



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 09:06 PM EST

PDB ID : 7RNR
EMDB ID : EMD-24581
Title : Yeast CTP Synthase (Ura8) Bundle Bound to Substrates at Low pH
Authors : Hansen, J.M.; Lynch, E.M.; Farrell, D.P.; DiMaio, F.; Quispe, J.; Kollman, J.M.
Deposited on : 2021-07-29
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

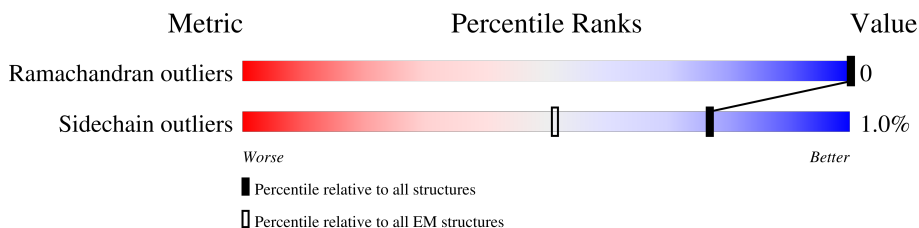
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)
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 ≥ 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	559	96% •
1	B	559	72% 96% •
1	E	559	72% 96% •
1	F	559	96% •
1	I	559	98% 96% •
1	J	559	15% 96% •
1	M	559	93% 96% •
1	N	559	88% 96% •
1	Q	559	10% 96% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	R	559	
1	S	559	
1	T	559	
1	Y	559	
1	Z	559	
1	a	559	
1	b	559	
1	g	559	
1	h	559	
1	k	559	
1	l	559	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UTP	A	605	X	-	-	-
4	UTP	B	601	X	-	-	-
4	UTP	E	603	X	-	-	-
4	UTP	F	601	X	-	-	-
4	UTP	I	605	X	-	-	-
4	UTP	J	601	X	-	-	-
4	UTP	M	603	X	-	-	-
4	UTP	N	601	X	-	-	-
4	UTP	Q	605	X	-	-	-
4	UTP	R	605	X	-	-	-
4	UTP	S	601	X	-	-	-
4	UTP	T	601	X	-	-	-
4	UTP	Y	603	X	-	-	-
4	UTP	Z	603	X	-	-	-
4	UTP	a	601	X	-	-	-
4	UTP	b	601	X	-	-	-
4	UTP	g	605	X	-	-	-
4	UTP	h	601	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UTP	k	603	X	-	-	-
4	UTP	l	601	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 177180 atoms, of which 88240 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 CTP synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	559	8778	2775	4393	757	833	20	0	0
1	E	559	8778	2775	4393	757	833	20	0	0
1	B	559	8778	2775	4393	757	833	20	0	0
1	F	559	8778	2775	4393	757	833	20	0	0
1	Q	559	8778	2775	4393	757	833	20	0	0
1	Y	559	8778	2775	4393	757	833	20	0	0
1	S	559	8778	2775	4393	757	833	20	0	0
1	a	559	8778	2775	4393	757	833	20	0	0
1	I	559	8778	2775	4393	757	833	20	0	0
1	M	559	8778	2775	4393	757	833	20	0	0
1	J	559	8778	2775	4393	757	833	20	0	0
1	N	559	8778	2775	4393	757	833	20	0	0
1	R	559	8778	2775	4393	757	833	20	0	0
1	Z	559	8778	2775	4393	757	833	20	0	0
1	T	559	8778	2775	4393	757	833	20	0	0
1	b	559	8778	2775	4393	757	833	20	0	0
1	g	559	8778	2775	4393	757	833	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	k	559	8778	2775	4393	757	833	20	0	0
1	h	559	8778	2775	4393	757	833	20	0	0
1	l	559	8778	2775	4393	757	833	20	0	0

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A6A5PYW3
A	?	-	MET	deletion	UNP A0A6A5PYW3
A	?	-	PRO	deletion	UNP A0A6A5PYW3
A	?	-	GLU	deletion	UNP A0A6A5PYW3
A	?	-	ILE	deletion	UNP A0A6A5PYW3
A	?	-	ASP	deletion	UNP A0A6A5PYW3
A	?	-	LYS	deletion	UNP A0A6A5PYW3
A	?	-	GLU	deletion	UNP A0A6A5PYW3
A	?	-	HIS	deletion	UNP A0A6A5PYW3
A	?	-	MET	deletion	UNP A0A6A5PYW3
A	?	-	GLY	deletion	UNP A0A6A5PYW3
A	?	-	GLY	deletion	UNP A0A6A5PYW3
E	?	-	TYR	deletion	UNP A0A6A5PYW3
E	?	-	MET	deletion	UNP A0A6A5PYW3
E	?	-	PRO	deletion	UNP A0A6A5PYW3
E	?	-	GLU	deletion	UNP A0A6A5PYW3
E	?	-	ILE	deletion	UNP A0A6A5PYW3
E	?	-	ASP	deletion	UNP A0A6A5PYW3
E	?	-	LYS	deletion	UNP A0A6A5PYW3
E	?	-	GLU	deletion	UNP A0A6A5PYW3
E	?	-	HIS	deletion	UNP A0A6A5PYW3
E	?	-	MET	deletion	UNP A0A6A5PYW3
E	?	-	GLY	deletion	UNP A0A6A5PYW3
E	?	-	GLY	deletion	UNP A0A6A5PYW3
B	?	-	TYR	deletion	UNP A0A6A5PYW3
B	?	-	MET	deletion	UNP A0A6A5PYW3
B	?	-	PRO	deletion	UNP A0A6A5PYW3
B	?	-	GLU	deletion	UNP A0A6A5PYW3
B	?	-	ILE	deletion	UNP A0A6A5PYW3
B	?	-	ASP	deletion	UNP A0A6A5PYW3
B	?	-	LYS	deletion	UNP A0A6A5PYW3
B	?	-	GLU	deletion	UNP A0A6A5PYW3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	HIS	deletion	UNP A0A6A5PYW3
B	?	-	MET	deletion	UNP A0A6A5PYW3
B	?	-	GLY	deletion	UNP A0A6A5PYW3
B	?	-	GLY	deletion	UNP A0A6A5PYW3
F	?	-	TYR	deletion	UNP A0A6A5PYW3
F	?	-	MET	deletion	UNP A0A6A5PYW3
F	?	-	PRO	deletion	UNP A0A6A5PYW3
F	?	-	GLU	deletion	UNP A0A6A5PYW3
F	?	-	ILE	deletion	UNP A0A6A5PYW3
F	?	-	ASP	deletion	UNP A0A6A5PYW3
F	?	-	LYS	deletion	UNP A0A6A5PYW3
F	?	-	GLU	deletion	UNP A0A6A5PYW3
F	?	-	HIS	deletion	UNP A0A6A5PYW3
F	?	-	MET	deletion	UNP A0A6A5PYW3
F	?	-	GLY	deletion	UNP A0A6A5PYW3
F	?	-	GLY	deletion	UNP A0A6A5PYW3
Q	?	-	TYR	deletion	UNP A0A6A5PYW3
Q	?	-	MET	deletion	UNP A0A6A5PYW3
Q	?	-	PRO	deletion	UNP A0A6A5PYW3
Q	?	-	GLU	deletion	UNP A0A6A5PYW3
Q	?	-	ILE	deletion	UNP A0A6A5PYW3
Q	?	-	ASP	deletion	UNP A0A6A5PYW3
Q	?	-	LYS	deletion	UNP A0A6A5PYW3
Q	?	-	GLU	deletion	UNP A0A6A5PYW3
Q	?	-	HIS	deletion	UNP A0A6A5PYW3
Q	?	-	MET	deletion	UNP A0A6A5PYW3
Q	?	-	GLY	deletion	UNP A0A6A5PYW3
Q	?	-	GLY	deletion	UNP A0A6A5PYW3
Y	?	-	TYR	deletion	UNP A0A6A5PYW3
Y	?	-	MET	deletion	UNP A0A6A5PYW3
Y	?	-	PRO	deletion	UNP A0A6A5PYW3
Y	?	-	GLU	deletion	UNP A0A6A5PYW3
Y	?	-	ILE	deletion	UNP A0A6A5PYW3
Y	?	-	ASP	deletion	UNP A0A6A5PYW3
Y	?	-	LYS	deletion	UNP A0A6A5PYW3
Y	?	-	GLU	deletion	UNP A0A6A5PYW3
Y	?	-	HIS	deletion	UNP A0A6A5PYW3
Y	?	-	MET	deletion	UNP A0A6A5PYW3
Y	?	-	GLY	deletion	UNP A0A6A5PYW3
Y	?	-	GLY	deletion	UNP A0A6A5PYW3
S	?	-	TYR	deletion	UNP A0A6A5PYW3
S	?	-	MET	deletion	UNP A0A6A5PYW3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
S	?	-	PRO	deletion	UNP A0A6A5PYW3
S	?	-	GLU	deletion	UNP A0A6A5PYW3
S	?	-	ILE	deletion	UNP A0A6A5PYW3
S	?	-	ASP	deletion	UNP A0A6A5PYW3
S	?	-	LYS	deletion	UNP A0A6A5PYW3
S	?	-	GLU	deletion	UNP A0A6A5PYW3
S	?	-	HIS	deletion	UNP A0A6A5PYW3
S	?	-	MET	deletion	UNP A0A6A5PYW3
S	?	-	GLY	deletion	UNP A0A6A5PYW3
S	?	-	GLY	deletion	UNP A0A6A5PYW3
a	?	-	TYR	deletion	UNP A0A6A5PYW3
a	?	-	MET	deletion	UNP A0A6A5PYW3
a	?	-	PRO	deletion	UNP A0A6A5PYW3
a	?	-	GLU	deletion	UNP A0A6A5PYW3
a	?	-	ILE	deletion	UNP A0A6A5PYW3
a	?	-	ASP	deletion	UNP A0A6A5PYW3
a	?	-	LYS	deletion	UNP A0A6A5PYW3
a	?	-	GLU	deletion	UNP A0A6A5PYW3
a	?	-	HIS	deletion	UNP A0A6A5PYW3
a	?	-	MET	deletion	UNP A0A6A5PYW3
a	?	-	GLY	deletion	UNP A0A6A5PYW3
a	?	-	GLY	deletion	UNP A0A6A5PYW3
I	?	-	TYR	deletion	UNP A0A6A5PYW3
I	?	-	MET	deletion	UNP A0A6A5PYW3
I	?	-	PRO	deletion	UNP A0A6A5PYW3
I	?	-	GLU	deletion	UNP A0A6A5PYW3
I	?	-	ILE	deletion	UNP A0A6A5PYW3
I	?	-	ASP	deletion	UNP A0A6A5PYW3
I	?	-	LYS	deletion	UNP A0A6A5PYW3
I	?	-	GLU	deletion	UNP A0A6A5PYW3
I	?	-	HIS	deletion	UNP A0A6A5PYW3
I	?	-	MET	deletion	UNP A0A6A5PYW3
I	?	-	GLY	deletion	UNP A0A6A5PYW3
I	?	-	GLY	deletion	UNP A0A6A5PYW3
M	?	-	TYR	deletion	UNP A0A6A5PYW3
M	?	-	MET	deletion	UNP A0A6A5PYW3
M	?	-	PRO	deletion	UNP A0A6A5PYW3
M	?	-	GLU	deletion	UNP A0A6A5PYW3
M	?	-	ILE	deletion	UNP A0A6A5PYW3
M	?	-	ASP	deletion	UNP A0A6A5PYW3
M	?	-	LYS	deletion	UNP A0A6A5PYW3
M	?	-	GLU	deletion	UNP A0A6A5PYW3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	HIS	deletion	UNP A0A6A5PYW3
M	?	-	MET	deletion	UNP A0A6A5PYW3
M	?	-	GLY	deletion	UNP A0A6A5PYW3
M	?	-	GLY	deletion	UNP A0A6A5PYW3
J	?	-	TYR	deletion	UNP A0A6A5PYW3
J	?	-	MET	deletion	UNP A0A6A5PYW3
J	?	-	PRO	deletion	UNP A0A6A5PYW3
J	?	-	GLU	deletion	UNP A0A6A5PYW3
J	?	-	ILE	deletion	UNP A0A6A5PYW3
J	?	-	ASP	deletion	UNP A0A6A5PYW3
J	?	-	LYS	deletion	UNP A0A6A5PYW3
J	?	-	GLU	deletion	UNP A0A6A5PYW3
J	?	-	HIS	deletion	UNP A0A6A5PYW3
J	?	-	MET	deletion	UNP A0A6A5PYW3
J	?	-	GLY	deletion	UNP A0A6A5PYW3
J	?	-	GLY	deletion	UNP A0A6A5PYW3
N	?	-	TYR	deletion	UNP A0A6A5PYW3
N	?	-	MET	deletion	UNP A0A6A5PYW3
N	?	-	PRO	deletion	UNP A0A6A5PYW3
N	?	-	GLU	deletion	UNP A0A6A5PYW3
N	?	-	ILE	deletion	UNP A0A6A5PYW3
N	?	-	ASP	deletion	UNP A0A6A5PYW3
N	?	-	LYS	deletion	UNP A0A6A5PYW3
N	?	-	GLU	deletion	UNP A0A6A5PYW3
N	?	-	HIS	deletion	UNP A0A6A5PYW3
N	?	-	MET	deletion	UNP A0A6A5PYW3
N	?	-	GLY	deletion	UNP A0A6A5PYW3
N	?	-	GLY	deletion	UNP A0A6A5PYW3
R	?	-	TYR	deletion	UNP A0A6A5PYW3
R	?	-	MET	deletion	UNP A0A6A5PYW3
R	?	-	PRO	deletion	UNP A0A6A5PYW3
R	?	-	GLU	deletion	UNP A0A6A5PYW3
R	?	-	ILE	deletion	UNP A0A6A5PYW3
R	?	-	ASP	deletion	UNP A0A6A5PYW3
R	?	-	LYS	deletion	UNP A0A6A5PYW3
R	?	-	GLU	deletion	UNP A0A6A5PYW3
R	?	-	HIS	deletion	UNP A0A6A5PYW3
R	?	-	MET	deletion	UNP A0A6A5PYW3
R	?	-	GLY	deletion	UNP A0A6A5PYW3
R	?	-	GLY	deletion	UNP A0A6A5PYW3
Z	?	-	TYR	deletion	UNP A0A6A5PYW3
Z	?	-	MET	deletion	UNP A0A6A5PYW3

Continued on next page...

Continued from previous page...

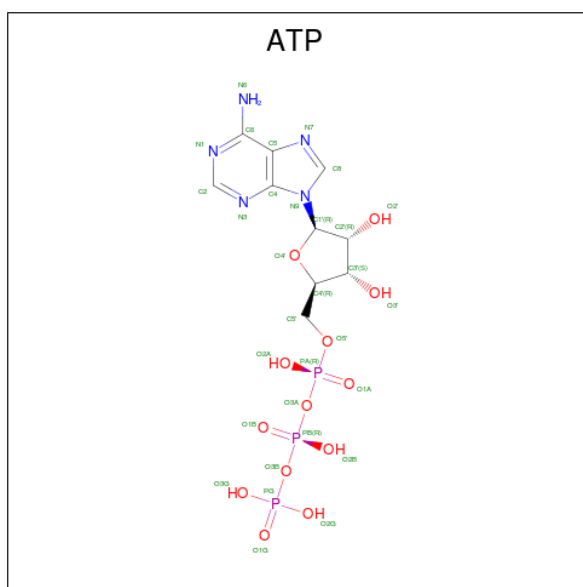
Chain	Residue	Modelled	Actual	Comment	Reference
Z	?	-	PRO	deletion	UNP A0A6A5PYW3
Z	?	-	GLU	deletion	UNP A0A6A5PYW3
Z	?	-	ILE	deletion	UNP A0A6A5PYW3
Z	?	-	ASP	deletion	UNP A0A6A5PYW3
Z	?	-	LYS	deletion	UNP A0A6A5PYW3
Z	?	-	GLU	deletion	UNP A0A6A5PYW3
Z	?	-	HIS	deletion	UNP A0A6A5PYW3
Z	?	-	MET	deletion	UNP A0A6A5PYW3
Z	?	-	GLY	deletion	UNP A0A6A5PYW3
Z	?	-	GLY	deletion	UNP A0A6A5PYW3
T	?	-	TYR	deletion	UNP A0A6A5PYW3
T	?	-	MET	deletion	UNP A0A6A5PYW3
T	?	-	PRO	deletion	UNP A0A6A5PYW3
T	?	-	GLU	deletion	UNP A0A6A5PYW3
T	?	-	ILE	deletion	UNP A0A6A5PYW3
T	?	-	ASP	deletion	UNP A0A6A5PYW3
T	?	-	LYS	deletion	UNP A0A6A5PYW3
T	?	-	GLU	deletion	UNP A0A6A5PYW3
T	?	-	HIS	deletion	UNP A0A6A5PYW3
T	?	-	MET	deletion	UNP A0A6A5PYW3
T	?	-	GLY	deletion	UNP A0A6A5PYW3
T	?	-	GLY	deletion	UNP A0A6A5PYW3
b	?	-	TYR	deletion	UNP A0A6A5PYW3
b	?	-	MET	deletion	UNP A0A6A5PYW3
b	?	-	PRO	deletion	UNP A0A6A5PYW3
b	?	-	GLU	deletion	UNP A0A6A5PYW3
b	?	-	ILE	deletion	UNP A0A6A5PYW3
b	?	-	ASP	deletion	UNP A0A6A5PYW3
b	?	-	LYS	deletion	UNP A0A6A5PYW3
b	?	-	GLU	deletion	UNP A0A6A5PYW3
b	?	-	HIS	deletion	UNP A0A6A5PYW3
b	?	-	MET	deletion	UNP A0A6A5PYW3
b	?	-	GLY	deletion	UNP A0A6A5PYW3
b	?	-	GLY	deletion	UNP A0A6A5PYW3
g	?	-	TYR	deletion	UNP A0A6A5PYW3
g	?	-	MET	deletion	UNP A0A6A5PYW3
g	?	-	PRO	deletion	UNP A0A6A5PYW3
g	?	-	GLU	deletion	UNP A0A6A5PYW3
g	?	-	ILE	deletion	UNP A0A6A5PYW3
g	?	-	ASP	deletion	UNP A0A6A5PYW3
g	?	-	LYS	deletion	UNP A0A6A5PYW3
g	?	-	GLU	deletion	UNP A0A6A5PYW3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
g	?	-	HIS	deletion	UNP A0A6A5PYW3
g	?	-	MET	deletion	UNP A0A6A5PYW3
g	?	-	GLY	deletion	UNP A0A6A5PYW3
g	?	-	GLY	deletion	UNP A0A6A5PYW3
k	?	-	TYR	deletion	UNP A0A6A5PYW3
k	?	-	MET	deletion	UNP A0A6A5PYW3
k	?	-	PRO	deletion	UNP A0A6A5PYW3
k	?	-	GLU	deletion	UNP A0A6A5PYW3
k	?	-	ILE	deletion	UNP A0A6A5PYW3
k	?	-	ASP	deletion	UNP A0A6A5PYW3
k	?	-	LYS	deletion	UNP A0A6A5PYW3
k	?	-	GLU	deletion	UNP A0A6A5PYW3
k	?	-	HIS	deletion	UNP A0A6A5PYW3
k	?	-	MET	deletion	UNP A0A6A5PYW3
k	?	-	GLY	deletion	UNP A0A6A5PYW3
k	?	-	GLY	deletion	UNP A0A6A5PYW3
h	?	-	TYR	deletion	UNP A0A6A5PYW3
h	?	-	MET	deletion	UNP A0A6A5PYW3
h	?	-	PRO	deletion	UNP A0A6A5PYW3
h	?	-	GLU	deletion	UNP A0A6A5PYW3
h	?	-	ILE	deletion	UNP A0A6A5PYW3
h	?	-	ASP	deletion	UNP A0A6A5PYW3
h	?	-	LYS	deletion	UNP A0A6A5PYW3
h	?	-	GLU	deletion	UNP A0A6A5PYW3
h	?	-	HIS	deletion	UNP A0A6A5PYW3
h	?	-	MET	deletion	UNP A0A6A5PYW3
h	?	-	GLY	deletion	UNP A0A6A5PYW3
h	?	-	GLY	deletion	UNP A0A6A5PYW3
l	?	-	TYR	deletion	UNP A0A6A5PYW3
l	?	-	MET	deletion	UNP A0A6A5PYW3
l	?	-	PRO	deletion	UNP A0A6A5PYW3
l	?	-	GLU	deletion	UNP A0A6A5PYW3
l	?	-	ILE	deletion	UNP A0A6A5PYW3
l	?	-	ASP	deletion	UNP A0A6A5PYW3
l	?	-	LYS	deletion	UNP A0A6A5PYW3
l	?	-	GLU	deletion	UNP A0A6A5PYW3
l	?	-	HIS	deletion	UNP A0A6A5PYW3
l	?	-	MET	deletion	UNP A0A6A5PYW3
l	?	-	GLY	deletion	UNP A0A6A5PYW3
l	?	-	GLY	deletion	UNP A0A6A5PYW3

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
2	A	1	43	10	12	5	13	3	0
2	E	1	43	10	12	5	13	3	0
2	B	1	43	10	12	5	13	3	0
2	F	1	43	10	12	5	13	3	0
2	Q	1	43	10	12	5	13	3	0
2	Y	1	43	10	12	5	13	3	0
2	S	1	43	10	12	5	13	3	0
2	a	1	43	10	12	5	13	3	0
2	I	1	43	10	12	5	13	3	0
2	M	1	43	10	12	5	13	3	0
2	J	1	43	10	12	5	13	3	0
2	N	1	43	10	12	5	13	3	0
2	R	1	43	10	12	5	13	3	0
2	Z	1	43	10	12	5	13	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
2	T	1	43	10	12	5	13	3	0
2	b	1	43	10	12	5	13	3	0
2	g	1	43	10	12	5	13	3	0
2	k	1	43	10	12	5	13	3	0
2	h	1	43	10	12	5	13	3	0
2	l	1	43	10	12	5	13	3	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

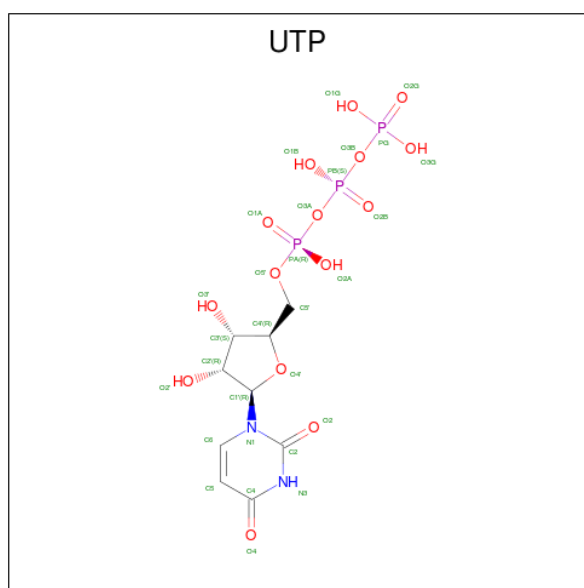
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	3	3	3	0
3	E	1	1	1	0
3	B	3	3	3	0
3	F	1	1	1	0
3	Q	3	3	3	0
3	Y	1	1	1	0
3	S	3	3	3	0
3	a	1	1	1	0
3	I	3	3	3	0
3	M	1	1	1	0
3	J	3	3	3	0
3	N	1	1	1	0
3	R	3	3	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
3	Z	1	Total	Mg	0
			1	1	
3	T	3	Total	Mg	0
			3	3	
3	b	1	Total	Mg	0
			1	1	
3	g	3	Total	Mg	0
			3	3	
3	k	1	Total	Mg	0
			1	1	
3	h	3	Total	Mg	0
			3	3	
3	l	1	Total	Mg	0
			1	1	

- Molecule 4 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



Mol	Chain	Residues	Atoms					AltConf	
4	A	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	E	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	B	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	F	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	

Continued on next page...

