



# wwPDB EM Validation Summary Report ⓘ

May 26, 2024 – 03:28 AM EDT

PDB ID : 7RS5  
EMDB ID : EMD-24666  
Title : Cryo-EM structure of Kip3 (AMPPNP) bound to Taxol-Stabilized Microtubules  
Authors : Hernandez-Lopez, R.A.; Leschziner, A.E.; Arellano-Santoyo, H.; Pellman, D.; Stokasimov, E.; Wang, R.Y.-R.  
Deposited on : 2021-08-10  
Resolution : 3.90 Å (reported)  
Based on initial models : 4FRZ, 3JAT

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

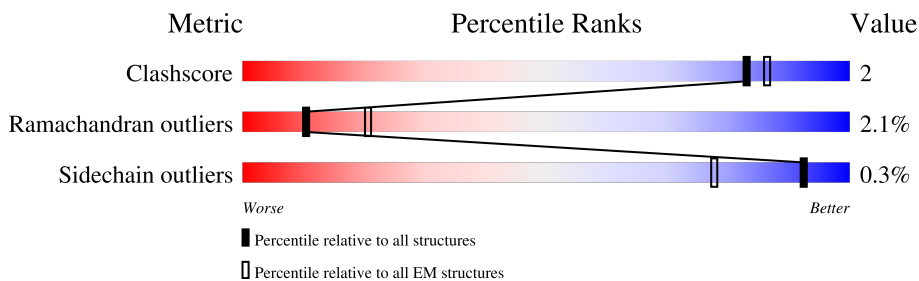
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
1	E	451	
1	G	451	
1	I	451	
1	L	451	
1	N	451	
1	P	451	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	R	451	78% 89% 5% 5%
2	B	445	89% 6% .
2	D	445	90% 5% .
2	F	445	90% 5% . .
2	H	445	37% 89% 6% .
2	J	445	89% 6% .
2	M	445	60% 90% 5% . .
2	O	445	90% 5% .
2	Q	445	17% 90% 5% .
2	S	445	90% 5% . .
3	K	355	33% 91% 6% . .
3	a	355	30% 95% . .
3	b	355	36% 95% . .
3	c	355	39% 95% . .
3	d	355	40% 95% . .
3	e	355	51% 95% . .
3	f	355	40% 95% . .
3	g	355	30% 95% . .
3	h	355	46% 95% . .

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 169884 atoms, of which 83763 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 Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	427	6594	2118	3251	569	635	21	0	0
1	C	427	6594	2118	3251	569	635	21	0	0
1	E	427	6594	2118	3251	569	635	21	0	0
1	G	427	6594	2118	3251	569	635	21	0	0
1	I	427	6594	2118	3251	569	635	21	0	0
1	L	427	6594	2118	3251	569	635	21	0	0
1	N	427	6594	2118	3251	569	635	21	0	0
1	P	427	6594	2118	3251	569	635	21	0	0
1	R	427	6594	2118	3251	569	635	21	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	conflict	UNP P02550
C	265	GLY	ALA	conflict	UNP P02550
E	265	GLY	ALA	conflict	UNP P02550
G	265	GLY	ALA	conflict	UNP P02550
I	265	GLY	ALA	conflict	UNP P02550
L	265	GLY	ALA	conflict	UNP P02550
N	265	GLY	ALA	conflict	UNP P02550
P	265	GLY	ALA	conflict	UNP P02550
R	265	GLY	ALA	conflict	UNP P02550

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	426	6581	2105	3230	575	646	25	0	0
2	D	426	6581	2105	3230	575	646	25	0	0
2	F	426	6581	2105	3230	575	646	25	0	0
2	H	426	6581	2105	3230	575	646	25	0	0
2	J	426	6581	2105	3230	575	646	25	0	0
2	M	426	6581	2105	3230	575	646	25	0	0
2	O	426	6581	2105	3230	575	646	25	0	0
2	Q	426	6581	2105	3230	575	646	25	0	0
2	S	426	6581	2105	3230	575	646	25	0	0

- Molecule 3 is a protein called yeast kinesin-8/ Kip3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	K	346	5458	1692	2738	490	525	13	0	0
3	a	346	5458	1692	2738	490	525	13	0	0
3	b	346	5458	1692	2738	490	525	13	0	0
3	c	346	5458	1692	2738	490	525	13	0	0
3	d	346	5458	1692	2738	490	525	13	0	0
3	e	346	5458	1692	2738	490	525	13	0	0
3	f	346	5458	1692	2738	490	525	13	0	0
3	g	346	5458	1692	2738	490	525	13	0	0
3	h	346	5458	1692	2738	490	525	13	0	0

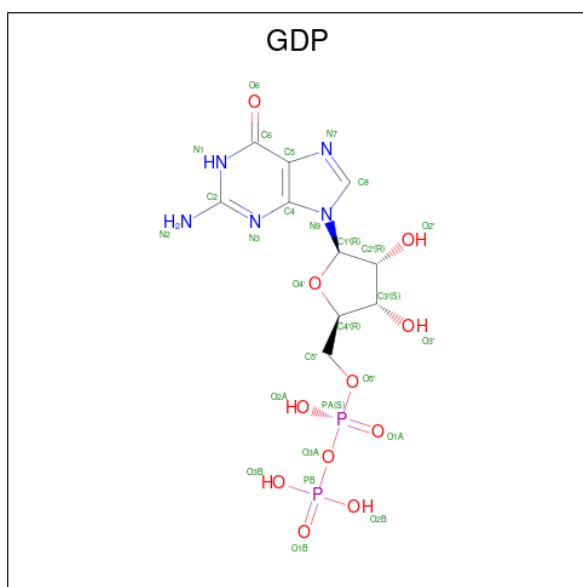
- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total 1	Mg 1	0
5	a	1	Total 1	Mg 1	0
5	E	1	Total 1	Mg 1	0
5	b	1	Total 1	Mg 1	0
5	G	1	Total 1	Mg 1	0
5	c	1	Total 1	Mg 1	0
5	I	1	Total 1	Mg 1	0
5	d	1	Total 1	Mg 1	0
5	L	1	Total 1	Mg 1	0
5	e	1	Total 1	Mg 1	0
5	N	1	Total 1	Mg 1	0
5	f	1	Total 1	Mg 1	0
5	P	1	Total 1	Mg 1	0
5	g	1	Total 1	Mg 1	0
5	R	1	Total 1	Mg 1	0
5	h	1	Total 1	Mg 1	0

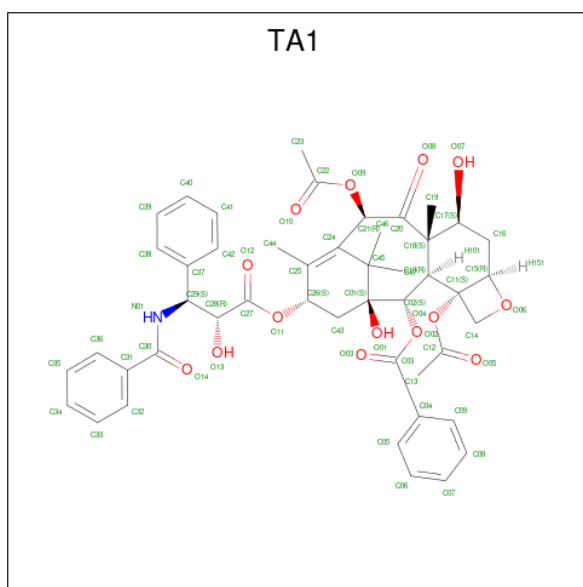
- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
6	B	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	
6	D	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	
6	F	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	
6	H	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	
6	J	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	
6	M	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	
6	O	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	
6	Q	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	
6	S	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	

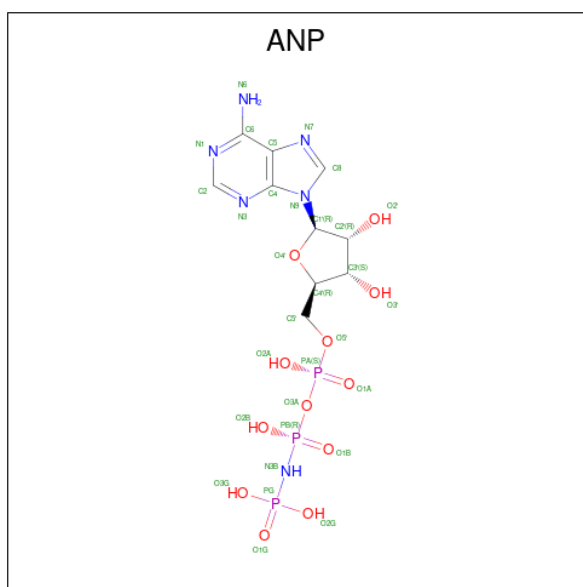
- Molecule 7 is TAXOL (three-letter code: TA1) (formula: C<sub>47</sub>H<sub>51</sub>NO<sub>14</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				AltConf	
			Total	C	H	N		O
7	B	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	D	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	F	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	H	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	J	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	M	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	O	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	Q	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	S	1	Total	C	H	N	O	0
			113	47	51	1	14	

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ) (labeled as "Ligand of Interest" by depositor).

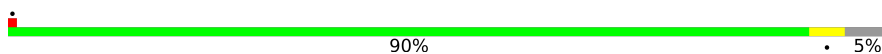


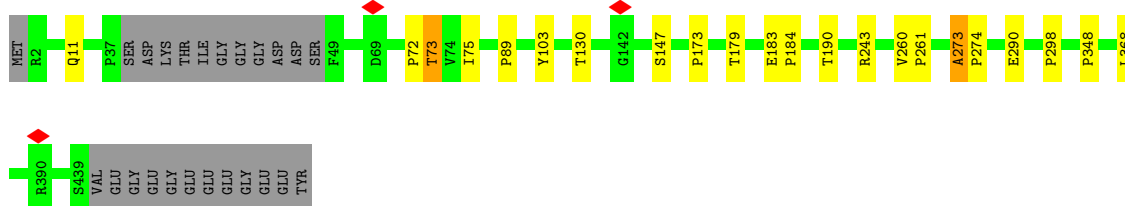
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
8	K	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
8	a	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
8	b	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
8	c	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
8	d	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
8	e	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
8	f	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
8	g	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
8	h	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

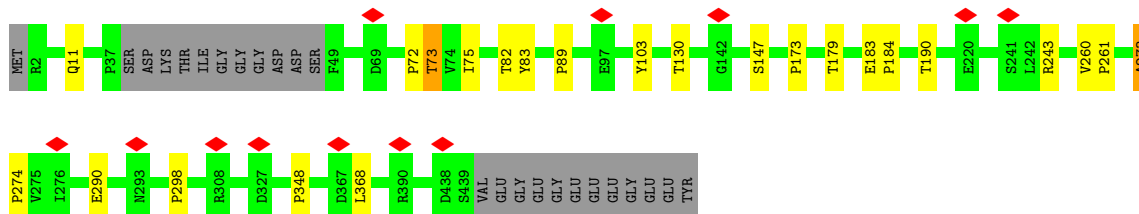
- Molecule 1: Tubulin alpha-1A chain

Chain A:  90% 5%



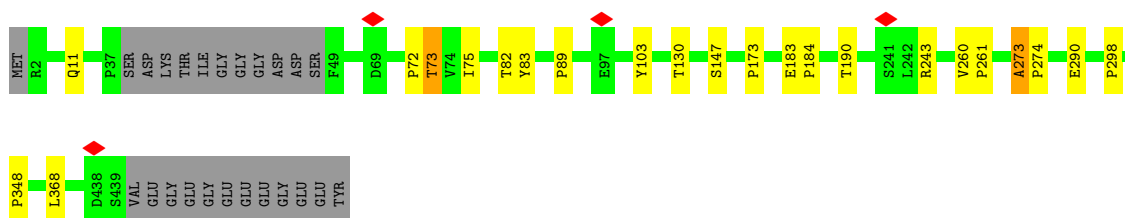
- Molecule 1: Tubulin alpha-1A chain

Chain C:  89% 5% 5%

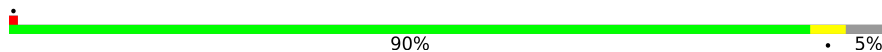


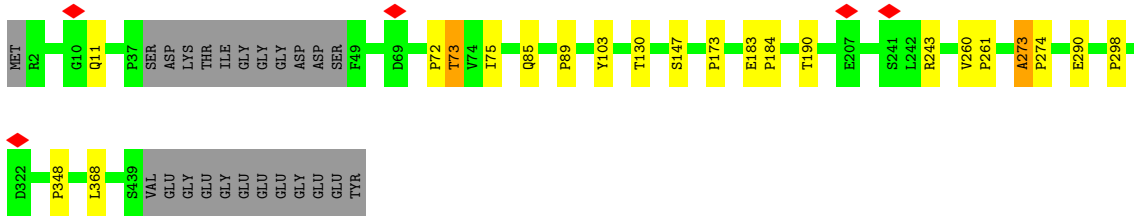
- Molecule 1: Tubulin alpha-1A chain

Chain E:  90% 5% 5%

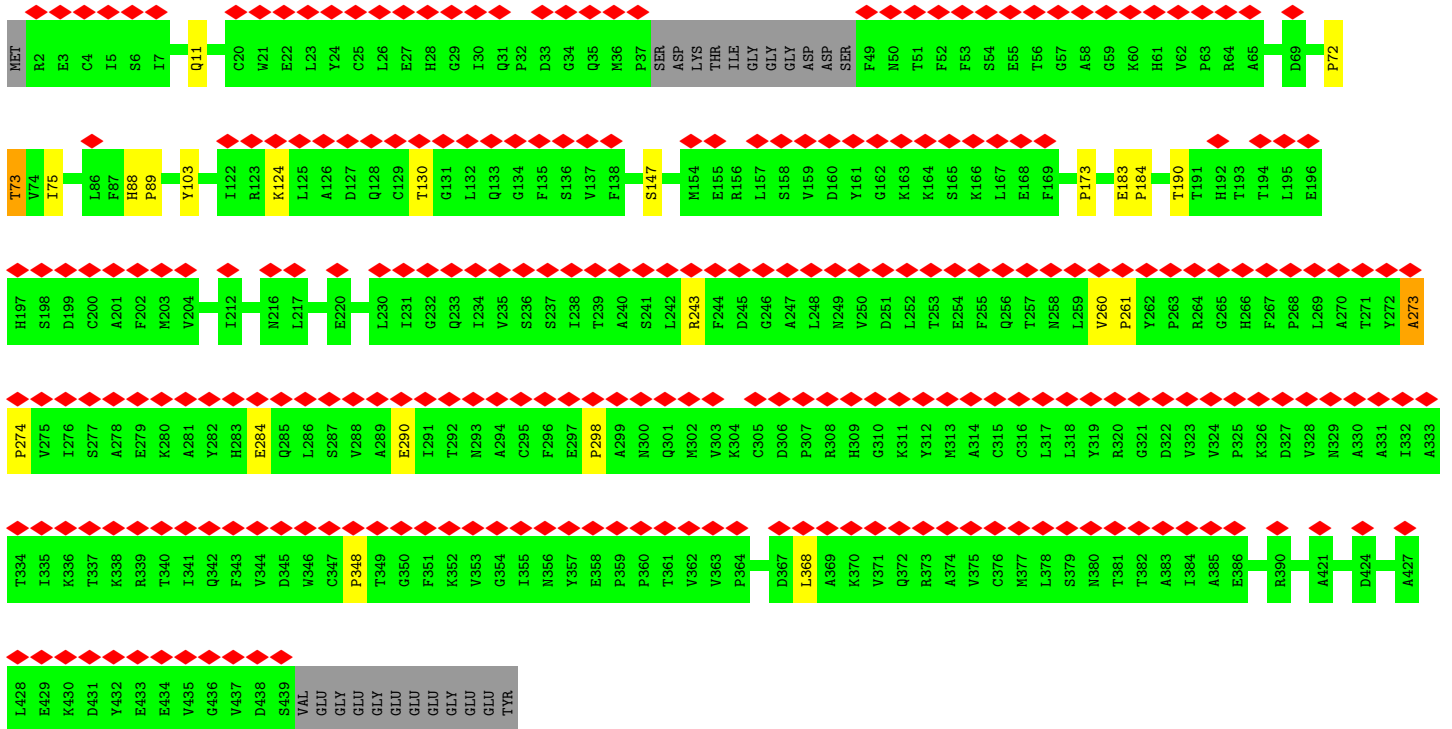
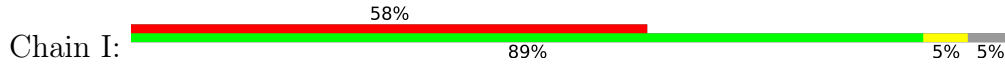


- Molecule 1: Tubulin alpha-1A chain

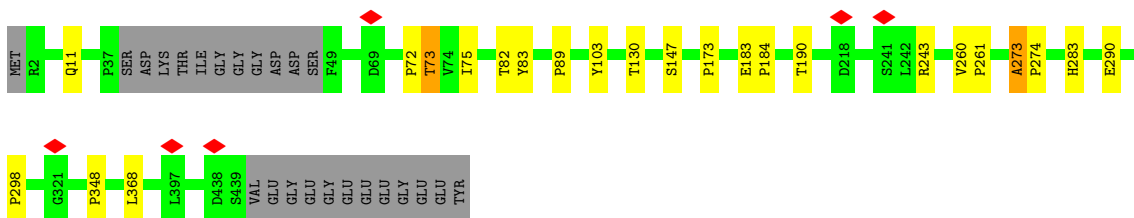
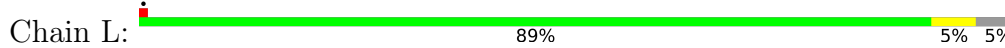
Chain G:  90% 5%



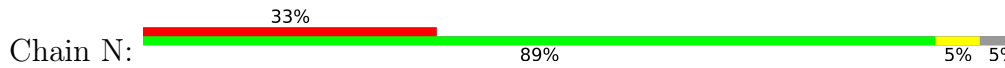
• Molecule 1: Tubulin alpha-1A chain

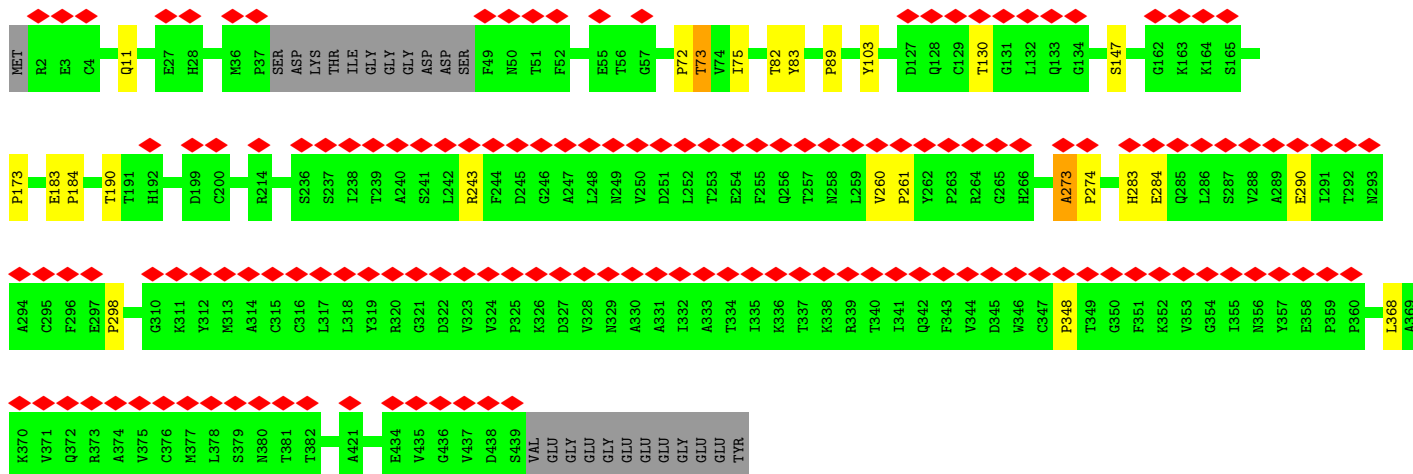


• Molecule 1: Tubulin alpha-1A chain

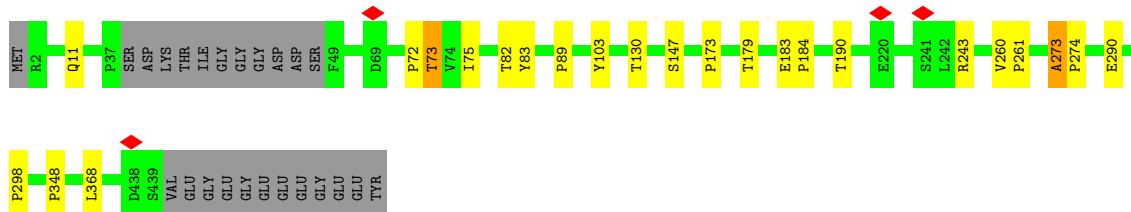
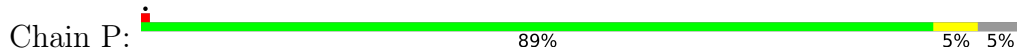


• Molecule 1: Tubulin alpha-1A chain

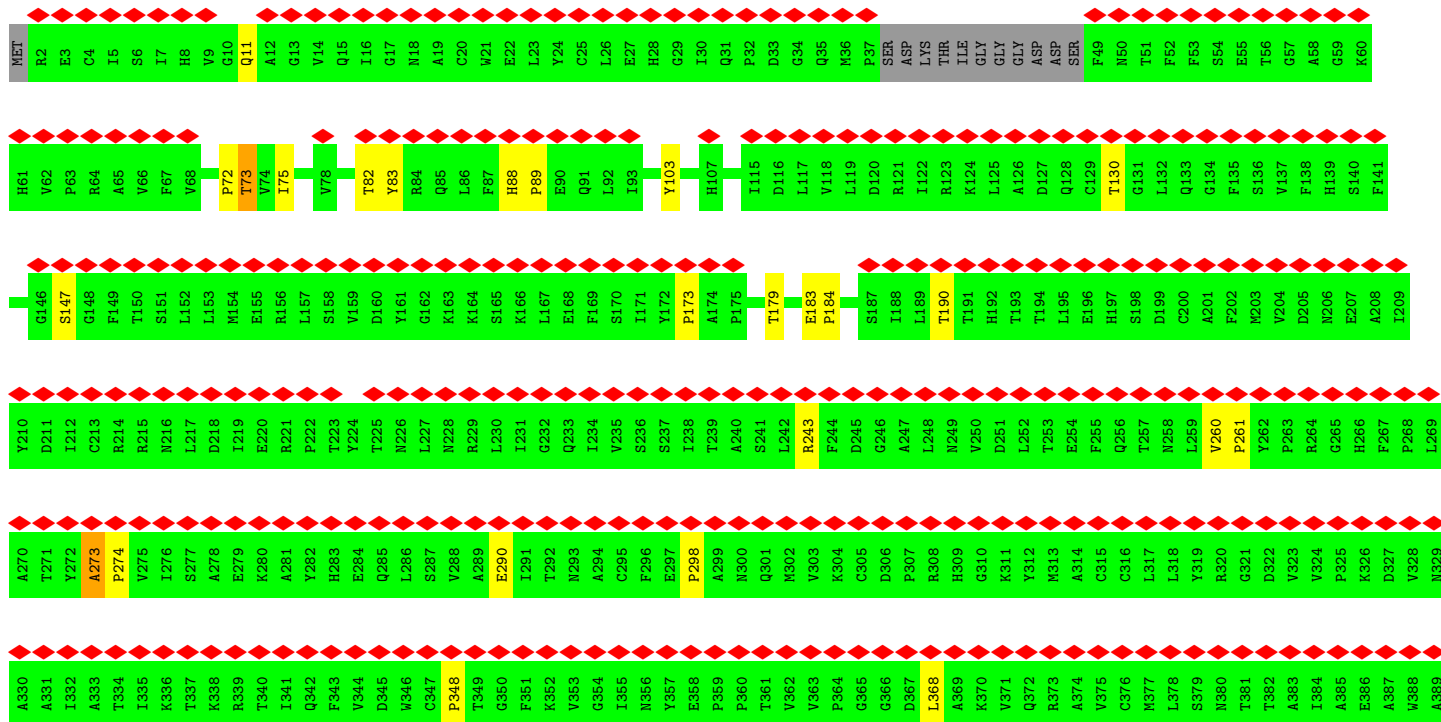
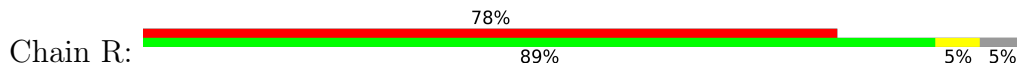




