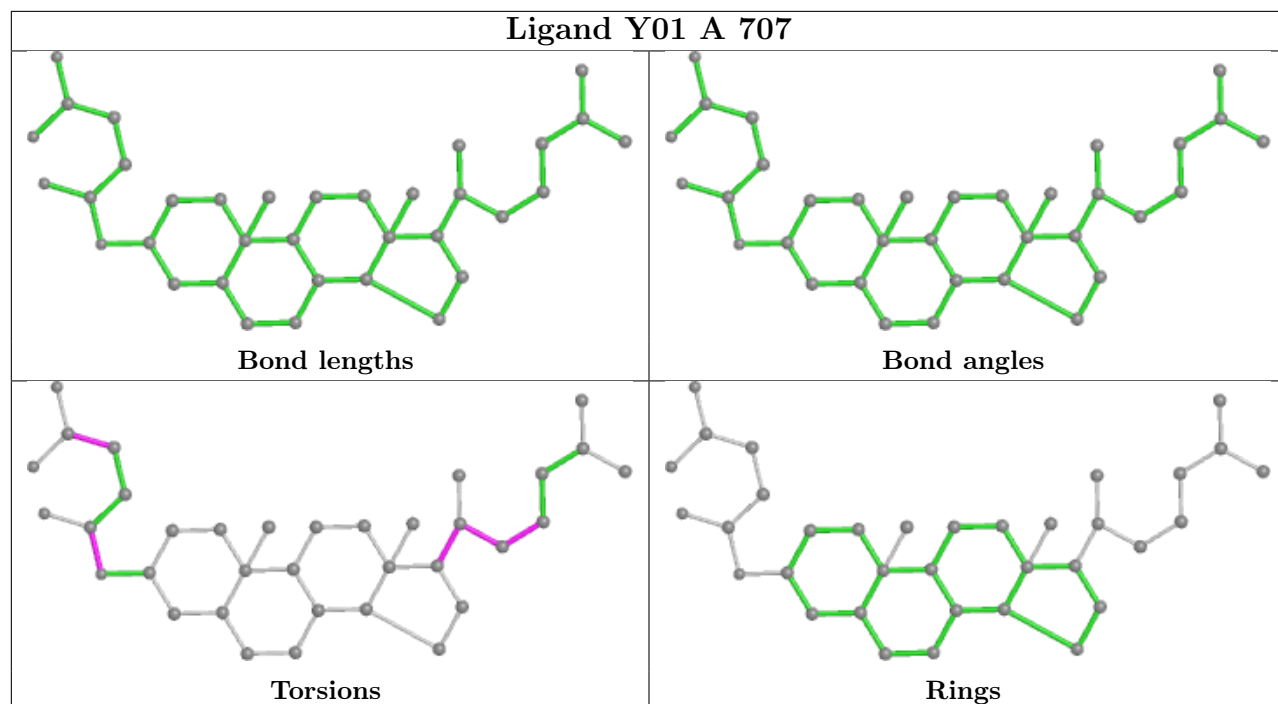
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