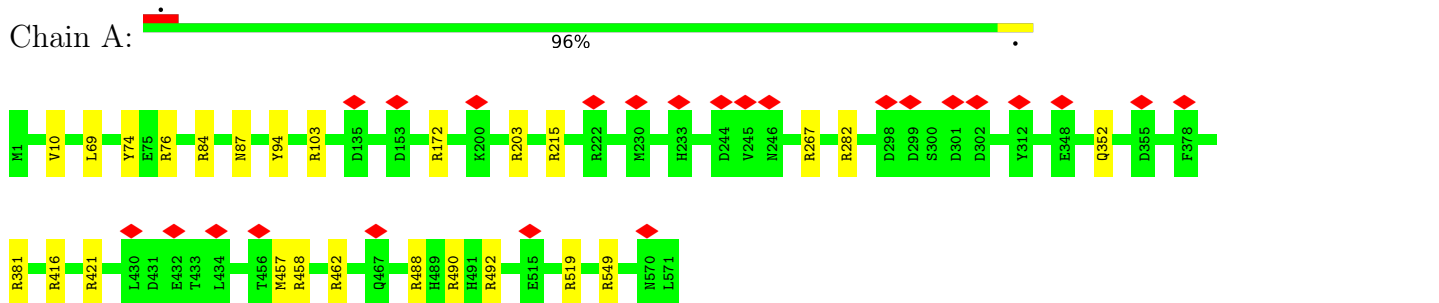
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
4	Q	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	Y	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	S	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	a	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	I	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	M	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	J	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	N	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	R	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	Z	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	T	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	b	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	g	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	k	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	h	1	Total 36	C 9	H 7	N 2	O 15	P 3	0
4	l	1	Total 36	C 9	H 7	N 2	O 15	P 3	0

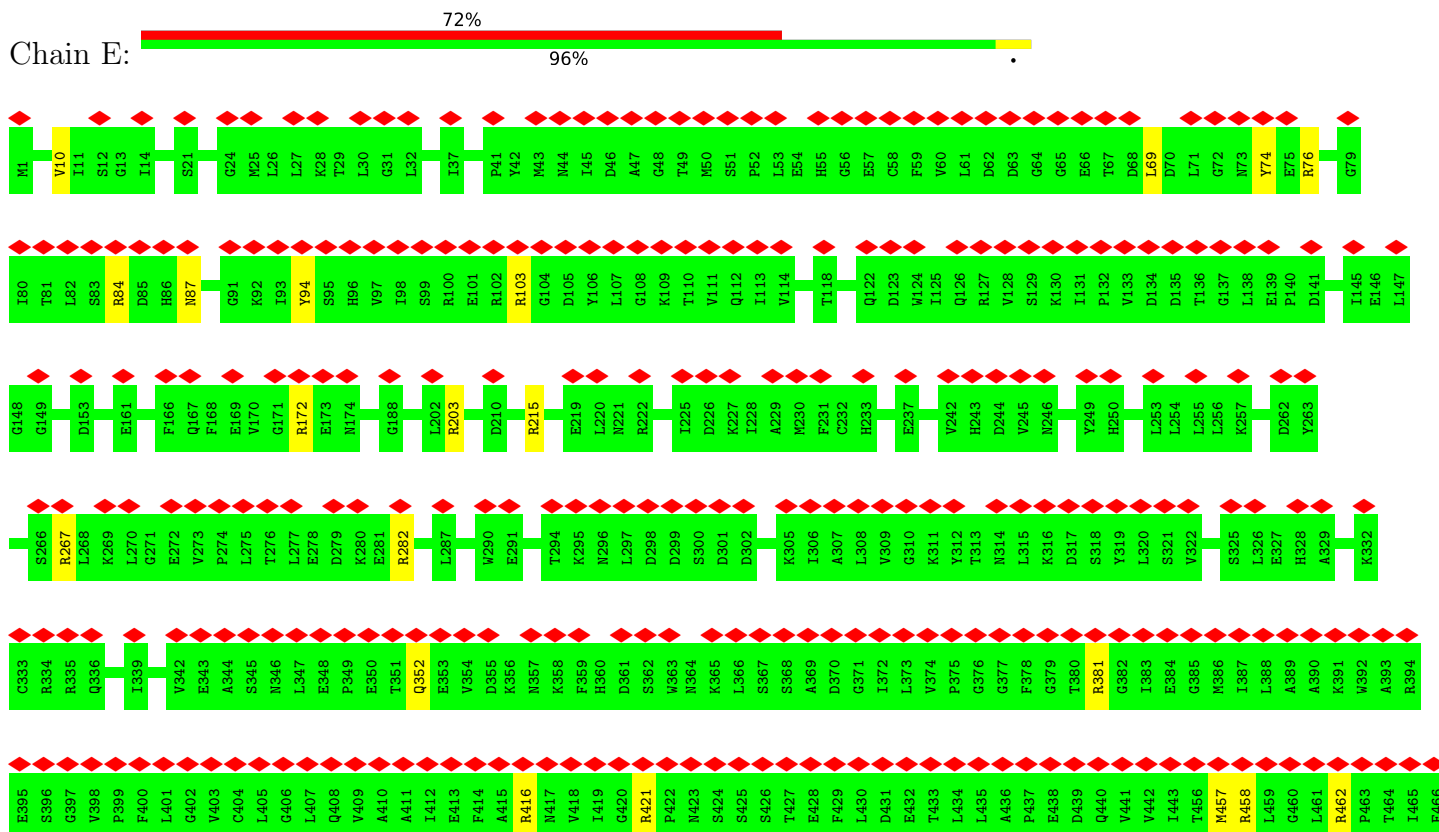
3 Residue-property plots [i](#)

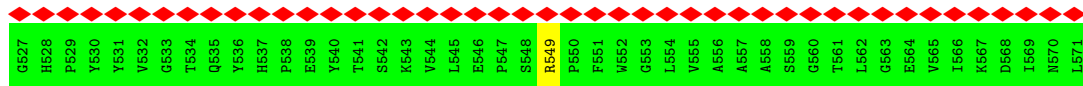
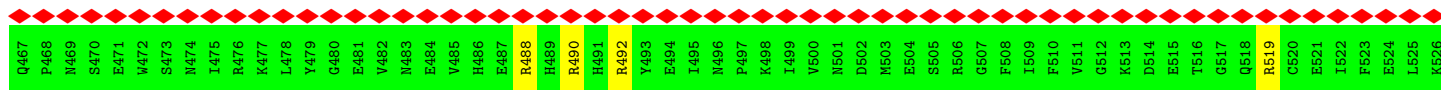
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CTP synthase

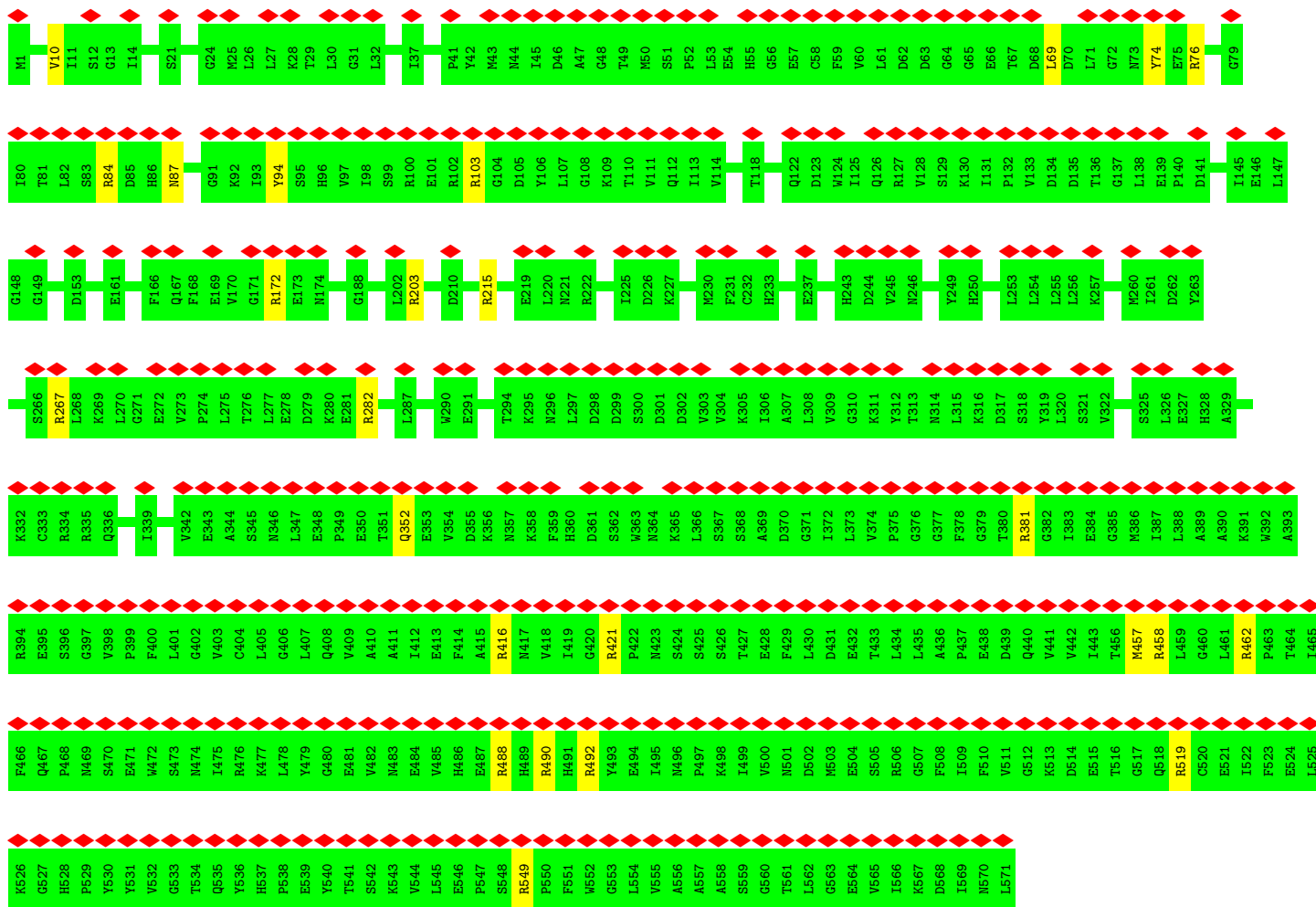


- Molecule 1: CTP synthase

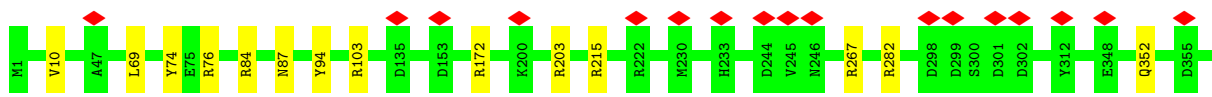


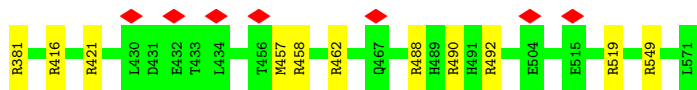


• Molecule 1: CTP synthase

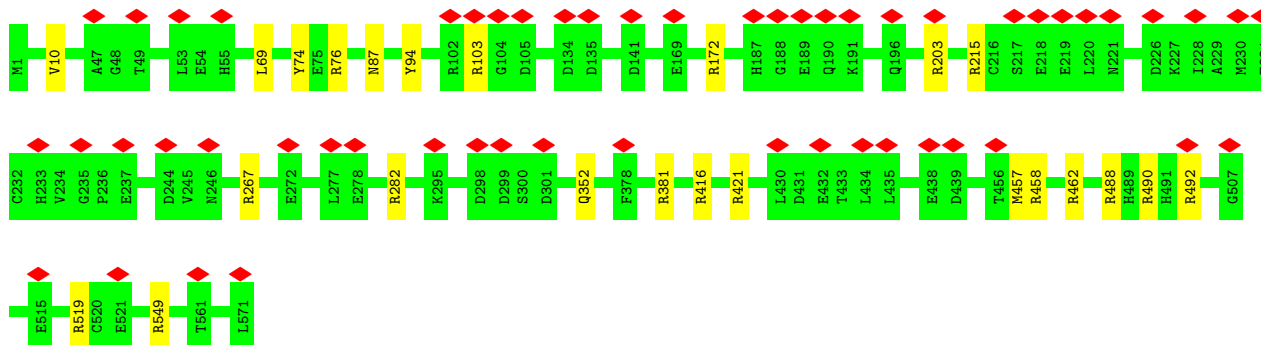


• Molecule 1: CTP synthase

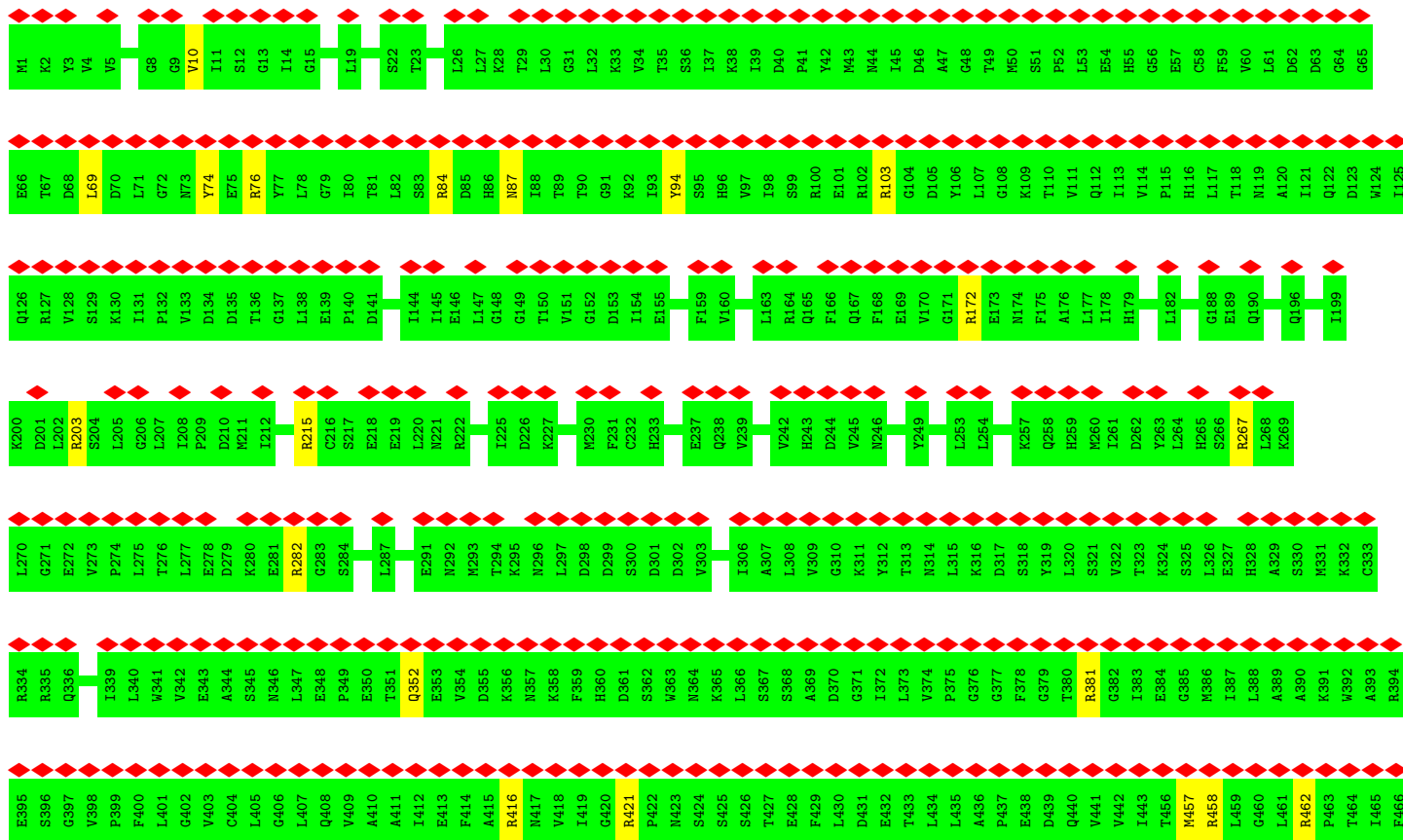
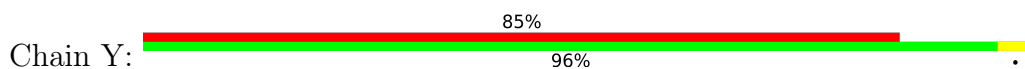


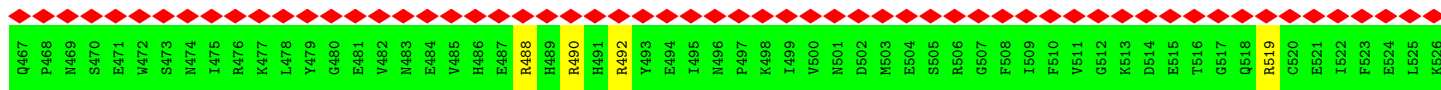


• Molecule 1: CTP synthase

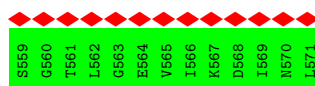
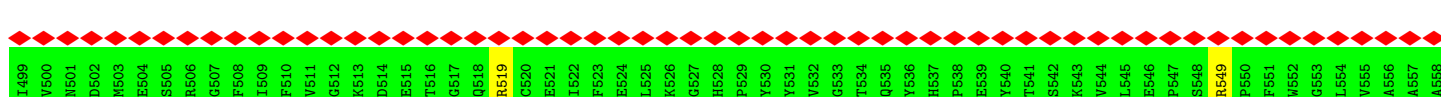
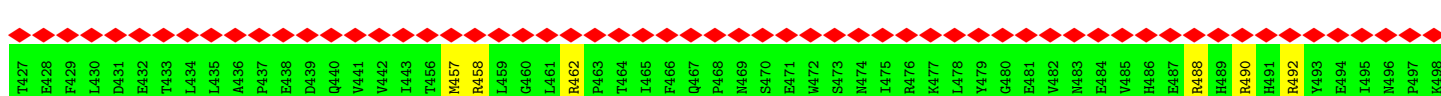
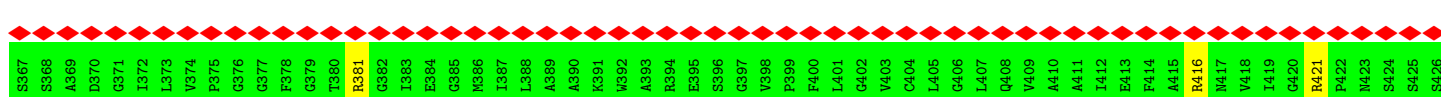
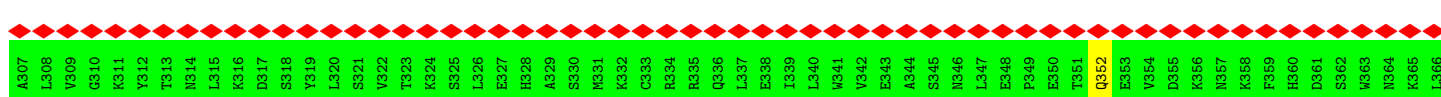
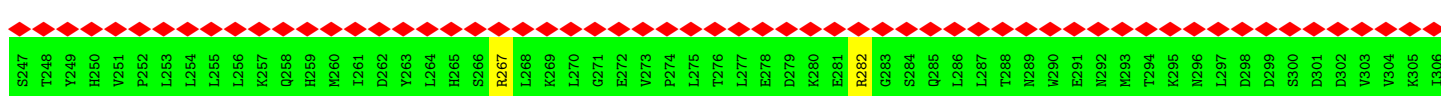
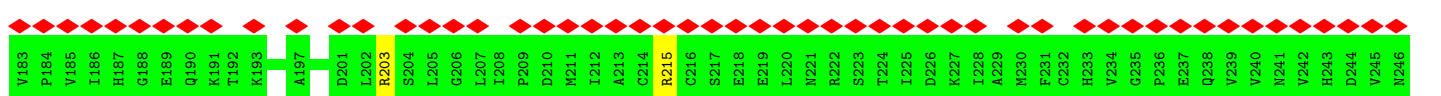
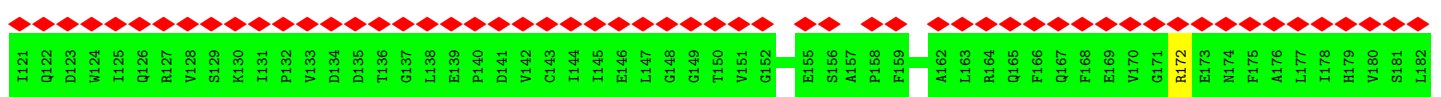
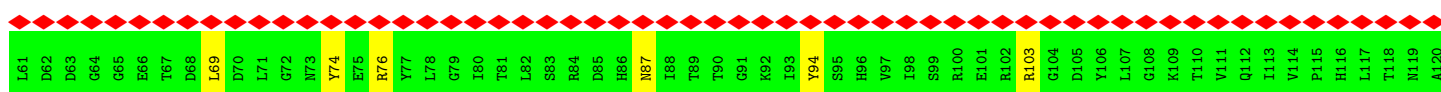
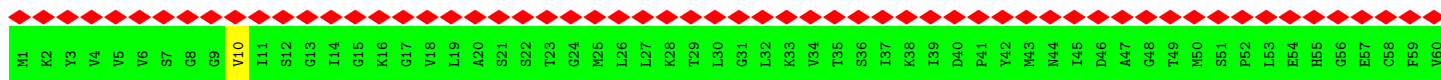
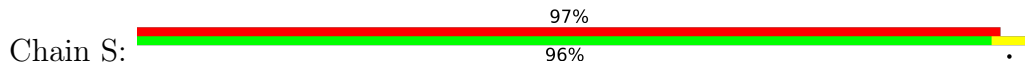


• Molecule 1: CTP synthase

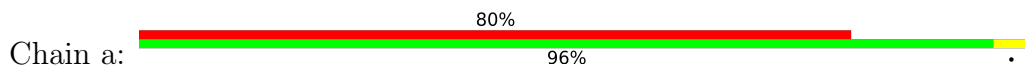


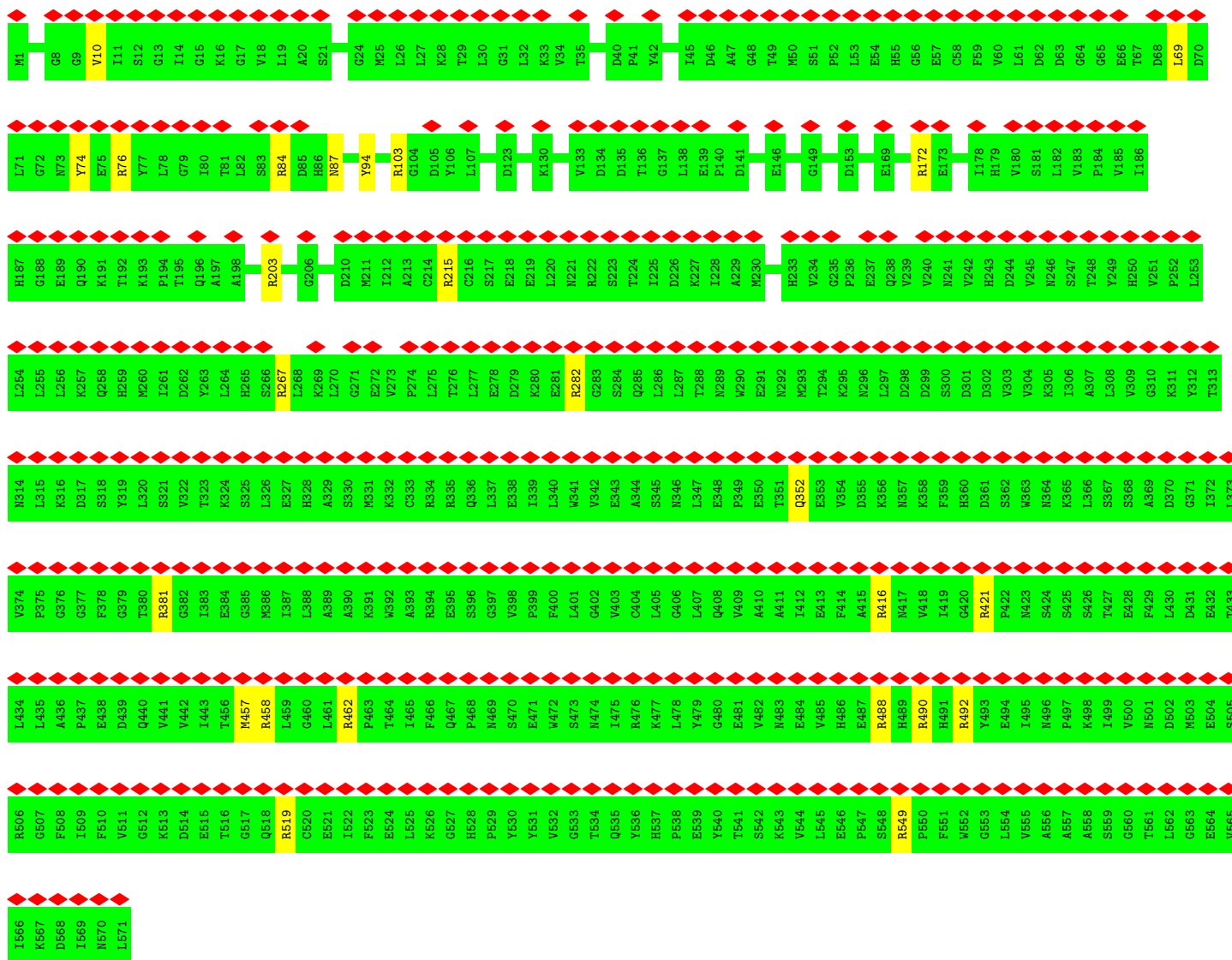


• Molecule 1: CTP synthase

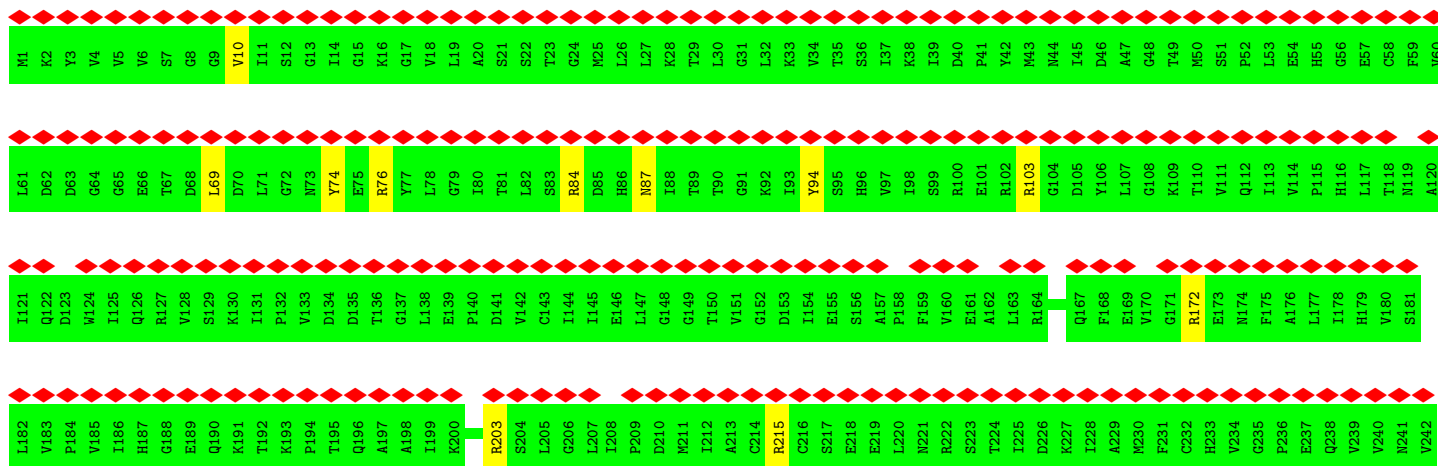
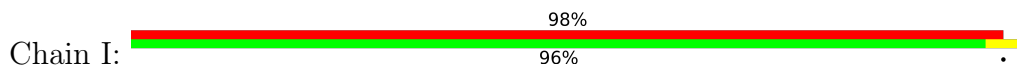


• Molecule 1: CTP synthase





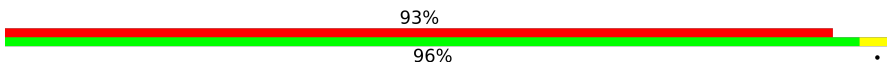
• Molecule 1: CTP synthase



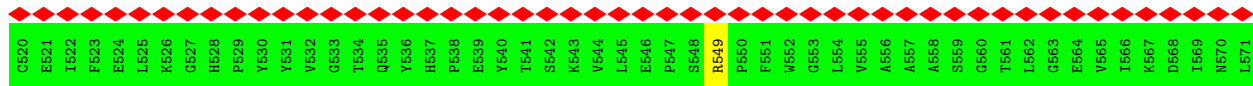
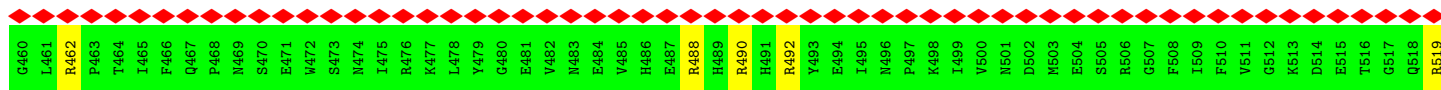
H243	H244	V303	V304	V306	V307	L308	V309	G310	K311	Y312	T313	N314	L315	K316	D317	S318	Y319	L320	S321	V322	T323	K324	S325	L326	R267	L268	K269	L270	G271	E272	V273	P274	L275	T276	L277	E278	D279	K280	E281	R282	G283	S284	Q285	L286	L287	L288	N289	V290	E291	N292	M293	T294	K295	N296	L297	D298	D299	S300	D301	D302				
N363	N364	K365	L366	S367	A369	D370	G371	I372	L373	V374	P375	K316	G377	F378	G379	T380	R381	G382	L383	E384	G385	M386	I387	L388	A389	A390	S391	M391	K392	C393	R394	R395	S396	G397	V398	P399	F400	L401	G402	V403	A404	L405	G406	L407	Q408	V409	A410	A411	T351	Q352	E353	V354	D355	K356	N357	K358	F359	G360	D361	S362				
M423	S424	S425	S426	E428	F429	L430	D431	E432	T433	L434	L435	A436	P437	E438	D439	Q440	V441	V442	I443	V456	M457	R458	L459	G460	L461	R462	T463	L464	L465	F466	Q467	M468	M469	S470	W471	E472	S473	M474	I475	R476	L477	L478	Y479	G480	E481	V482	M483	E484	V485	H486	E487	R488	H489	R490	H491	L492	Y493	E494						
I495	M496	P497	K498	I499	V500	N501	D502	M503	S505	R506	G507	I509	F510	V511	G512	K513	D514	E515	T516	G517	Q518	R519	C520	E521	I522	F523	E524	L525	K526	G527	H528	P529	Y530	V531	Y532	G533	T534	Q535	V536	H537	P538	E539	V540	T541	S542	K543	V544	L545	E546	P547	S548	R549	P550	F551	N552	G553	L554							
V555	A556	A557	A558	S559	G560	T561	L562	G563	E564	V565	I566	K567	D568	I569	N570	L571																																																