• Molecule 1: Tubulin alpha-1A chain

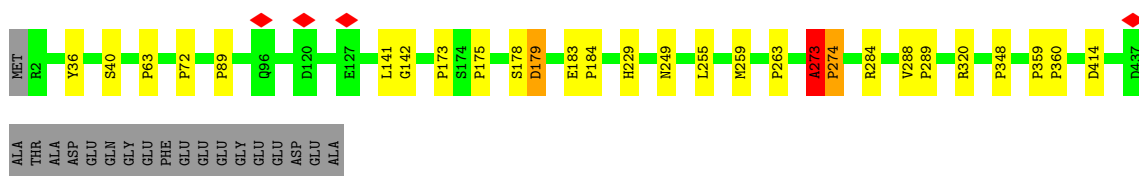
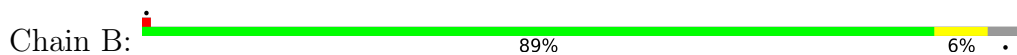


• Molecule 1: Tubulin alpha-1A chain

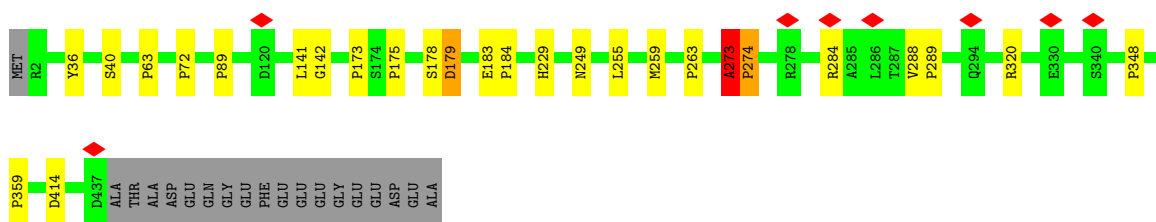
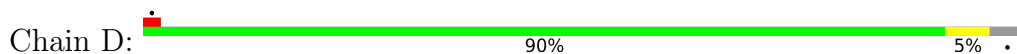




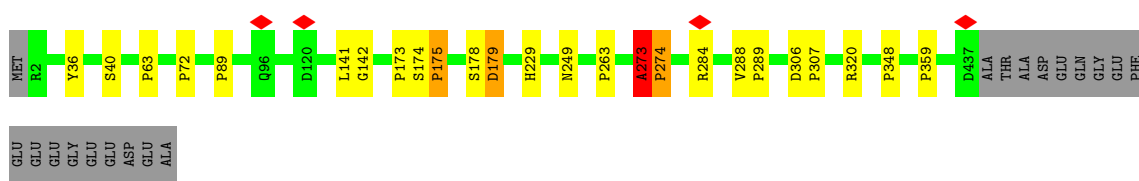
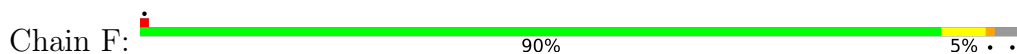
• Molecule 2: Tubulin beta chain



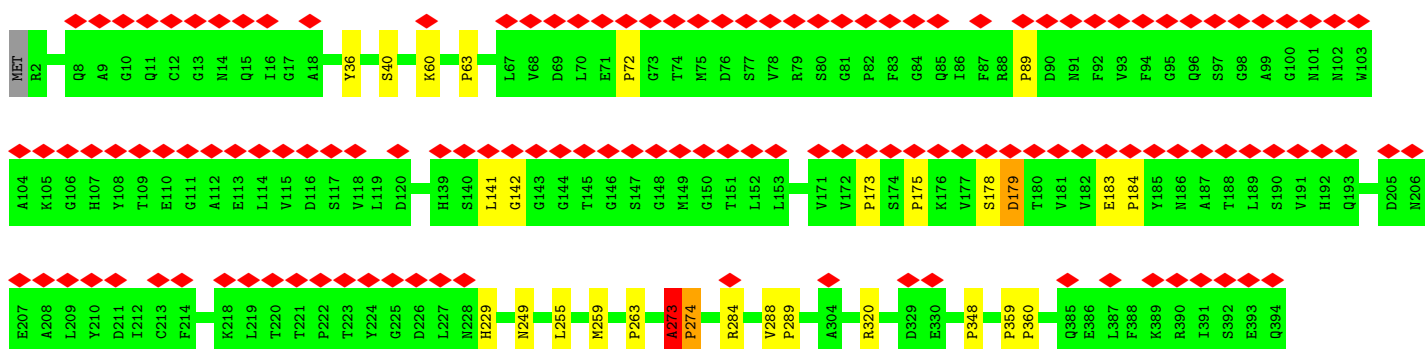
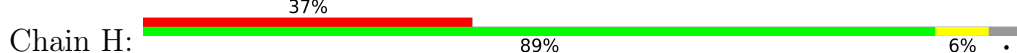
• Molecule 2: Tubulin beta chain

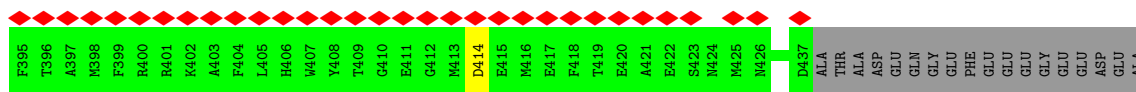


• Molecule 2: Tubulin beta chain

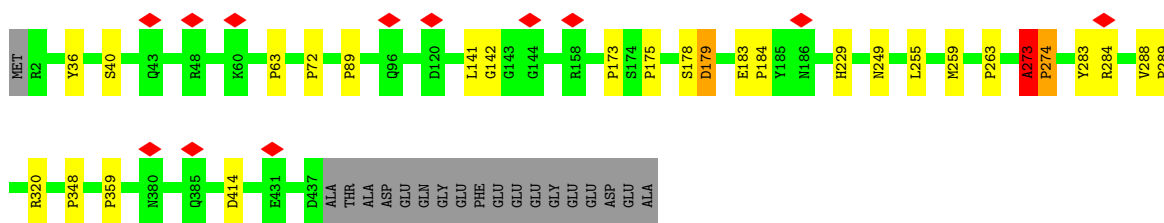
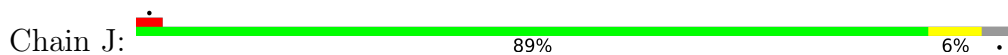


• Molecule 2: Tubulin beta chain

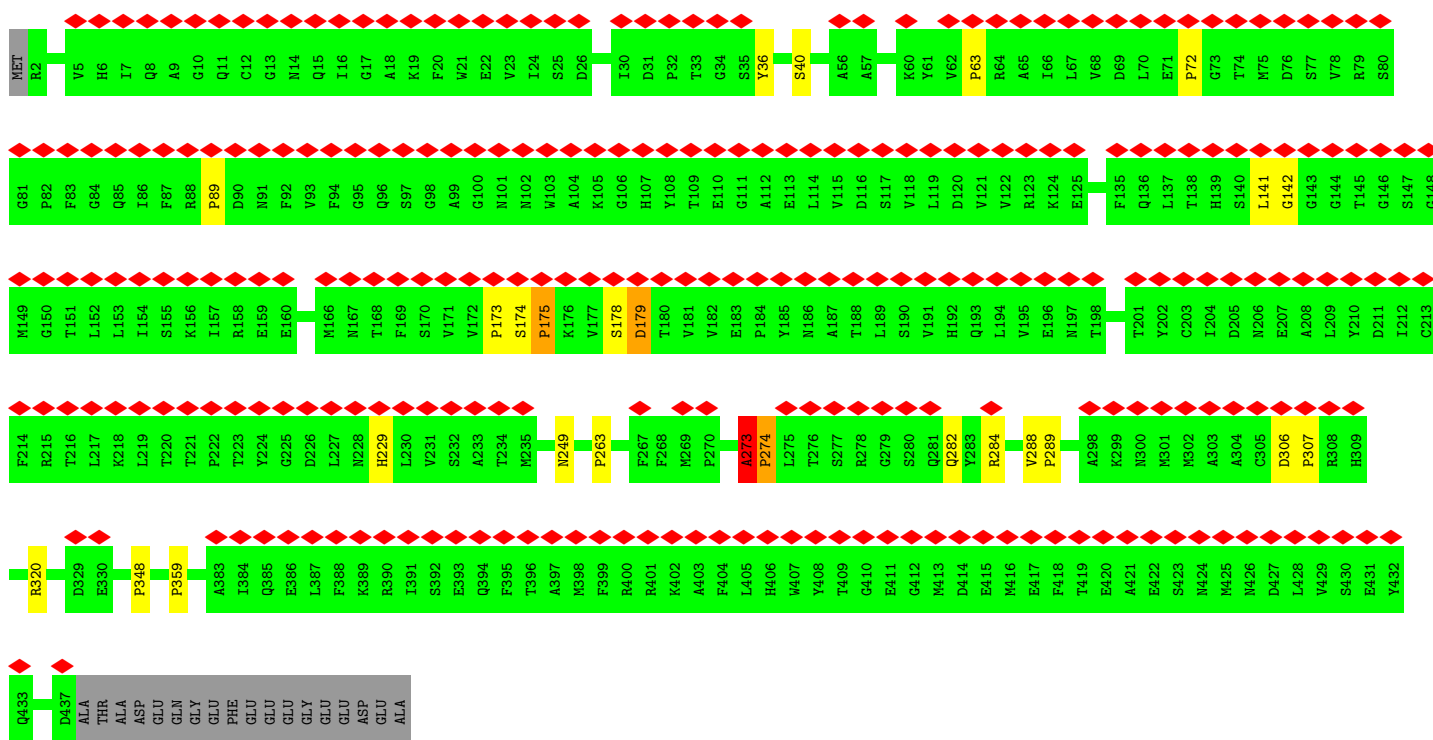
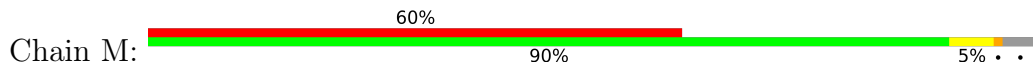




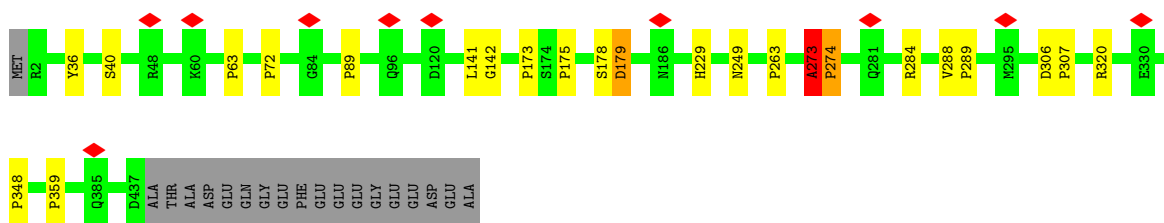
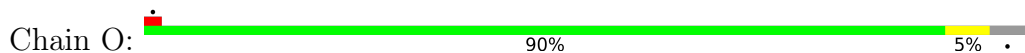
• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain

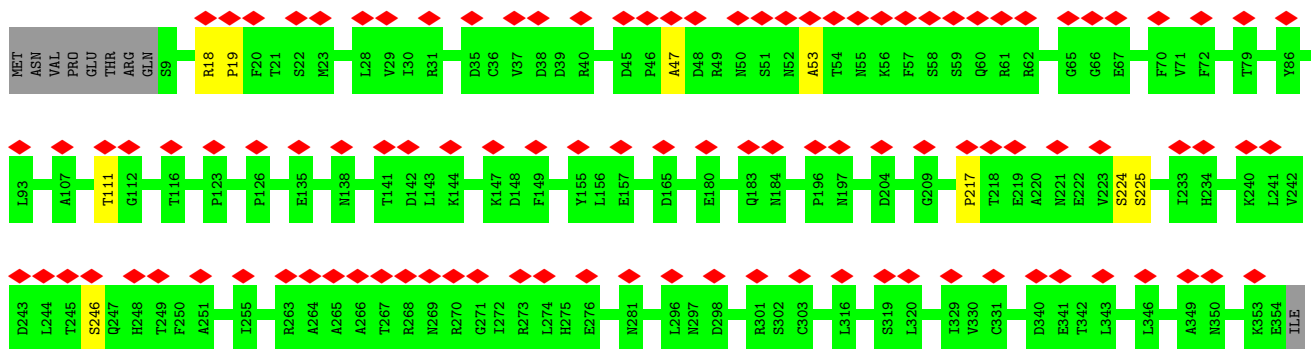


• Molecule 2: Tubulin beta chain

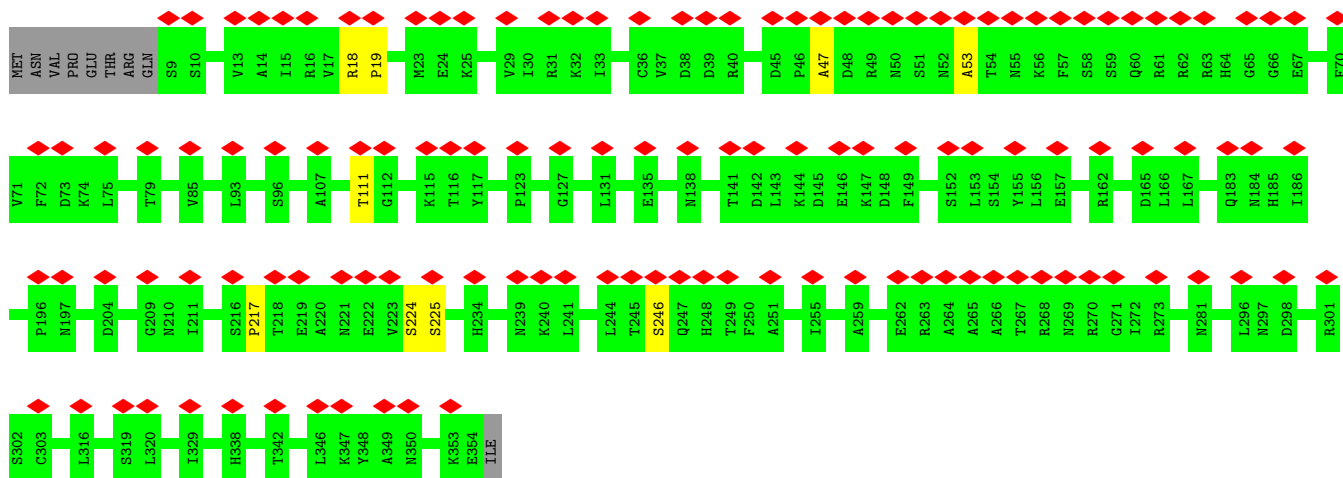




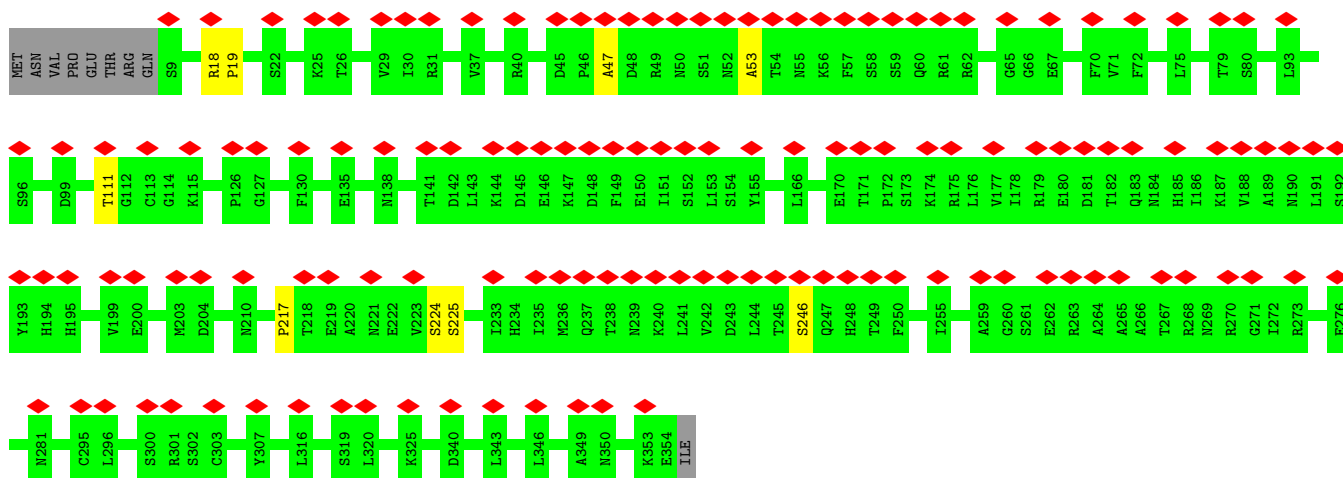
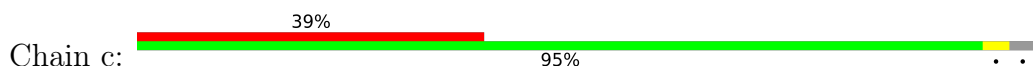




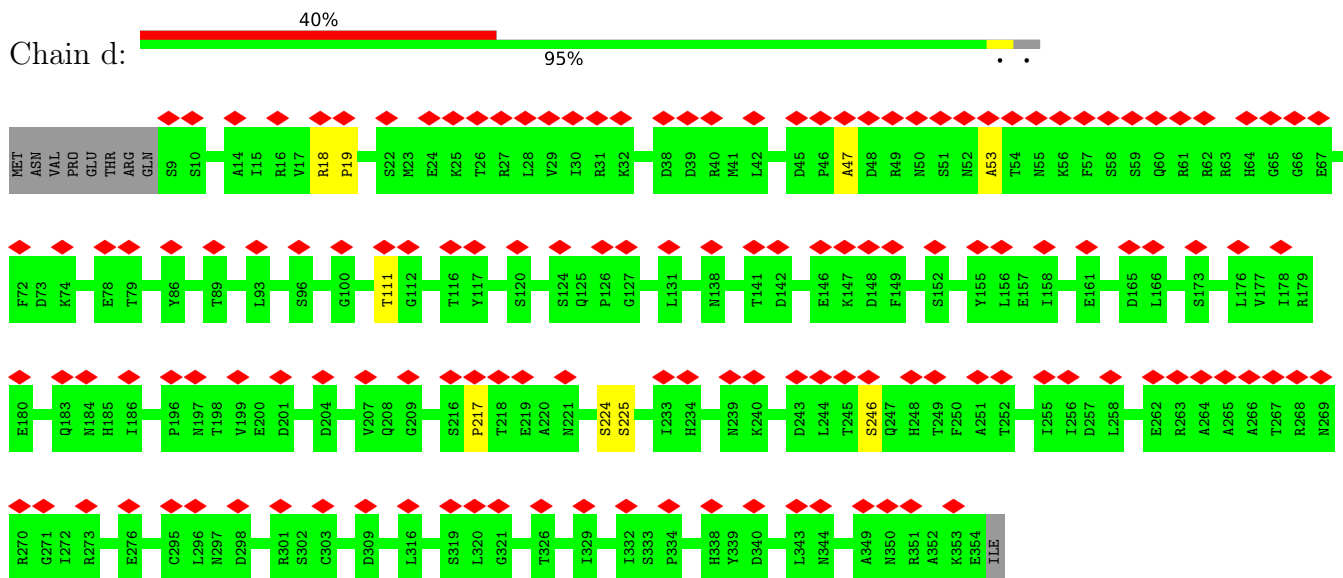
• Molecule 3: yeast kinesin-8/ Kip3



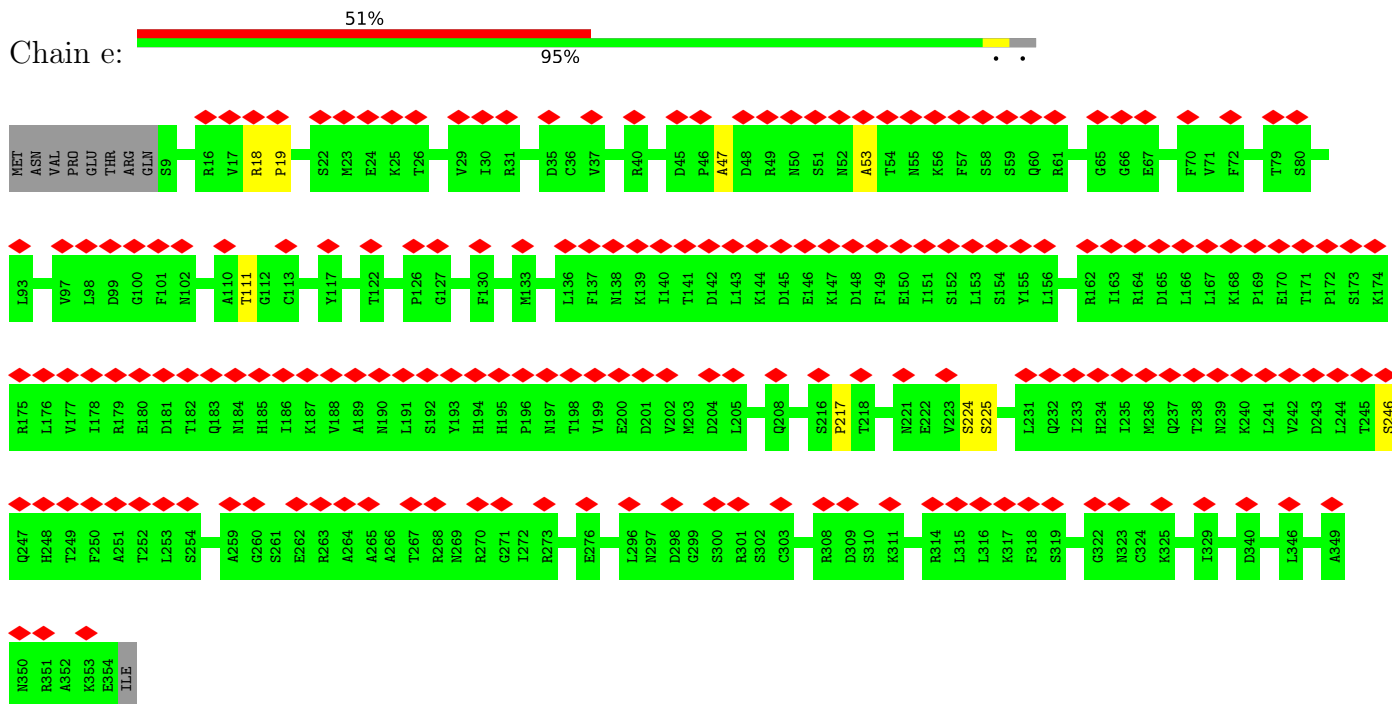
• Molecule 3: yeast kinesin-8/ Kip3



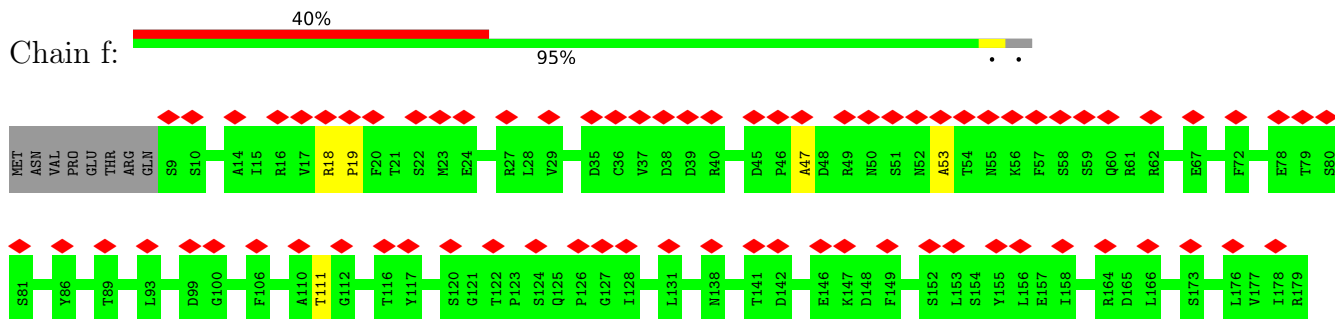
• Molecule 3: yeast kinesin-8/ Kip3

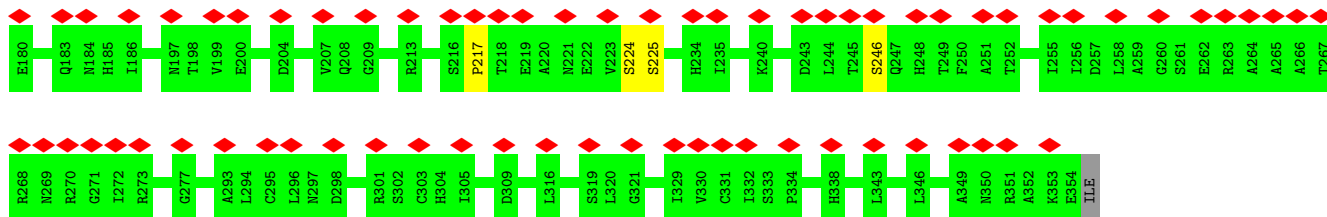


• Molecule 3: yeast kinesin-8/ Kip3

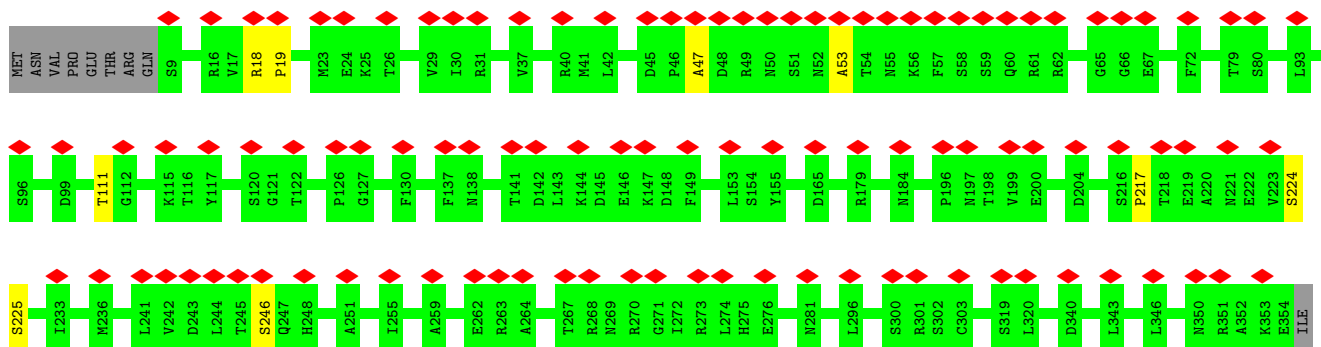
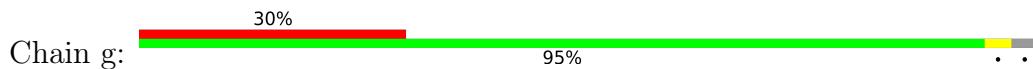


