



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:44 PM UTC

PDB ID : 7RNR / pdb_00007rnr
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

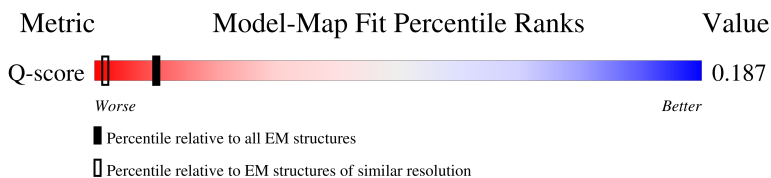
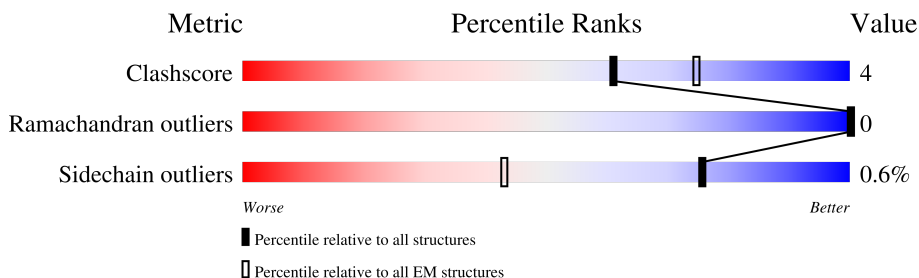
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	
1	B	559	
1	E	559	
1	F	559	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	559	98% 96% .
1	J	559	15% 95% .
1	M	559	93% 96% .
1	N	559	88% 96% .
1	Q	559	10% 96% .
1	R	559	10% 96% .
1	S	559	97% 96% .
1	T	559	97% 96% .
1	Y	559	85% 96% .
1	Z	559	85% 96% .
1	a	559	80% 96% .
1	b	559	79% 96% .
1	g	559	98% 96% .
1	h	559	15% 96% .
1	k	559	93% 96% .
1	l	559	88% 96% .

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
2	ATP	A	601	-	-	X	-
2	ATP	B	602	-	-	X	-
2	ATP	E	601	-	-	X	-
2	ATP	F	602	-	-	X	-
2	ATP	I	601	-	-	X	-
2	ATP	J	602	-	-	X	-
2	ATP	M	601	-	-	X	-
2	ATP	N	602	-	-	X	-
2	ATP	Q	601	-	-	X	-
2	ATP	R	601	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	S	602	-	-	X	-
2	ATP	T	602	-	-	X	-
2	ATP	Y	601	-	-	X	-
2	ATP	Z	601	-	-	X	-
2	ATP	a	602	-	-	X	-
2	ATP	b	602	-	-	X	-
2	ATP	g	601	-	-	X	-
2	ATP	h	602	-	-	X	-
2	ATP	k	601	-	-	X	-
2	ATP	l	602	-	-	X	-
4	UTP	A	605	X	-	X	-
4	UTP	B	601	X	-	X	-
4	UTP	E	603	X	-	X	-
4	UTP	F	601	X	-	X	-
4	UTP	I	605	X	-	X	-
4	UTP	J	601	X	-	X	-
4	UTP	M	603	X	-	X	-
4	UTP	N	601	X	-	X	-
4	UTP	Q	605	X	-	X	-
4	UTP	R	605	X	-	X	-
4	UTP	S	601	X	-	X	-
4	UTP	T	601	X	-	X	-
4	UTP	Y	603	X	-	X	-
4	UTP	Z	603	X	-	X	-
4	UTP	a	601	X	-	X	-
4	UTP	b	601	X	-	X	-
4	UTP	g	605	X	-	X	-
4	UTP	h	601	X	-	X	-
4	UTP	k	603	X	-	X	-
4	UTP	l	601	X	-	X	-

2 Entry composition

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

Continued on next page...

Continued from previous page...

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

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...