• Molecule 1: CTP synthase

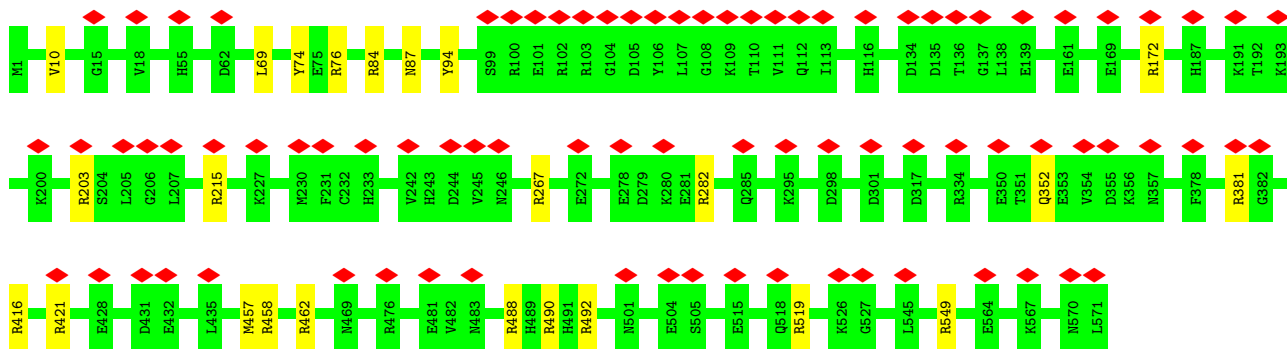
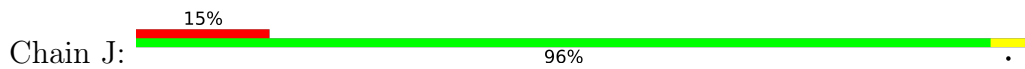
Chain M:



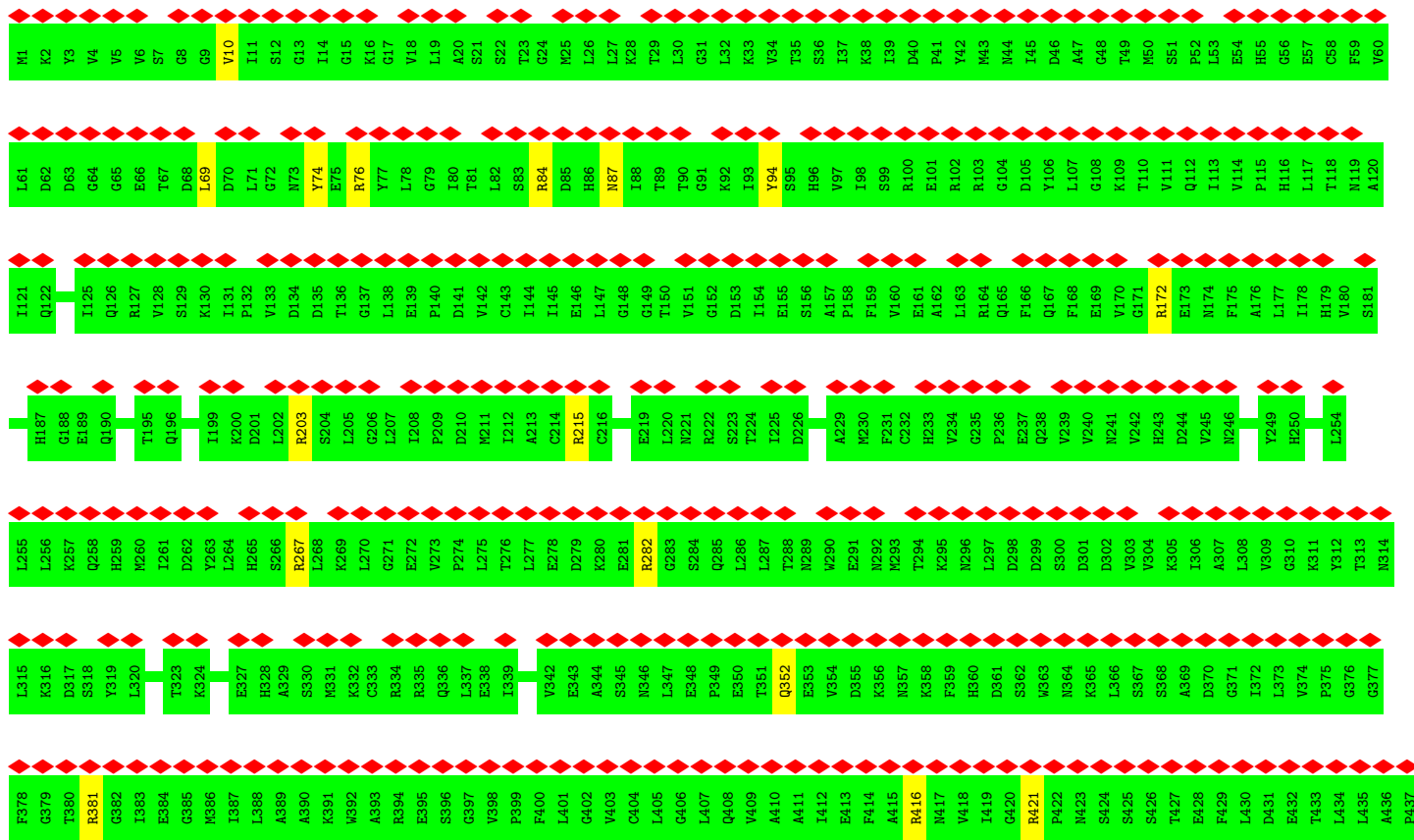
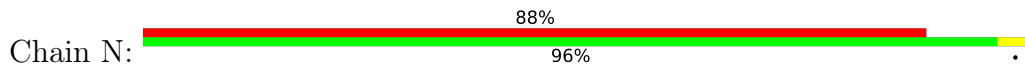
M1	K2	Y3	V4	W5	V6	S7	G8	S9	V10	I11	S12	G13	I14	G15	K16	G17	V18	L19	A20	S21	S22	T23	G24	M25	L26	L27	K28	T29	L30	G31	L32	K33	V34	T35	S36	I37	K38	L39	D40	P41	Y42	M43	N44	L45	D46	A47	O48	M50	S51	P52	L53	E54	H55	G56	E57	C58	F59	V60									
L61	D62	D63	G64	E65	G66	T67	D68	L69	D70	L71	G72	M73	Y74	E75	R76	Y77	L78	G79	I80	T81	L82	S83	H84	D85	H86	N87	I88	T89	T90	G91	K92	L93	I94	R95	V96	I97	L98	L99	D100	P101	I102	I103	L104	L105	L106	L107	G108	D123	W124	I125	Q126	R127	V128	S129	K130	I131	F132	V133	D134	D135	T136	L137	L138	E139	F140	D141	V142
C143	I144	I145	E146	L147	G148	G149	T150	V151	G152	D153	I154	E155	S156	L163	R164	Q165	F166	Q167	F168	E169	V170	G171	R172	E173	M174	F175	A176	L177	T178	E179	H180	V181	S182	L183	V184	P185	I186	H187	G188	E189	Q190	K191	T192	K193	P194	T195	Q196	A197	I198	I199	K200	D201	L202	R203	S204	L205	G206	L207									
I208	P209	D210	M211	L212	A213	C214	R215	C216	S217	E218	E219	L220	N221	R222	S223	T224	I225	D226	K227	I228	A229	M230	F231	C232	H233	V234	G235	E236	E237	Q238	D239	V240	N241	V242	H243	D244	V245	N246	S247	T248	Y249	H250	V251	P252	L253	L254	L255	L256	K257	Q258	H259	M260	T261	D262	V263	L264	H265	S266	R267								
L268	K269	L270	G271	E272	V273	P274	L275	T276	L277	E278	D279	K280	E281	R282	G283	S284	Q285	L286	L287	T288	M289	W290	E291	M292	K293	T294	K295	N296	E297	D298	D299	S300	D301	D302	V303	V304	K305	I306	A307	L308	V309	G310	K311	V312	T313	N314	L315	K316	D317	S318	Y319	L320	S321	V322	T323	K324	S325	L326	E327								
H328	A329	S330	M331	K332	C333	R334	R335	Q336	L337	E338	I339	L340	W341	V342	E343	A344	S345	N346	L347	E348	P349	E350	T351	Q352	E353	V354	D355	K356	N357	K358	F359	H360	D361	S362	W363	N364	K365	L366	S367	S368	A369	D370	G371	I372	L373	V374	P375	G376	G377	F378	G379	T380	R381	G382	I383	E384	S385	M386	I387								
L388	A389	K391	W392	A393	R394	R395	L396	T427	E428	F429	L430	D431	E432	L434	A436	P437	G378	G379	Q440	V441	V442	I443	V456	M457	R458	L459	G460	L461	R462	T463	L464	L465	F466	Q467	M468	M469	S470	W471	E472	S473	M474	I475	R476	L477	L478	Y479	G480	E481	V482	M483	E484	V485	H486	E487	R488	H489	R490	H491	L492	Y493	E494						

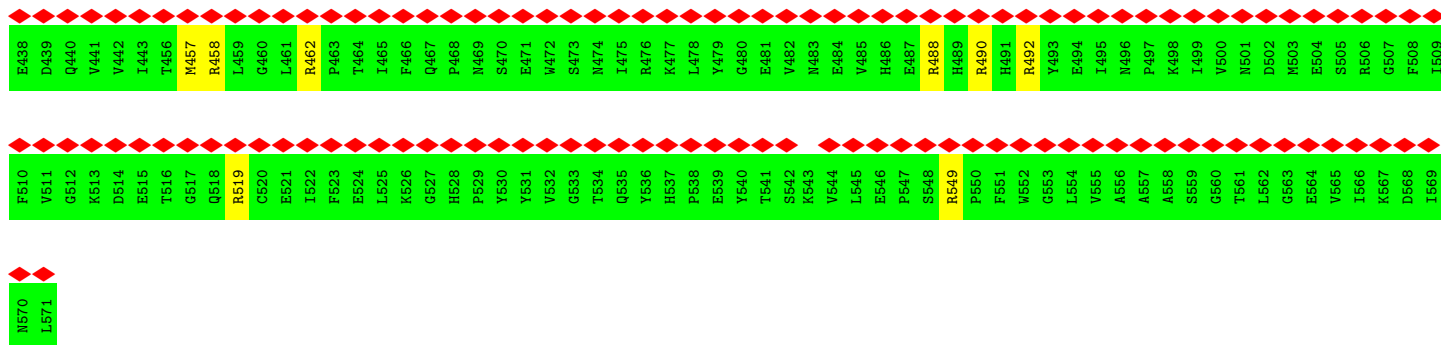


• Molecule 1: CTP synthase

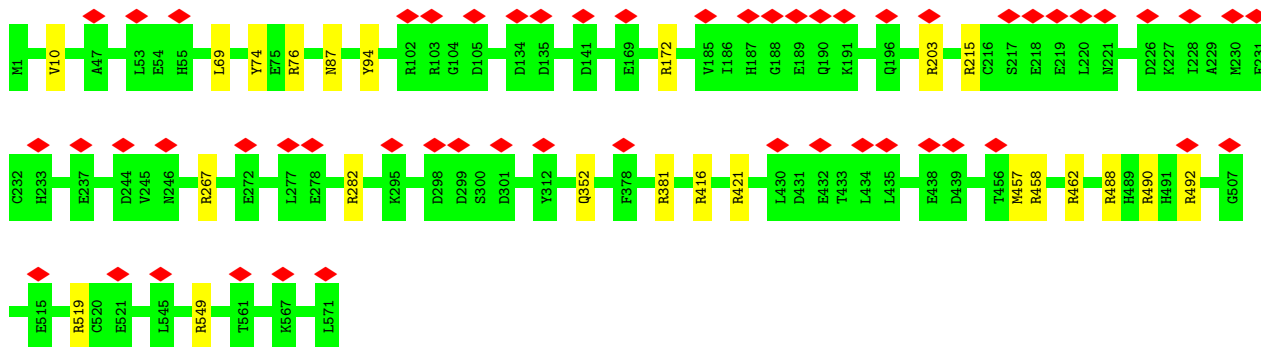


• Molecule 1: CTP synthase

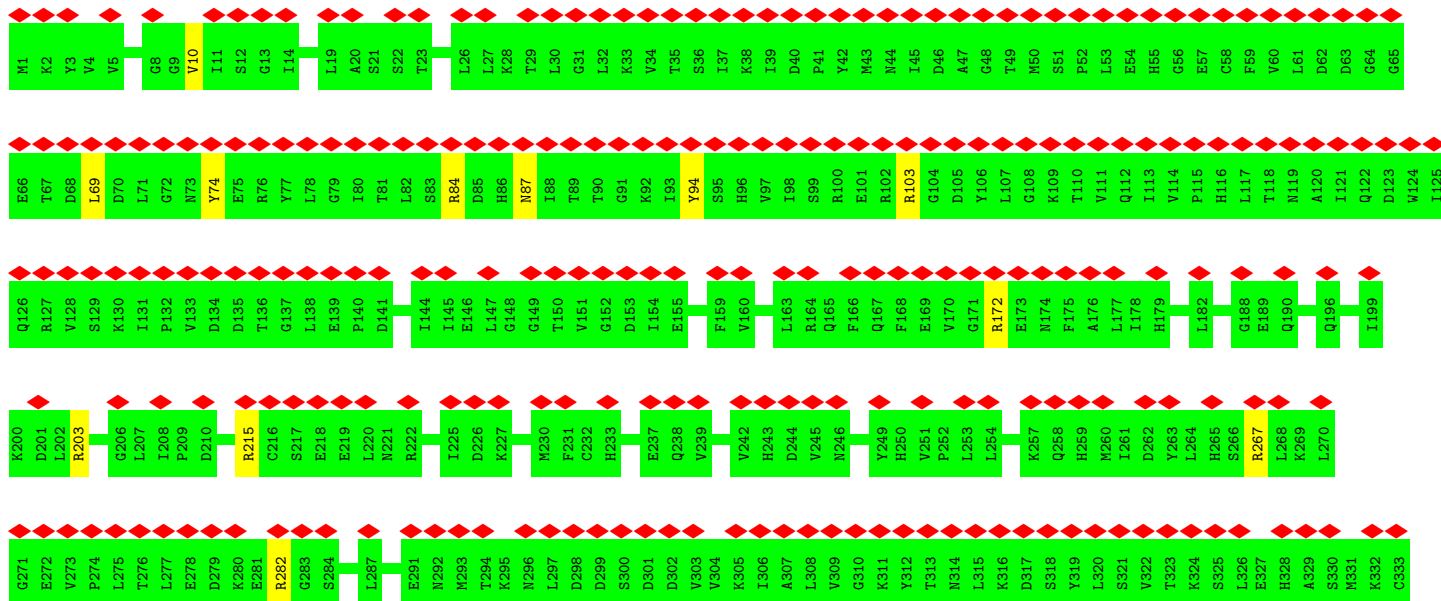
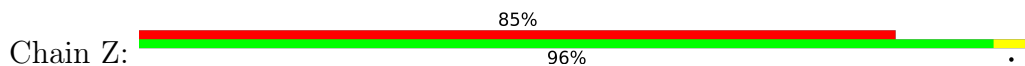




• Molecule 1: CTP synthase



• Molecule 1: CTP synthase

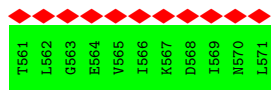


R334	R335	Q336	I339	L340	W341	V342	E343	A344	S345	N346	L347	E348	P349	E350	T351	Q352	E353	V354	D355	K356	M357	K358	F359	H360	D361	S362	W363	N364	K365	L366	S367	S368	A369	D370	G371	I372	L373	V374	P375	G376	G377	F378	T380	R381	G382	I383	E384	G385	M386	I387	L388	A389	A390	K391	W392	A393	R394		
E396	S396	G397	V398	P399	F400	L401	G402	V403	L405	G406	L407	Q408	V409	A410	A411	I412	E413	F414	A415	R416	M417	V418	I419	G420	R421	P422	M423	S424	S425	S426	T427	E428	V500	F429	L430	D431	E432	T433	L434	L436	G507	F508	I509	F510	V511	G512	K513	D514	E515	T516	M457	R458	L459	G460	L461	R462	F463	I465	F466
Q467	P468	N469	S470	E471	W472	S473	N474	I475	K476	K477	L478	Y479	G480	E481	V482	N483	E484	V485	H486	A487	R488	H489	R490	H491	R492	Y493	E494	I495	N496	P497	K498	I499	G500	N501	D502	M503	E504	S505	R506	G507	F508	I509	F510	V511	G512	K513	D514	E515	T516	G517	Q518	R519	C520	E521	I522	F523	E524	L525	K526
G527	H528	P529	Y530	V531	W532	G533	T534	Q535	H537	P538	E539	Y540	T541	S542	K543	V544	L545	E546	P547	S548	R549	P550	F551	W552	G553	L554	V555	A556	A557	A558	S559	G560	T561	L562	G563	E564	V565	I566	K567	L569	N570	L571																	

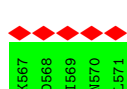
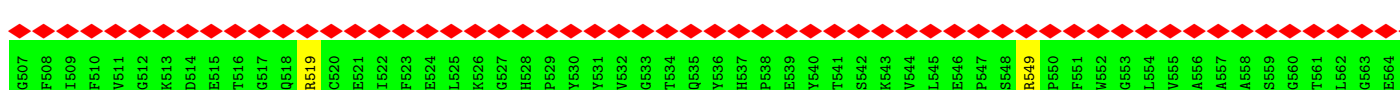
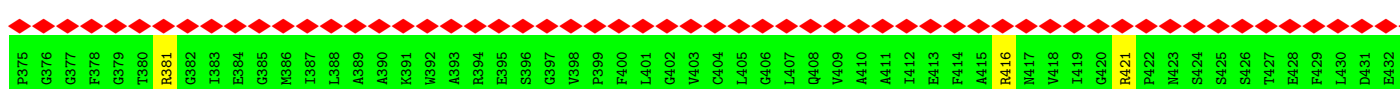
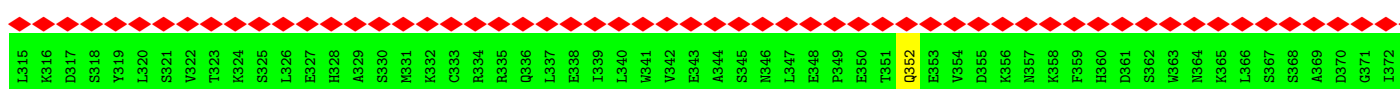
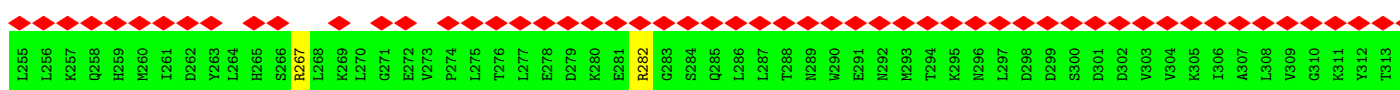
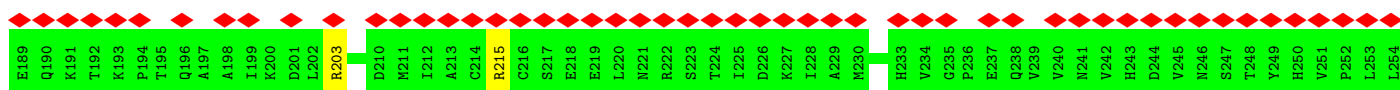
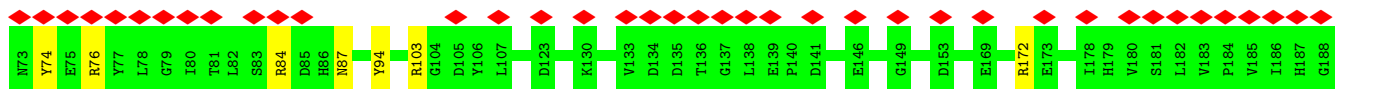
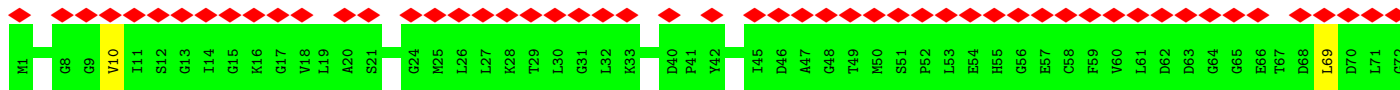
• Molecule 1: CTP synthase



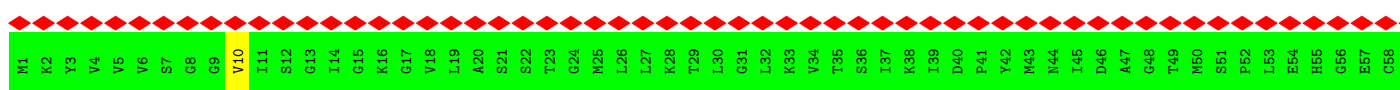
M1	K2	Y3	V4	W5	V6	S7	G8	G9	V10	I11	S12	G13	I14	G15	K16	G17	V18	L19	A20	S21	S22	T23	G24	M25	R26	L27	K28	T29	L30	G31	L32	K33	V34	T35	S36	I37	K38	I39	D40	P41	V42	M43	N44	I45	D46	A47	G48	T49	M50	S51	P52	L53	E54	H55	G56	E57	C58	F59	A120																																																														
L61	D62	D63	G64	G65	E66	T67	D68	L69	D70	L71	G72	M73	Y74	E75	R76	Y77	L78	G79	T80	T81	L82	S83	H84	D85	H86	N87	L88	T89	T90	G91	K92	I93	Y94	S95	H96	V97	I98	S99	R100	E101	R102	R103	G104	D105	V106	L107	G108	K109	T110	V111	Q112	I113	V114	P115	H116	L117	T118	M119	A120																																																														
I121	Q122	D123	W124	I125	Q126	R127	V128	S129	K130	I131	P132	I133	D134	D135	T136	G137	L138	E139	P140	D141	V142	C143	I144	I145	I146	L147	G148	G149	T150	V151	G152	E155	S156	A157	P158	F159	A162	L163	R164	Q165	Q166	Q167	F168	E169	V170	G171	R172	E173	M174	F175	A176	L177	I178	H179	V180	S181	L182																																																																
W183	P184	V185	I186	H187	G188	E189	Q190	K191	T192	K193	K200	D201	L202	R203	S204	L205	G206	F209	D210	M211	T212	A213	C214	R215	C216	S217	E218	E219	L220	M221	R222	S223	T224	L225	D226	K227	L228	A229	M230	F231	C232	H233	V234	G235	P236	E237	Q238	V239	V240	M241	V242	H243	D244	V245	M246	S247	T248																																																																
Y249	H250	W251	P252	L253	L254	L255	L256	K257	Q258	H259	M260	I261	D262	Y263	L264	H265	S266	R267	L268	K269	A329	M211	G271	E272	V273	L275	T276	L277	E278	D279	K280	E281	R282	G283	S284	Q285	L286	L287	T288	M289	W290	C292	E291	M292	M293	T294	K295	N296	L297	D298	D299	S300	D301	S302	V303	V304	K305	A307	L308																																																														
V309	G310	K311	Y312	T313	N314	L315	K316	D317	S318	Y319	L320	S321	V322	T323	K324	S325	L326	E327	H328	A329	S330	M331	K332	C333	R334	R335	Q336	L337	E338	I339	L340	W341	V342	E343	A344	S345	N346	L347	E348	P349	E350	T351	Q352	E353	F354	D355	K356	N357	D358	F359	H360	D361	S362	W363	N364	K365	L366	S367	S368																																																														
A369	D370	G371	I372	L373	V374	P375	G376	P377	F378	G379	T380	R381	G382	I383	E384	G385	M386	I387	L388	A389	A390	K391	W392	A393	R394	E395	S396	G397	V398	F399	F400	L401	G402	V403	O404	L405	L406	L407	O408	V409	A410	A411	I412	E413	F414	A415	R416	M417	V418	I419	G420	R421	P422	M423	S424	M425	S426	S427	F428	S429	Y530	Y531	W532	S473	M474	L475	R476	K477	L478	Y479	G480	E481	V482	M483	E484	V485	H486	E487	R488	H489	R490	H491	R492	Y493	L554	I495	M496	A497	A498	S499	E500	F501	V502	I499	G500	N501	D502	M503	E504	S505	R506	G507	F508	I509	F510	V511	G512	K513	D514	E515	T516	G517	Q518	R519	C520	E521	I522	F523	E524	L525	K526
F429	L430	D431	F432	T433	L434	L435	A436	P437	F438	D439	Q440	V441	V442	I443	T444	T445	M447	R448	L449	G440	L461	R462	P463	T464	L465	F466	Q467	P468	M469	S470	E471	W472	S473	M474	L475	R476	K477	L478	Y479	G480	E481	V482	M483	E484	V485	H486	E487	R488	H489	R490	H491	R492	Y493	L554	I495	M496	A497	A498	S499	E500	F501	V502	I499	G500	N501	D502	M503	E504	S505	R506	G507	F508	I509	F510	V511	G512	K513	D514	E515	T516	G517	Q518	R519	C520	E521	I522	F523	E524	L525	K526																															
M501	D502	M503	E504	S505	G507	F508	I509	F510	V511	G512	K513	D514	E515	T516	G517	Q518	R519	C520	E521	I522	F523	E524	L525	K526	G527	H528	P529	Y530	Y531	W532	S473	M474	L475	R476	K477	L478	Y479	G480	E481	V482	M483	E484	V485	H486	E487	R488	H489	R490	H491	R492	Y493	L554	I495	M496	A497	A498	S499	E500	F501	V502	I499	G500	N501	D502	M503	E504	S505	R506	G507	F508	I509	F510	V511	G512	K513	D514	E515	T516	G517	Q518	R519	C520	E521	I522	F523	E524	L525	K526																																	