• Molecule 3: yeast kinesin-8/ Kip3

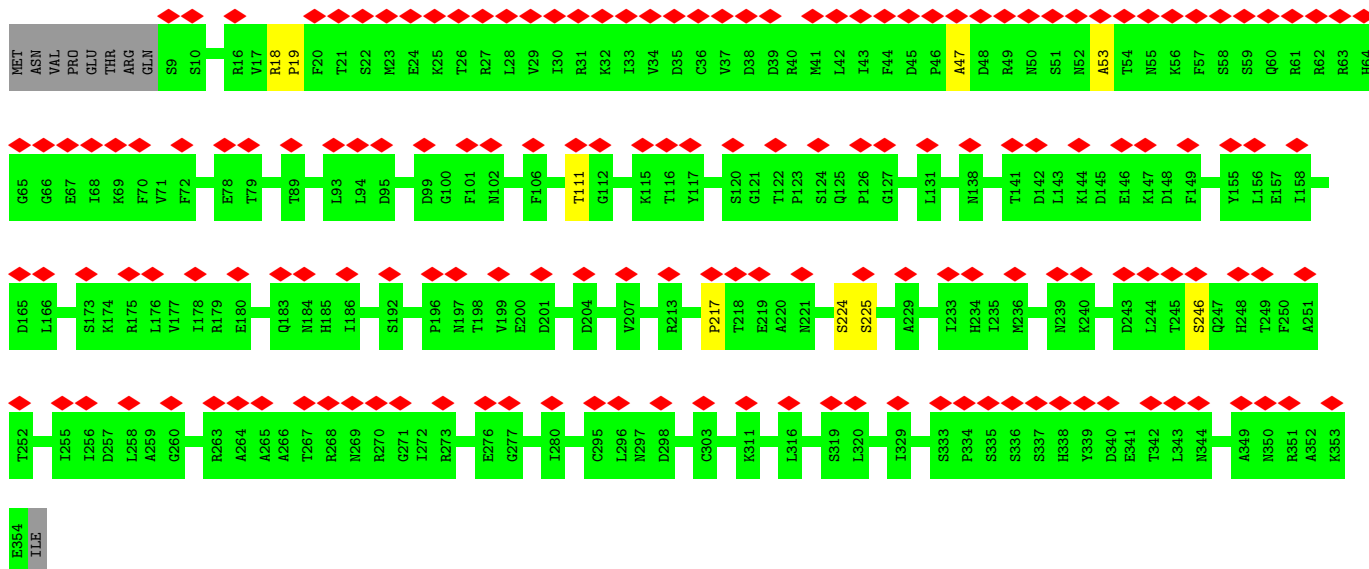
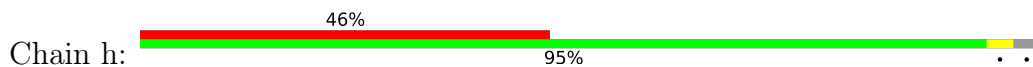




• Molecule 3: yeast kinesin-8/ Kip3



• Molecule 3: yeast kinesin-8/ Kip3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.76°, rise=8.55 Å, axial sym=C14	Depositor
Number of segments used	14934	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The contrast transfer function (CTF) was estimated using CTFFIND4 [(Rohou and Grigorieff, 2015) CTFFIND4: Fast and accurate] with a 500 um step search. A second CTFFIND run with a 100 um step search was carried out to refine the initial defocus values. Micrographs whose estimated resolution was lower than 8 Angstrom with 0.8 confidence were excluded.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	12.936	Depositor
Minimum map value	-9.617	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.408	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GDP, ANP, MG, TA1

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	0.74	0/3420	0.54	0/4643
1	C	0.74	0/3420	0.54	0/4643
1	E	0.74	0/3420	0.54	0/4643
1	G	0.74	0/3420	0.54	0/4643
1	I	0.74	0/3420	0.54	0/4643
1	L	0.74	0/3420	0.54	0/4643
1	N	0.74	0/3420	0.54	0/4643
1	P	0.74	0/3420	0.54	0/4643
1	R	0.74	0/3420	0.54	0/4643
2	B	0.72	0/3426	0.54	0/4642
2	D	0.72	0/3426	0.54	0/4642
2	F	0.72	0/3426	0.54	0/4642
2	H	0.72	0/3426	0.54	0/4642
2	J	0.72	0/3426	0.54	0/4642
2	M	0.72	0/3426	0.54	0/4642
2	O	0.72	0/3426	0.54	0/4642
2	Q	0.72	0/3426	0.54	0/4642
2	S	0.72	0/3426	0.54	0/4642
3	K	0.69	0/2762	0.53	0/3733
3	a	0.69	0/2762	0.53	0/3733
3	b	0.69	0/2762	0.53	0/3733
3	c	0.69	0/2762	0.53	0/3733
3	d	0.69	0/2762	0.53	0/3733
3	e	0.69	0/2762	0.53	0/3733
3	f	0.69	0/2762	0.53	0/3733
3	g	0.69	0/2762	0.53	0/3733
3	h	0.69	0/2762	0.53	0/3733
All	All	0.72	0/86472	0.54	0/117162

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1
2	M	0	1
2	O	0	1
2	Q	0	1
2	S	0	1
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	273	ALA	Peptide
2	D	273	ALA	Peptide
2	F	273	ALA	Peptide
2	H	273	ALA	Peptide
2	J	273	ALA	Peptide

## 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	3343	3251	3249	11	0
1	C	3343	3251	3249	12	0
1	E	3343	3251	3249	11	0
1	G	3343	3251	3249	11	0
1	I	3343	3251	3249	14	0
1	L	3343	3251	3249	12	0
1	N	3343	3251	3249	14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	3343	3251	3249	12	0
1	R	3343	3251	3249	13	0
2	B	3351	3230	3229	16	0
2	D	3351	3230	3229	16	0
2	F	3351	3230	3229	14	0
2	H	3351	3230	3229	18	0
2	J	3351	3230	3229	17	0
2	M	3351	3230	3229	15	0
2	O	3351	3230	3229	13	0
2	Q	3351	3230	3229	16	0
2	S	3351	3230	3229	17	0
3	K	2720	2738	2735	14	0
3	a	2720	2738	2735	0	0
3	b	2720	2738	2735	0	0
3	c	2720	2738	2735	0	0
3	d	2720	2738	2735	0	0
3	e	2720	2738	2735	0	0
3	f	2720	2738	2735	0	0
3	g	2720	2738	2735	0	0
3	h	2720	2738	2735	0	0
4	A	32	12	12	2	0
4	C	32	12	12	2	0
4	E	32	12	12	1	0
4	G	32	12	12	1	0
4	I	32	12	12	1	0
4	L	32	12	12	1	0
4	N	32	12	12	1	0
4	P	32	12	12	2	0
4	R	32	12	12	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	N	1	0	0	0	0
5	P	1	0	0	0	0
5	R	1	0	0	0	0
5	a	1	0	0	0	0
5	b	1	0	0	0	0
5	c	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	d	1	0	0	0	0
5	e	1	0	0	0	0
5	f	1	0	0	0	0
5	g	1	0	0	0	0
5	h	1	0	0	0	0
6	B	28	12	12	0	0
6	D	28	12	12	0	0
6	F	28	12	12	0	0
6	H	28	12	12	0	0
6	J	28	12	12	0	0
6	M	28	12	12	0	0
6	O	28	12	12	0	0
6	Q	28	12	12	0	0
6	S	28	12	12	0	0
7	B	62	51	51	3	0
7	D	62	51	51	3	0
7	F	62	51	51	3	0
7	H	62	51	51	3	0
7	J	62	51	51	3	0
7	M	62	51	51	3	0
7	O	62	51	51	3	0
7	Q	62	51	51	3	0
7	S	62	51	51	3	0
8	K	31	13	13	3	0
8	a	31	13	13	0	0
8	b	31	13	13	0	0
8	c	31	13	13	0	0
8	d	31	13	13	0	0
8	e	31	13	13	0	0
8	f	31	13	13	0	0
8	g	31	13	13	0	0
8	h	31	13	13	0	0
All	All	86121	83763	83709	278	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 2.

The worst 5 of 278 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:R:290:GLU:OE1	1:R:290:GLU:N	2.17	0.78

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:GLU:OE1	1:C:290:GLU:N	2.17	0.77
1:P:290:GLU:N	1:P:290:GLU:OE1	2.17	0.77
1:A:290:GLU:OE1	1:A:290:GLU:N	2.17	0.77
1:I:290:GLU:N	1:I:290:GLU:OE1	2.17	0.77

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	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	9	43
1	C	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	9	43
1	E	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	9	43
1	G	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	9	43
1	I	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	9	43
1	L	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	9	43
1	N	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	9	43
1	P	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	9	43
1	R	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	9	43
2	B	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	6	37
2	D	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	6	37
2	F	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	6	37
2	H	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	6	37
2	J	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	6	37
2	M	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	6	37
2	O	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	6	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	6	37
2	S	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	6	37
3	K	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	6	38
3	a	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	6	38
3	b	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	6	38
3	c	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	6	38
3	d	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	6	38
3	e	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	6	38
3	f	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	6	38
3	g	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	6	38
3	h	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	6	38
All	All	10719/11259 (95%)	9963 (93%)	531 (5%)	225 (2%)	10	39

5 of 225 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	179	ASP
2	B	273	ALA
3	K	18	ARG
3	K	19	PRO
3	K	103	ALA

### 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	359/377 (95%)	358 (100%)	1 (0%)	92	95
1	C	359/377 (95%)	358 (100%)	1 (0%)	92	95
1	E	359/377 (95%)	358 (100%)	1 (0%)	92	95
1	G	359/377 (95%)	358 (100%)	1 (0%)	92	95
1	I	359/377 (95%)	358 (100%)	1 (0%)	92	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	359/377 (95%)	358 (100%)	1 (0%)	92	95
1	N	359/377 (95%)	358 (100%)	1 (0%)	92	95
1	P	359/377 (95%)	358 (100%)	1 (0%)	92	95
1	R	359/377 (95%)	358 (100%)	1 (0%)	92	95
2	B	367/381 (96%)	366 (100%)	1 (0%)	92	95
2	D	367/381 (96%)	366 (100%)	1 (0%)	92	95
2	F	367/381 (96%)	366 (100%)	1 (0%)	92	95
2	H	367/381 (96%)	366 (100%)	1 (0%)	92	95
2	J	367/381 (96%)	366 (100%)	1 (0%)	92	95
2	M	367/381 (96%)	366 (100%)	1 (0%)	92	95
2	O	367/381 (96%)	366 (100%)	1 (0%)	92	95
2	Q	367/381 (96%)	366 (100%)	1 (0%)	92	95
2	S	367/381 (96%)	366 (100%)	1 (0%)	92	95
3	K	310/319 (97%)	309 (100%)	1 (0%)	92	95
3	a	310/319 (97%)	309 (100%)	1 (0%)	92	95
3	b	310/319 (97%)	309 (100%)	1 (0%)	92	95
3	c	310/319 (97%)	309 (100%)	1 (0%)	92	95
3	d	310/319 (97%)	309 (100%)	1 (0%)	92	95
3	e	310/319 (97%)	309 (100%)	1 (0%)	92	95
3	f	310/319 (97%)	309 (100%)	1 (0%)	92	95
3	g	310/319 (97%)	309 (100%)	1 (0%)	92	95
3	h	310/319 (97%)	309 (100%)	1 (0%)	92	95
All	All	9324/9693 (96%)	9297 (100%)	27 (0%)	92	95

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

Mol	Chain	Res	Type
3	d	111	THR
3	e	111	THR
1	R	89	PRO
2	M	89	PRO
1	N	89	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	192	HIS
2	S	8	GLN
2	M	8	GLN
2	Q	136	GLN
1	L	107	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 18 are monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	TA1	F	502	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	12 (11%)
4	GTP	G	501	5	26,34,34	1.38	2 (7%)	32,54,54	1.72	6 (18%)
7	TA1	H	502	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
6	GDP	B	501	-	24,30,30	1.06	1 (4%)	30,47,47	1.39	5 (16%)
6	GDP	M	501	-	24,30,30	1.06	1 (4%)	30,47,47	1.39	5 (16%)
8	ANP	c	401	5	29,33,33	1.82	6 (20%)	31,52,52	3.20	17 (54%)
8	ANP	g	401	5	29,33,33	1.82	6 (20%)	31,52,52	3.20	17 (54%)
7	TA1	D	502	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	12 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GTP	A	501	5	26,34,34	1.39	3 (11%)	32,54,54	1.72	6 (18%)
6	GDP	Q	501	-	24,30,30	1.07	1 (4%)	30,47,47	1.39	5 (16%)
7	TA1	B	502	-	68,68,68	2.01	19 (27%)	105,105,105	1.40	12 (11%)
4	GTP	E	501	5	26,34,34	1.38	2 (7%)	32,54,54	1.72	6 (18%)
7	TA1	M	502	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
8	ANP	d	401	5	29,33,33	1.82	6 (20%)	31,52,52	3.20	17 (54%)
8	ANP	b	401	5	29,33,33	1.82	6 (20%)	31,52,52	3.20	17 (54%)
4	GTP	L	501	5	26,34,34	1.38	2 (7%)	32,54,54	1.72	6 (18%)
6	GDP	J	501	-	24,30,30	1.07	1 (4%)	30,47,47	1.39	5 (16%)
7	TA1	O	502	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	12 (11%)
6	GDP	D	501	-	24,30,30	1.06	1 (4%)	30,47,47	1.39	5 (16%)
7	TA1	Q	502	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
7	TA1	S	502	-	68,68,68	2.01	19 (27%)	105,105,105	1.40	12 (11%)
4	GTP	P	501	5	26,34,34	1.39	3 (11%)	32,54,54	1.72	6 (18%)
8	ANP	a	401	5	29,33,33	1.81	7 (24%)	31,52,52	3.20	17 (54%)
7	TA1	J	502	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
6	GDP	F	501	-	24,30,30	1.07	1 (4%)	30,47,47	1.40	5 (16%)
4	GTP	R	501	5	26,34,34	1.39	3 (11%)	32,54,54	1.72	6 (18%)
4	GTP	I	501	5	26,34,34	1.38	2 (7%)	32,54,54	1.72	6 (18%)
8	ANP	h	401	5	29,33,33	1.81	6 (20%)	31,52,52	3.20	17 (54%)
6	GDP	S	501	-	24,30,30	1.07	1 (4%)	30,47,47	1.39	5 (16%)
6	GDP	O	501	-	24,30,30	1.07	1 (4%)	30,47,47	1.39	5 (16%)
4	GTP	C	501	5	26,34,34	1.38	2 (7%)	32,54,54	1.73	6 (18%)
8	ANP	K	501	5	29,33,33	1.81	6 (20%)	31,52,52	3.20	17 (54%)
6	GDP	H	501	-	24,30,30	1.07	1 (4%)	30,47,47	1.39	5 (16%)
8	ANP	e	401	5	29,33,33	1.82	6 (20%)	31,52,52	3.20	17 (54%)
4	GTP	N	501	5	26,34,34	1.39	3 (11%)	32,54,54	1.72	6 (18%)
8	ANP	f	401	5	29,33,33	1.81	6 (20%)	31,52,52	3.20	17 (54%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TA1	F	502	-	-	9/41/127/127	0/7/7/7

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	G	501	5	-	5/18/38/38	0/3/3/3
7	TA1	H	502	-	-	9/41/127/127	0/7/7/7
6	GDP	B	501	-	-	3/12/32/32	0/3/3/3
6	GDP	M	501	-	-	3/12/32/32	0/3/3/3
8	ANP	c	401	5	-	3/14/38/38	0/3/3/3
8	ANP	g	401	5	-	3/14/38/38	0/3/3/3
7	TA1	D	502	-	-	9/41/127/127	0/7/7/7
4	GTP	A	501	5	-	5/18/38/38	0/3/3/3
6	GDP	Q	501	-	-	3/12/32/32	0/3/3/3
7	TA1	B	502	-	-	9/41/127/127	0/7/7/7
4	GTP	E	501	5	-	5/18/38/38	0/3/3/3
7	TA1	M	502	-	-	9/41/127/127	0/7/7/7
8	ANP	d	401	5	-	3/14/38/38	0/3/3/3
8	ANP	b	401	5	-	3/14/38/38	0/3/3/3
4	GTP	L	501	5	-	5/18/38/38	0/3/3/3
6	GDP	J	501	-	-	3/12/32/32	0/3/3/3
7	TA1	O	502	-	-	9/41/127/127	0/7/7/7
6	GDP	D	501	-	-	3/12/32/32	0/3/3/3
7	TA1	Q	502	-	-	9/41/127/127	0/7/7/7
7	TA1	S	502	-	-	9/41/127/127	0/7/7/7
4	GTP	P	501	5	-	5/18/38/38	0/3/3/3
8	ANP	a	401	5	-	3/14/38/38	0/3/3/3
7	TA1	J	502	-	-	9/41/127/127	0/7/7/7
6	GDP	F	501	-	-	3/12/32/32	0/3/3/3
4	GTP	R	501	5	-	5/18/38/38	0/3/3/3
4	GTP	I	501	5	-	5/18/38/38	0/3/3/3
8	ANP	h	401	5	-	3/14/38/38	0/3/3/3
6	GDP	S	501	-	-	3/12/32/32	0/3/3/3
6	GDP	O	501	-	-	3/12/32/32	0/3/3/3
4	GTP	C	501	5	-	5/18/38/38	0/3/3/3
8	ANP	K	501	5	-	3/14/38/38	0/3/3/3
6	GDP	H	501	-	-	3/12/32/32	0/3/3/3
8	ANP	e	401	5	-	3/14/38/38	0/3/3/3
4	GTP	N	501	5	-	5/18/38/38	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ANP	f	401	5	-	3/14/38/38	0/3/3/3

The worst 5 of 257 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	502	TA1	C08-C09	5.31	1.50	1.38
7	H	502	TA1	C08-C09	5.30	1.50	1.38
7	B	502	TA1	C08-C09	5.29	1.50	1.38
7	F	502	TA1	C08-C09	5.29	1.50	1.38
7	S	502	TA1	C08-C09	5.26	1.50	1.38

The worst 5 of 356 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	f	401	ANP	C5'-C4'-C3'	-7.25	88.00	115.18
8	e	401	ANP	C5'-C4'-C3'	-7.25	88.01	115.18
8	a	401	ANP	C5'-C4'-C3'	-7.25	88.02	115.18
8	d	401	ANP	C5'-C4'-C3'	-7.25	88.03	115.18
8	K	501	ANP	C5'-C4'-C3'	-7.25	88.03	115.18

There are no chirality outliers.

5 of 180 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	A	501	GTP	C3'-C4'-C5'-O5'
4	C	501	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

19 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	502	TA1	3	0
4	G	501	GTP	1	0
7	H	502	TA1	3	0
7	D	502	TA1	3	0
4	A	501	GTP	2	0
7	B	502	TA1	3	0
4	E	501	GTP	1	0