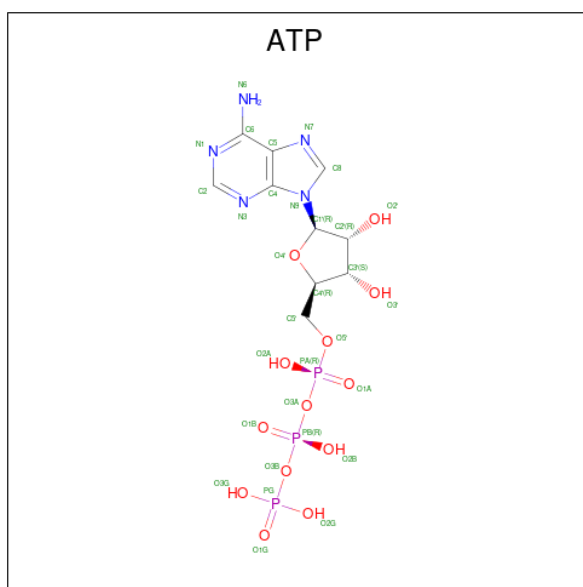
Chain	Residue	Modelled	Actual	Comment	Reference
Z	?	-	PRO	deletion	UNP A0A6A5PYW3
Z	?	-	GLU	deletion	UNP A0A6A5PYW3
Z	?	-	ILE	deletion	UNP A0A6A5PYW3
Z	?	-	ASP	deletion	UNP A0A6A5PYW3
Z	?	-	LYS	deletion	UNP A0A6A5PYW3
Z	?	-	GLU	deletion	UNP A0A6A5PYW3
Z	?	-	HIS	deletion	UNP A0A6A5PYW3
Z	?	-	MET	deletion	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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

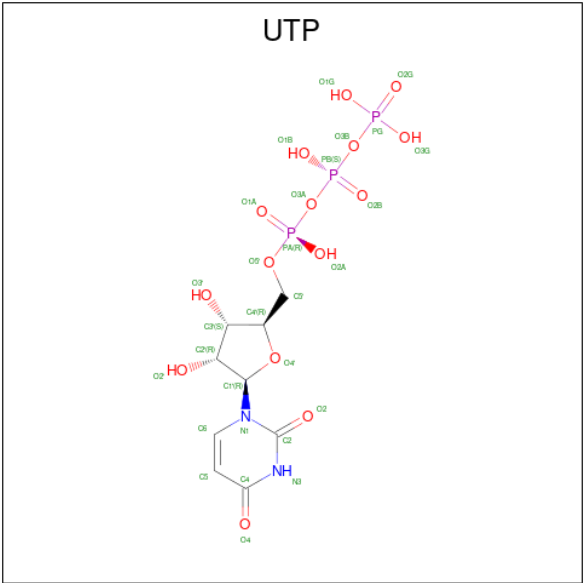
Mol	Chain	Residues	Atoms		AltConf
3	A	3	Total	Mg	0
			3	3	
3	E	1	Total	Mg	0
			1	1	
3	B	3	Total	Mg	0
			3	3	
3	F	1	Total	Mg	0
			1	1	
3	Q	3	Total	Mg	0
			3	3	
3	Y	1	Total	Mg	0
			1	1	
3	S	3	Total	Mg	0
			3	3	
3	a	1	Total	Mg	0
			1	1	
3	I	3	Total	Mg	0
			3	3	
3	M	1	Total	Mg	0
			1	1	
3	J	3	Total	Mg	0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

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 (CCD ID: 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...

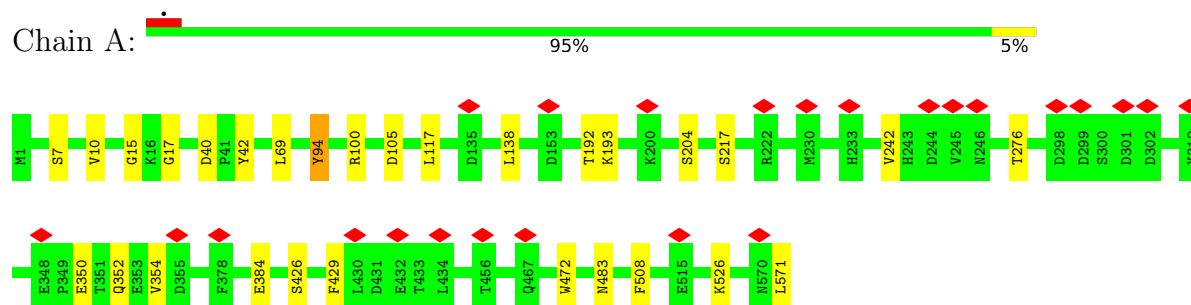
Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
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