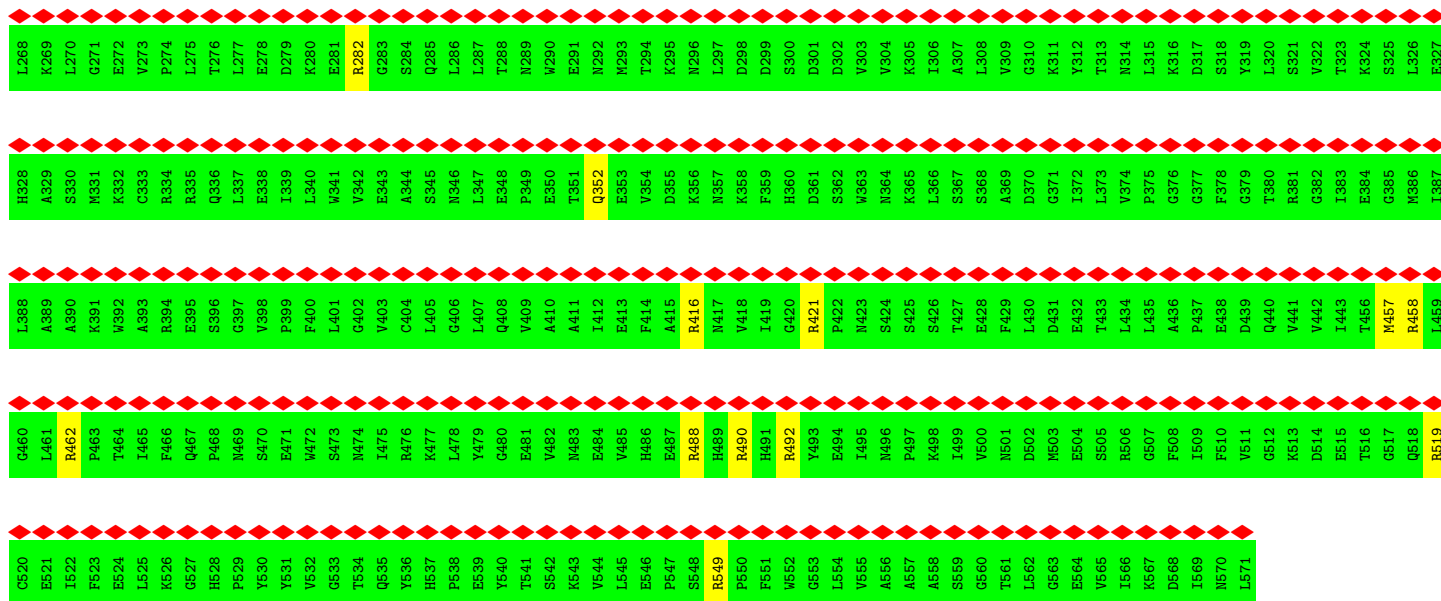


• Molecule 1: CTP synthase

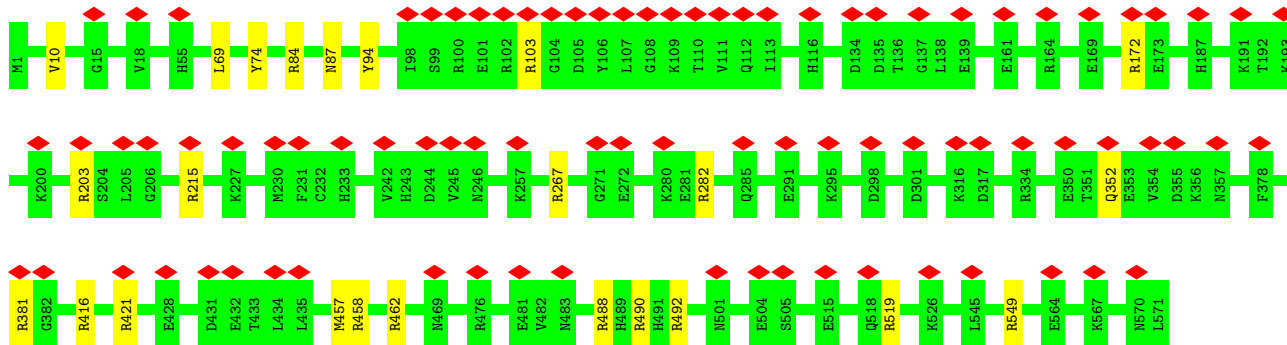


• Molecule 1: CTP synthase

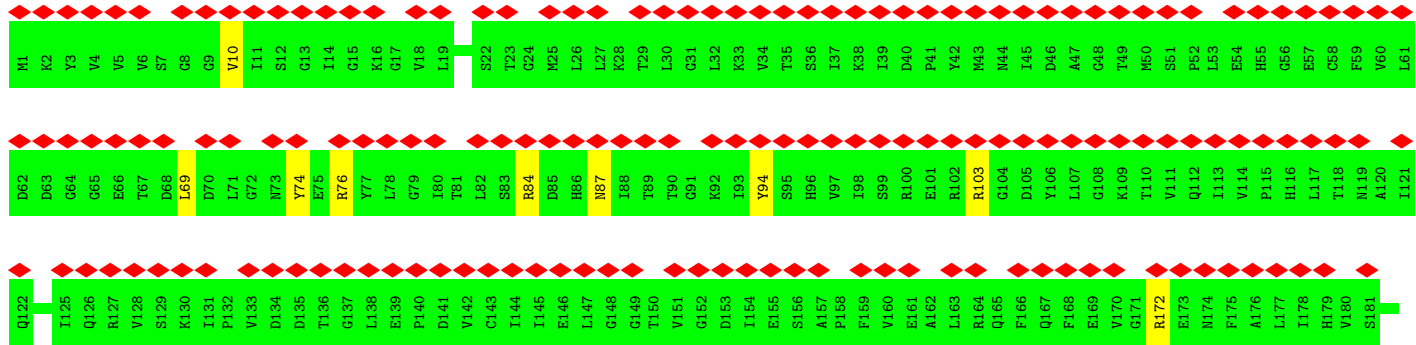
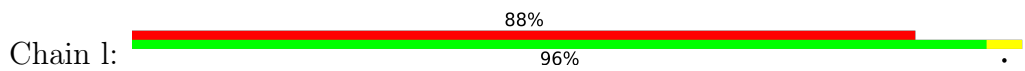




• Molecule 1: CTP synthase



• Molecule 1: CTP synthase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	21220	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	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	10.086	Depositor
Minimum map value	-6.069	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.120	Depositor
Recommended contour level	0.8	Depositor
Map size (\AA)	537.6, 537.6, 537.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	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, UTP, ATP

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	0.63	0/4471	1.04	19/6056 (0.3%)
1	B	0.63	0/4471	1.04	19/6056 (0.3%)
1	E	0.63	0/4471	1.04	19/6056 (0.3%)
1	F	0.63	0/4471	1.04	19/6056 (0.3%)
1	I	0.63	0/4471	1.04	20/6056 (0.3%)
1	J	0.63	0/4471	1.04	18/6056 (0.3%)
1	M	0.63	0/4471	1.04	18/6056 (0.3%)
1	N	0.63	0/4471	1.04	18/6056 (0.3%)
1	Q	0.63	0/4471	1.04	19/6056 (0.3%)
1	R	0.63	0/4471	1.04	17/6056 (0.3%)
1	S	0.63	0/4471	1.04	18/6056 (0.3%)
1	T	0.63	0/4471	1.04	19/6056 (0.3%)
1	Y	0.63	0/4471	1.04	19/6056 (0.3%)
1	Z	0.63	0/4471	1.04	18/6056 (0.3%)
1	a	0.63	0/4471	1.04	19/6056 (0.3%)
1	b	0.63	0/4471	1.04	19/6056 (0.3%)
1	g	0.63	0/4471	1.04	18/6056 (0.3%)
1	h	0.63	0/4471	1.04	18/6056 (0.3%)
1	k	0.63	0/4471	1.04	18/6056 (0.3%)
1	l	0.63	0/4471	1.04	19/6056 (0.3%)
All	All	0.63	0/89420	1.04	371/121120 (0.3%)

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
1	A	0	1
1	B	0	1
1	E	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	I	0	1
1	J	0	1
1	M	0	1
1	N	0	1
1	Q	0	1
1	R	0	1
1	S	0	1
1	T	0	1
1	Y	0	1
1	Z	0	1
1	a	0	1
1	b	0	1
1	g	0	1
1	h	0	1
1	k	0	1
1	l	0	1
All	All	0	20

There are no bond length outliers.

The worst 5 of 371 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	549	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	T	549	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	a	549	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	S	549	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	k	549	ARG	NE-CZ-NH1	8.06	124.33	120.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	TYR	Sidechain
1	B	94	TYR	Sidechain
1	E	94	TYR	Sidechain
1	F	94	TYR	Sidechain
1	Q	94	TYR	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	B	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	E	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	F	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	I	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	J	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	M	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	N	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	Q	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	R	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	S	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	T	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	Y	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	Z	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	a	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	b	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	g	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	h	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	k	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	l	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
All	All	11100/11180 (99%)	10820 (98%)	280 (2%)	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	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	B	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	E	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	F	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	I	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	J	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	M	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	N	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	Q	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	R	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	S	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	T	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	Y	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	Z	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	a	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	b	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	g	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	h	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	k	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	l	488/488 (100%)	483 (99%)	5 (1%)	76	86
All	All	9760/9760 (100%)	9660 (99%)	100 (1%)	77	86

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	87	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	69	LEU
1	l	457	MET
1	N	457	MET
1	Z	10	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	ASN
1	F	483	ASN
1	J	483	ASN
1	h	483	ASN

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 80 ligands modelled in this entry, 40 are monoatomic - leaving 40 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	ATP	h	602	3	26,33,33	1.14	2 (7%)	31,52,52	1.48	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	UTP	a	601	3	22,30,30	1.06	1 (4%)	27,47,47	1.44	5 (18%)
4	UTP	I	605	3	22,30,30	1.06	1 (4%)	27,47,47	1.46	5 (18%)
4	UTP	F	601	3	22,30,30	1.06	1 (4%)	27,47,47	1.46	5 (18%)
4	UTP	g	605	3	22,30,30	1.07	1 (4%)	27,47,47	1.46	5 (18%)
2	ATP	Z	601	3	26,33,33	1.13	2 (7%)	31,52,52	1.48	4 (12%)
2	ATP	T	602	3	26,33,33	1.14	2 (7%)	31,52,52	1.48	4 (12%)
4	UTP	B	601	3	22,30,30	1.07	1 (4%)	27,47,47	1.44	5 (18%)
4	UTP	E	603	3	22,30,30	1.07	1 (4%)	27,47,47	1.44	5 (18%)
2	ATP	N	602	3	26,33,33	1.14	2 (7%)	31,52,52	1.48	4 (12%)
4	UTP	Z	603	3	22,30,30	1.06	1 (4%)	27,47,47	1.47	5 (18%)
4	UTP	A	605	3	22,30,30	1.07	1 (4%)	27,47,47	1.46	5 (18%)
4	UTP	S	601	3	22,30,30	1.08	1 (4%)	27,47,47	1.45	5 (18%)
4	UTP	h	601	3	22,30,30	1.08	1 (4%)	27,47,47	1.44	5 (18%)
4	UTP	Y	603	3	22,30,30	1.07	1 (4%)	27,47,47	1.47	5 (18%)
2	ATP	F	602	3	26,33,33	1.14	2 (7%)	31,52,52	1.47	4 (12%)
2	ATP	I	601	3	26,33,33	1.14	2 (7%)	31,52,52	1.48	4 (12%)
2	ATP	g	601	3	26,33,33	1.14	2 (7%)	31,52,52	1.48	4 (12%)
2	ATP	b	602	3	26,33,33	1.14	2 (7%)	31,52,52	1.48	4 (12%)
4	UTP	R	605	3	22,30,30	1.06	1 (4%)	27,47,47	1.44	5 (18%)
4	UTP	J	601	3	22,30,30	1.07	1 (4%)	27,47,47	1.44	5 (18%)
4	UTP	Q	605	3	22,30,30	1.06	1 (4%)	27,47,47	1.44	5 (18%)
4	UTP	N	601	3	22,30,30	1.06	1 (4%)	27,47,47	1.46	5 (18%)
2	ATP	A	601	3	26,33,33	1.14	2 (7%)	31,52,52	1.48	4 (12%)
2	ATP	Q	601	3	26,33,33	1.14	2 (7%)	31,52,52	1.48	4 (12%)
4	UTP	l	601	3	22,30,30	1.06	1 (4%)	27,47,47	1.47	5 (18%)
2	ATP	J	602	3	26,33,33	1.14	2 (7%)	31,52,52	1.47	4 (12%)
2	ATP	S	602	3	26,33,33	1.14	2 (7%)	31,52,52	1.47	4 (12%)
4	UTP	k	603	3	22,30,30	1.07	1 (4%)	27,47,47	1.44	5 (18%)
4	UTP	T	601	3	22,30,30	1.08	1 (4%)	27,47,47	1.45	5 (18%)
2	ATP	E	601	3	26,33,33	1.13	2 (7%)	31,52,52	1.48	4 (12%)
2	ATP	R	601	3	26,33,33	1.15	2 (7%)	31,52,52	1.48	4 (12%)
2	ATP	Y	601	3	26,33,33	1.12	2 (7%)	31,52,52	1.47	4 (12%)
2	ATP	k	601	3	26,33,33	1.12	2 (7%)	31,52,52	1.47	4 (12%)
2	ATP	l	602	3	26,33,33	1.13	2 (7%)	31,52,52	1.48	4 (12%)
2	ATP	B	602	3	26,33,33	1.14	2 (7%)	31,52,52	1.48	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	M	601	3	26,33,33	1.13	2 (7%)	31,52,52	1.48	4 (12%)
4	UTP	b	601	3	22,30,30	1.07	1 (4%)	27,47,47	1.44	5 (18%)
2	ATP	a	602	3	26,33,33	1.15	2 (7%)	31,52,52	1.48	4 (12%)
4	UTP	M	603	3	22,30,30	1.06	1 (4%)	27,47,47	1.44	5 (18%)

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	ATP	h	602	3	-	0/18/38/38	0/3/3/3
4	UTP	a	601	3	2/2/7/7	6/20/38/38	0/2/2/2
4	UTP	I	605	3	2/2/7/7	11/20/38/38	0/2/2/2
4	UTP	F	601	3	2/2/7/7	11/20/38/38	0/2/2/2
4	UTP	g	605	3	2/2/7/7	11/20/38/38	0/2/2/2
2	ATP	Z	601	3	-	0/18/38/38	0/3/3/3
2	ATP	T	602	3	-	0/18/38/38	0/3/3/3
4	UTP	B	601	3	2/2/7/7	6/20/38/38	0/2/2/2
4	UTP	E	603	3	2/2/7/7	6/20/38/38	0/2/2/2
2	ATP	N	602	3	-	0/18/38/38	0/3/3/3
4	UTP	Z	603	3	2/2/7/7	10/20/38/38	0/2/2/2
4	UTP	A	605	3	2/2/7/7	11/20/38/38	0/2/2/2
4	UTP	S	601	3	2/2/7/7	8/20/38/38	0/2/2/2
4	UTP	h	601	3	2/2/7/7	6/20/38/38	0/2/2/2
4	UTP	Y	603	3	2/2/7/7	10/20/38/38	0/2/2/2
2	ATP	F	602	3	-	0/18/38/38	0/3/3/3
2	ATP	I	601	3	-	0/18/38/38	0/3/3/3
2	ATP	g	601	3	-	0/18/38/38	0/3/3/3
2	ATP	b	602	3	-	0/18/38/38	0/3/3/3
4	UTP	R	605	3	2/2/7/7	6/20/38/38	0/2/2/2
4	UTP	J	601	3	2/2/7/7	6/20/38/38	0/2/2/2
4	UTP	Q	605	3	2/2/7/7	6/20/38/38	0/2/2/2
4	UTP	N	601	3	2/2/7/7	10/20/38/38	0/2/2/2
2	ATP	A	601	3	-	0/18/38/38	0/3/3/3
2	ATP	Q	601	3	-	0/18/38/38	0/3/3/3
4	UTP	l	601	3	2/2/7/7	10/20/38/38	0/2/2/2
2	ATP	J	602	3	-	0/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	S	602	3	-	0/18/38/38	0/3/3/3
4	UTP	k	603	3	2/2/7/7	9/20/38/38	0/2/2/2
4	UTP	T	601	3	2/2/7/7	8/20/38/38	0/2/2/2
2	ATP	E	601	3	-	0/18/38/38	0/3/3/3
2	ATP	R	601	3	-	0/18/38/38	0/3/3/3
2	ATP	Y	601	3	-	0/18/38/38	0/3/3/3
2	ATP	k	601	3	-	0/18/38/38	0/3/3/3
2	ATP	l	602	3	-	0/18/38/38	0/3/3/3
2	ATP	B	602	3	-	0/18/38/38	0/3/3/3
2	ATP	M	601	3	-	0/18/38/38	0/3/3/3
4	UTP	b	601	3	2/2/7/7	6/20/38/38	0/2/2/2
2	ATP	a	602	3	-	0/18/38/38	0/3/3/3
4	UTP	M	603	3	2/2/7/7	9/20/38/38	0/2/2/2

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	601	UTP	C4-N3	3.02	1.38	1.33
2	I	601	ATP	O4'-C1'	3.00	1.45	1.41
4	h	601	UTP	C4-N3	3.00	1.38	1.33
4	k	603	UTP	C4-N3	3.00	1.38	1.33
4	Y	603	UTP	C4-N3	3.00	1.38	1.33

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	602	ATP	C4-C5-N7	4.18	113.75	109.40
2	I	601	ATP	C4-C5-N7	4.17	113.75	109.40
2	g	601	ATP	C4-C5-N7	4.17	113.74	109.40
2	Q	601	ATP	C4-C5-N7	4.17	113.74	109.40
2	Z	601	ATP	C4-C5-N7	4.17	113.74	109.40

5 of 40 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	605	UTP	C1'
4	A	605	UTP	C4'
4	E	603	UTP	C1'
4	E	603	UTP	C4'
4	B	601	UTP	C1'

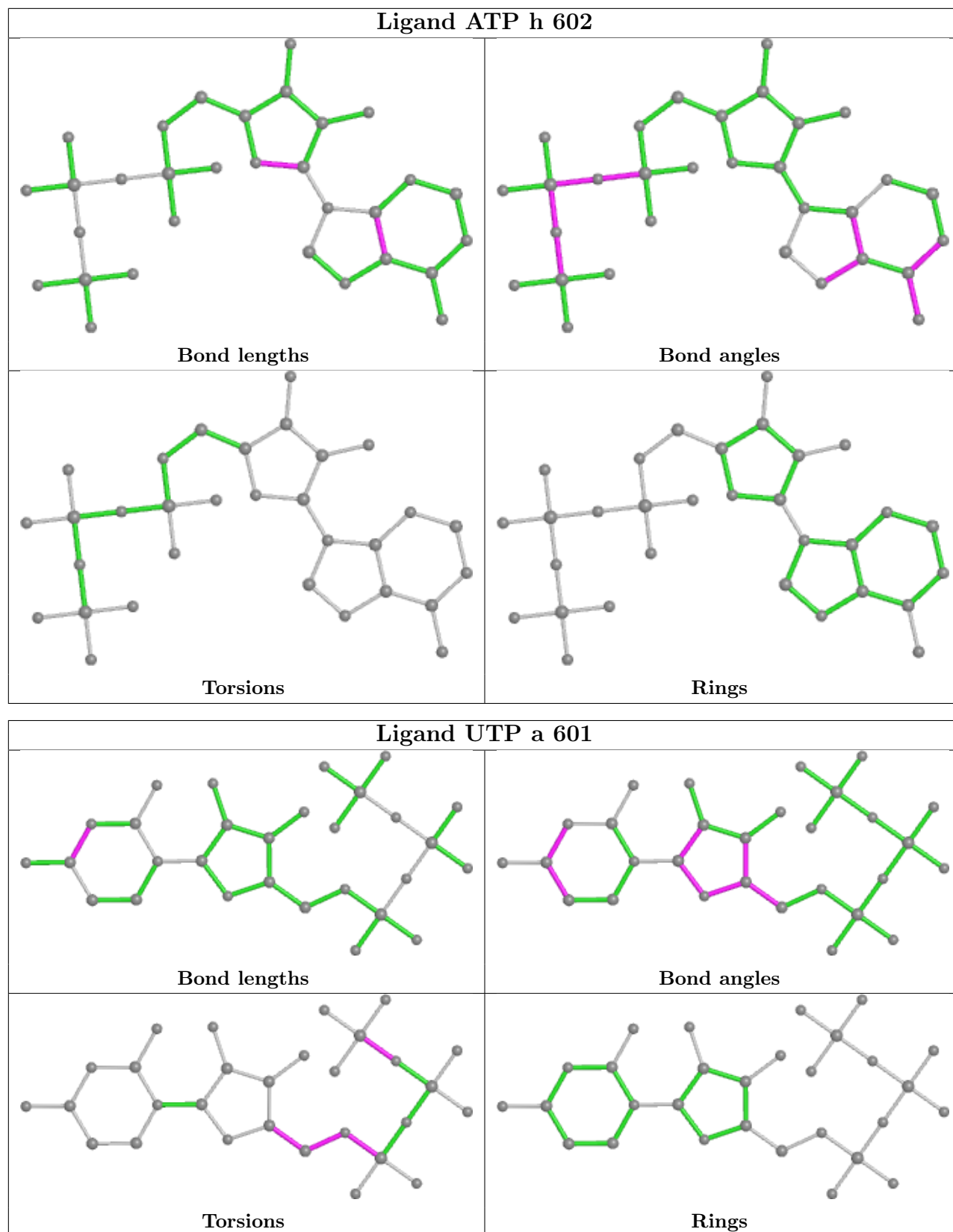
5 of 166 torsion outliers are listed below:

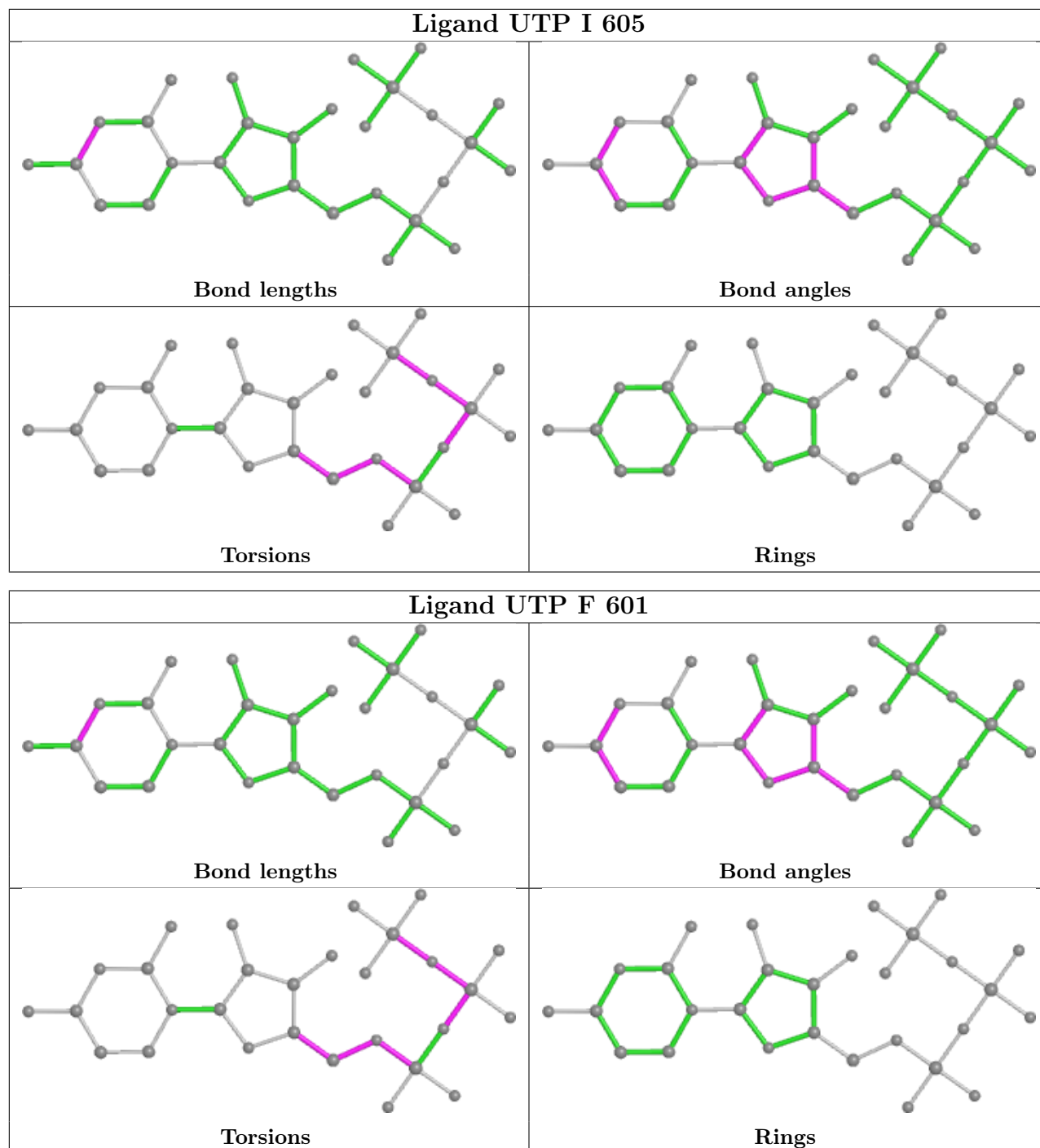
Mol	Chain	Res	Type	Atoms
4	A	605	UTP	C5'-O5'-PA-O1A
4	A	605	UTP	PB-O3B-PG-O1G
4	E	603	UTP	C5'-O5'-PA-O2A
4	B	601	UTP	C5'-O5'-PA-O2A
4	F	601	UTP	C5'-O5'-PA-O1A

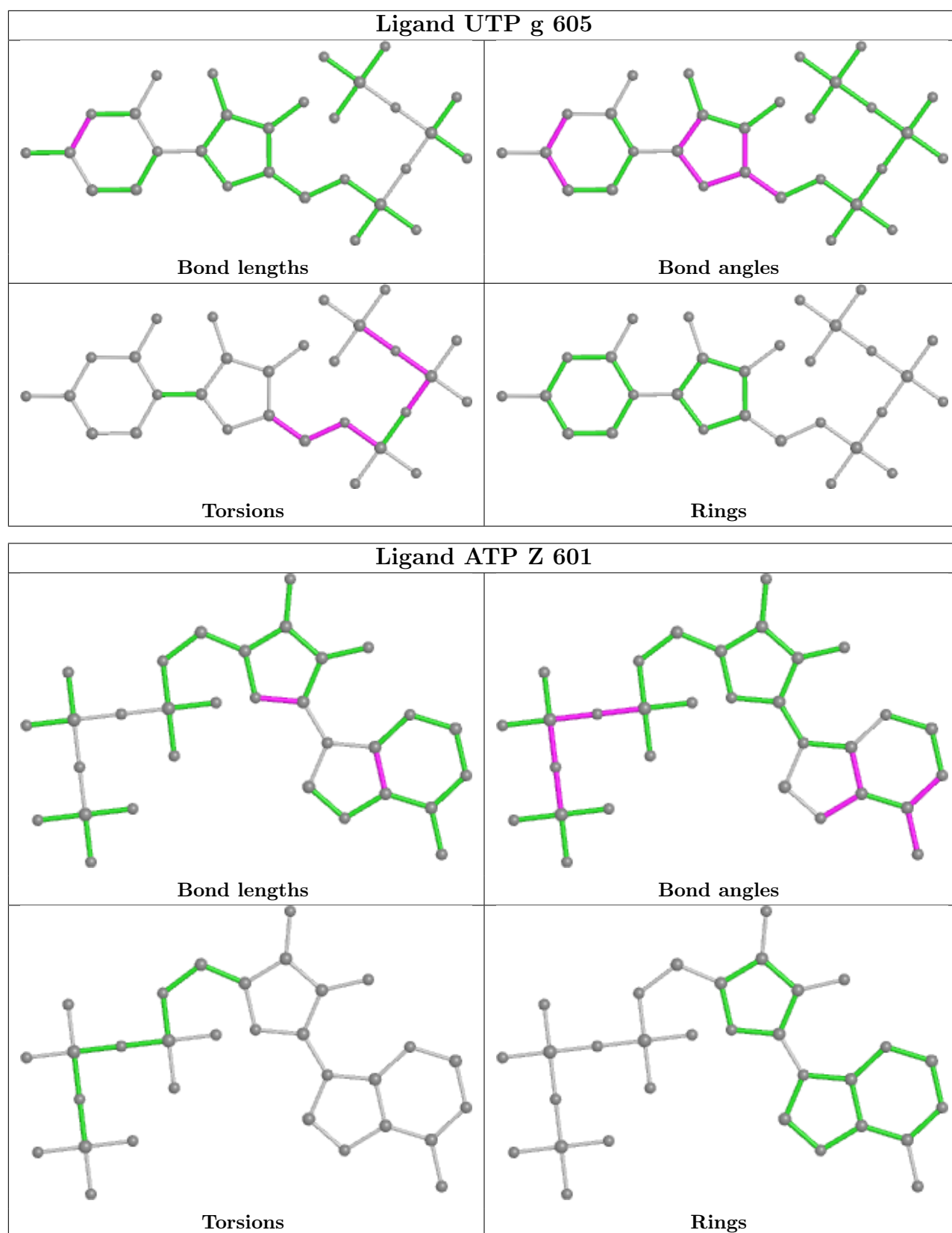
There are no ring outliers.