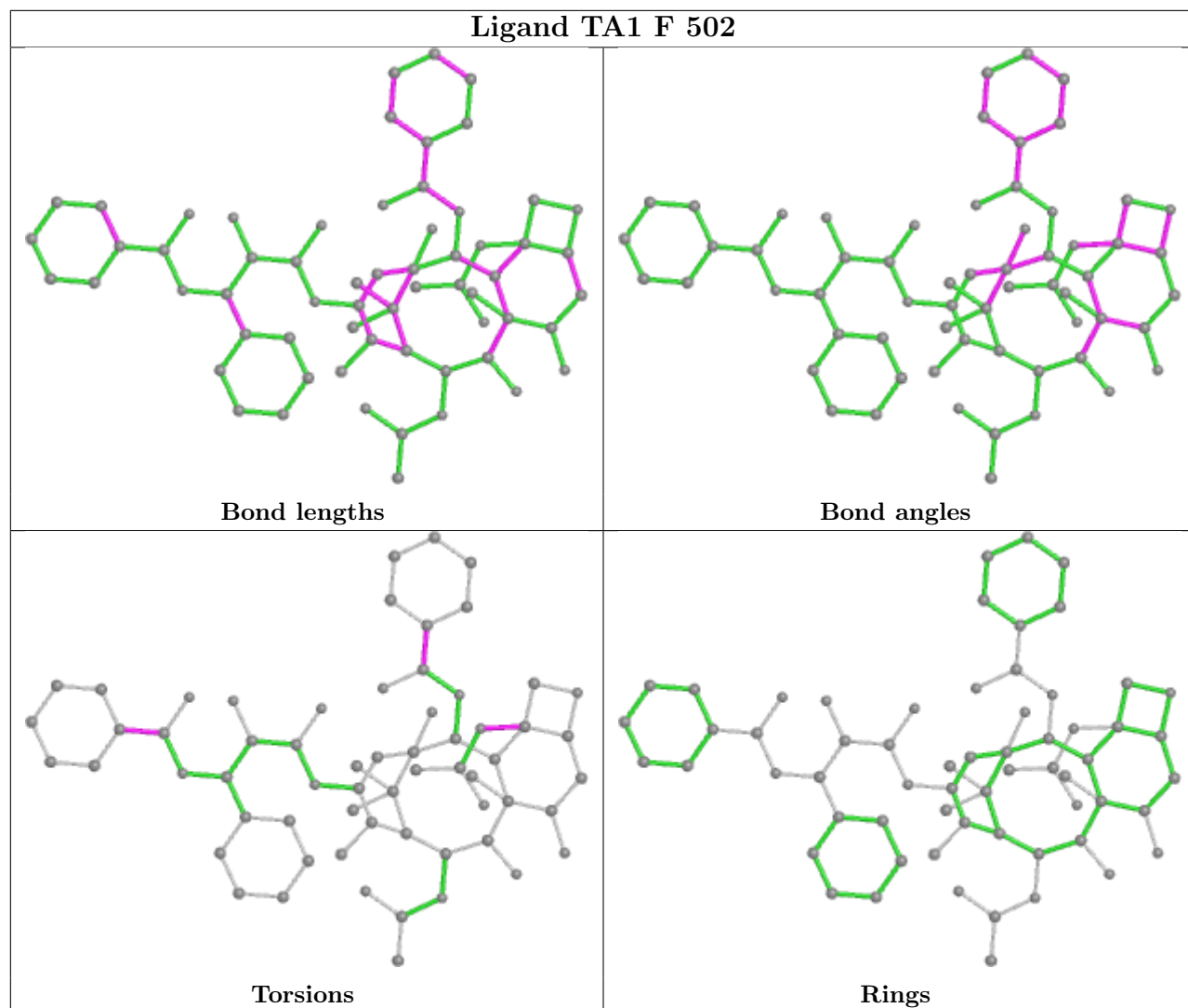
*Continued on next page...*

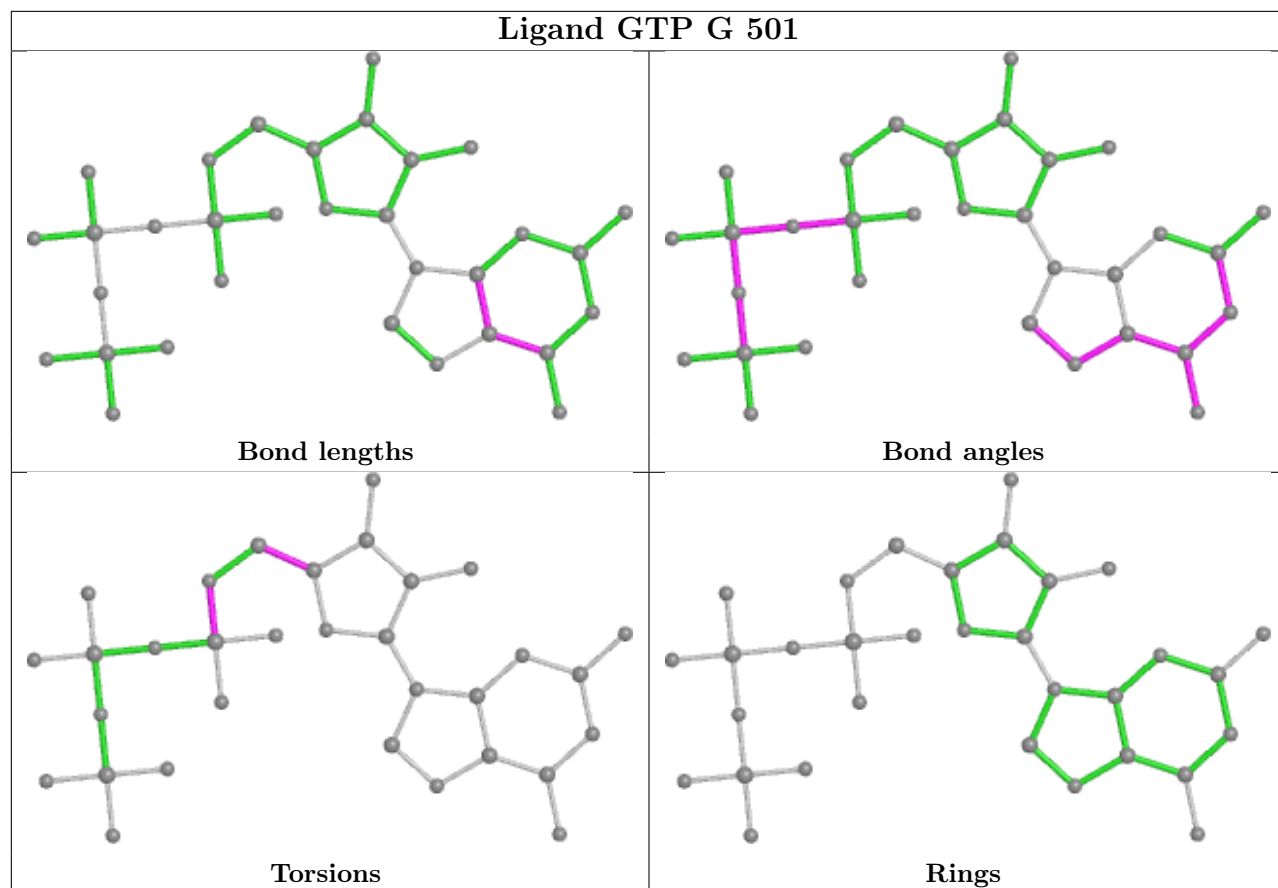
*Continued from previous page...*

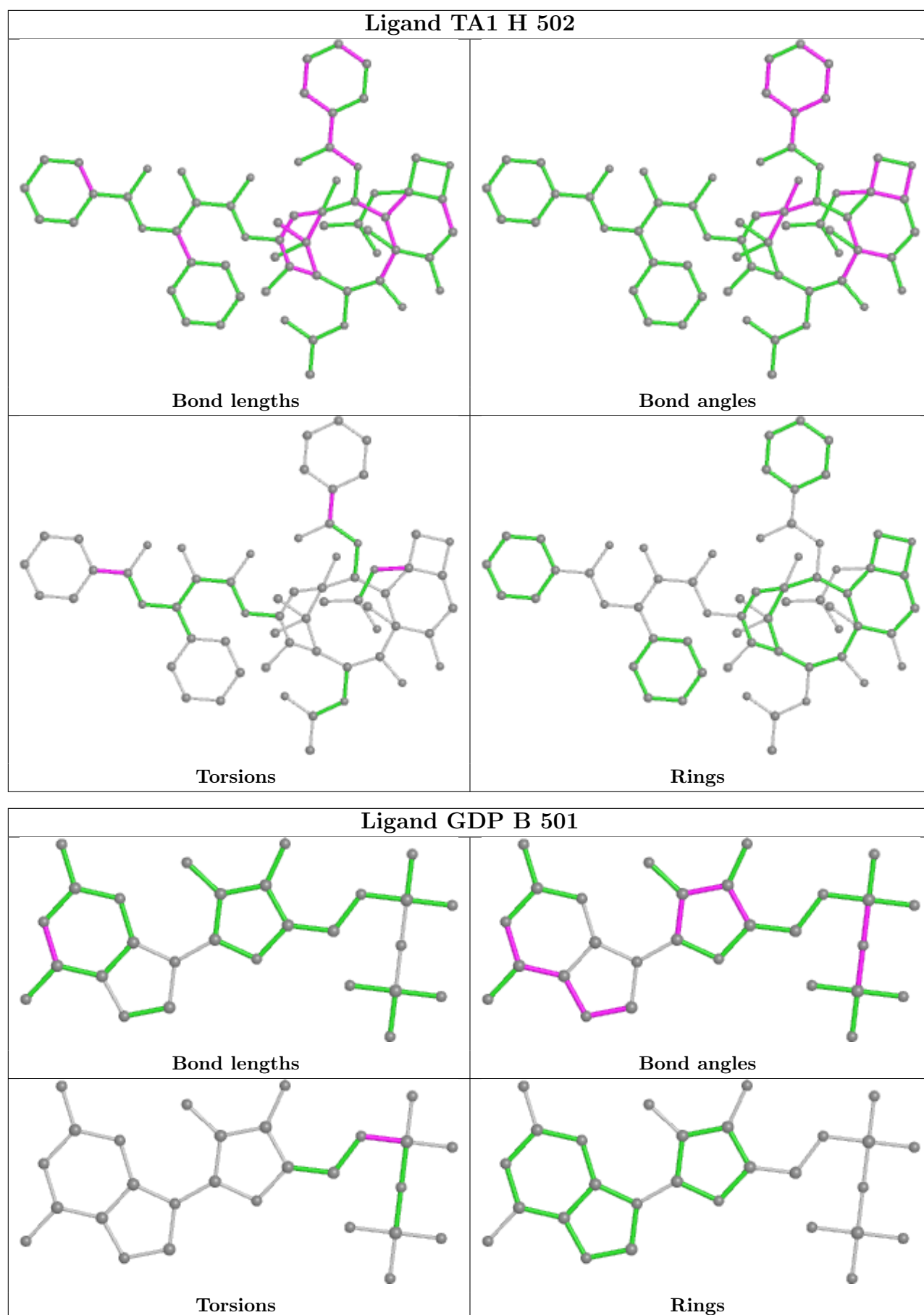
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	502	TA1	3	0
4	L	501	GTP	1	0
7	O	502	TA1	3	0
7	Q	502	TA1	3	0
7	S	502	TA1	3	0
4	P	501	GTP	2	0
7	J	502	TA1	3	0
4	R	501	GTP	2	0
4	I	501	GTP	1	0
4	C	501	GTP	2	0
8	K	501	ANP	3	0
4	N	501	GTP	1	0

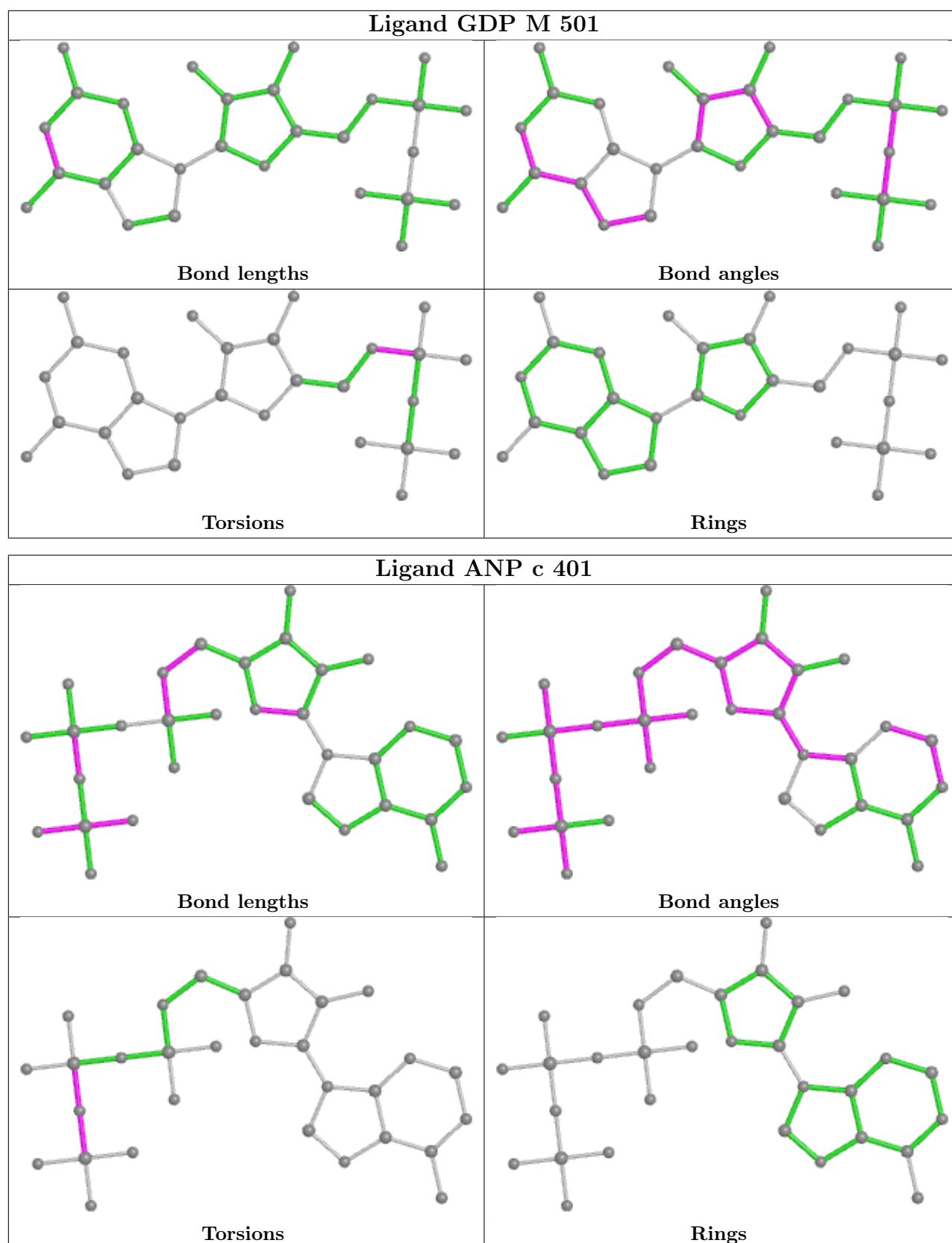
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