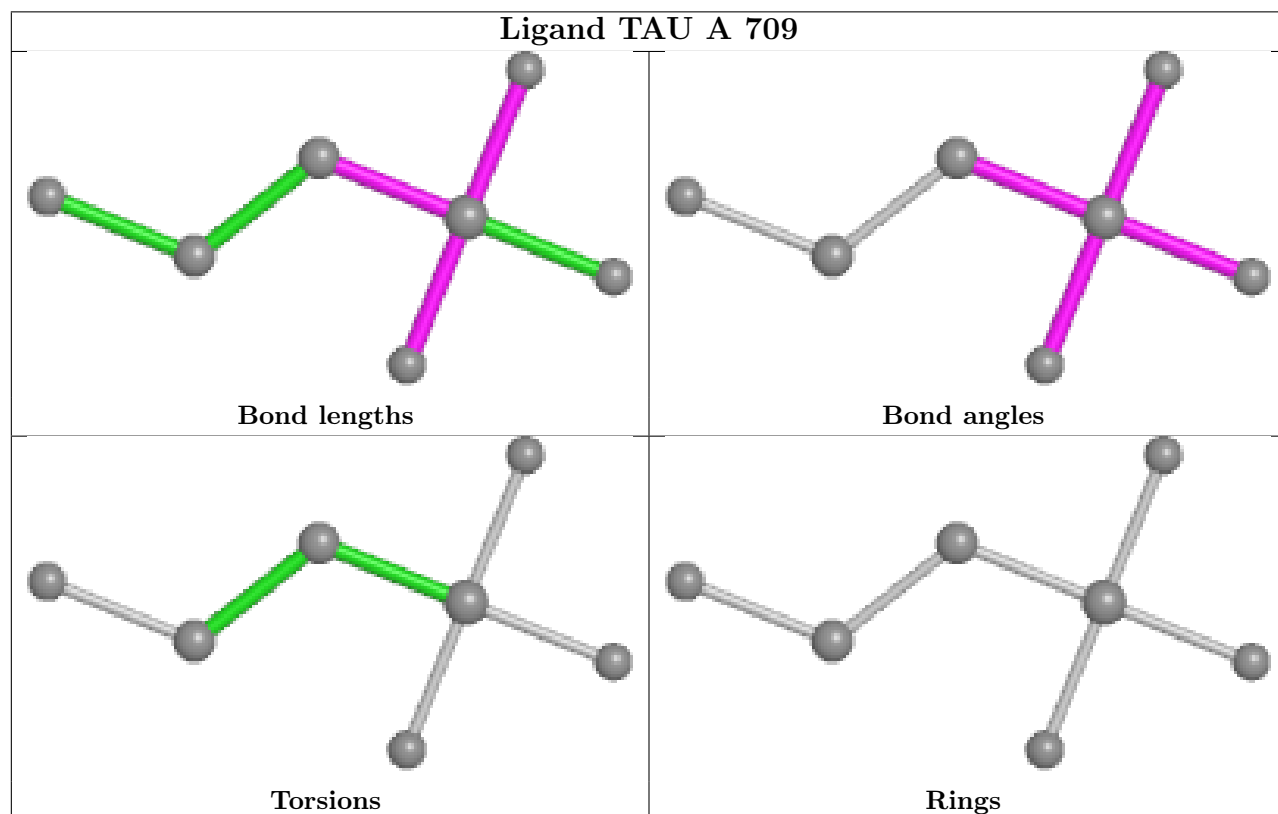


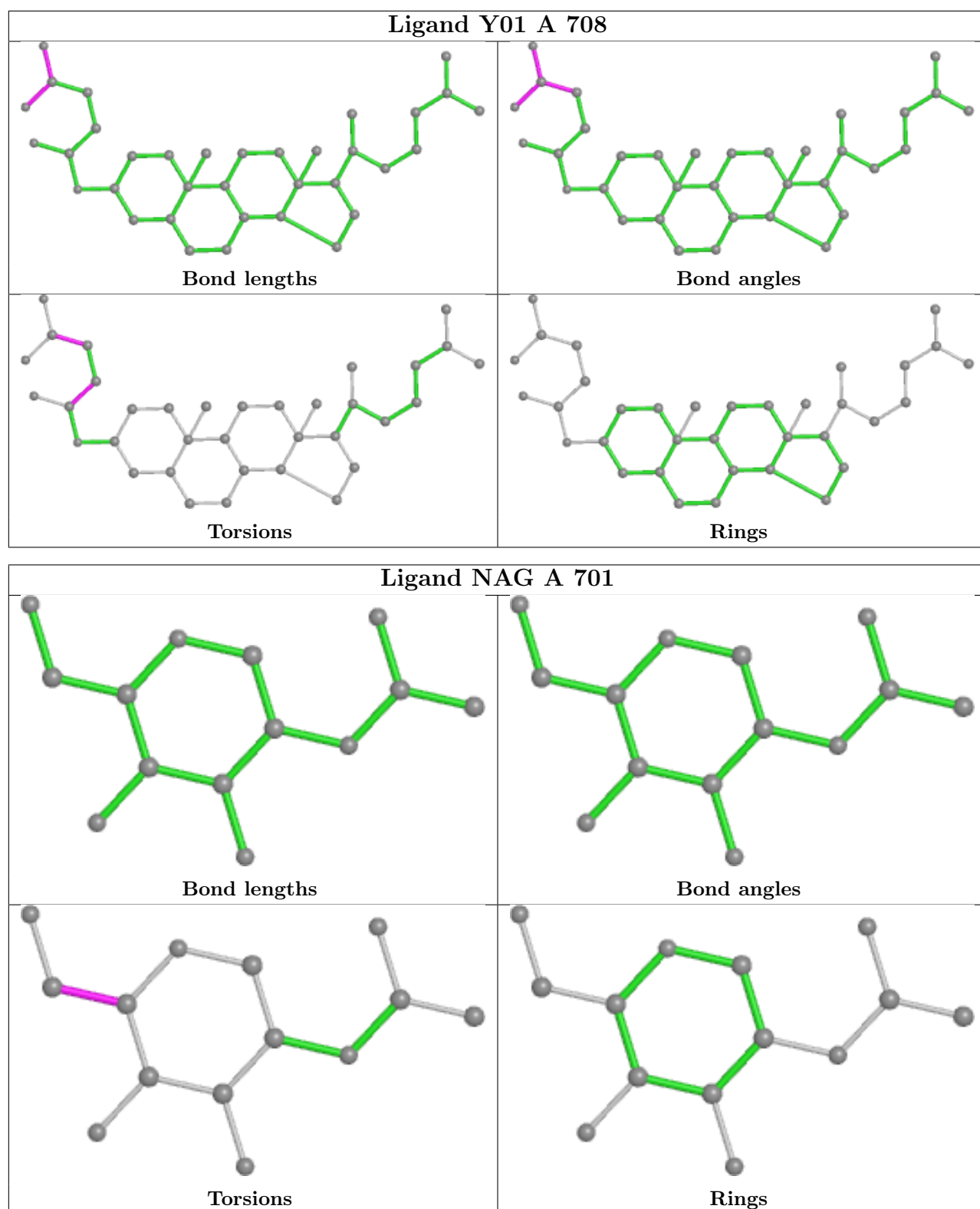


## Ligand Y01 A 707



## Ligand TAU A 709





## 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.