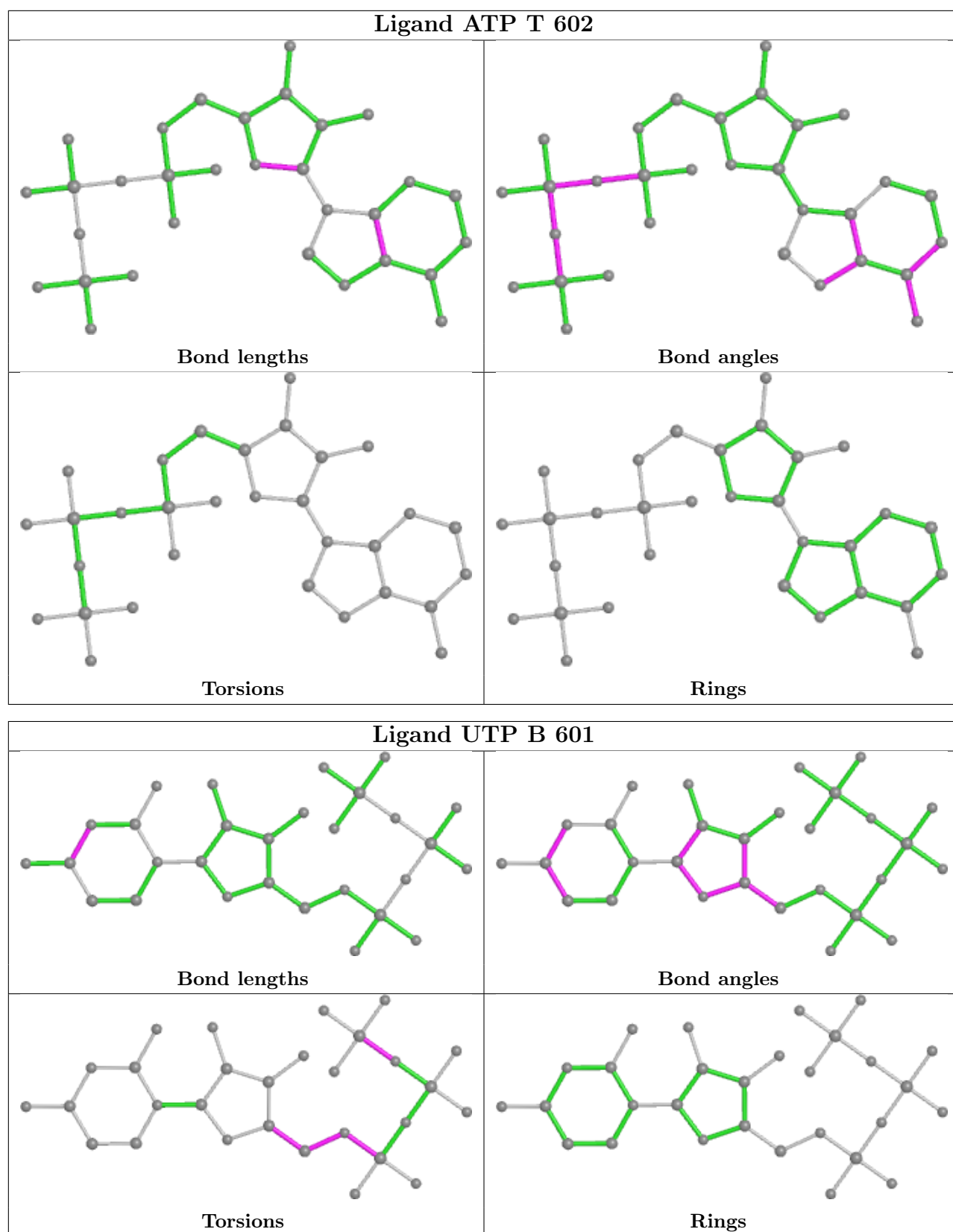
No monomer is involved in short contacts.

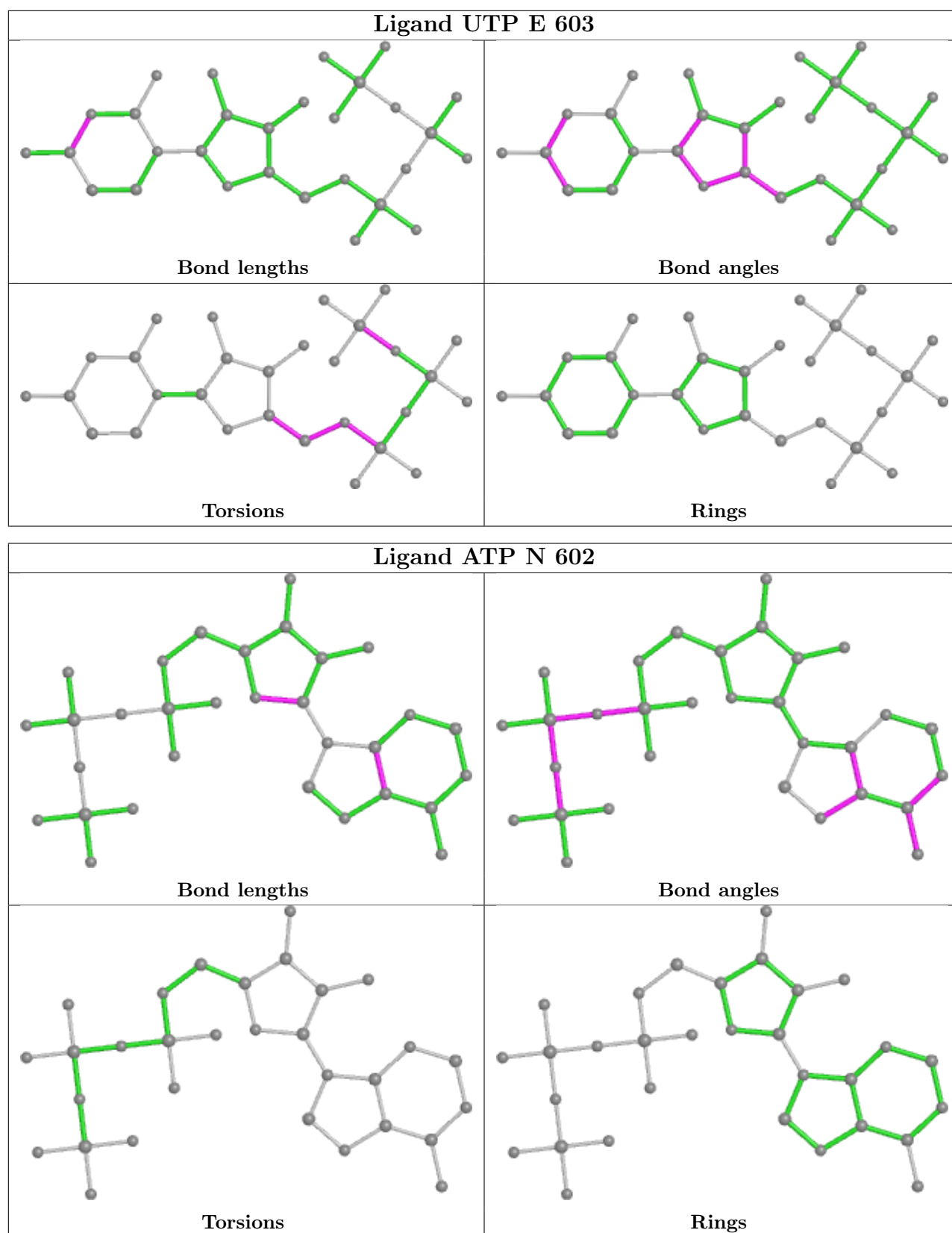
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