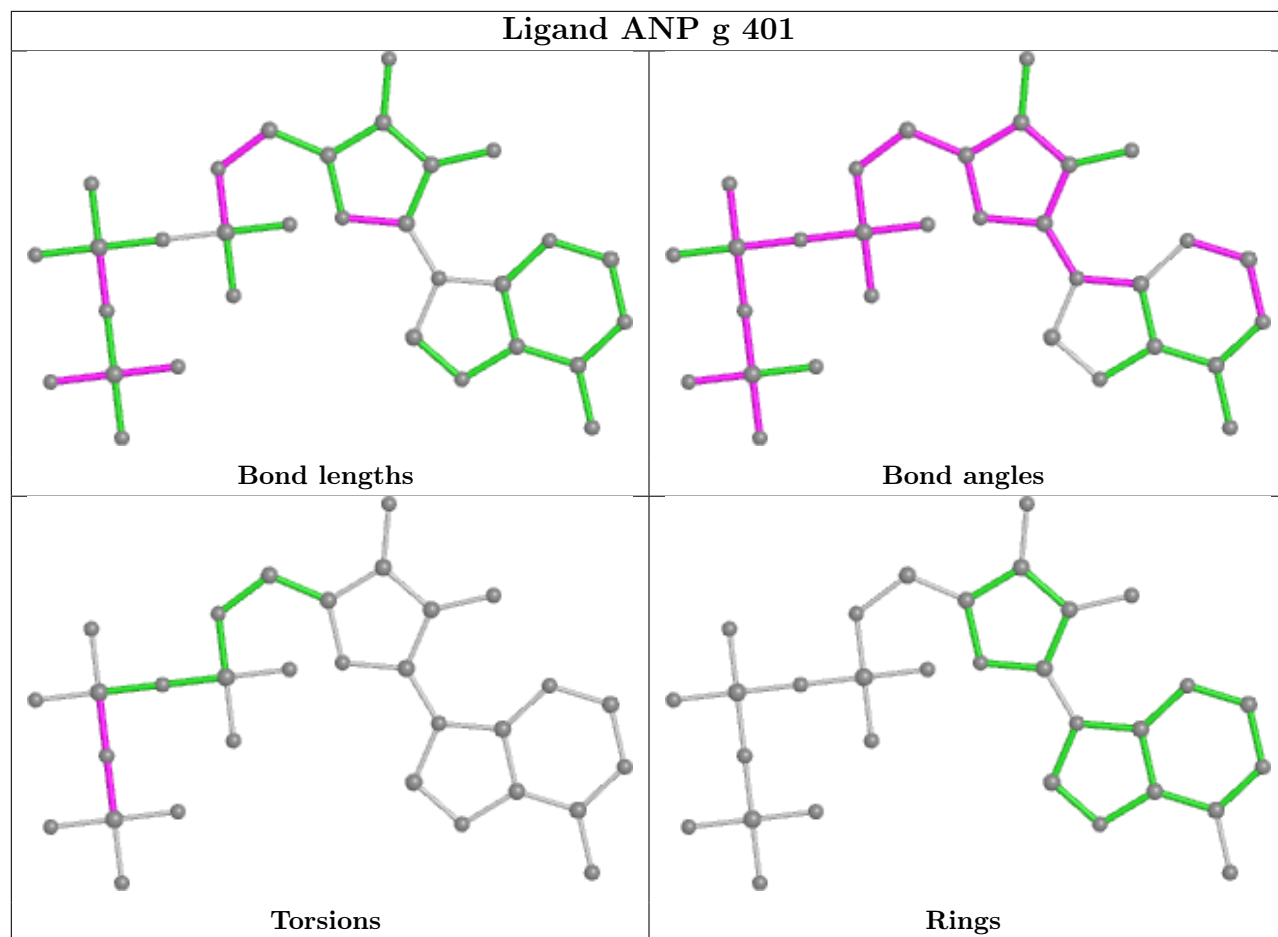


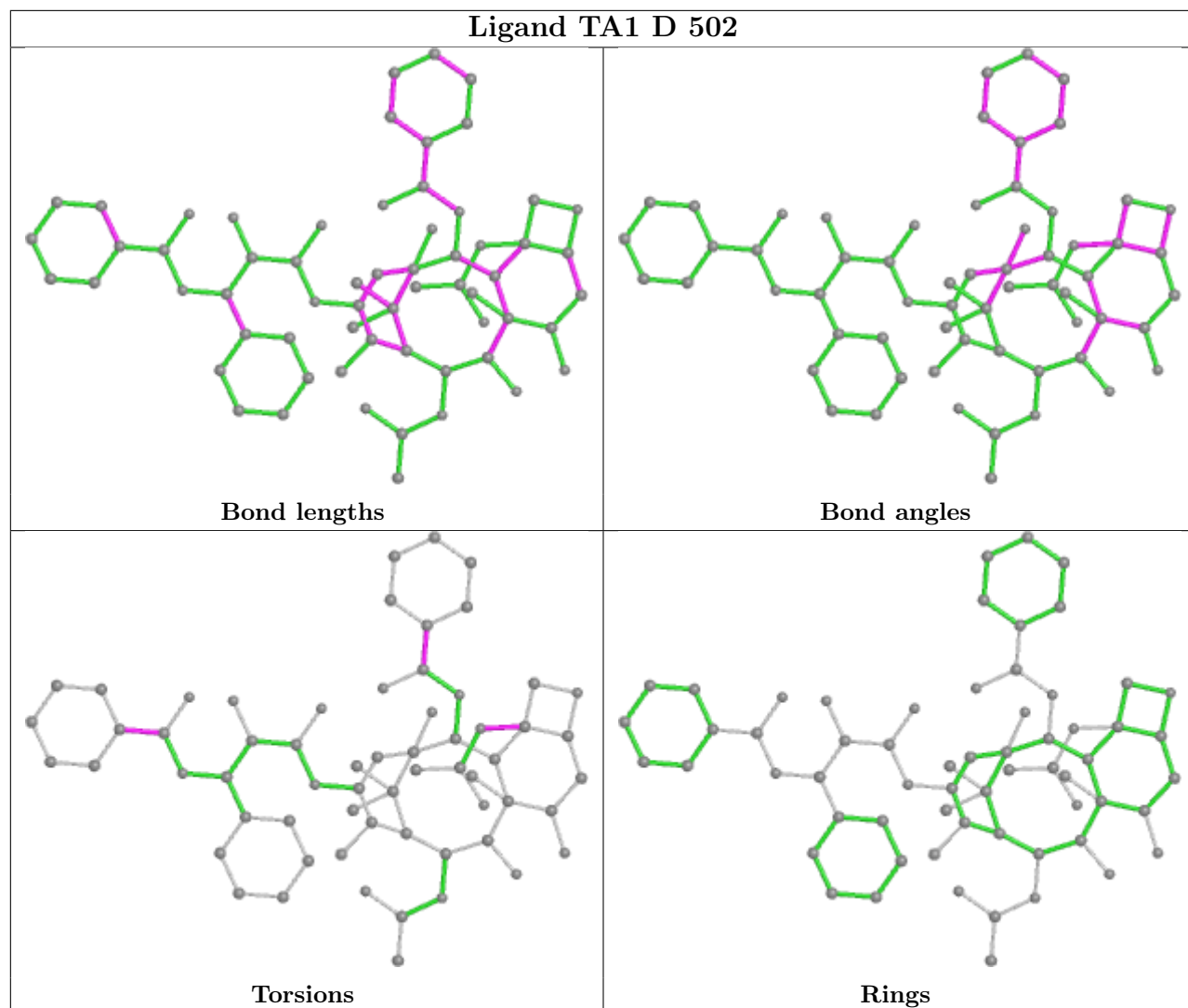


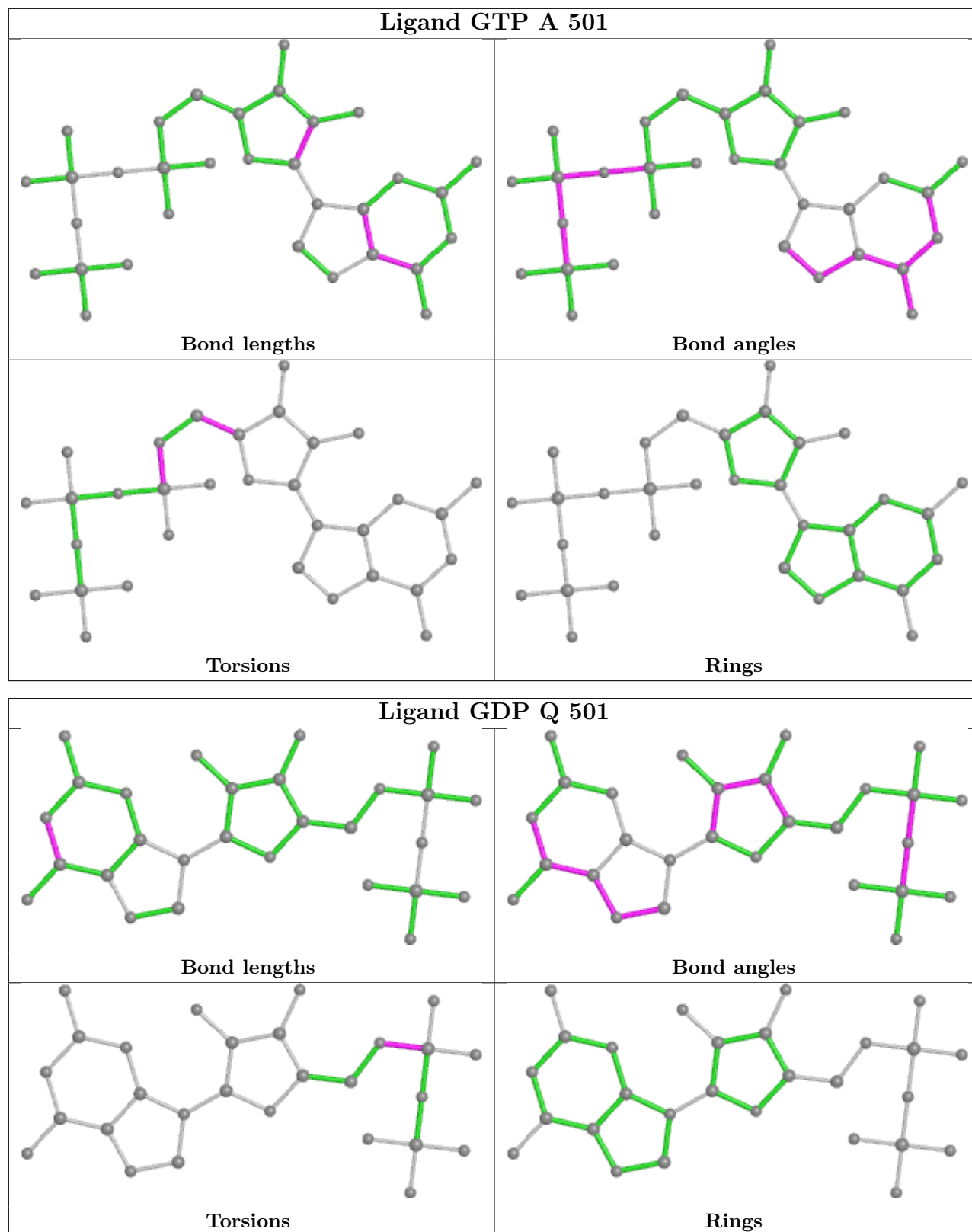


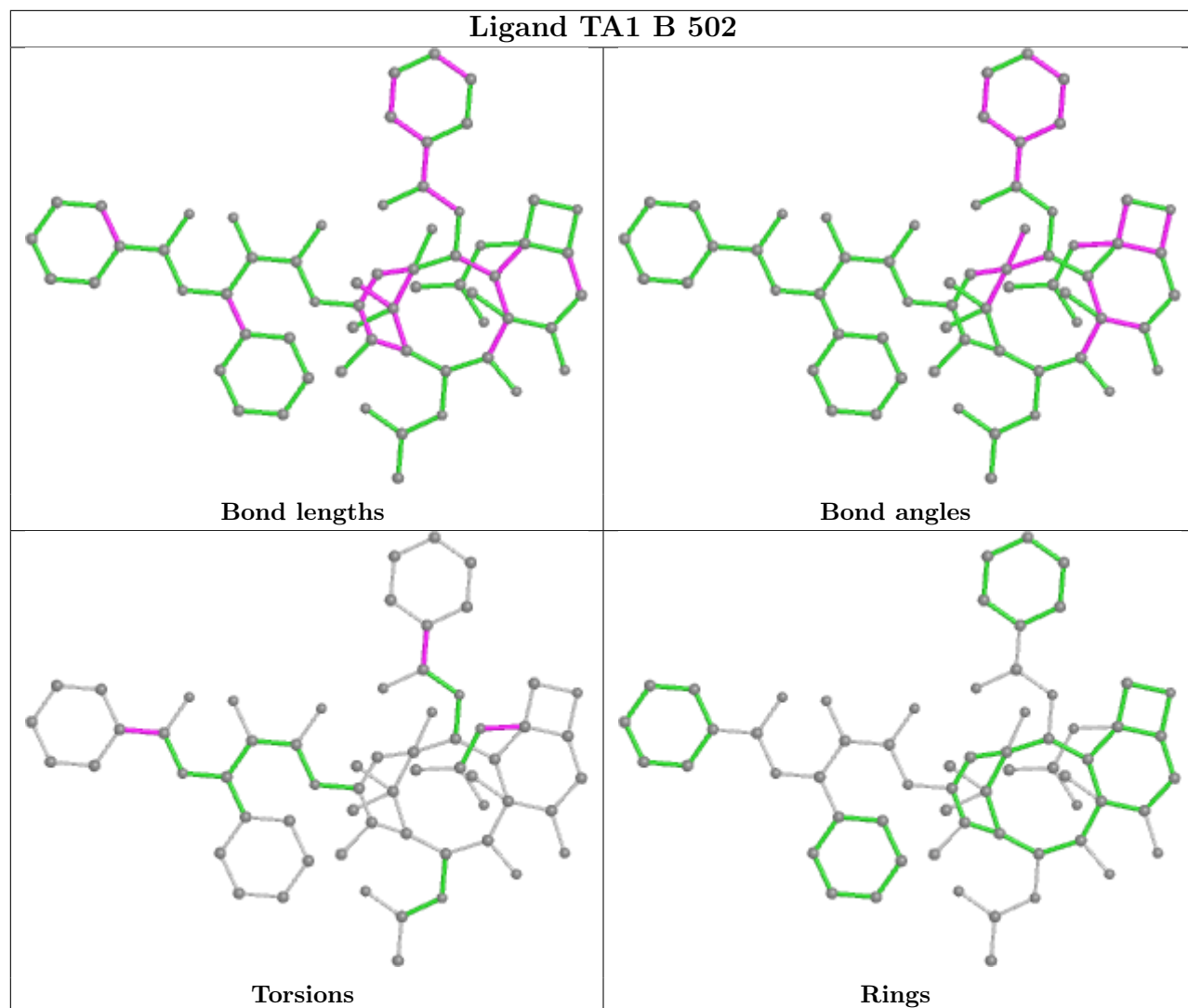




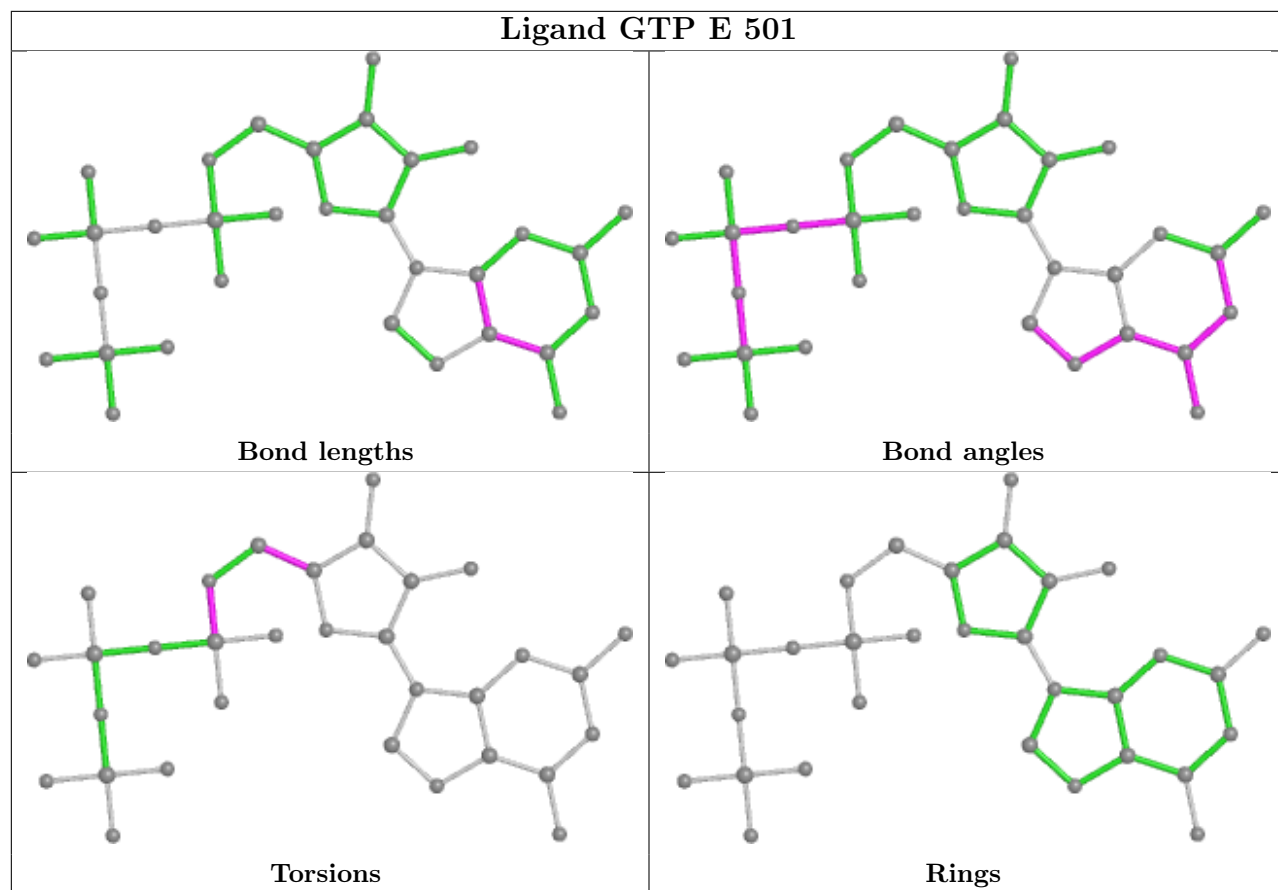


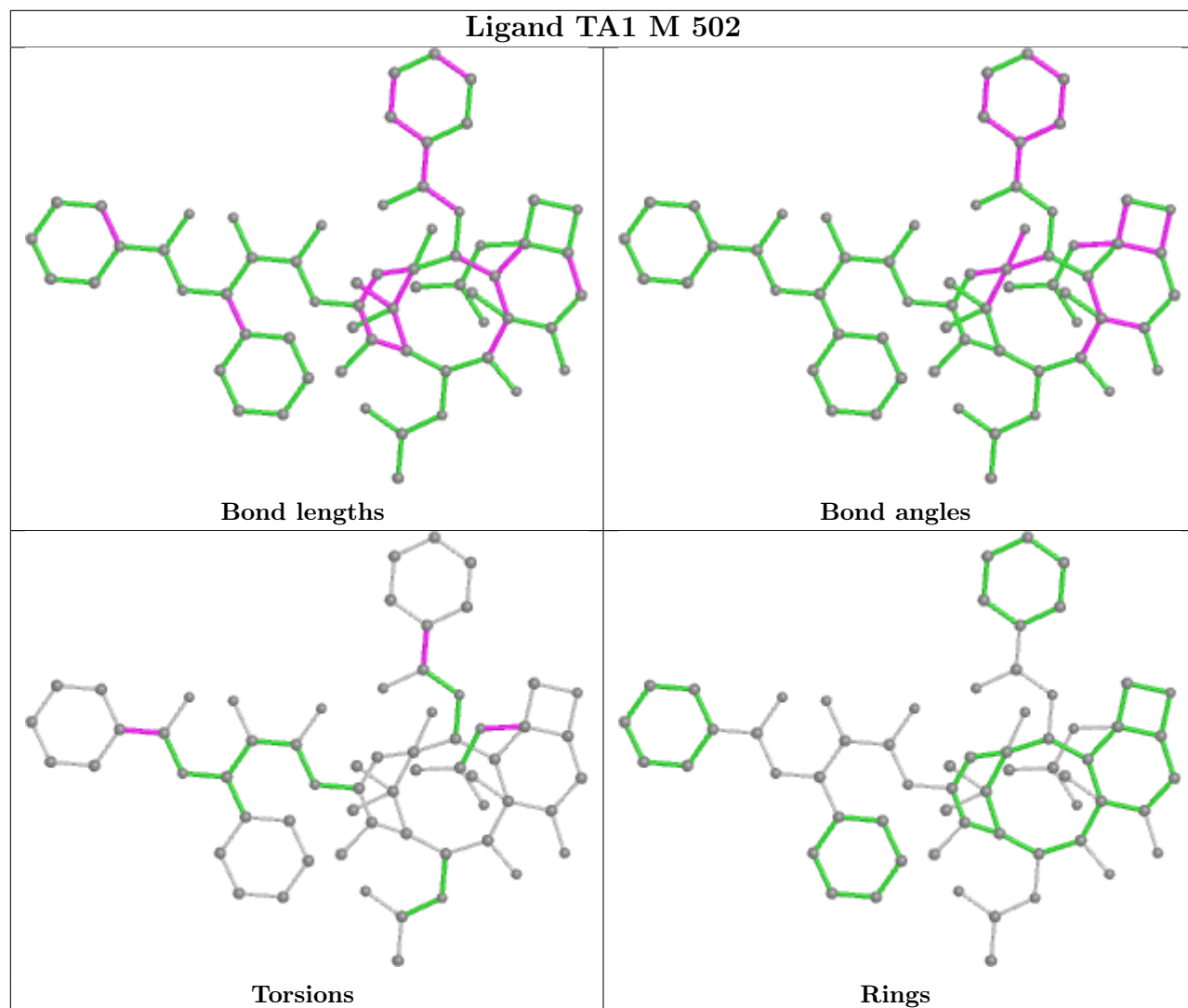


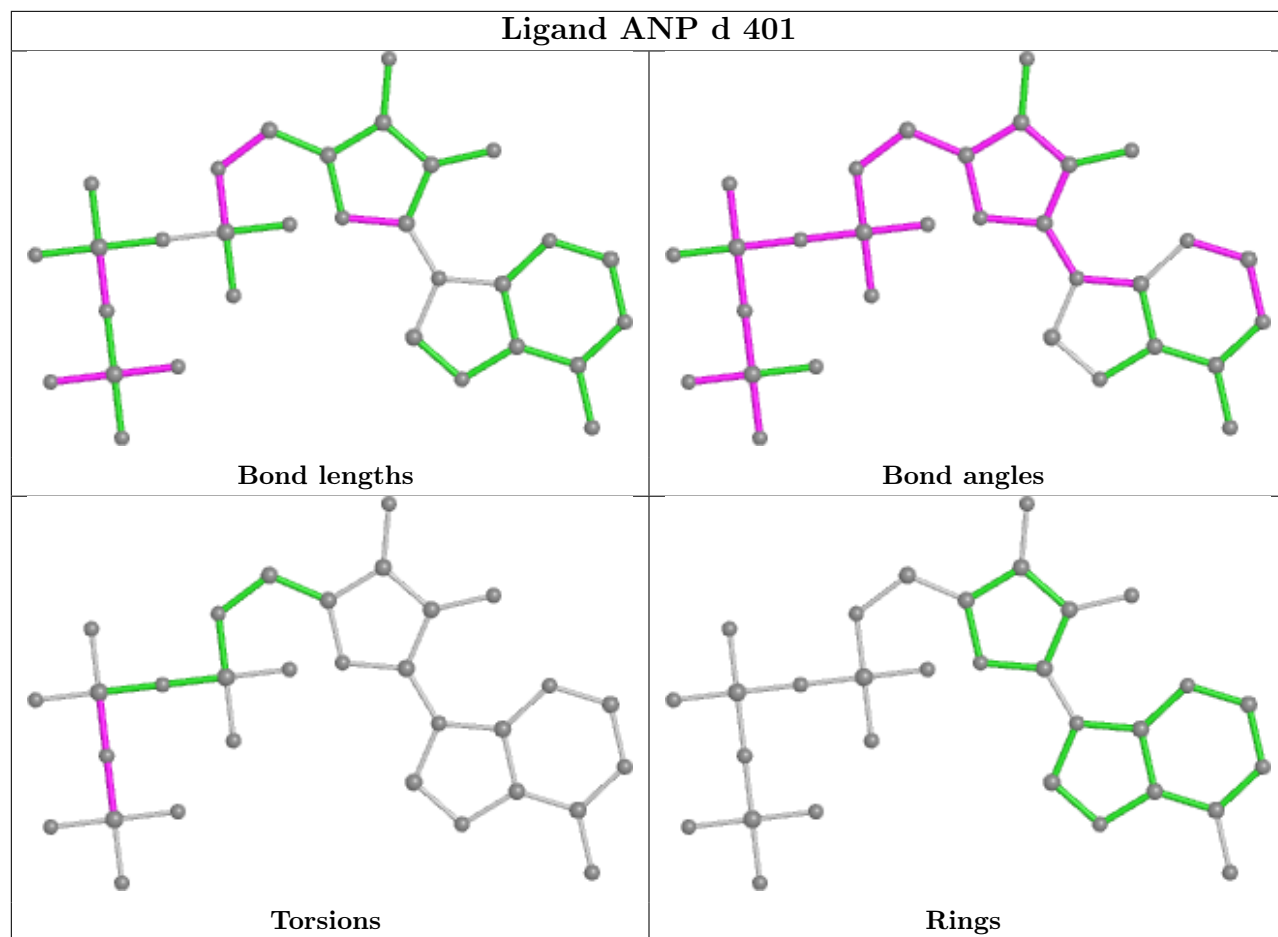


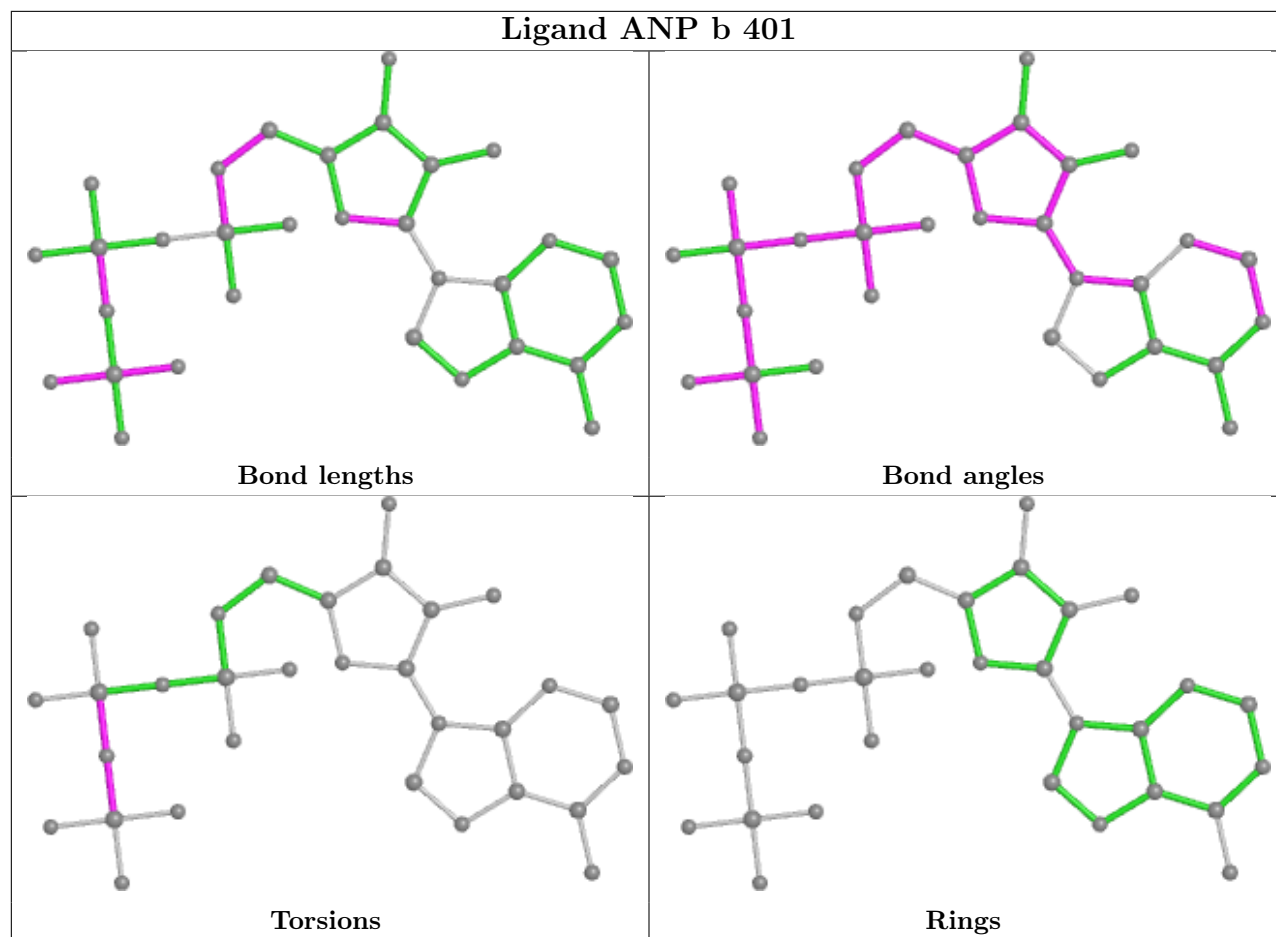


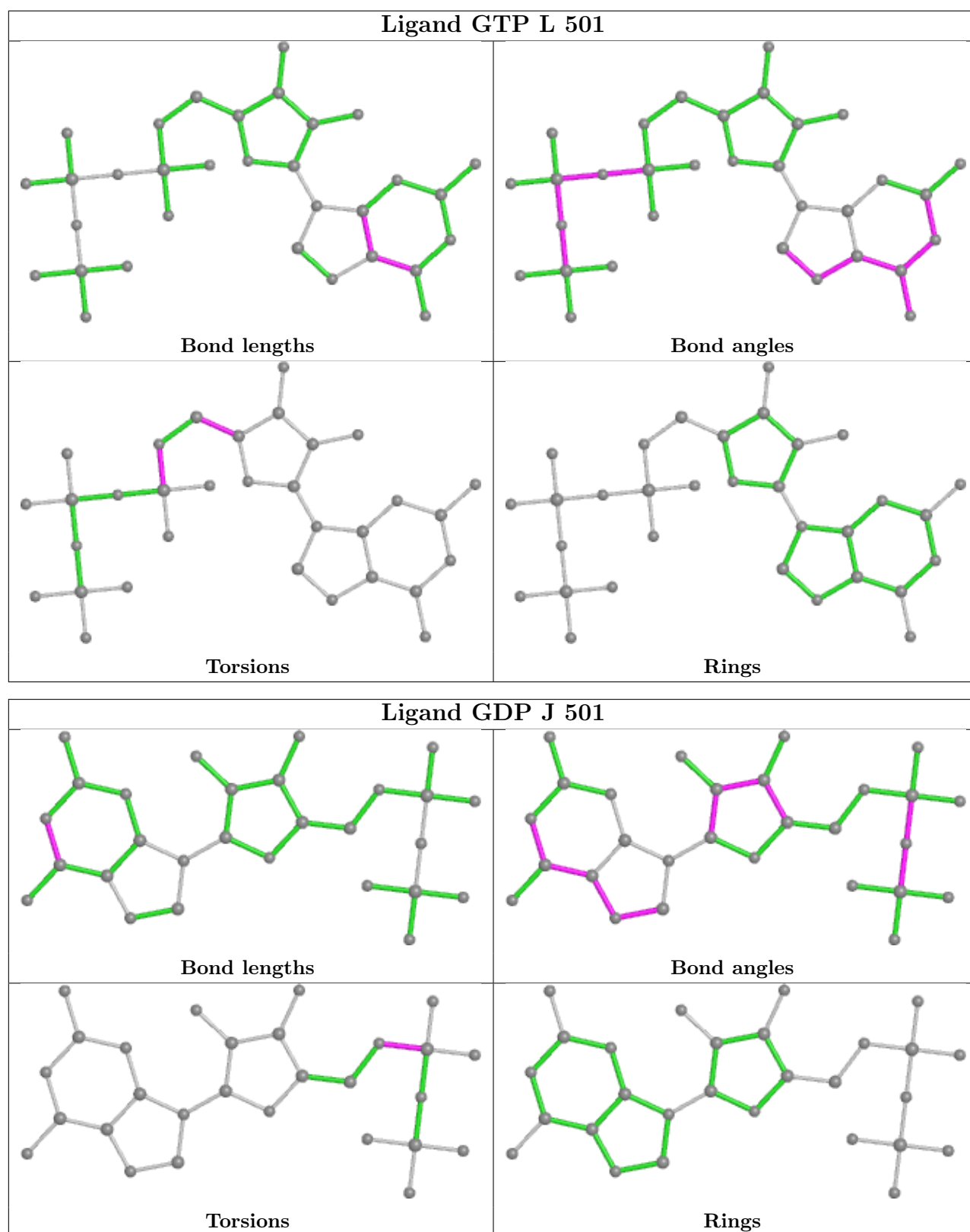


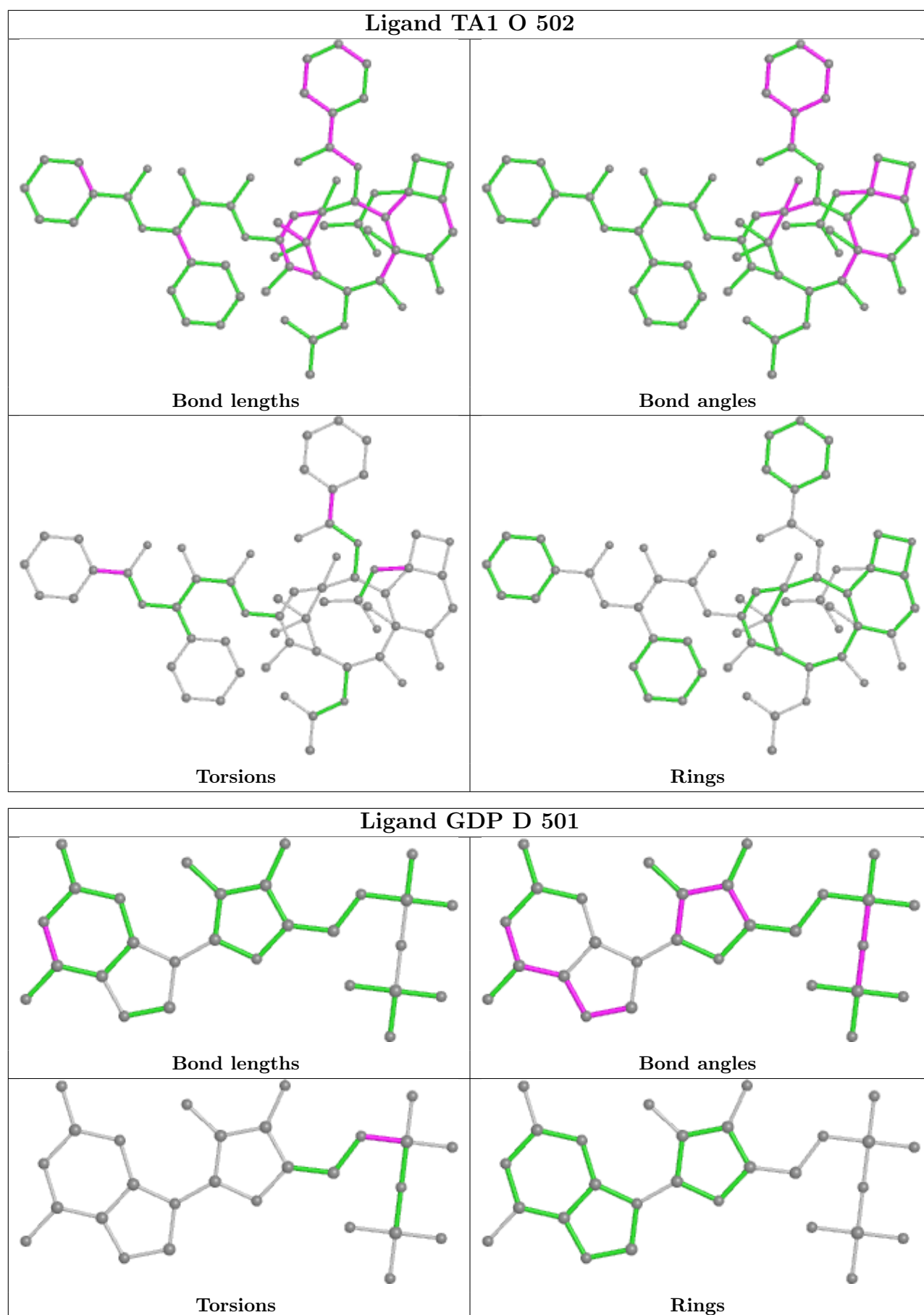


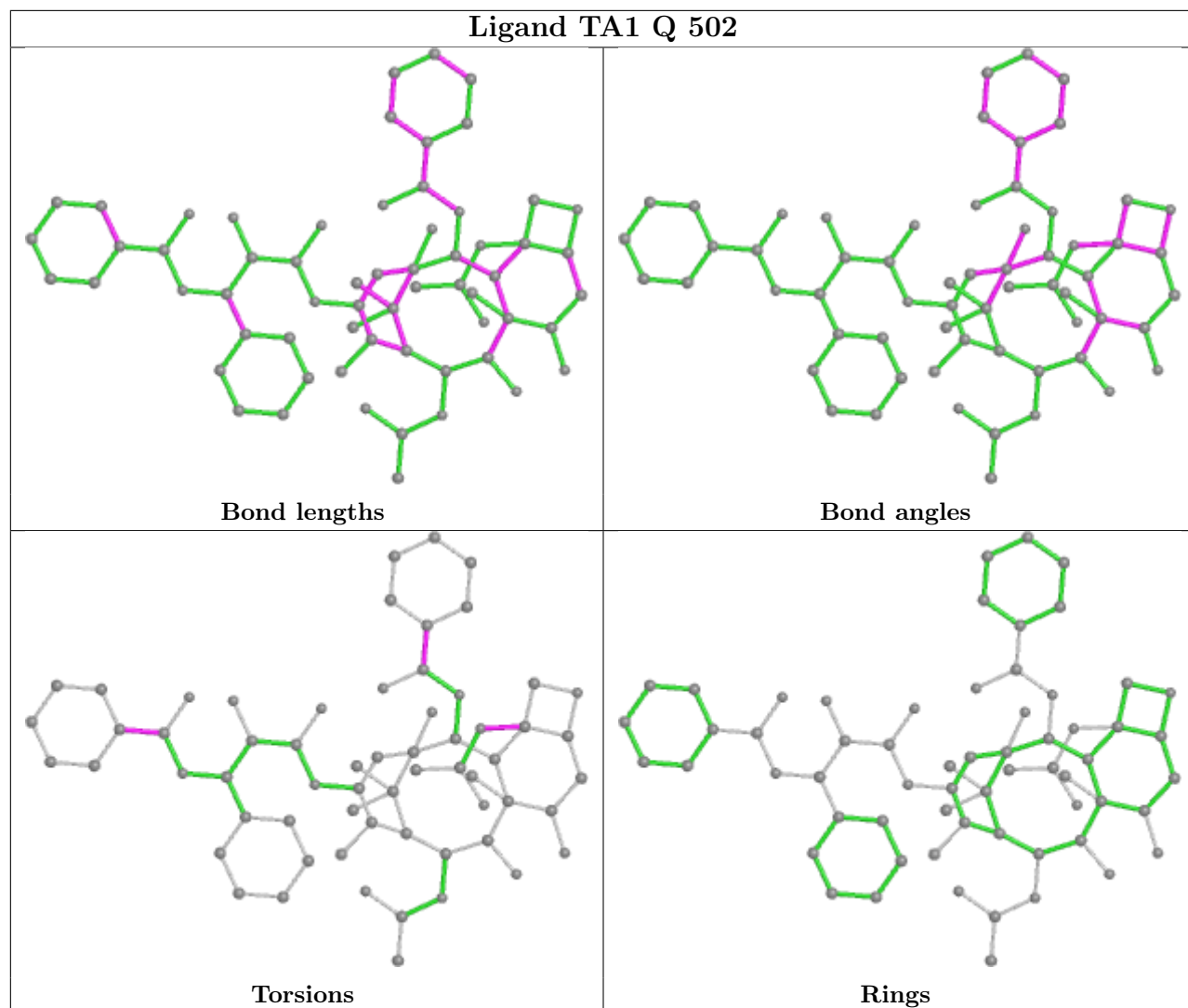


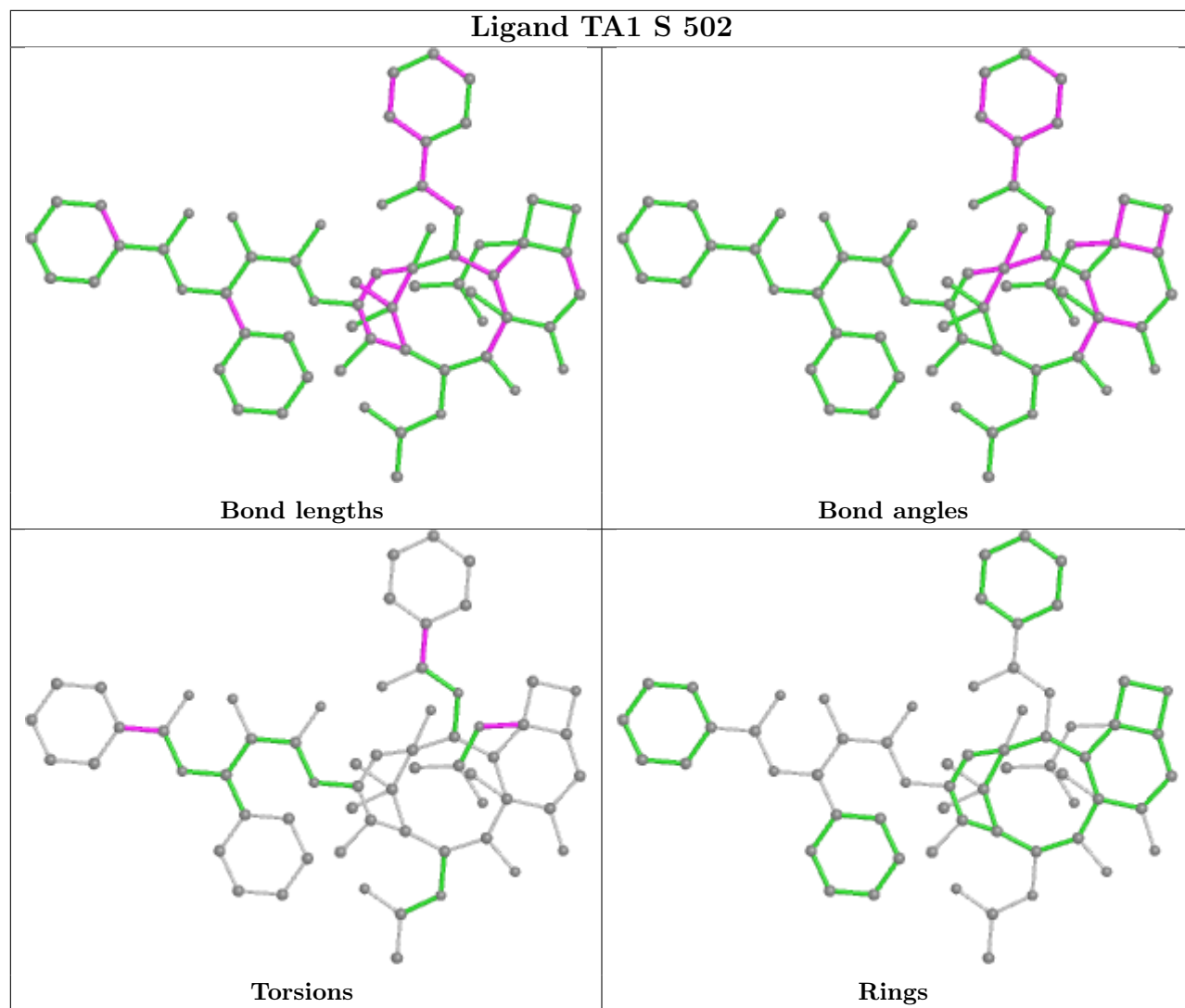




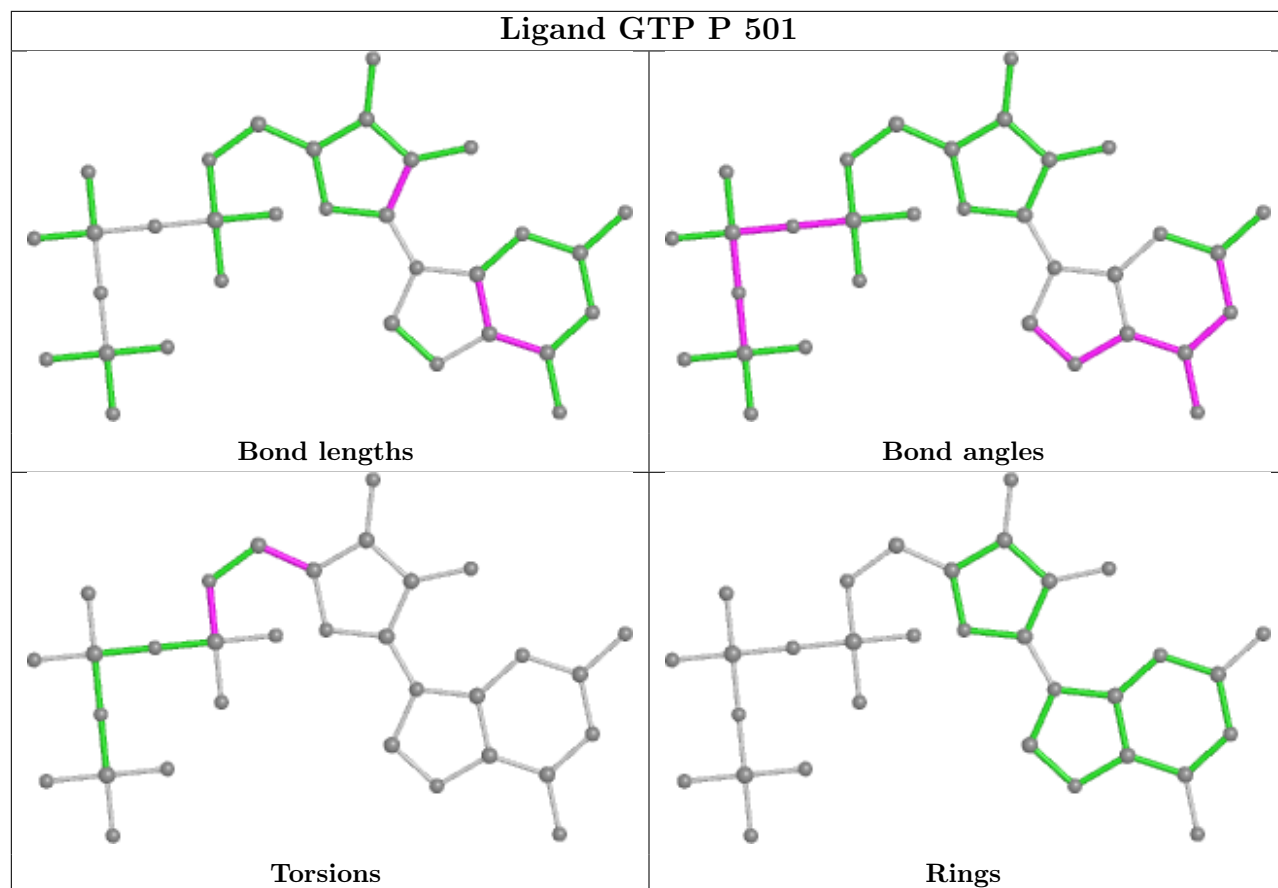


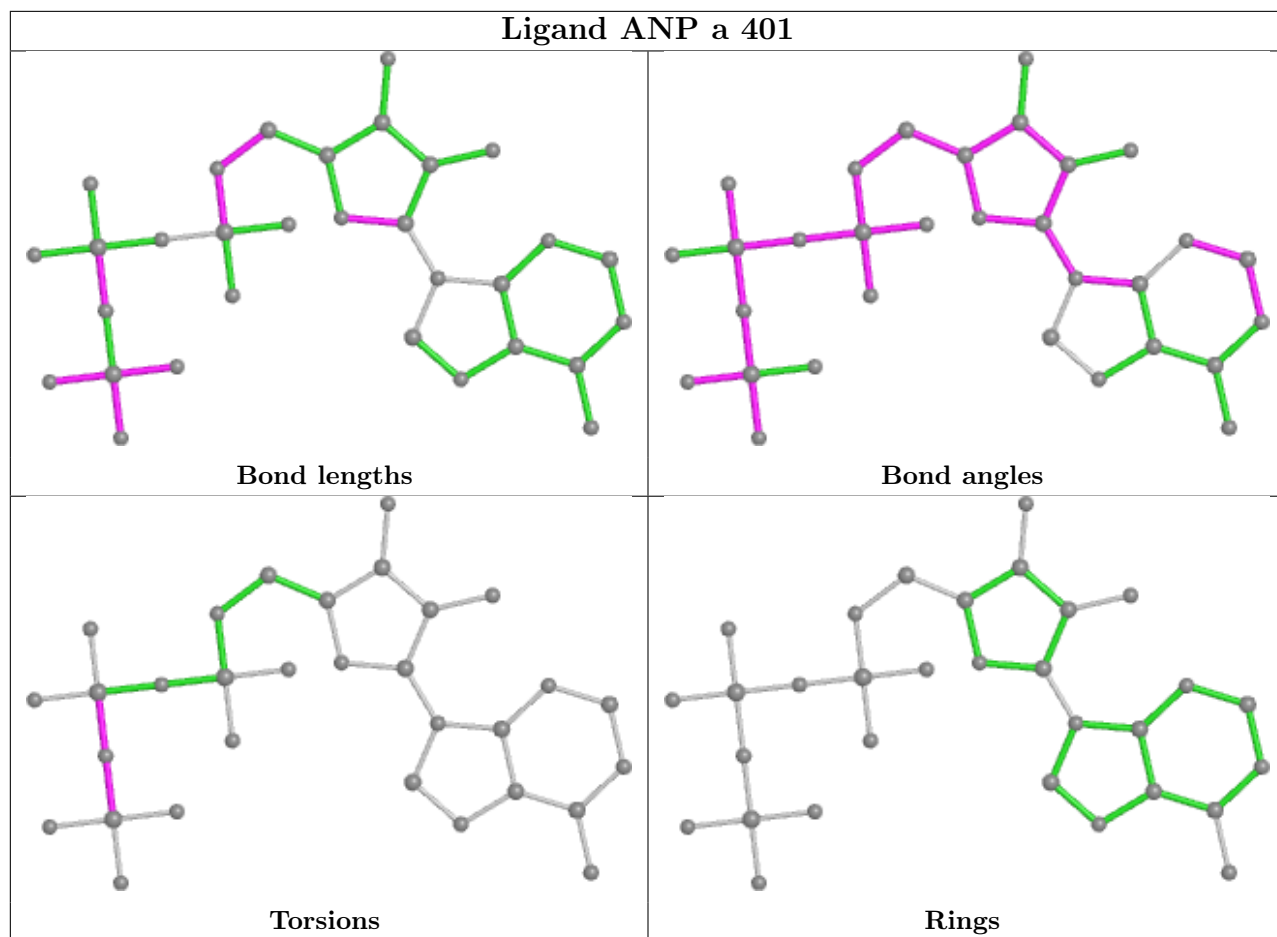


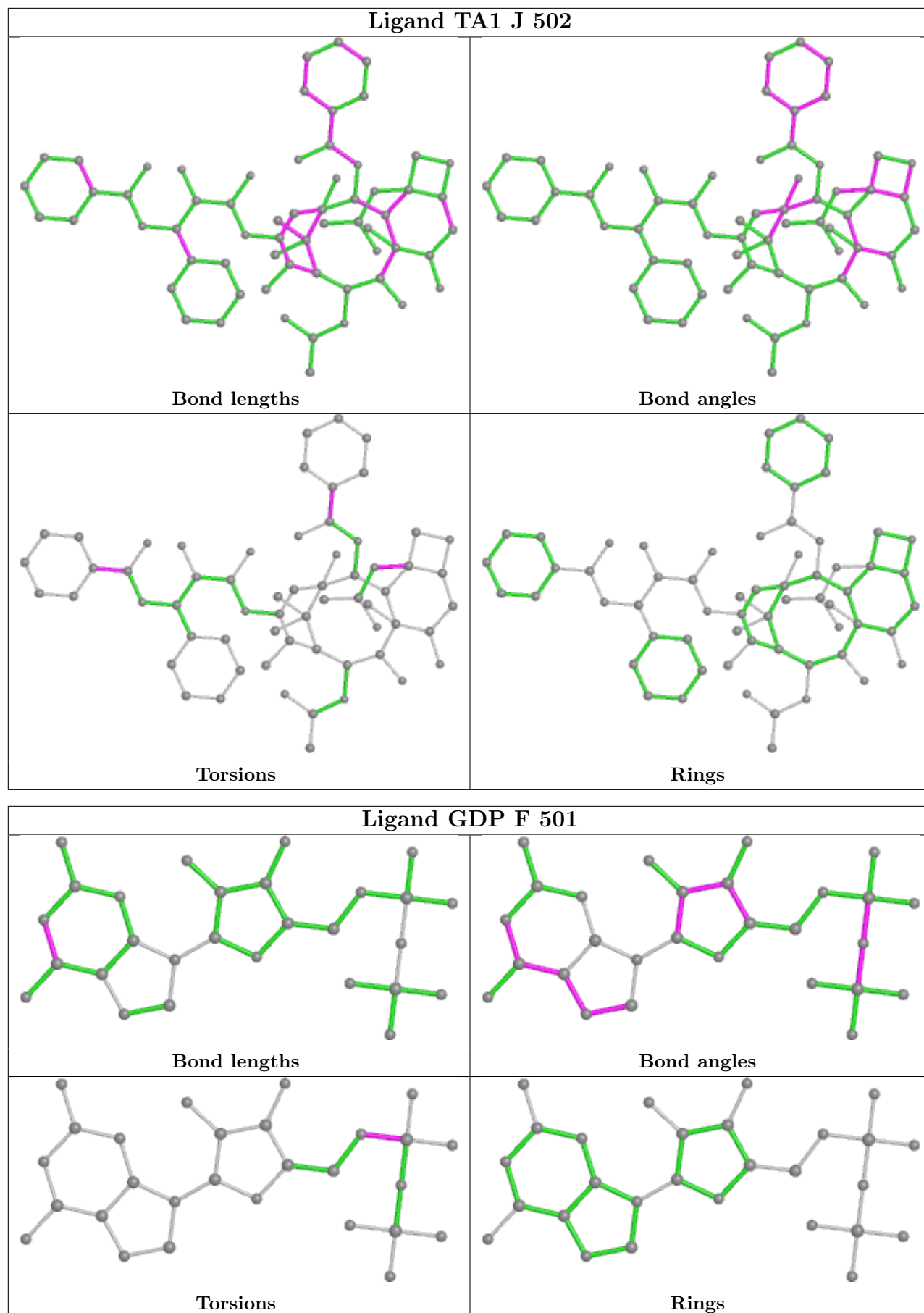


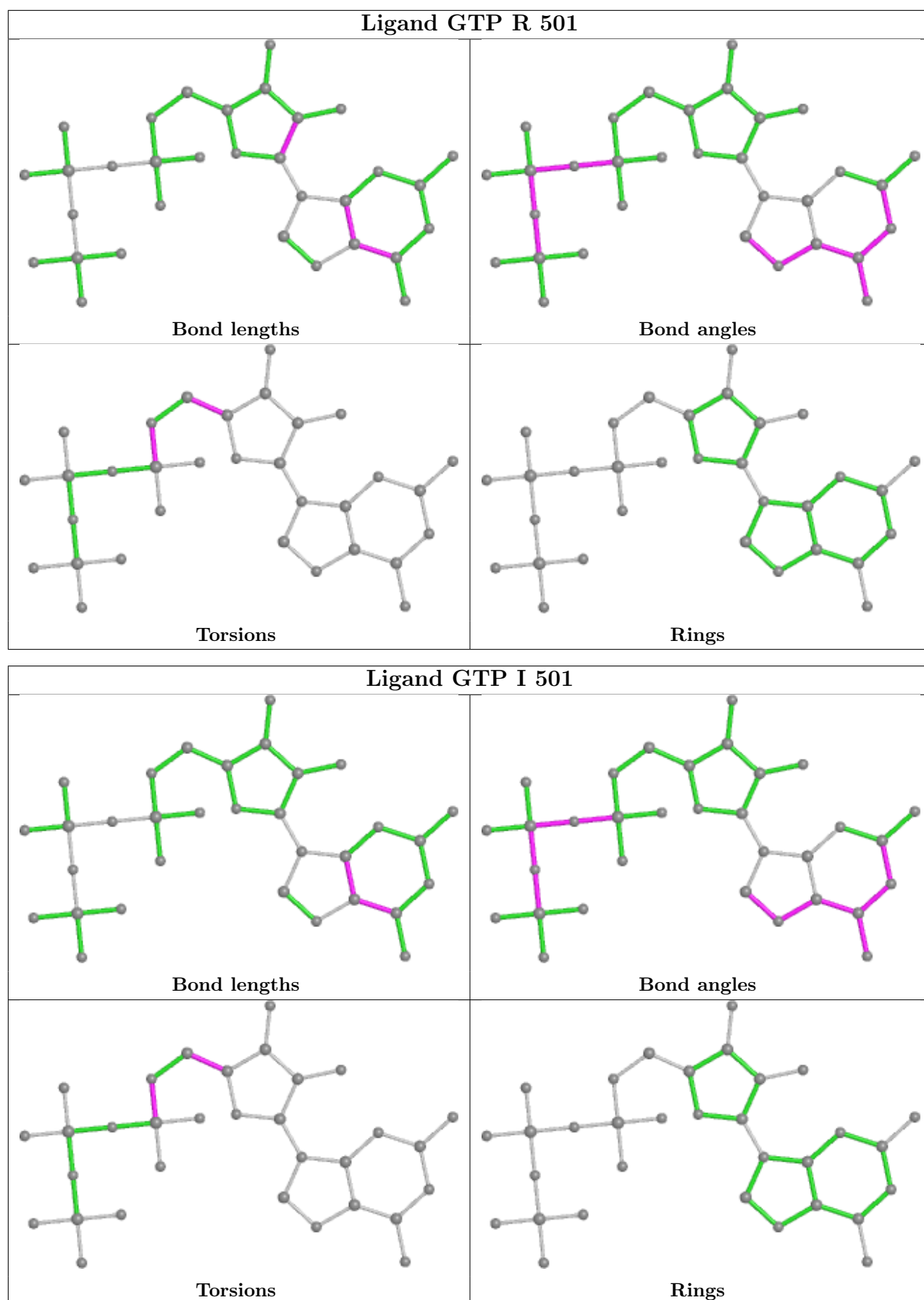


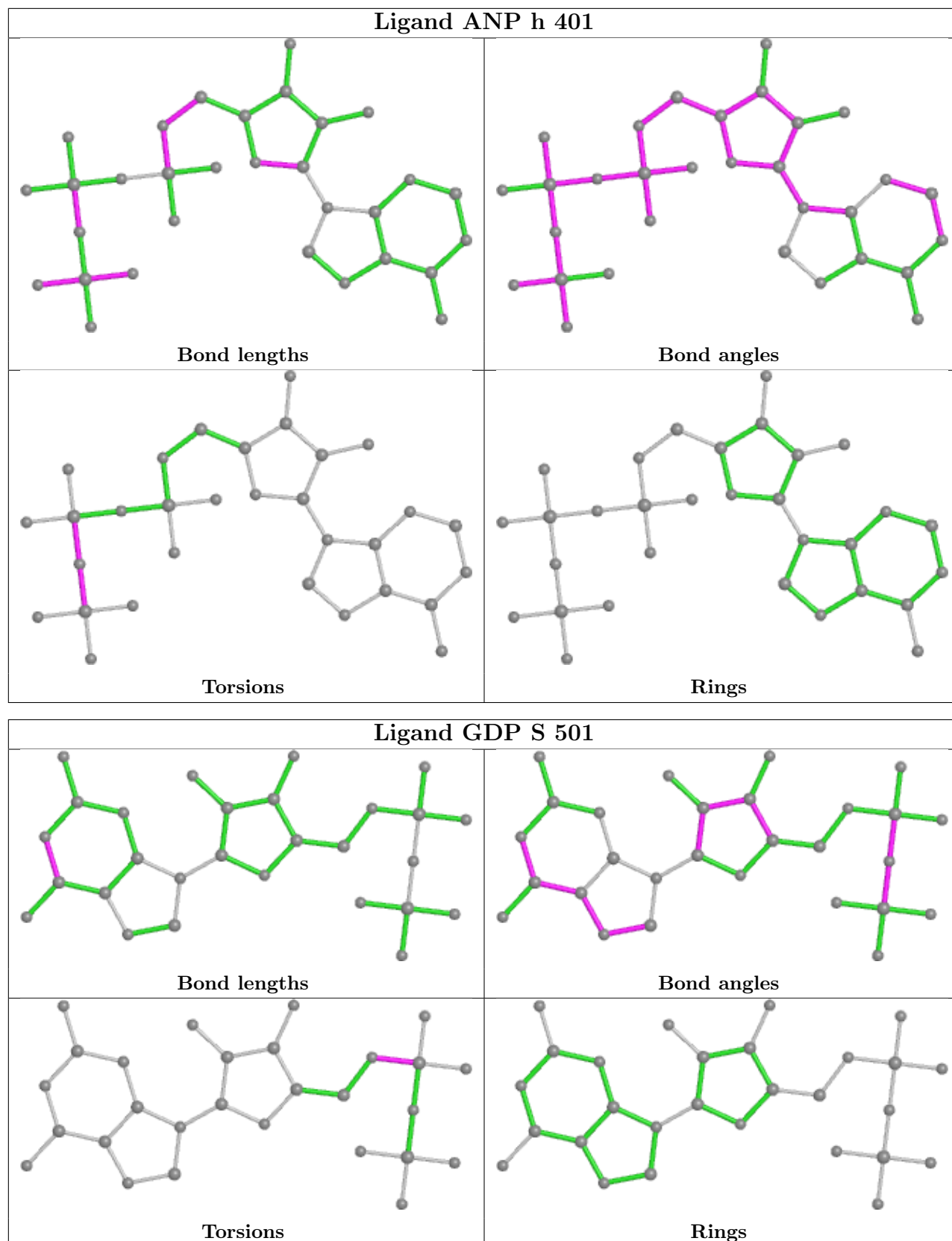


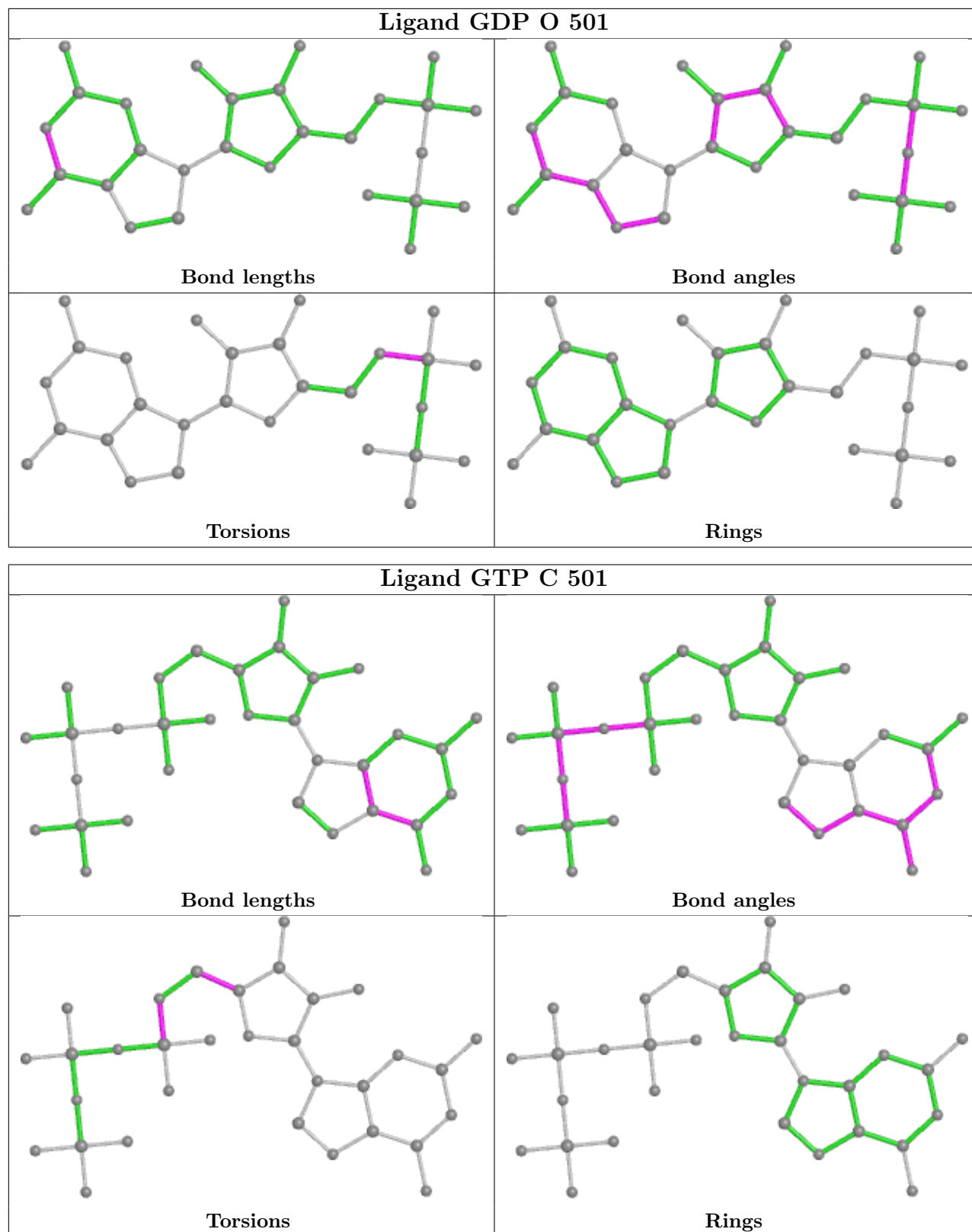


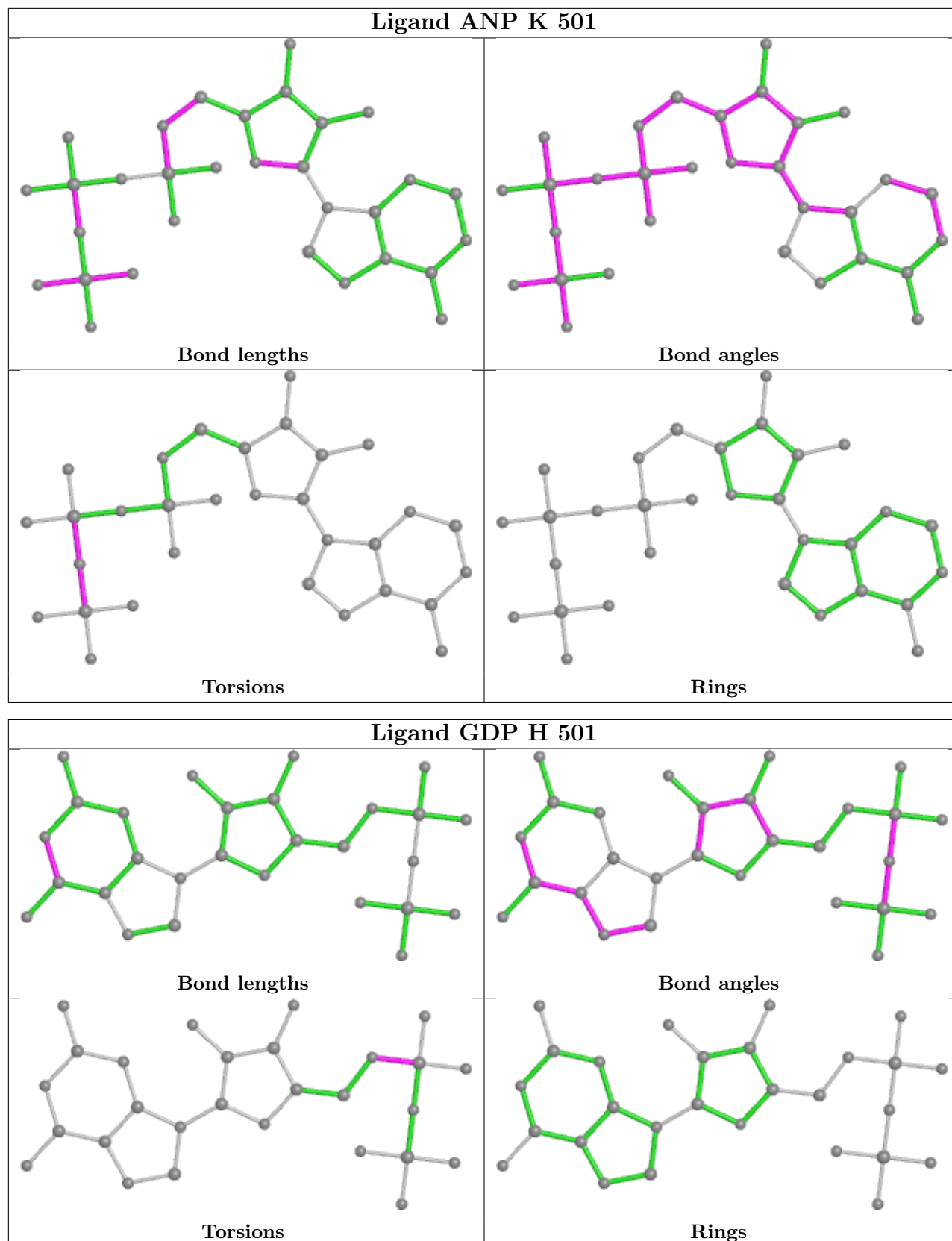


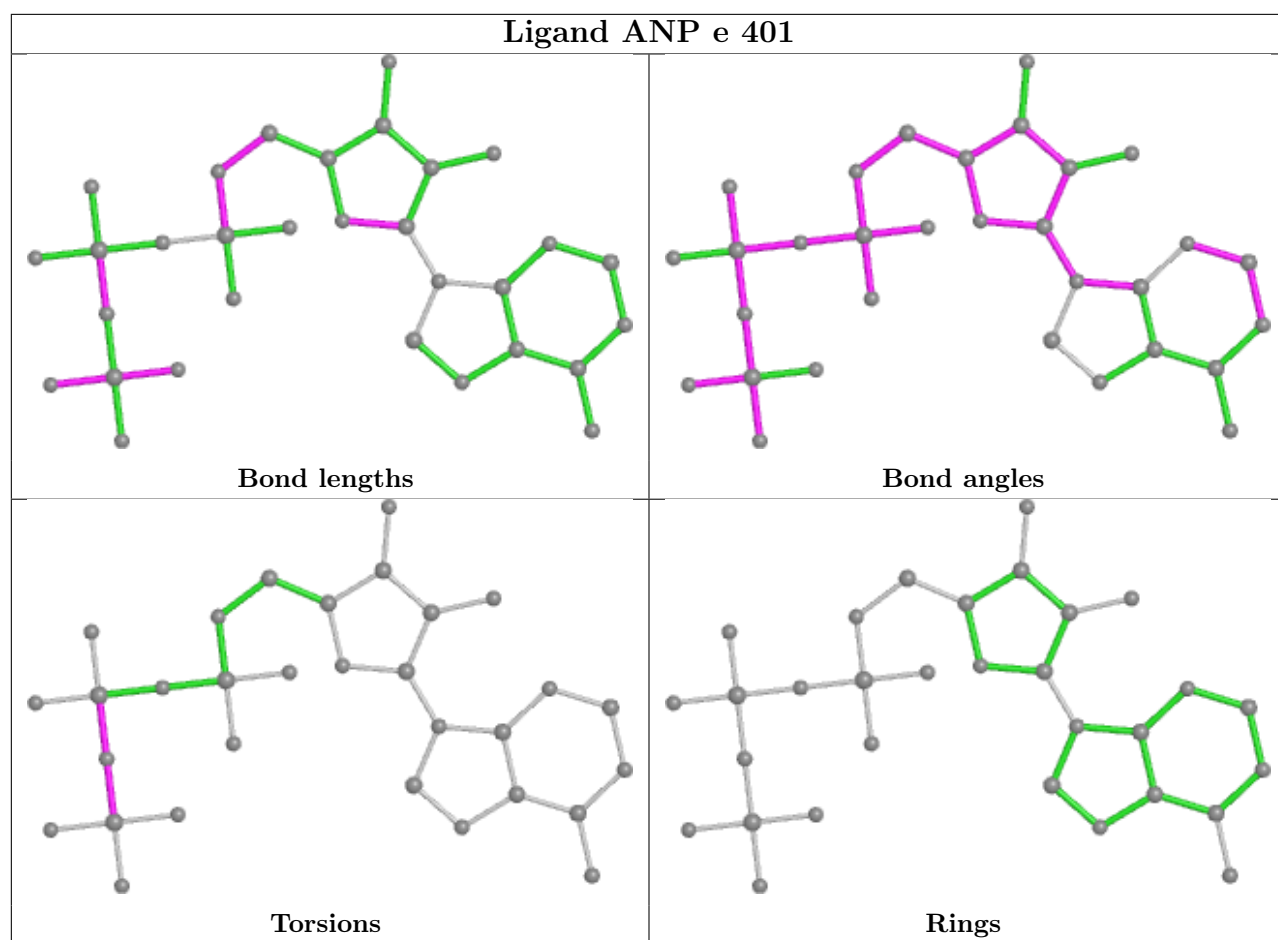




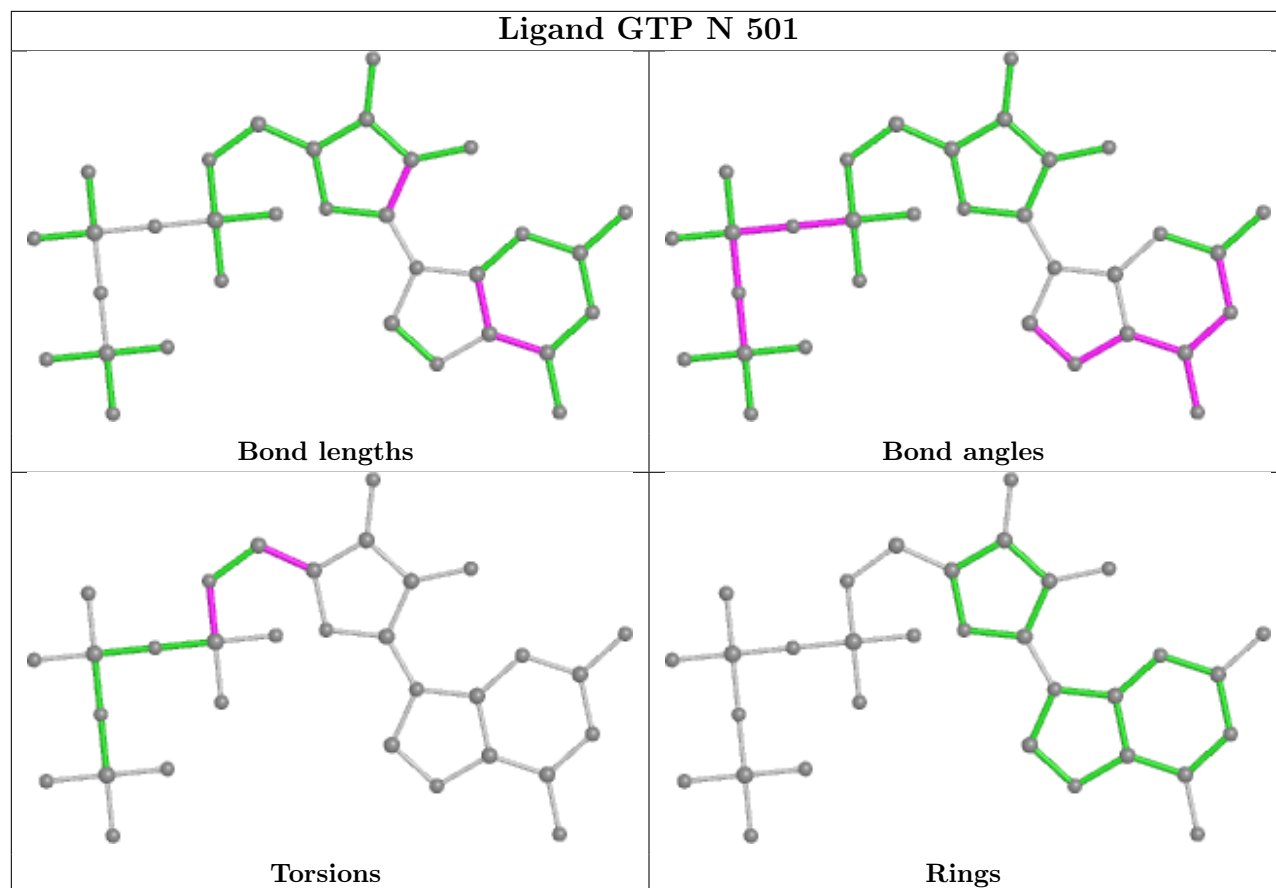


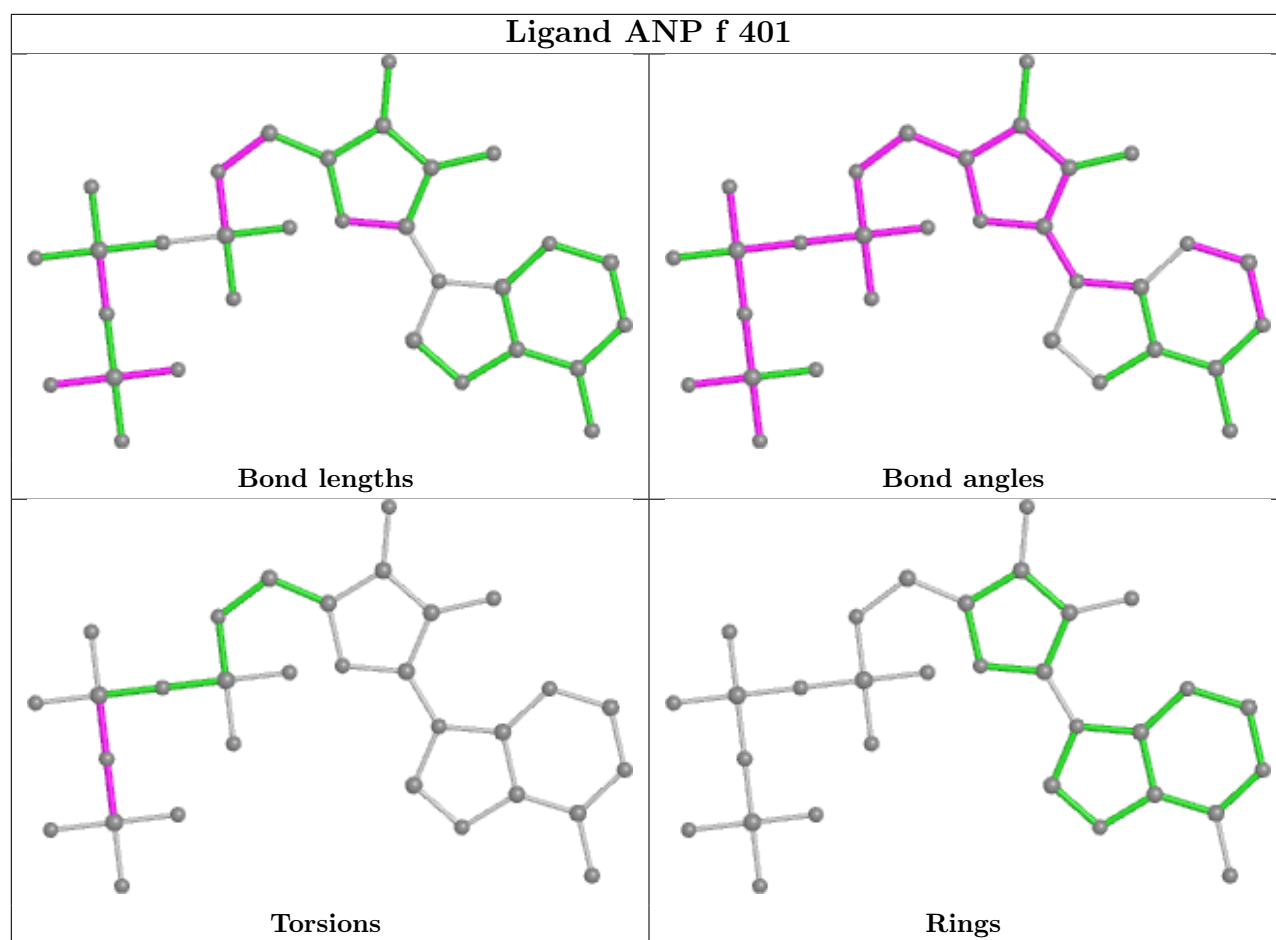












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

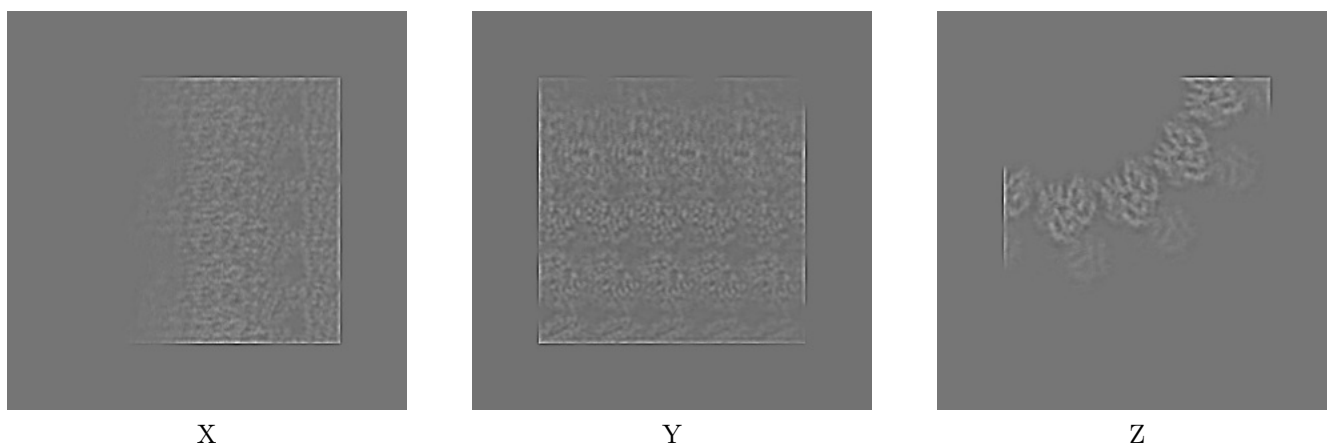
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24666. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