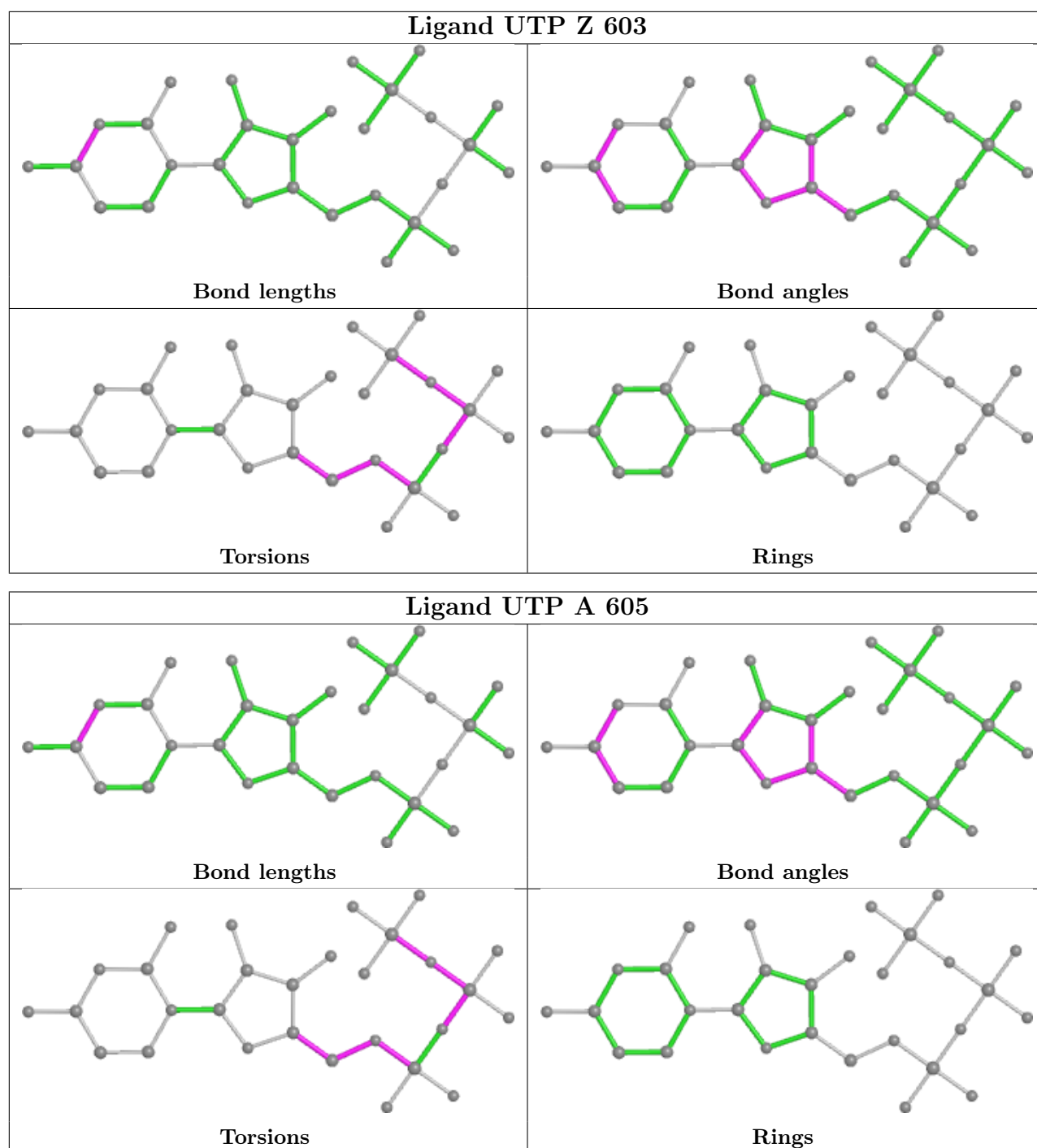


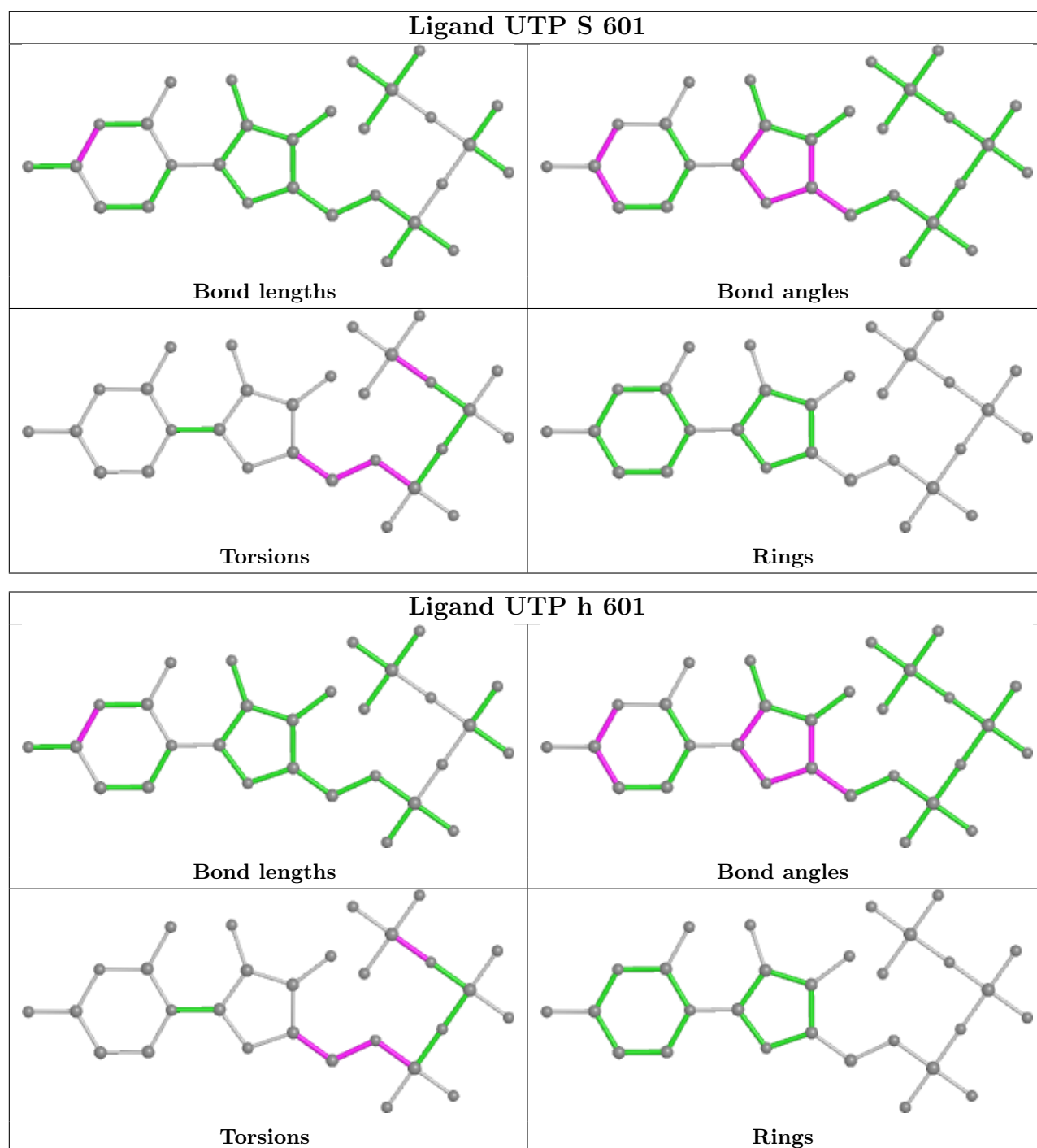


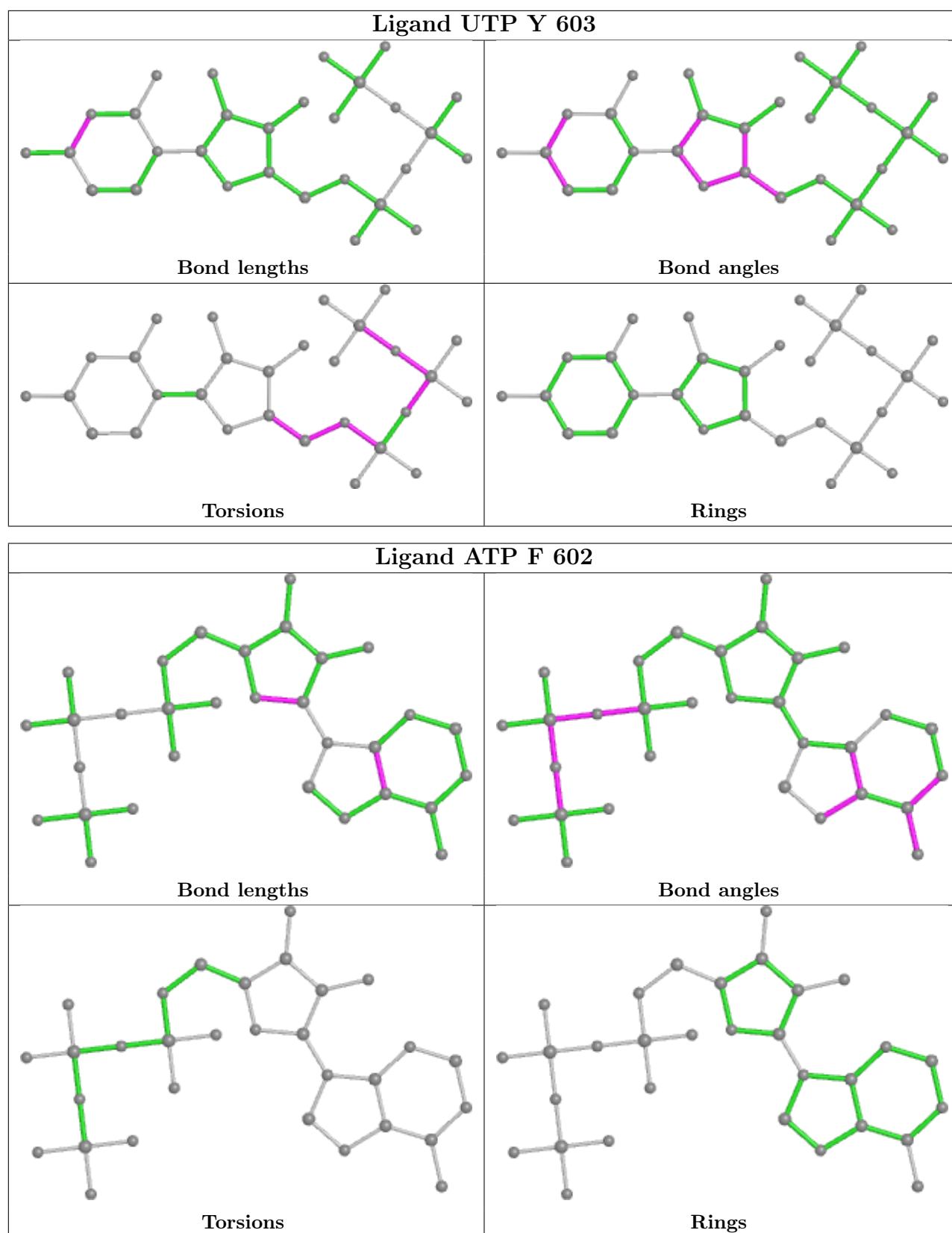


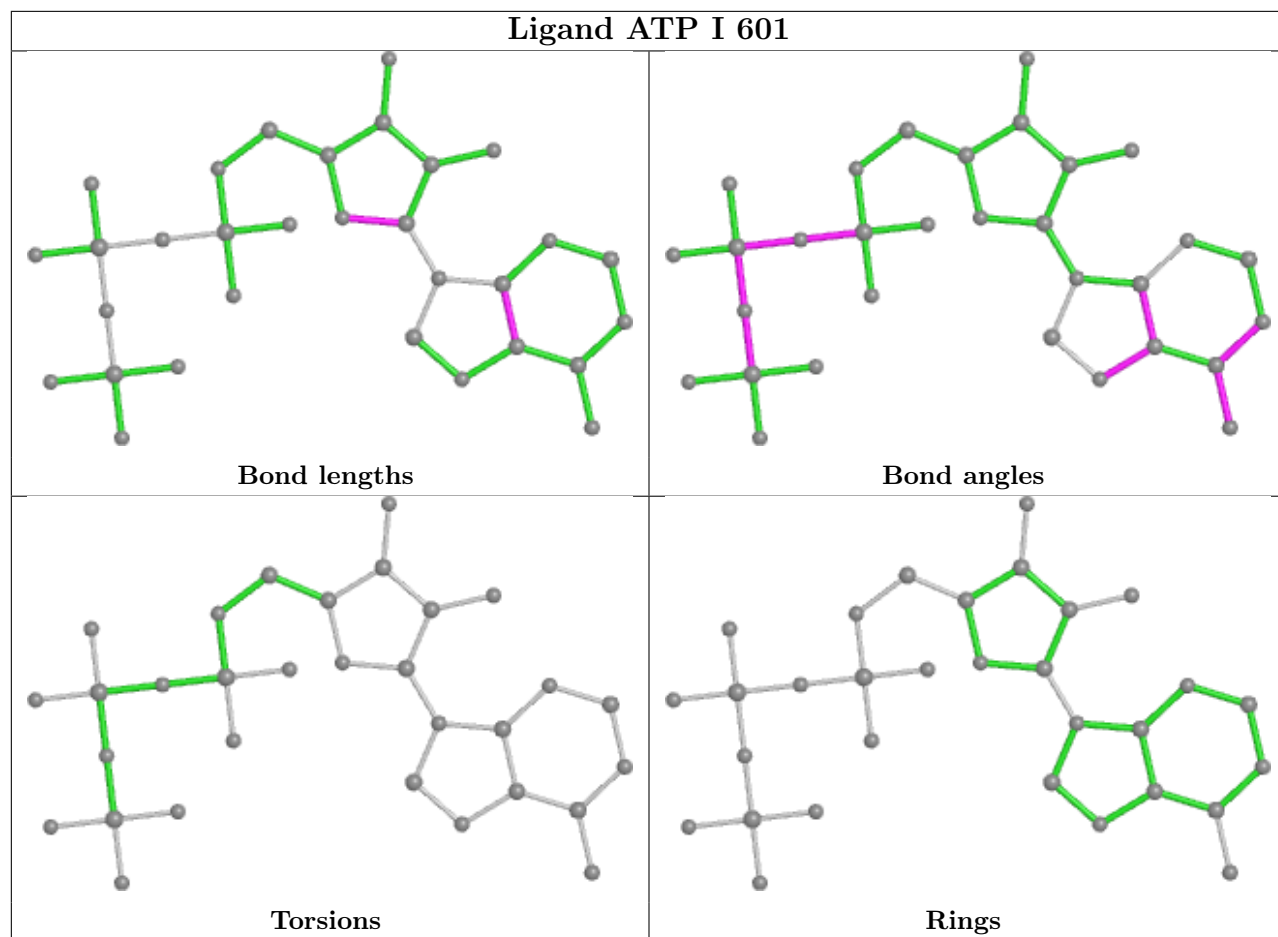


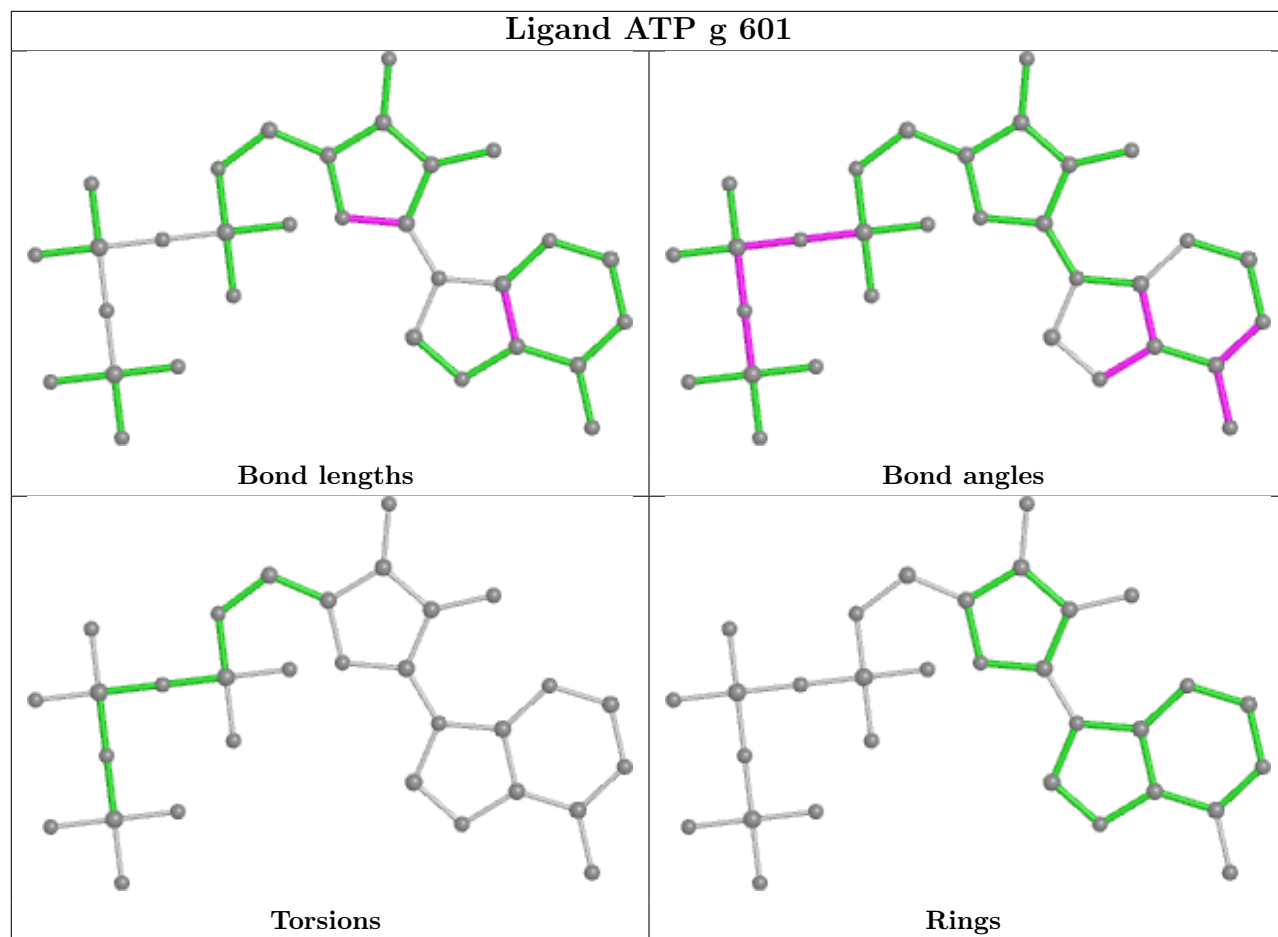


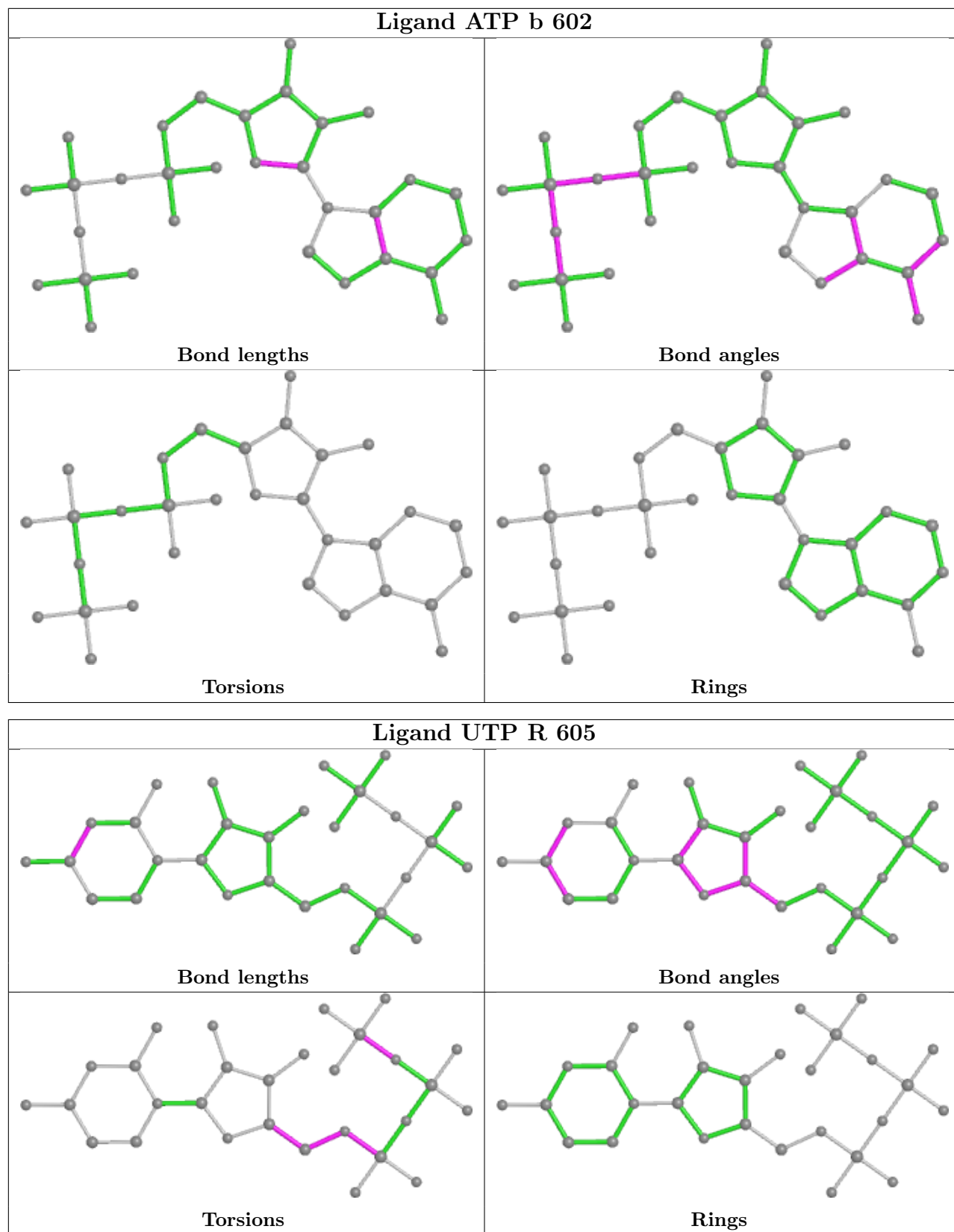


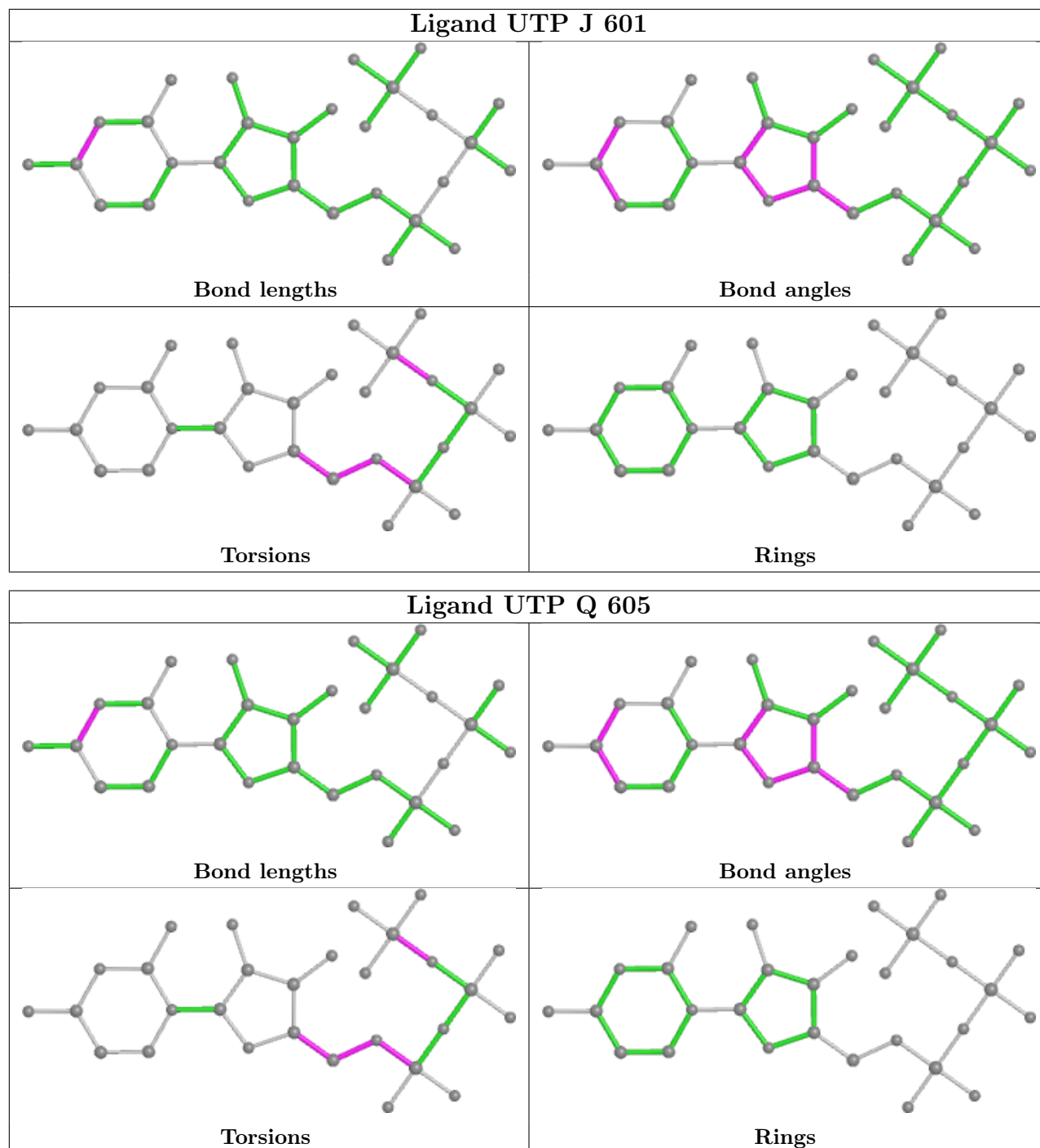


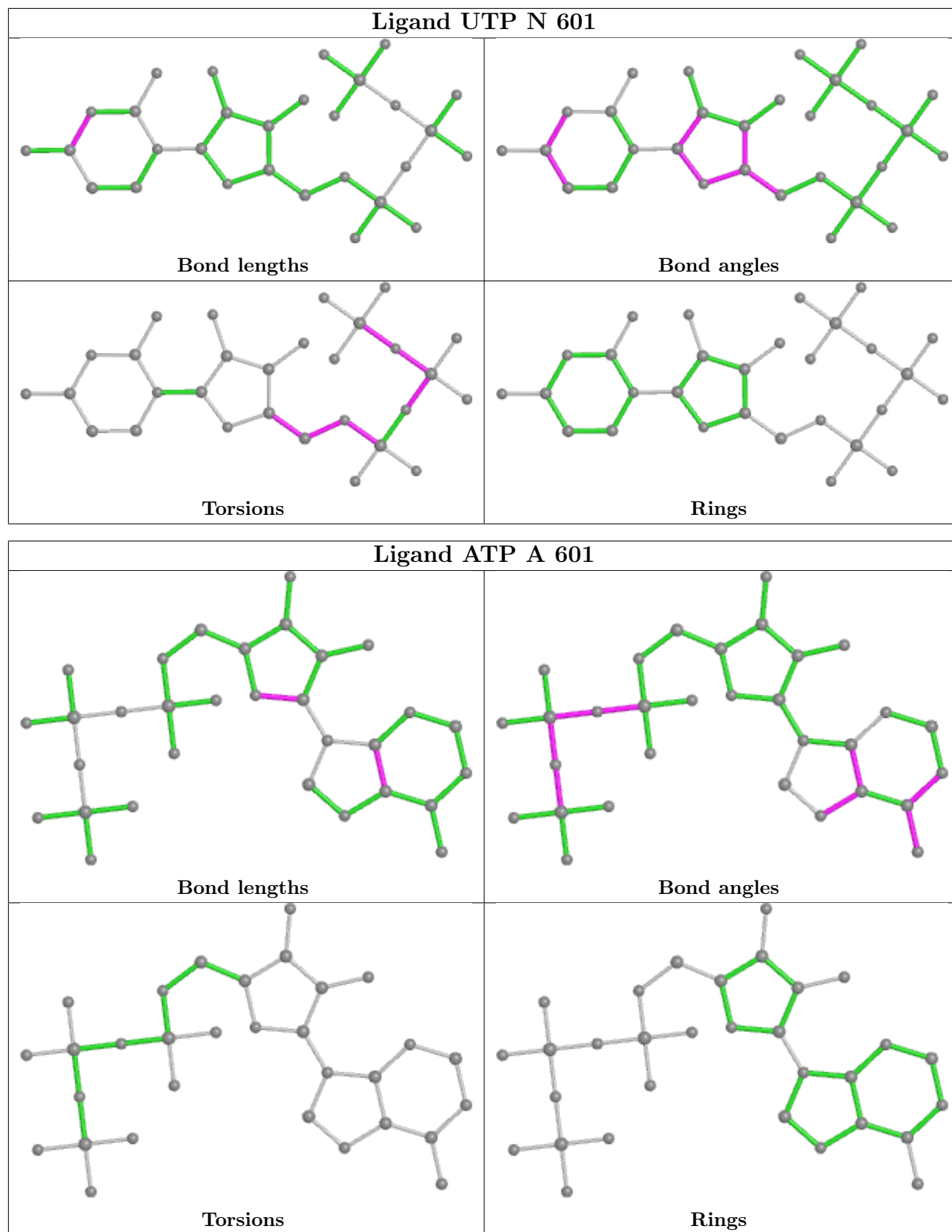


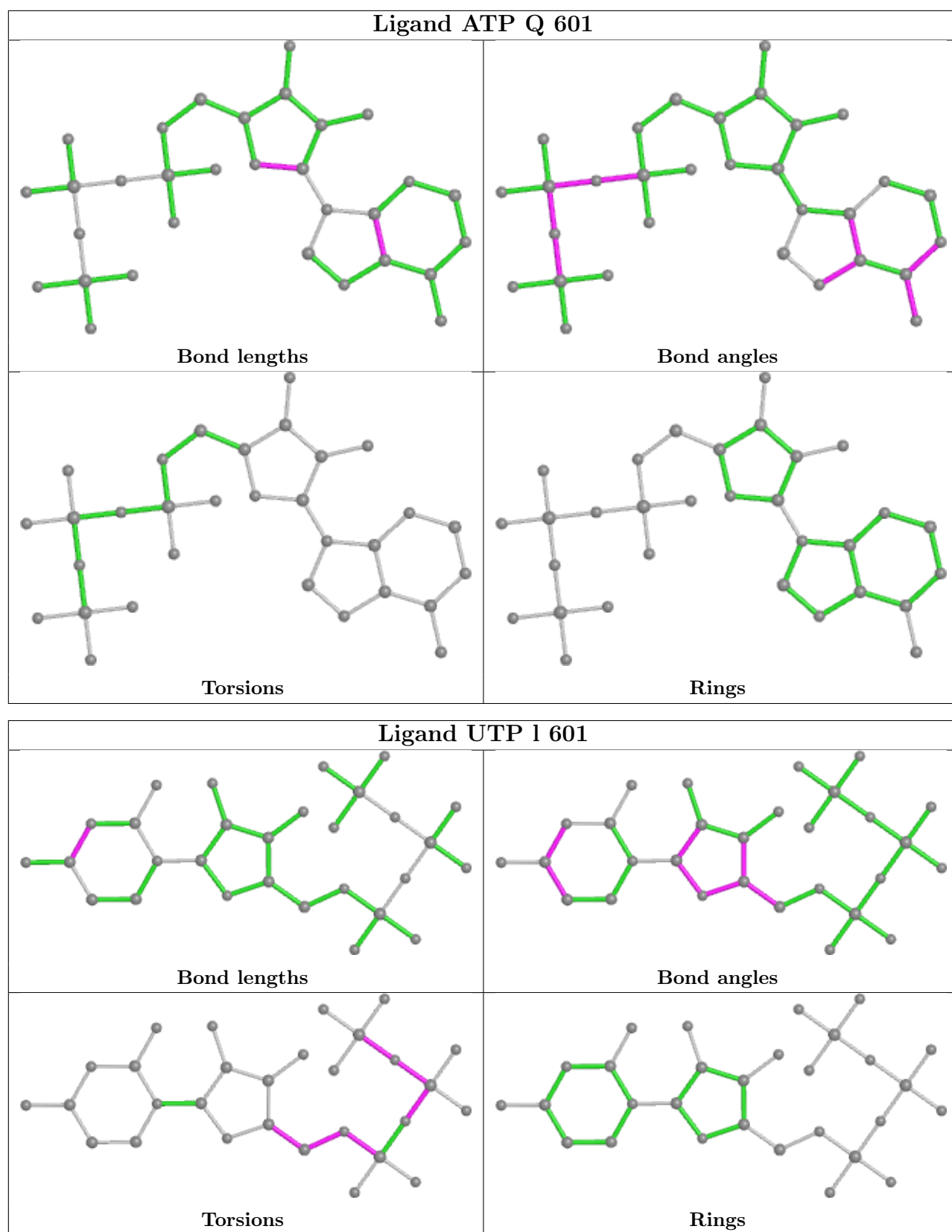


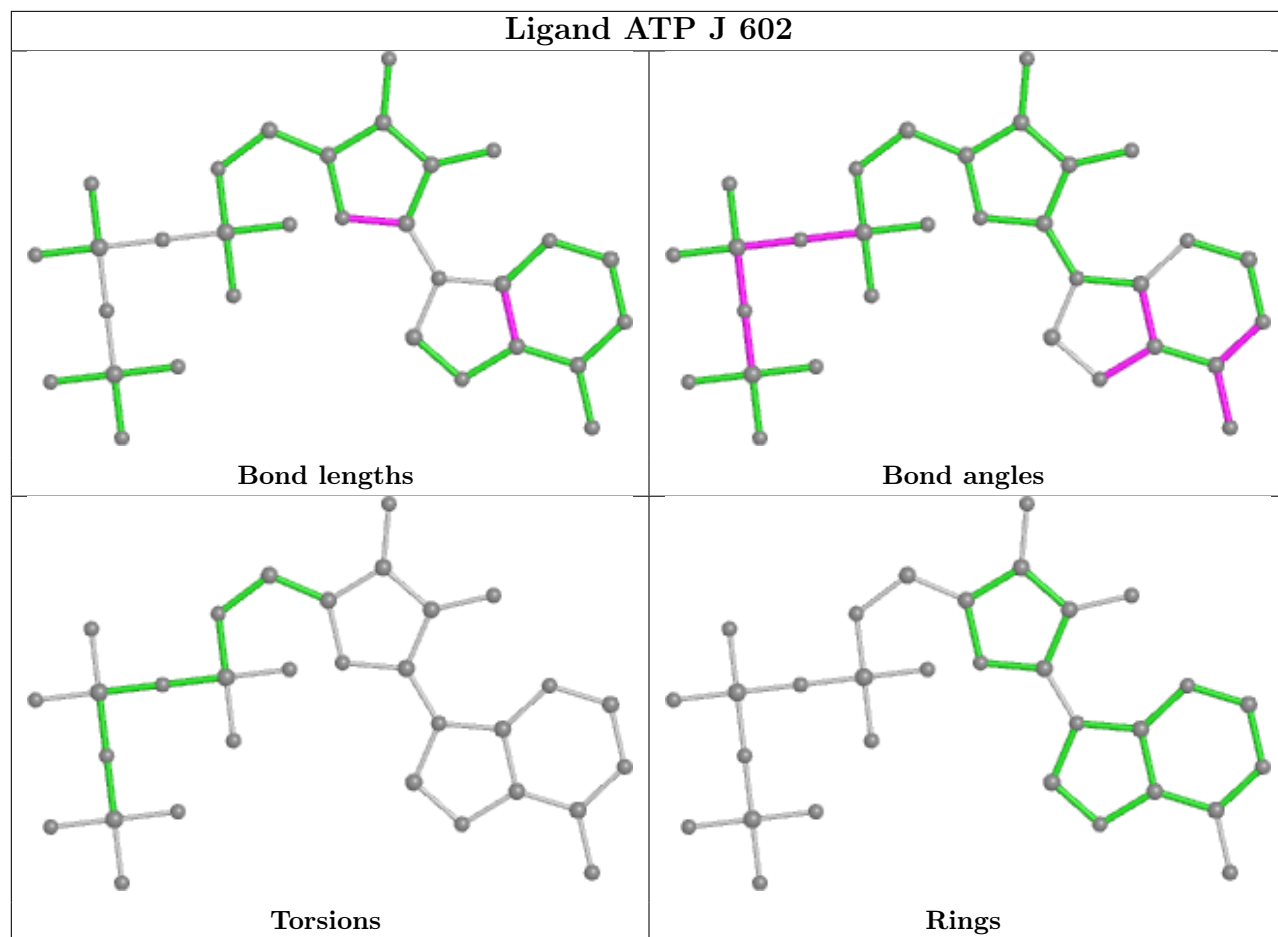


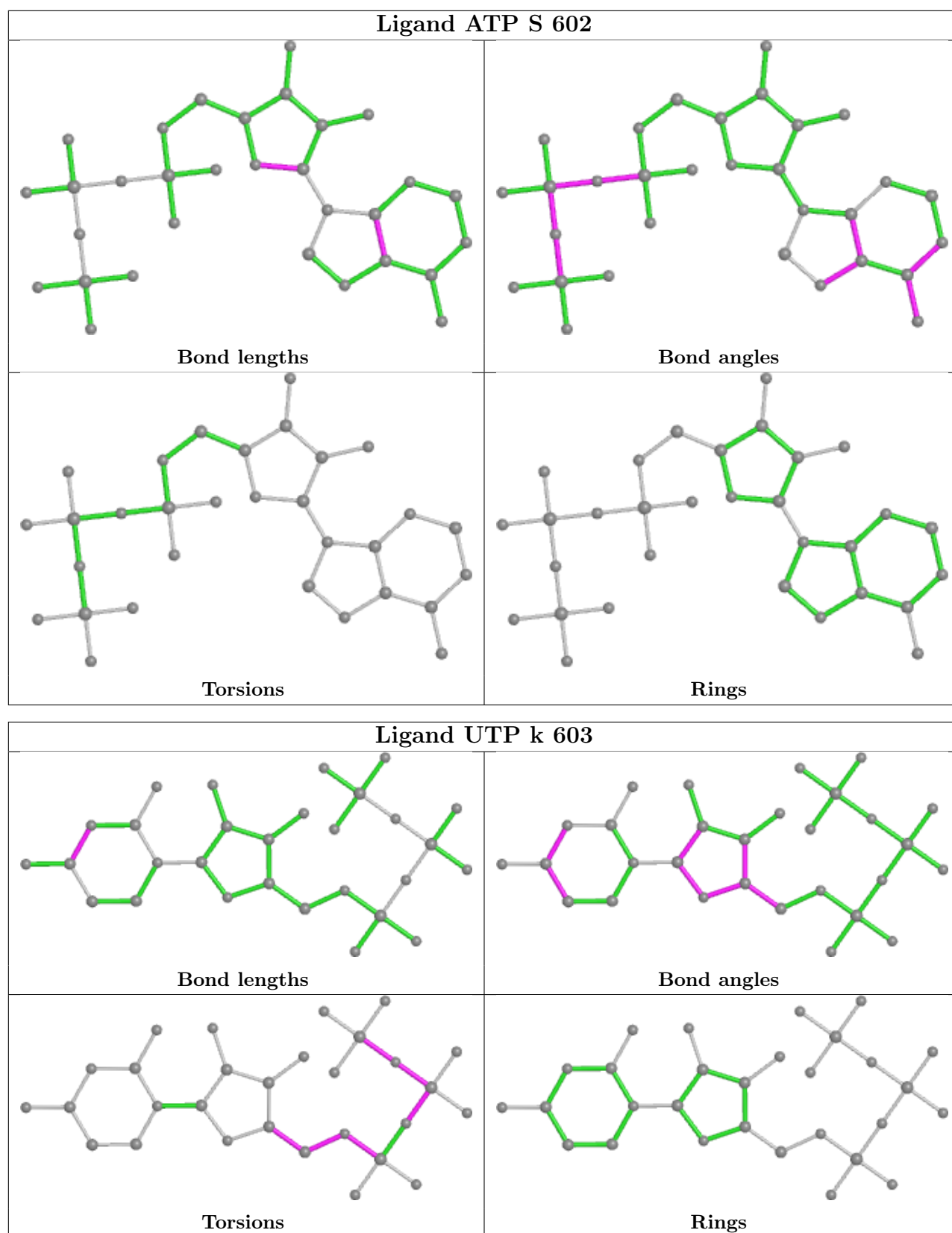


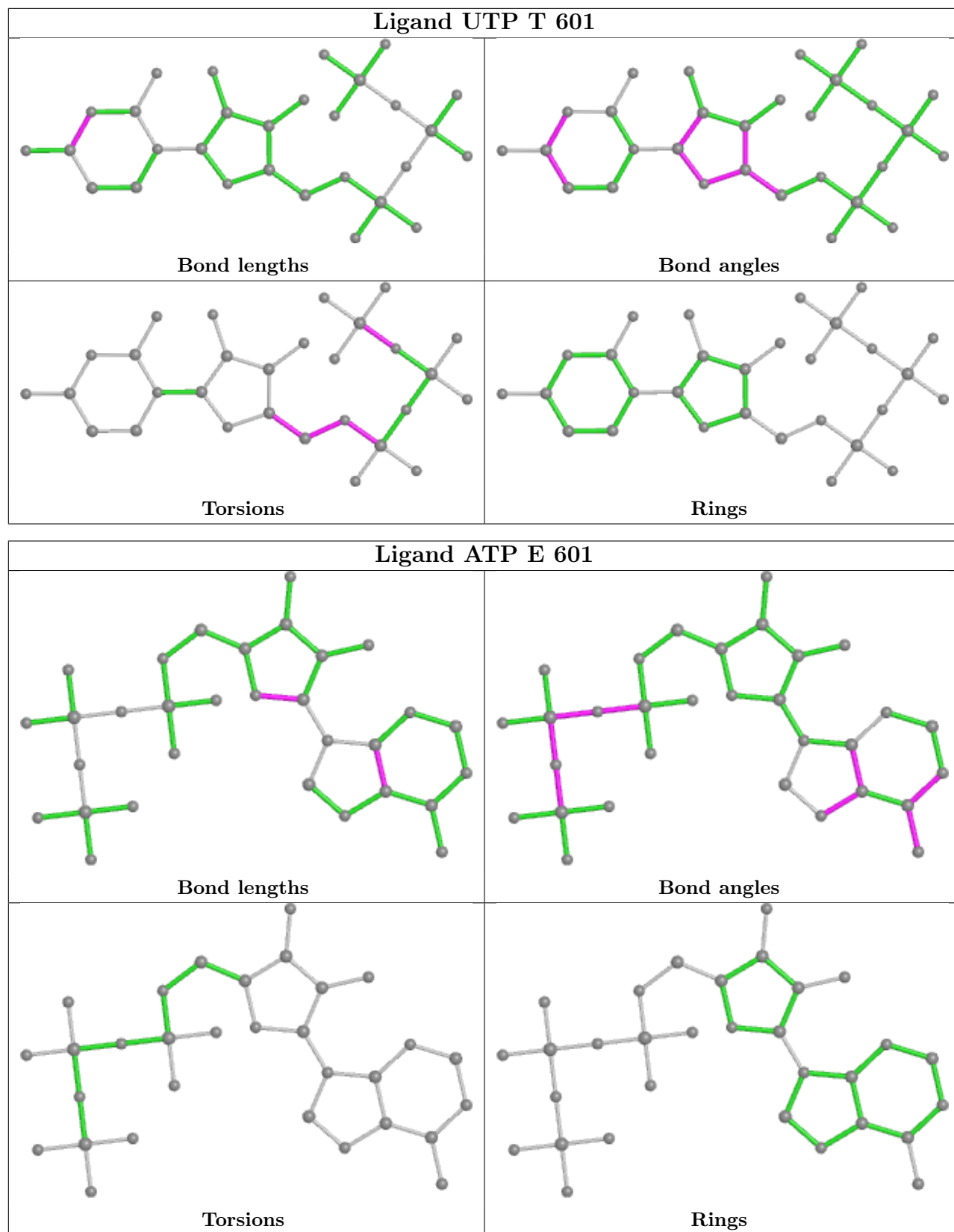


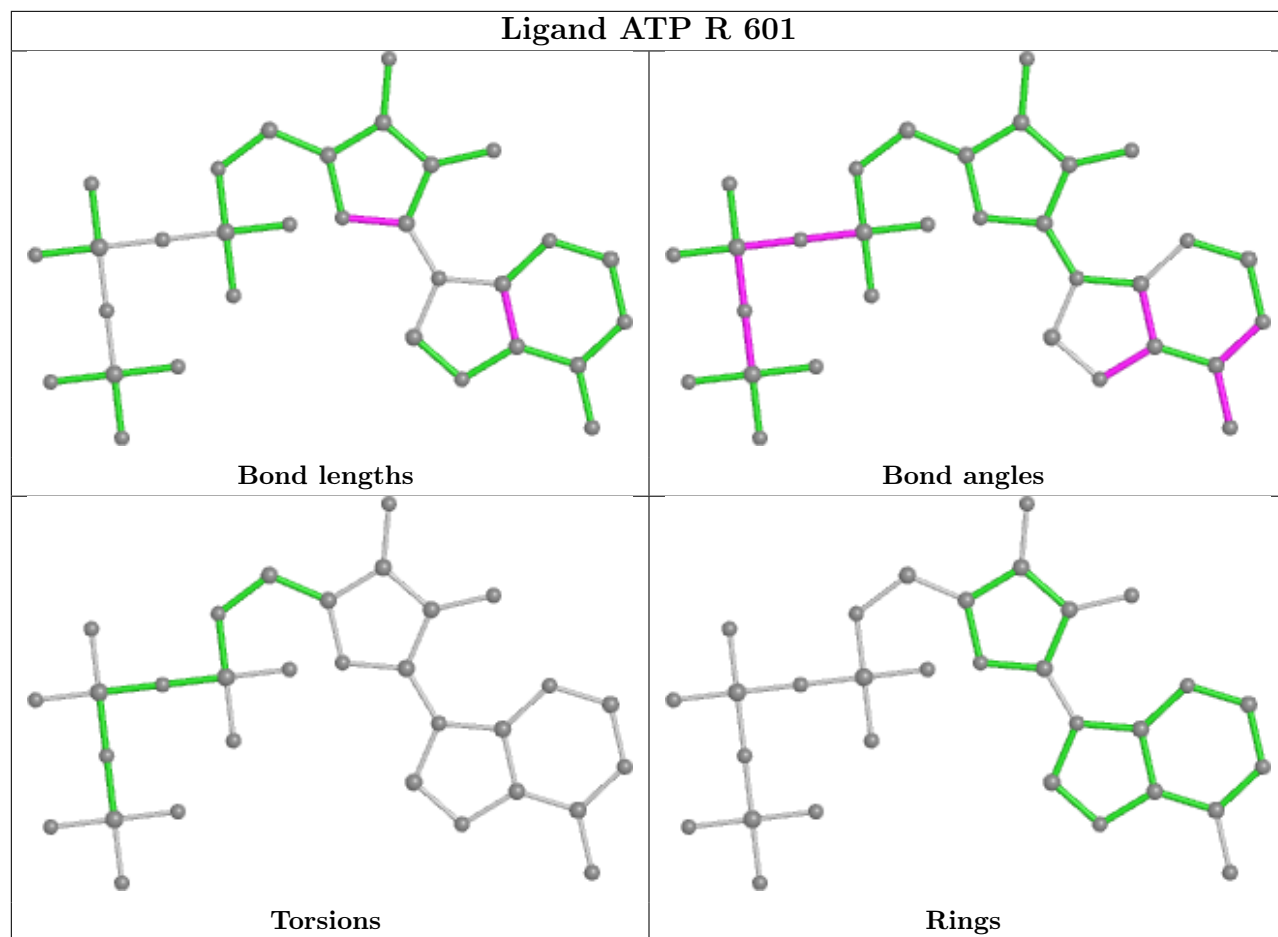


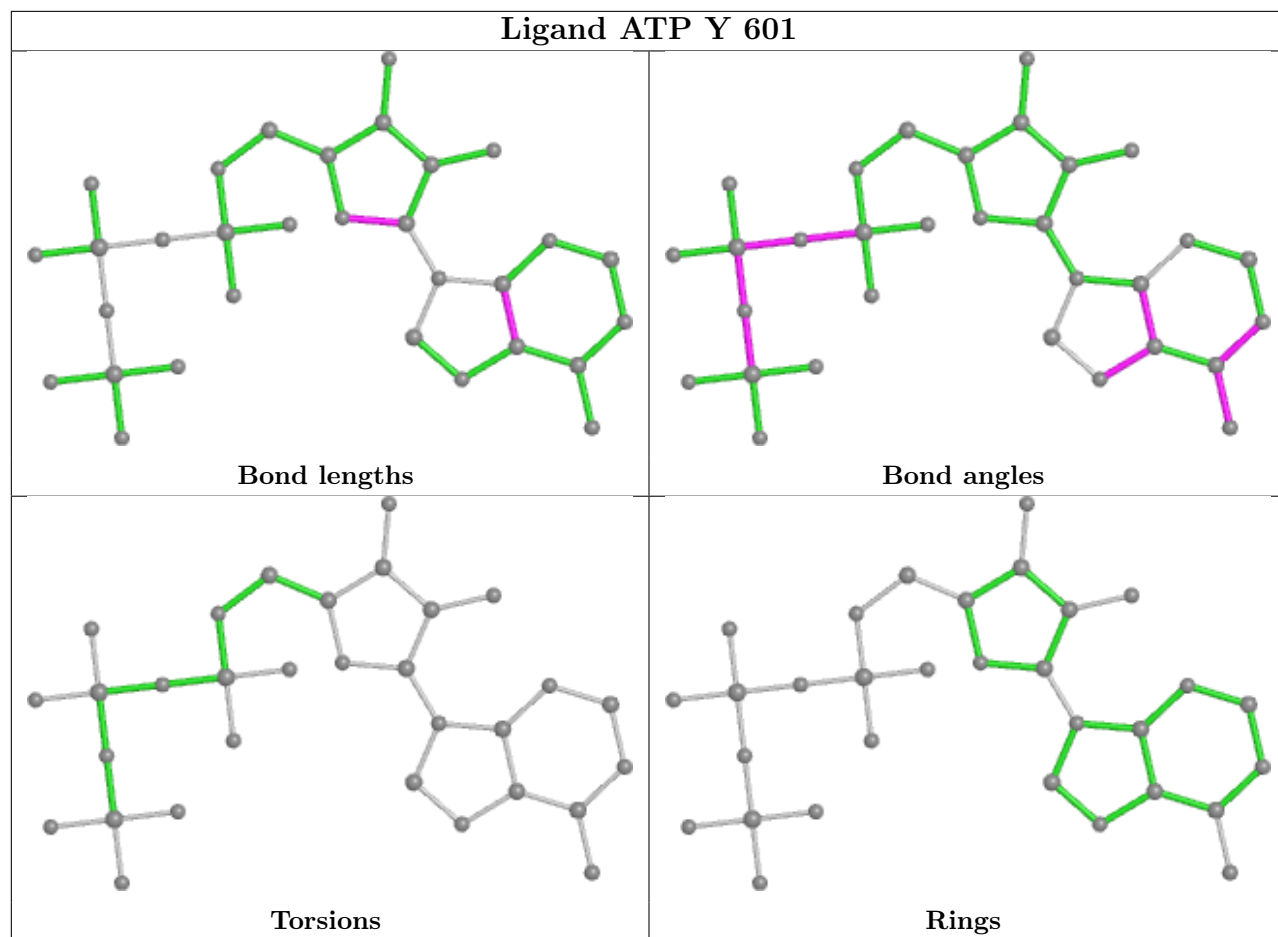