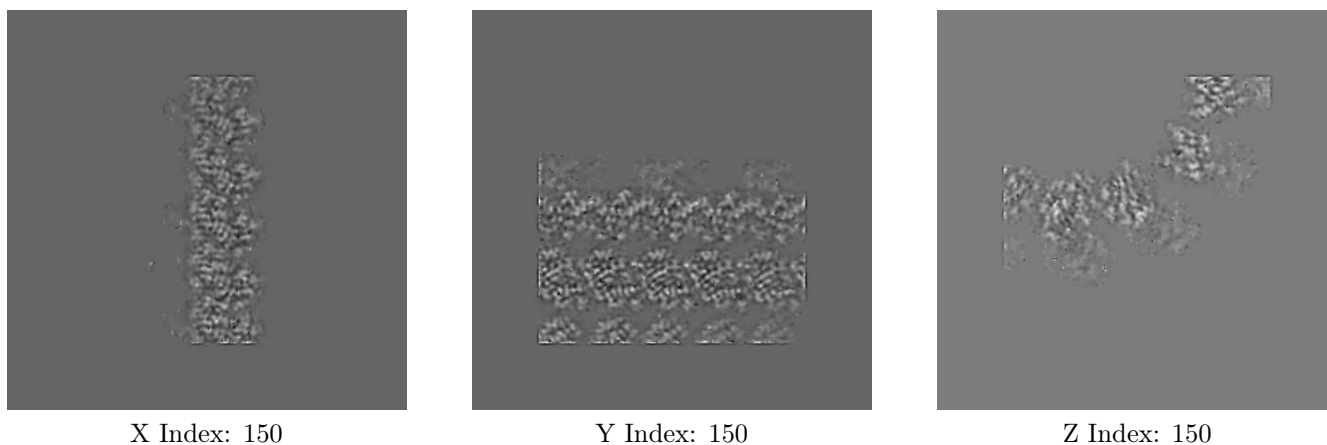
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

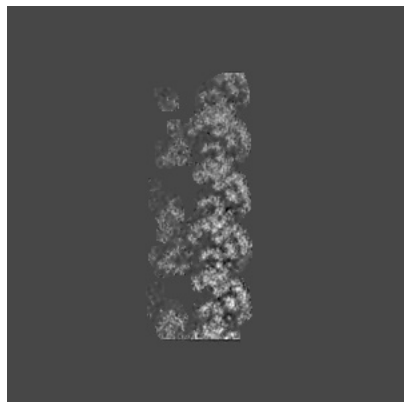
#### 6.2.1 Primary map



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

## 6.3 Largest variance slices [\(i\)](#)

### 6.3.1 Primary map



X Index: 50



Y Index: 249

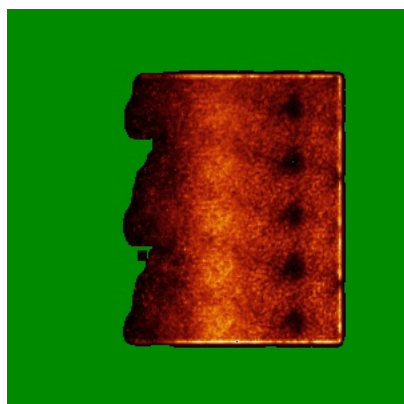


Z Index: 50

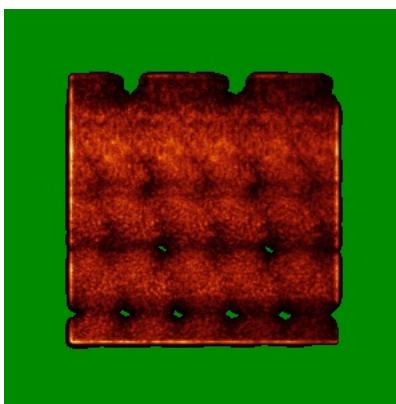
The images above show the largest variance slices of the map in three orthogonal directions.