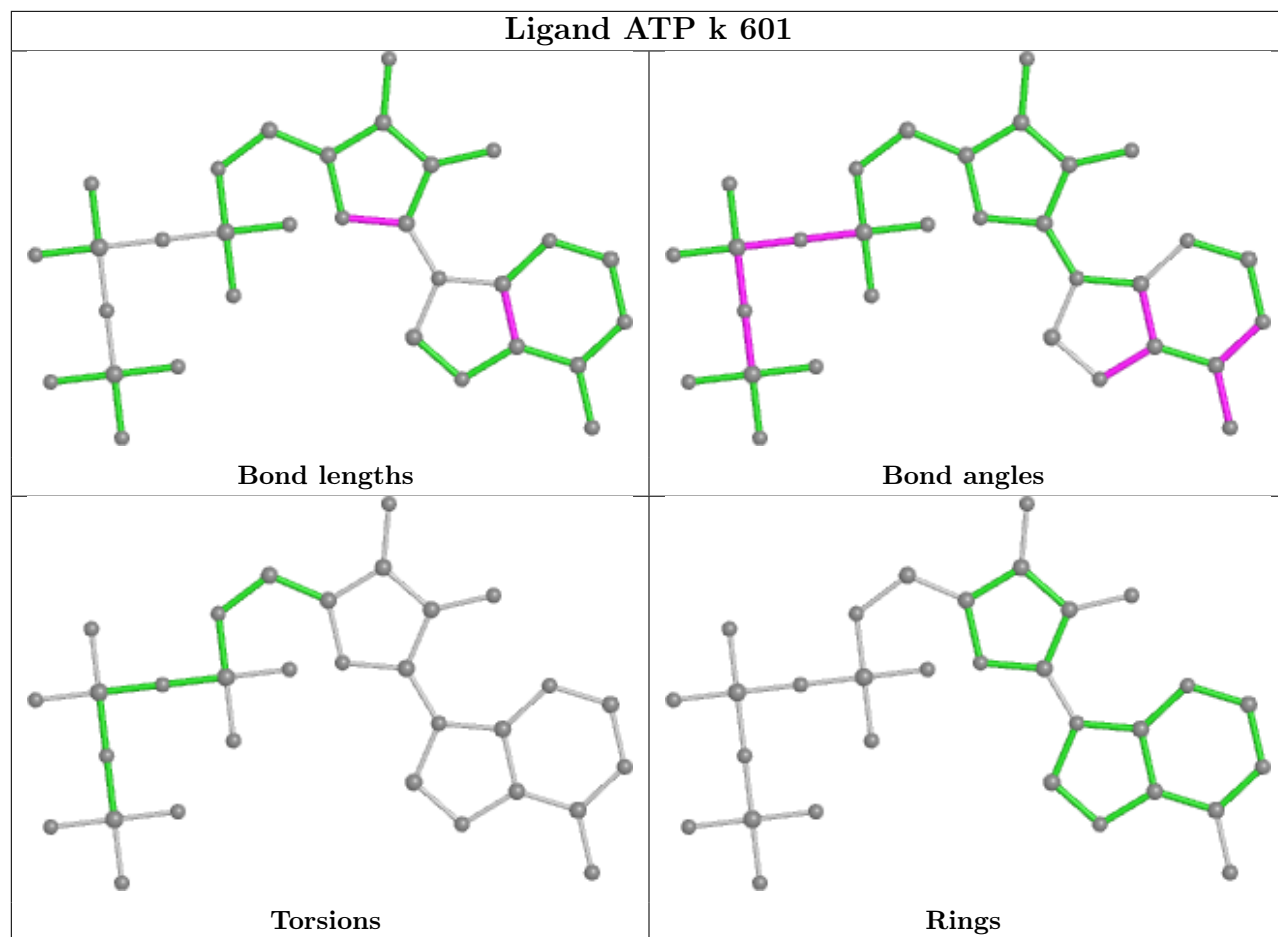


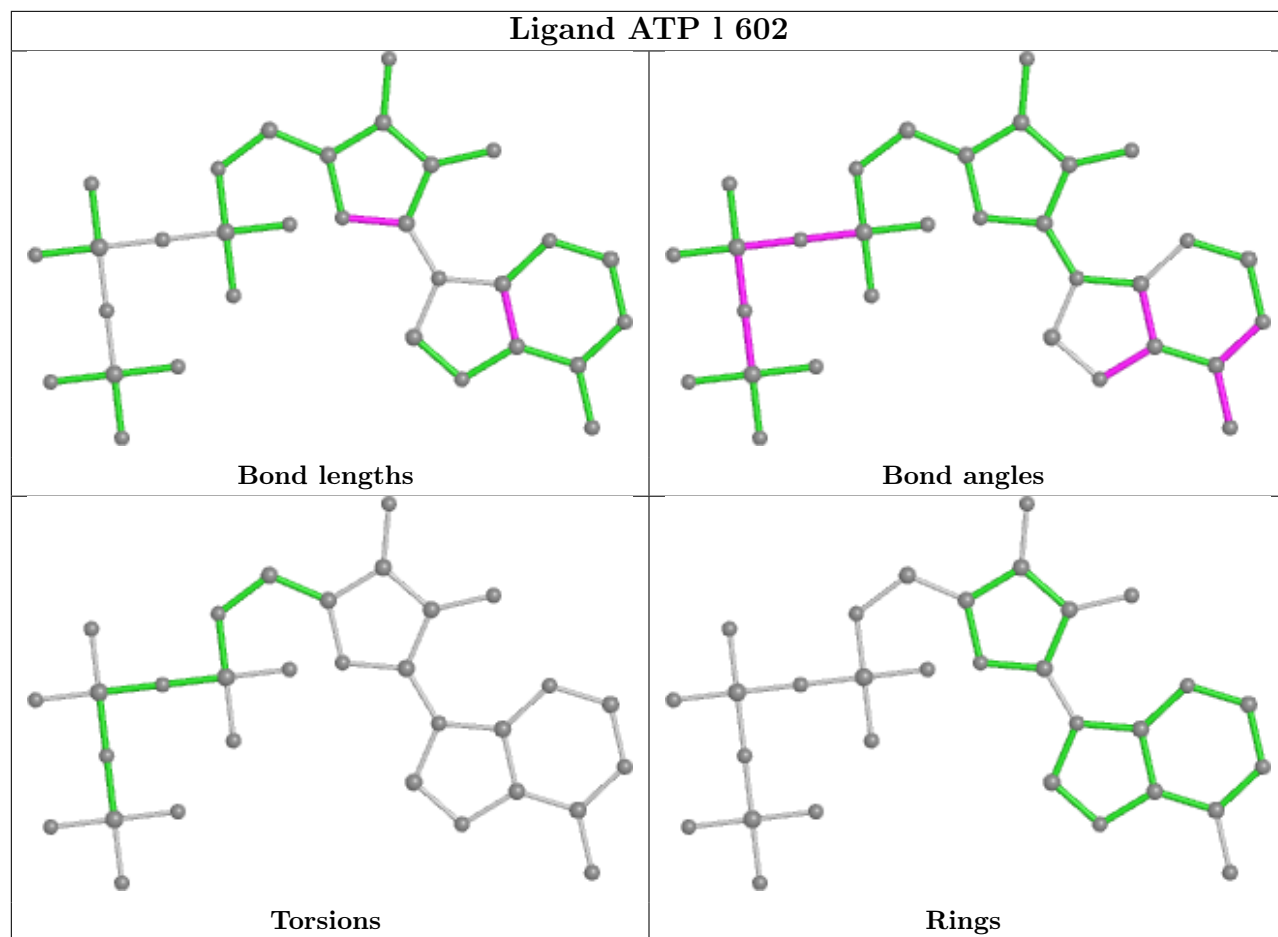


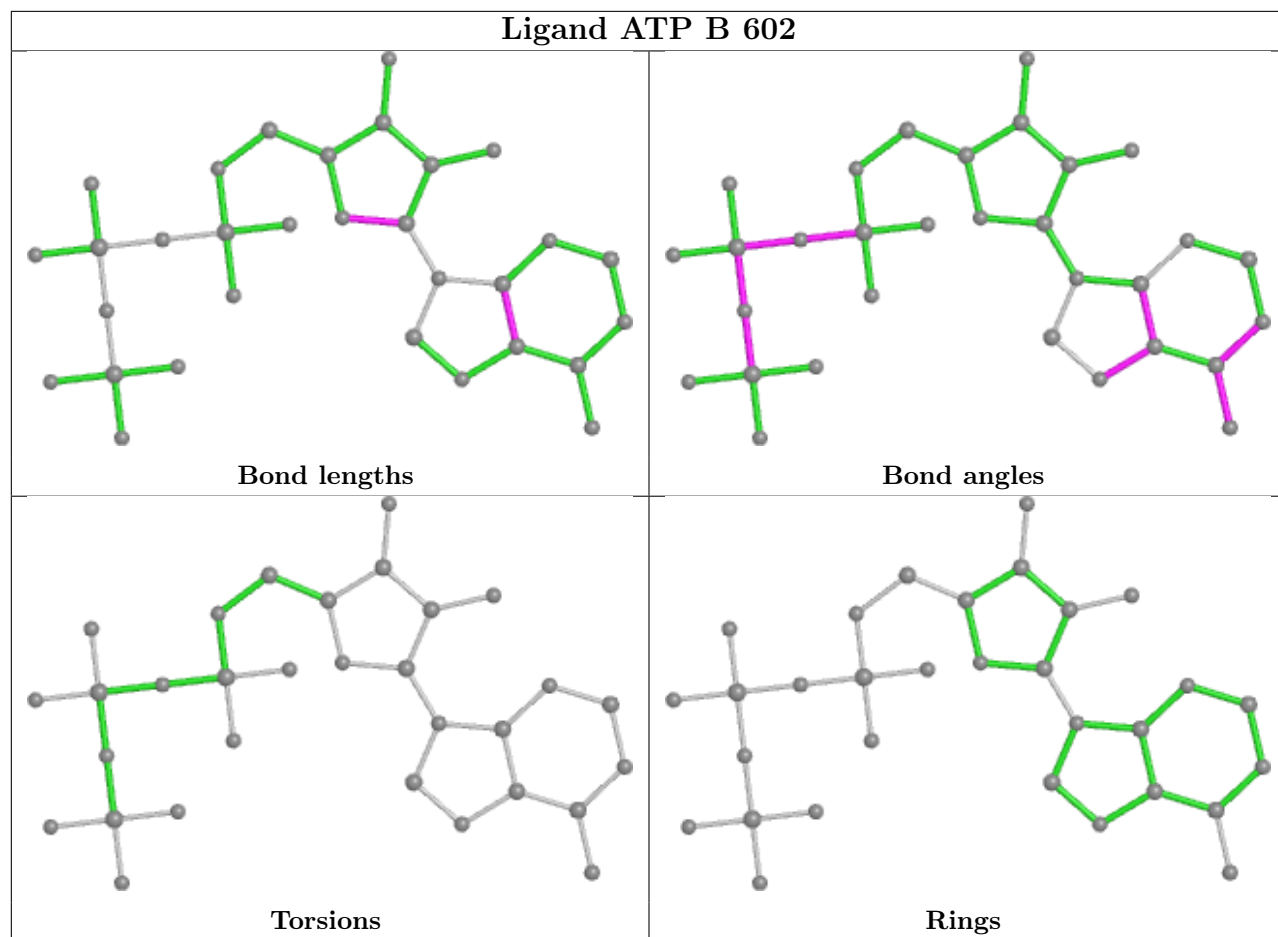


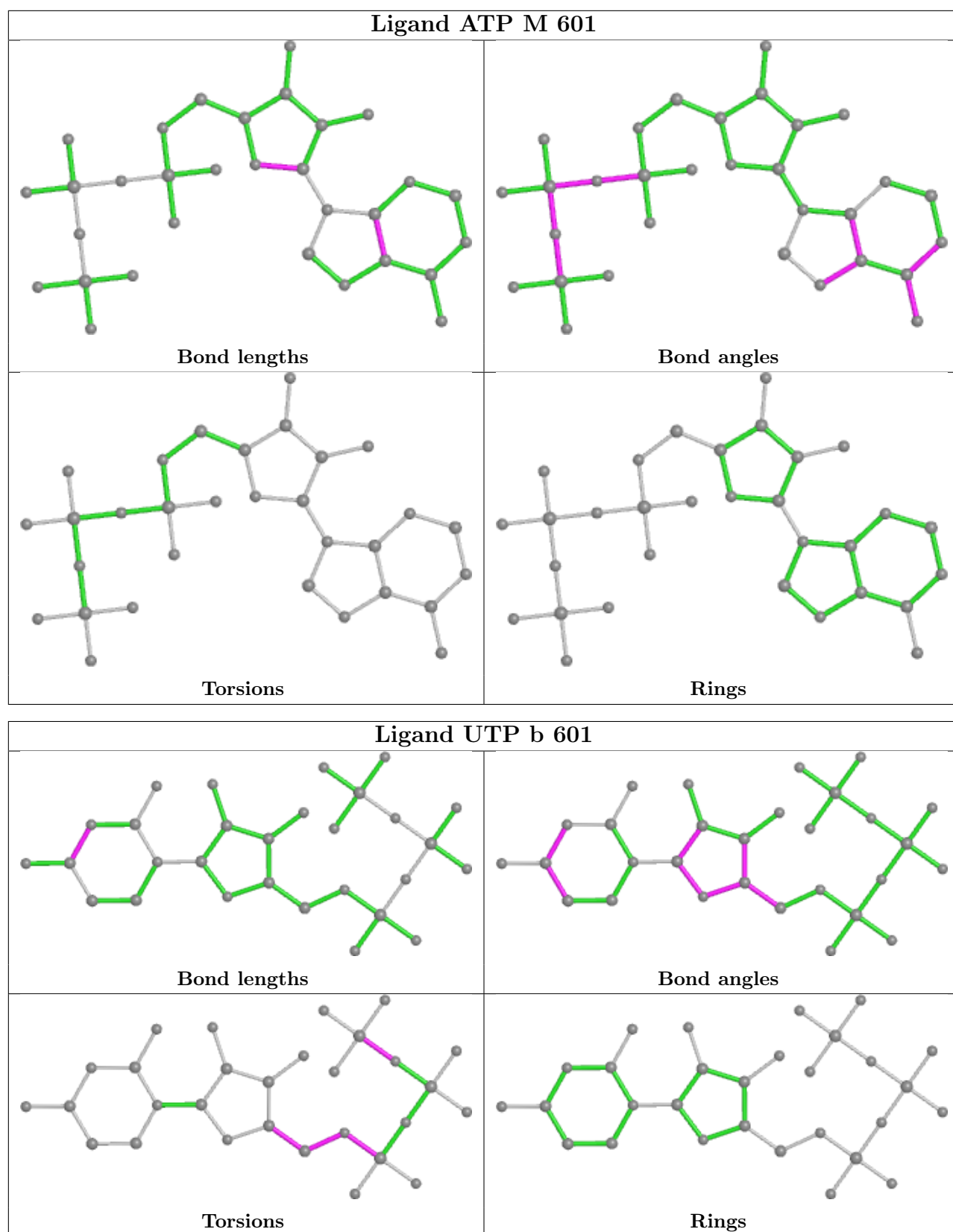


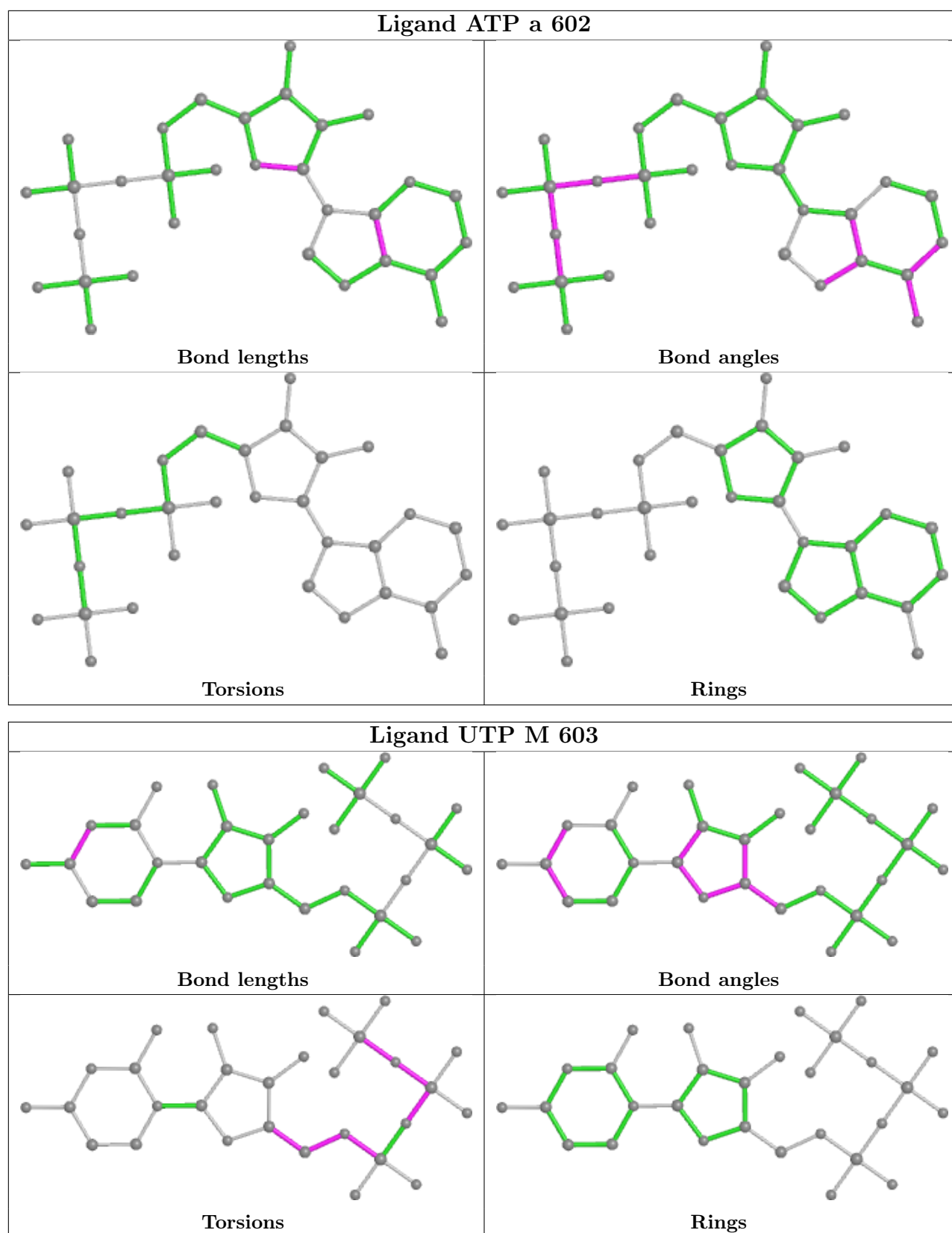












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	E	1
1	B	1
1	F	1
1	Q	1
1	Y	1
1	S	1
1	a	1
1	I	1
1	M	1
1	J	1
1	N	1
1	R	1
1	Z	1
1	T	1
1	b	1
1	g	1
1	k	1
1	h	1
1	l	1

The worst 5 of 20 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	443:ILE	C	456:THR	N	7.07
1	E	443:ILE	C	456:THR	N	7.07
1	B	443:ILE	C	456:THR	N	7.07
1	F	443:ILE	C	456:THR	N	7.07
1	Q	443:ILE	C	456:THR	N	7.07