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

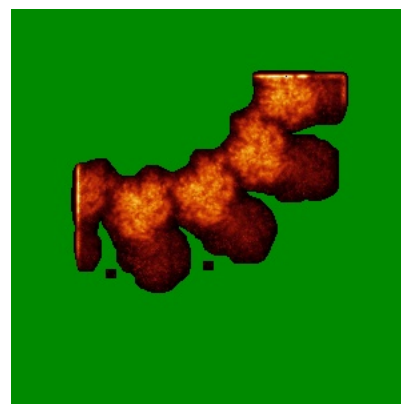
### 6.4.1 Primary map



X



Y

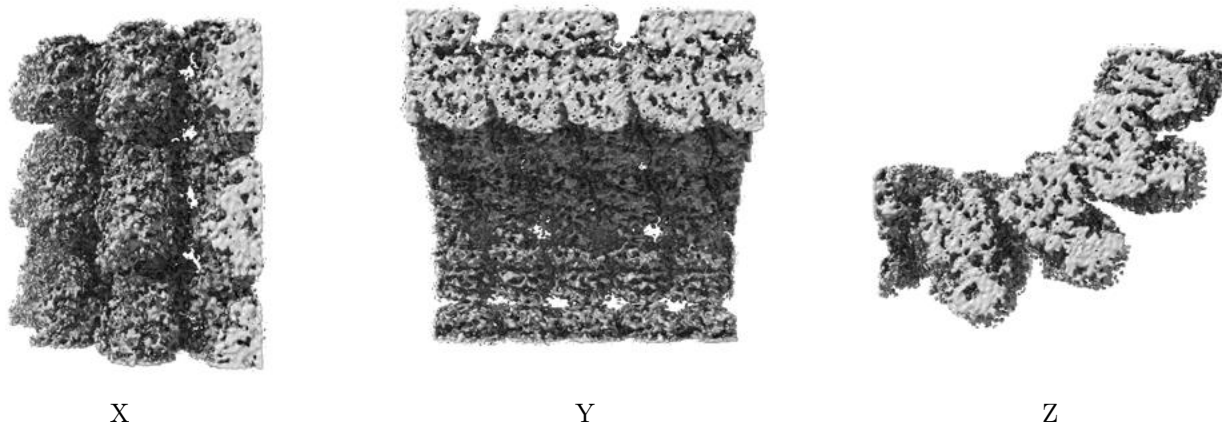


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

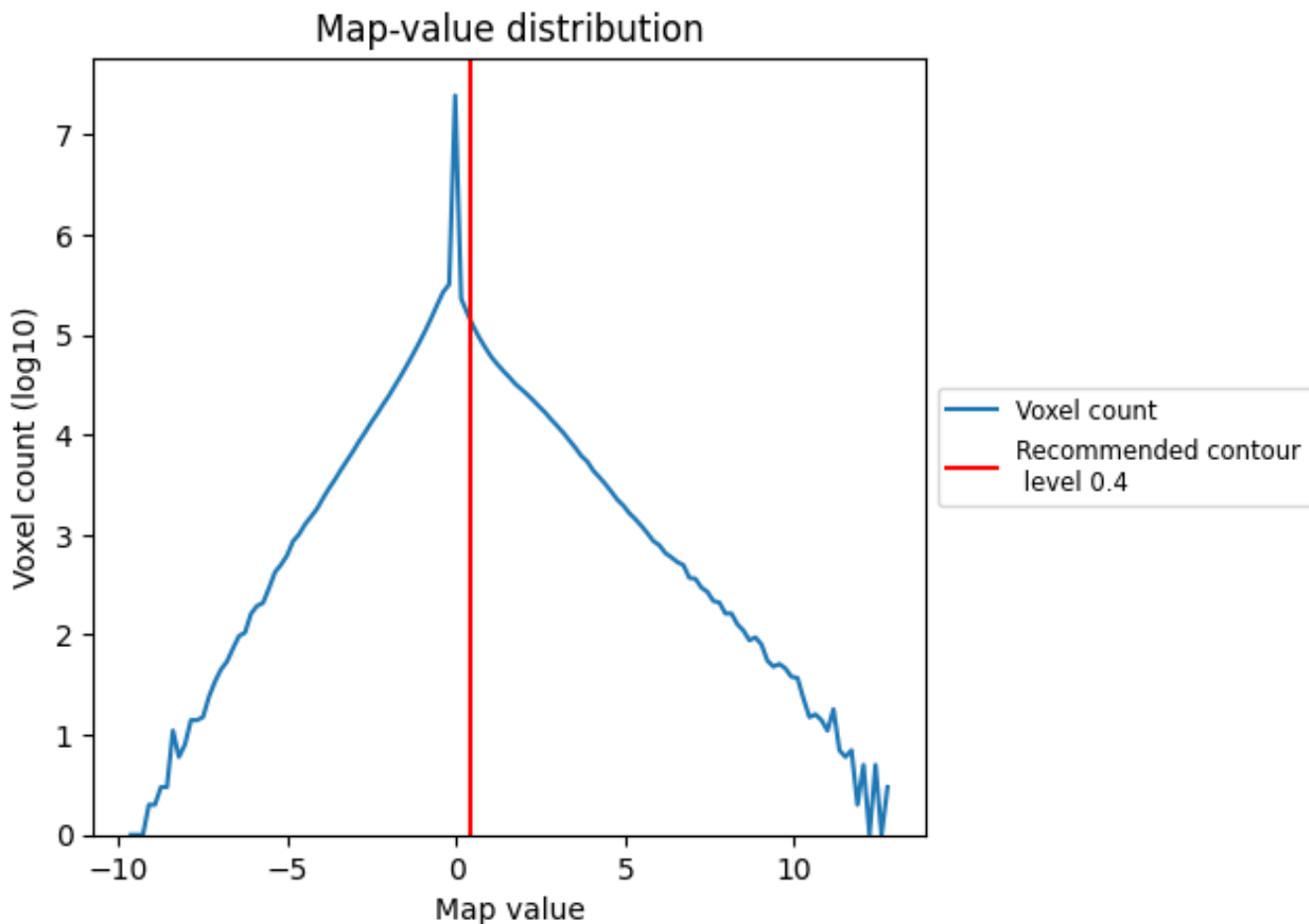
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

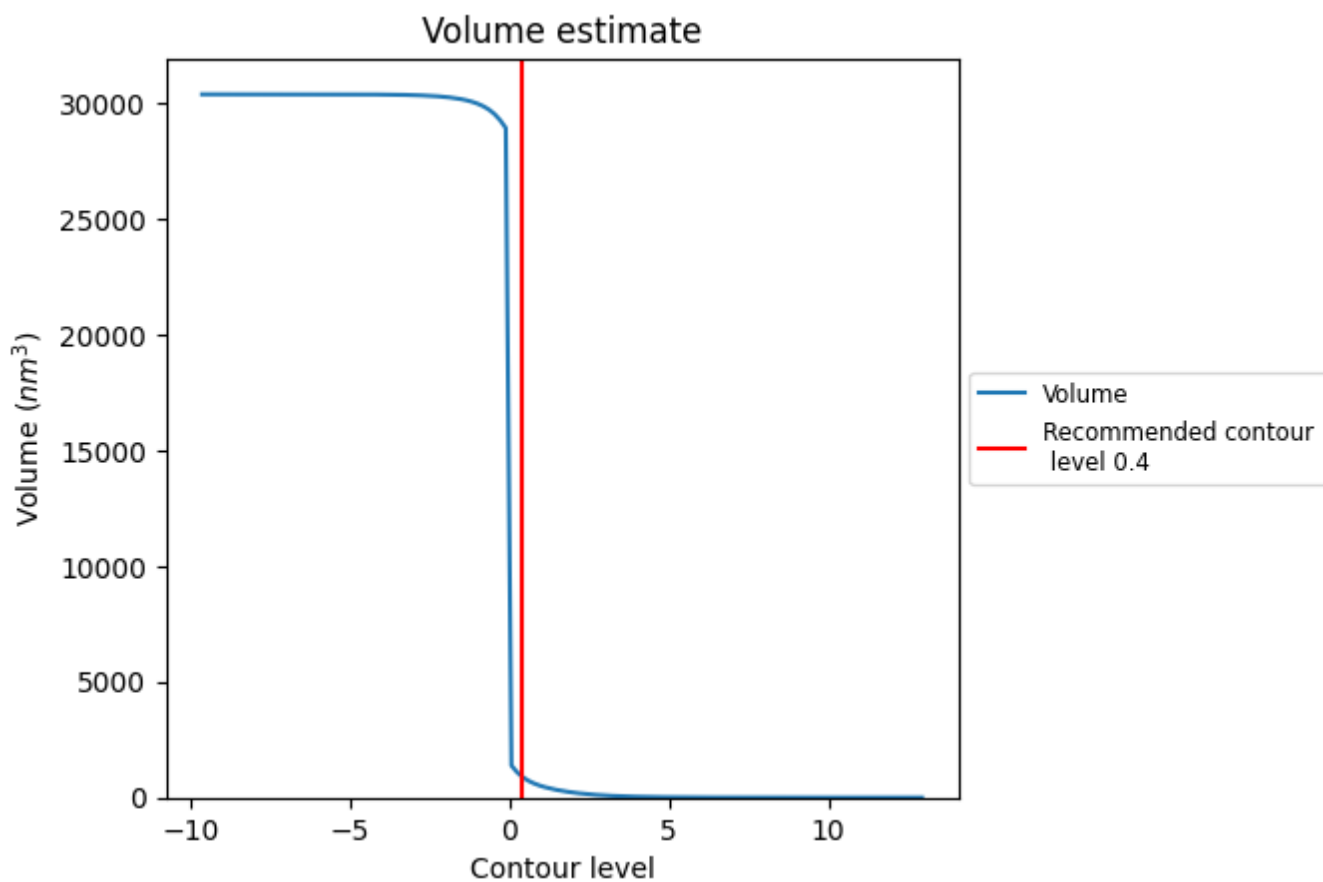
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

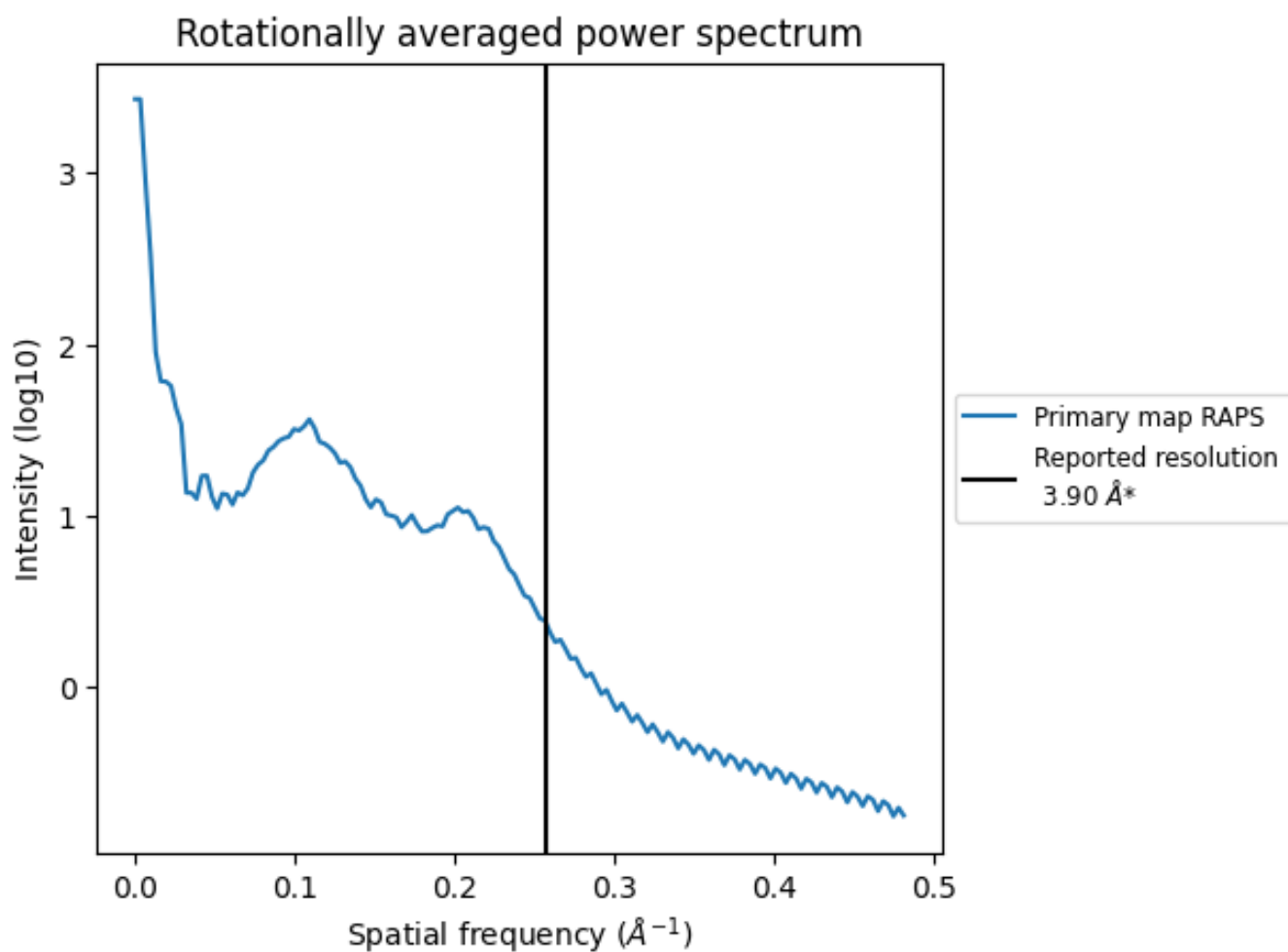
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 914 nm<sup>3</sup>; this corresponds to an approximate mass of 825 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum



\*Reported resolution corresponds to spatial frequency of  $0.256 \text{ \AA}^{-1}$



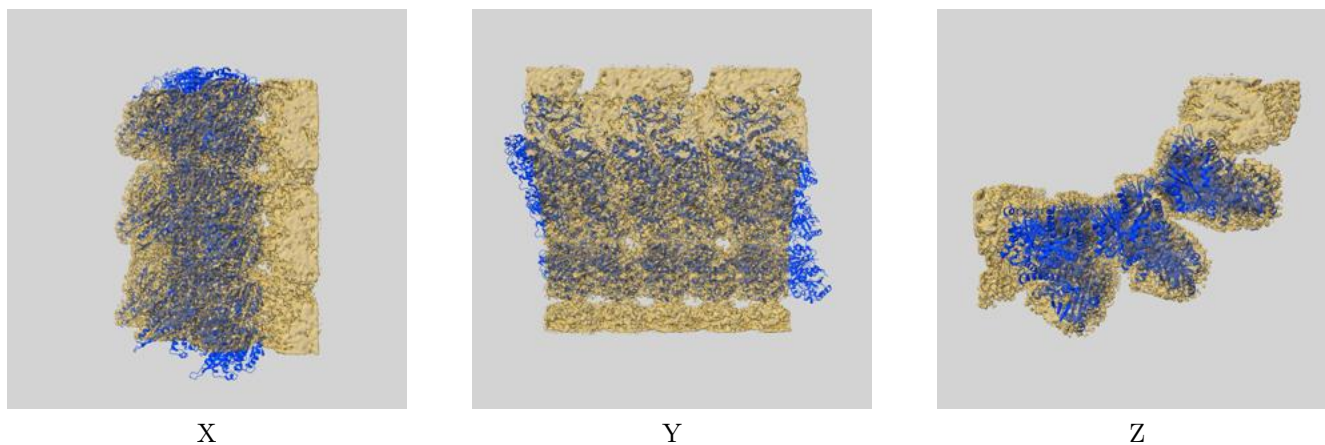
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

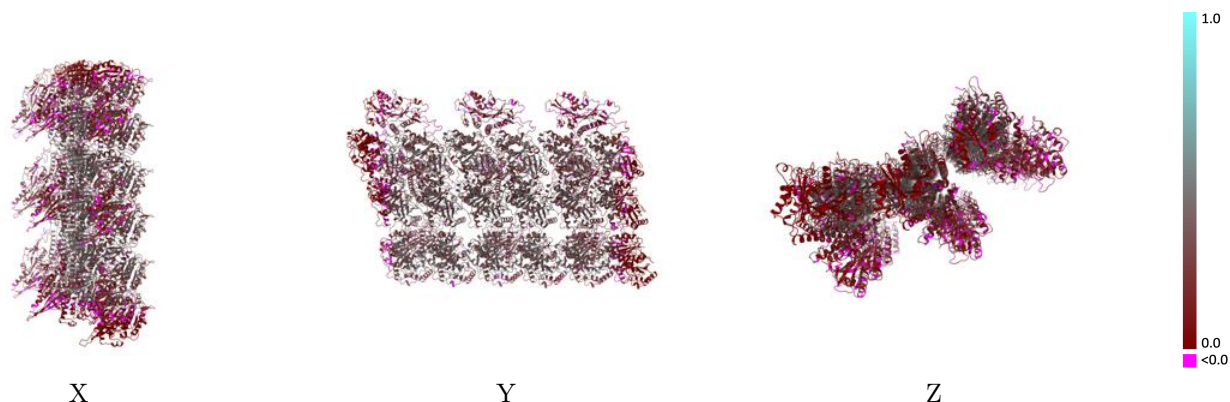
This section contains information regarding the fit between EMDB map EMD-24666 and PDB model 7RS5. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



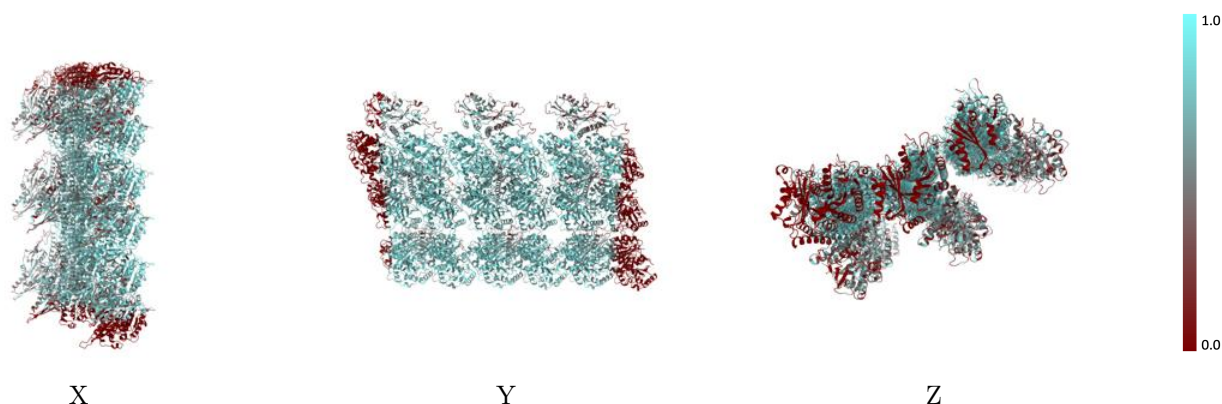
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



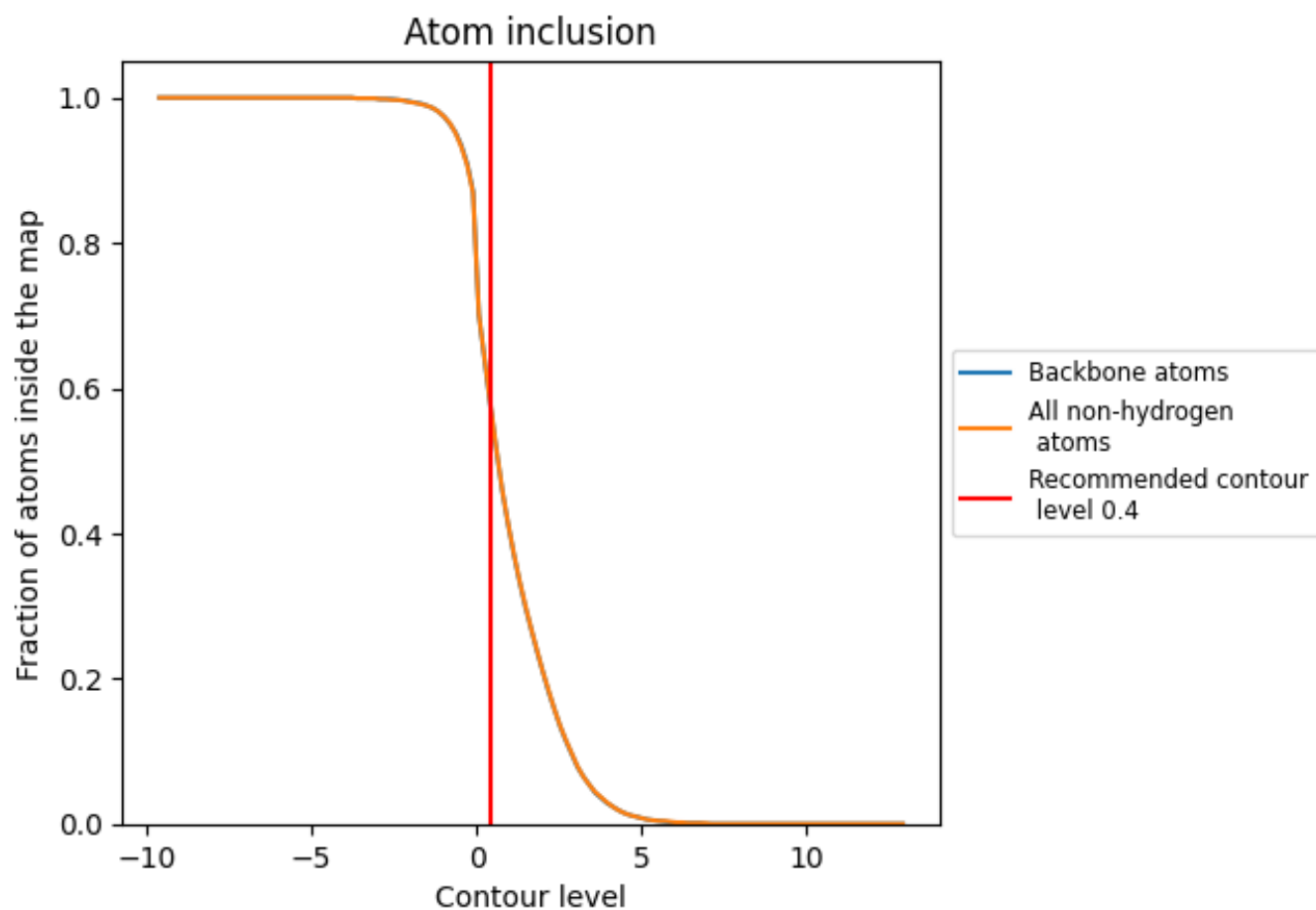
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5860	 0.2350
A	 0.7870	 0.3460
B	 0.7850	 0.3480
C	 0.7750	 0.3330
D	 0.7730	 0.3370
E	 0.7860	 0.3470
F	 0.7870	 0.3480
G	 0.7950	 0.3400
H	 0.5010	 0.2030
I	 0.3150	 0.1230
J	 0.7560	 0.3160
K	 0.4910	 0.1520
L	 0.7960	 0.3400
M	 0.3070	 0.1200
N	 0.5070	 0.1990
O	 0.7540	 0.3150
P	 0.7800	 0.3320
Q	 0.6550	 0.2690
R	 0.1420	 0.0560
S	 0.7440	 0.3050
a	 0.5060	 0.1490
b	 0.4880	 0.1540
c	 0.4640	 0.1270
d	 0.4360	 0.1210
e	 0.3620	 0.1000
f	 0.4440	 0.1190
g	 0.5310	 0.1540
h	 0.4030	 0.1030