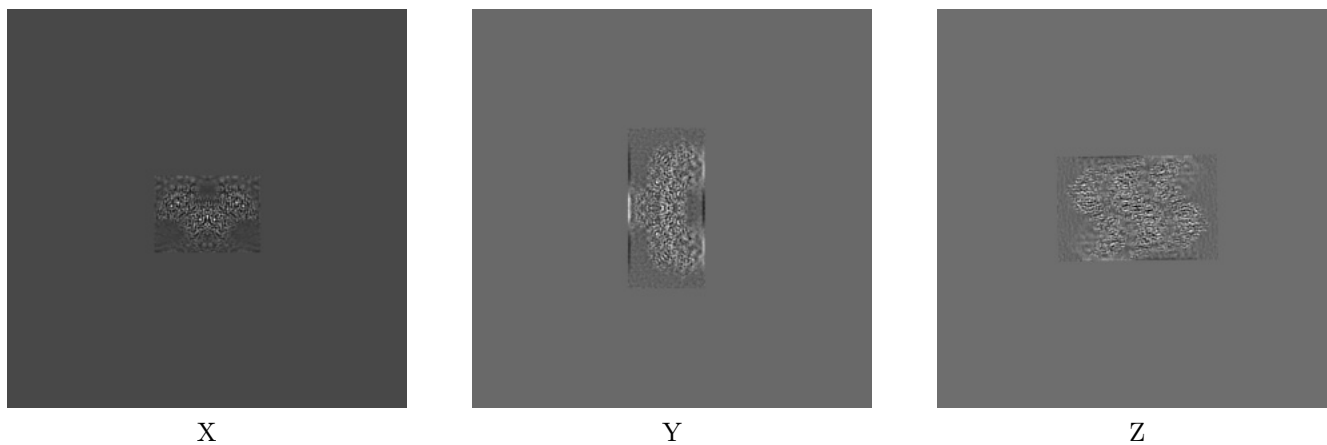
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24581. 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](#)

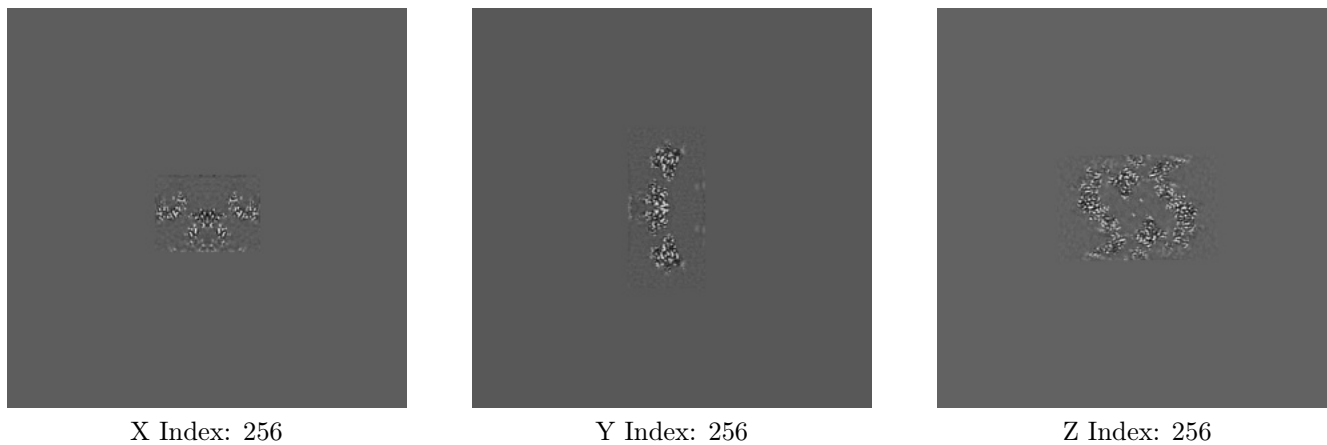
6.1.1 Primary map



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

6.2 Central slices [i](#)

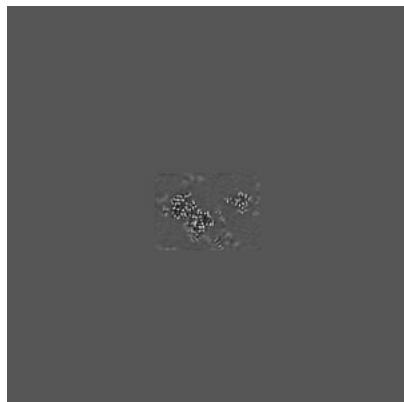
6.2.1 Primary map



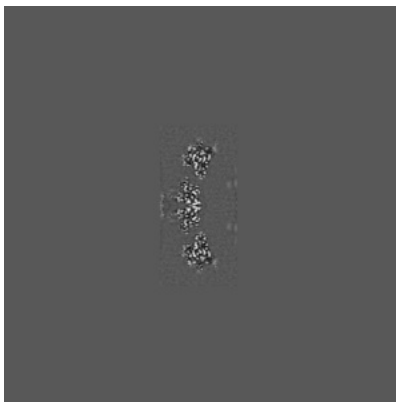
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

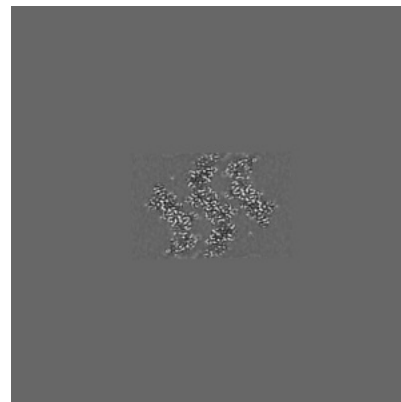
6.3.1 Primary map



X Index: 275



Y Index: 256

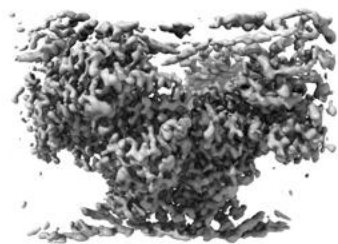


Z Index: 248

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

6.4 Orthogonal surface views [i](#)

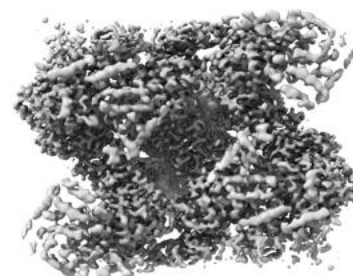
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

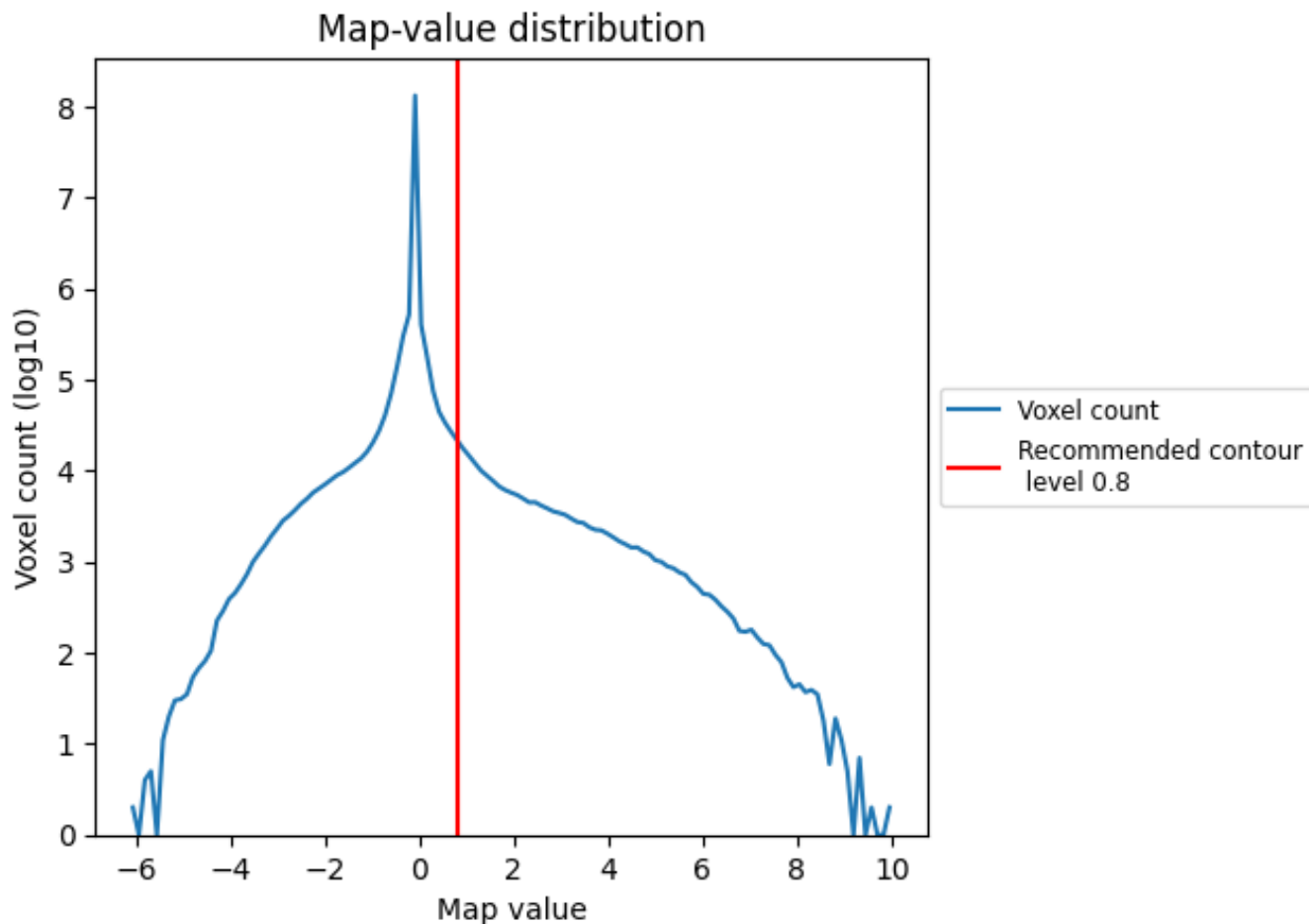
6.5 Mask visualisation

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

7 Map analysis [i](#)

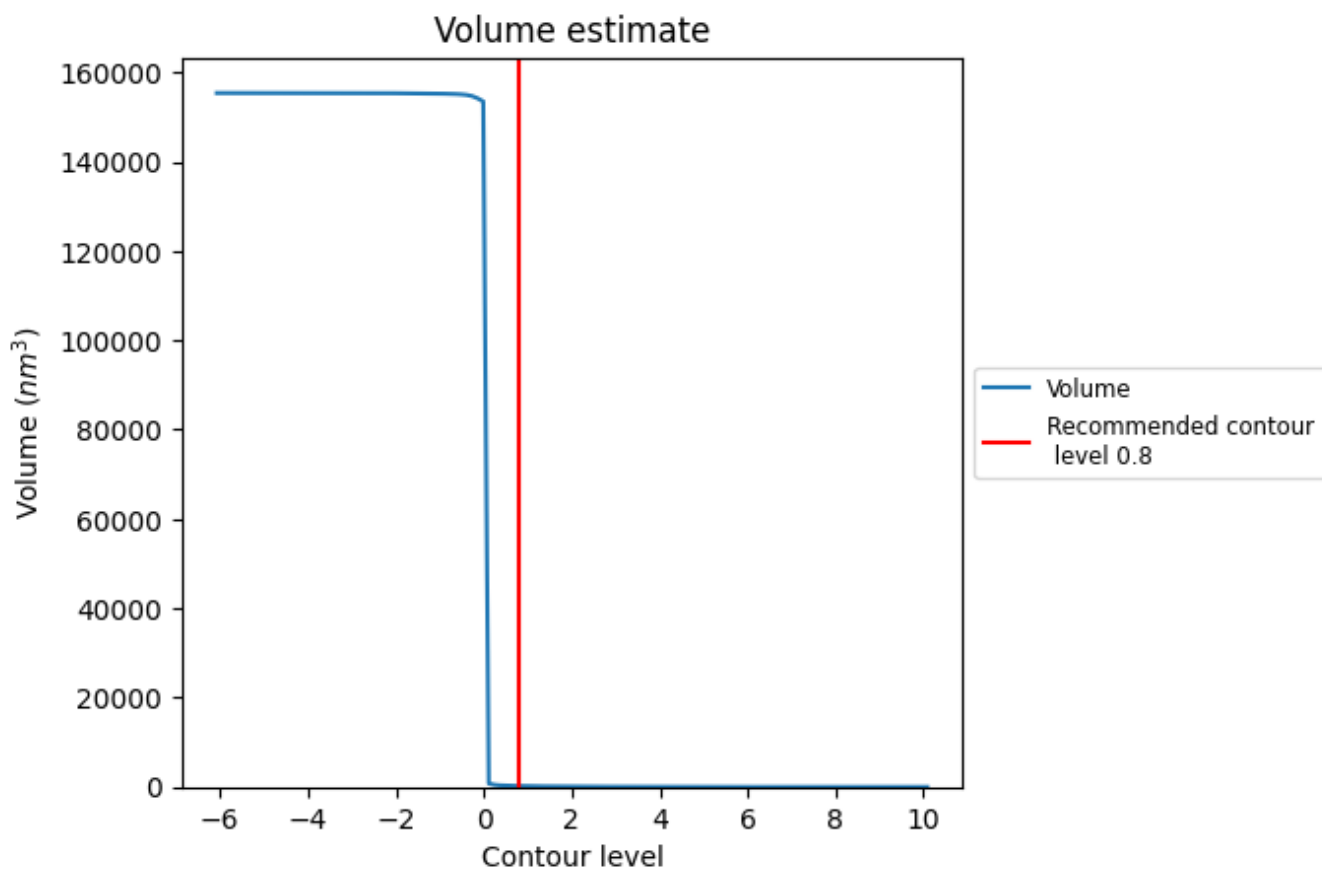
This section contains the results of statistical analysis of the map.

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.

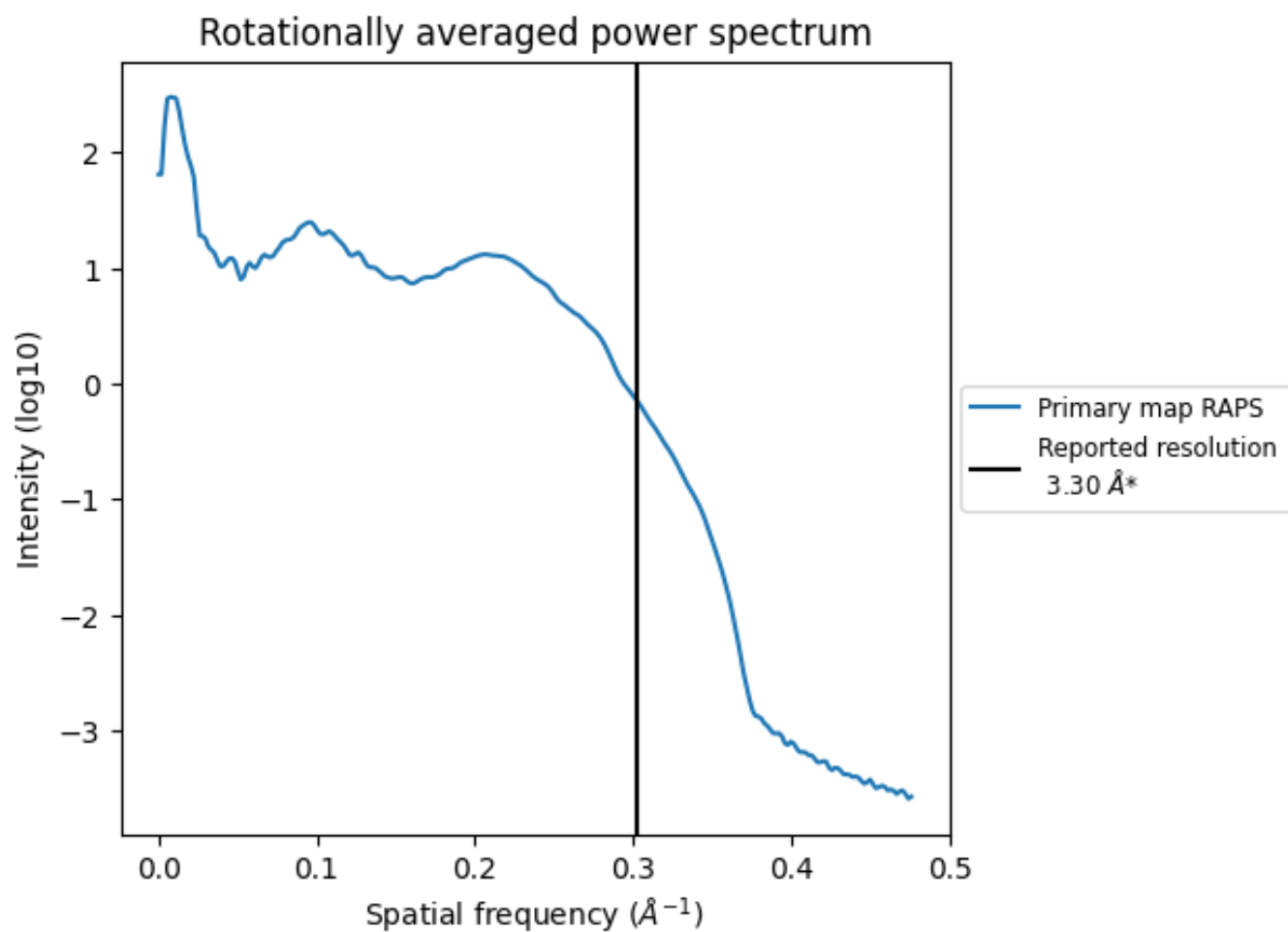
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 216 nm³; this corresponds to an approximate mass of 195 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 i



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

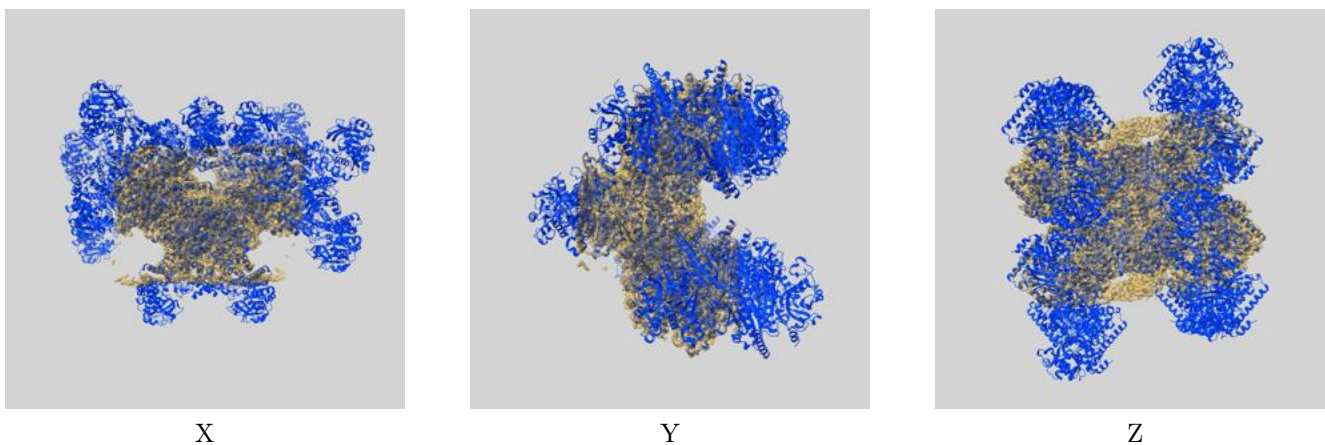
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

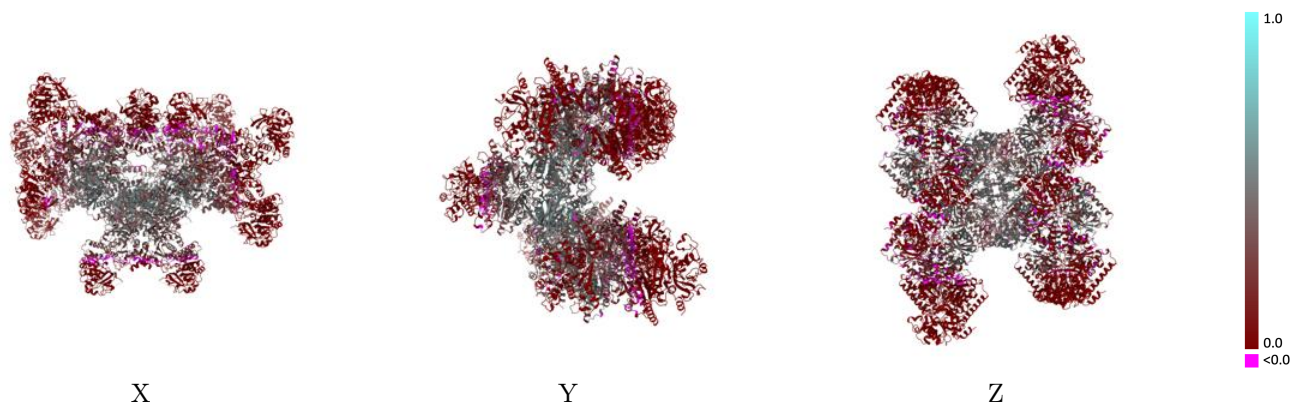
This section contains information regarding the fit between EMDB map EMD-24581 and PDB model 7RNR. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



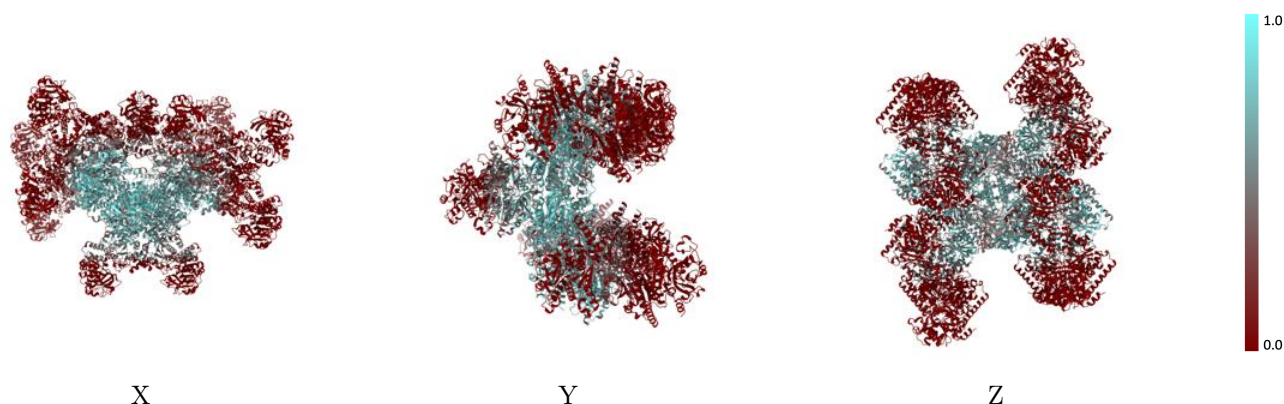
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



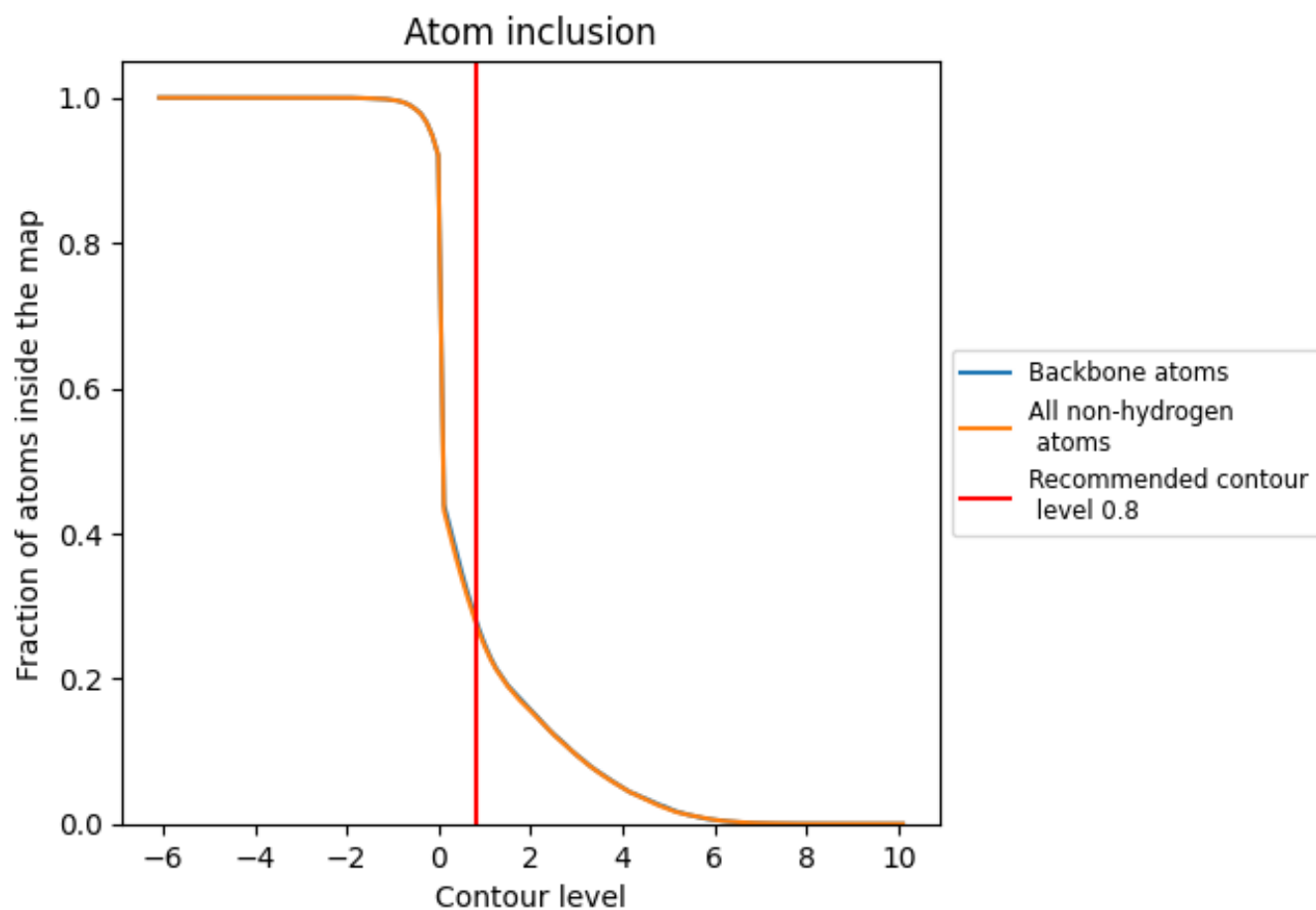
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 28% of all backbone atoms, 28% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2779	 0.1870
A	 0.7482	 0.4730
B	 0.2238	 0.1400
E	 0.2228	 0.1390
F	 0.7504	 0.4710
I	 0.0238	 0.0160
J	 0.6420	 0.3830
M	 0.0591	 0.0470
N	 0.1124	 0.0970
Q	 0.6912	 0.4150
R	 0.6912	 0.4130
S	 0.0316	 0.0420
T	 0.0311	 0.0420
Y	 0.1287	 0.0930
Z	 0.1324	 0.0930
a	 0.1699	 0.1610
b	 0.1738	 0.1640
g	 0.0247	 0.0160
h	 0.6434	 0.3870
k	 0.0605	 0.0490
l	 0.1140	 0.0970