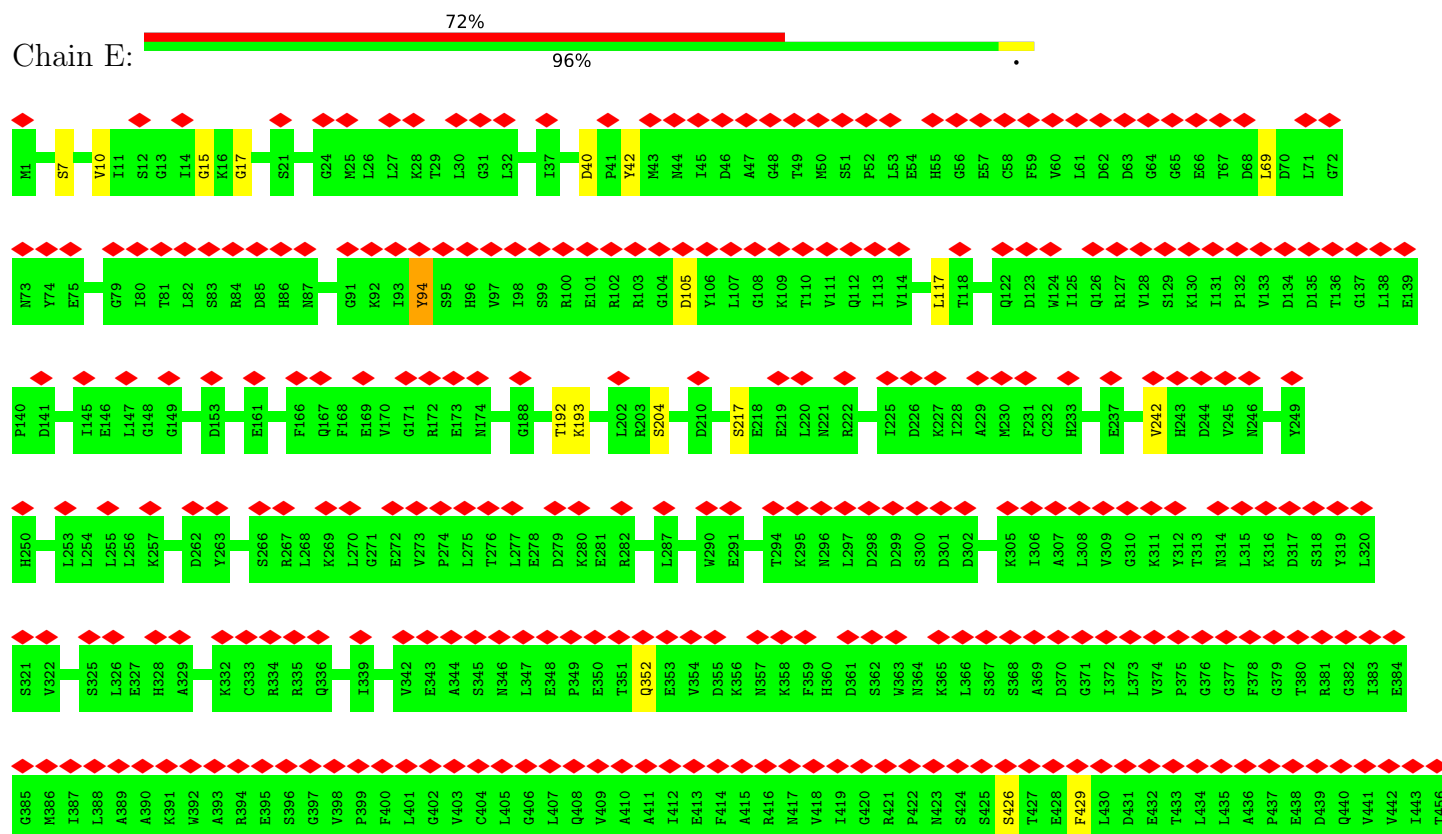
3 Residue-property plots [i](#)

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

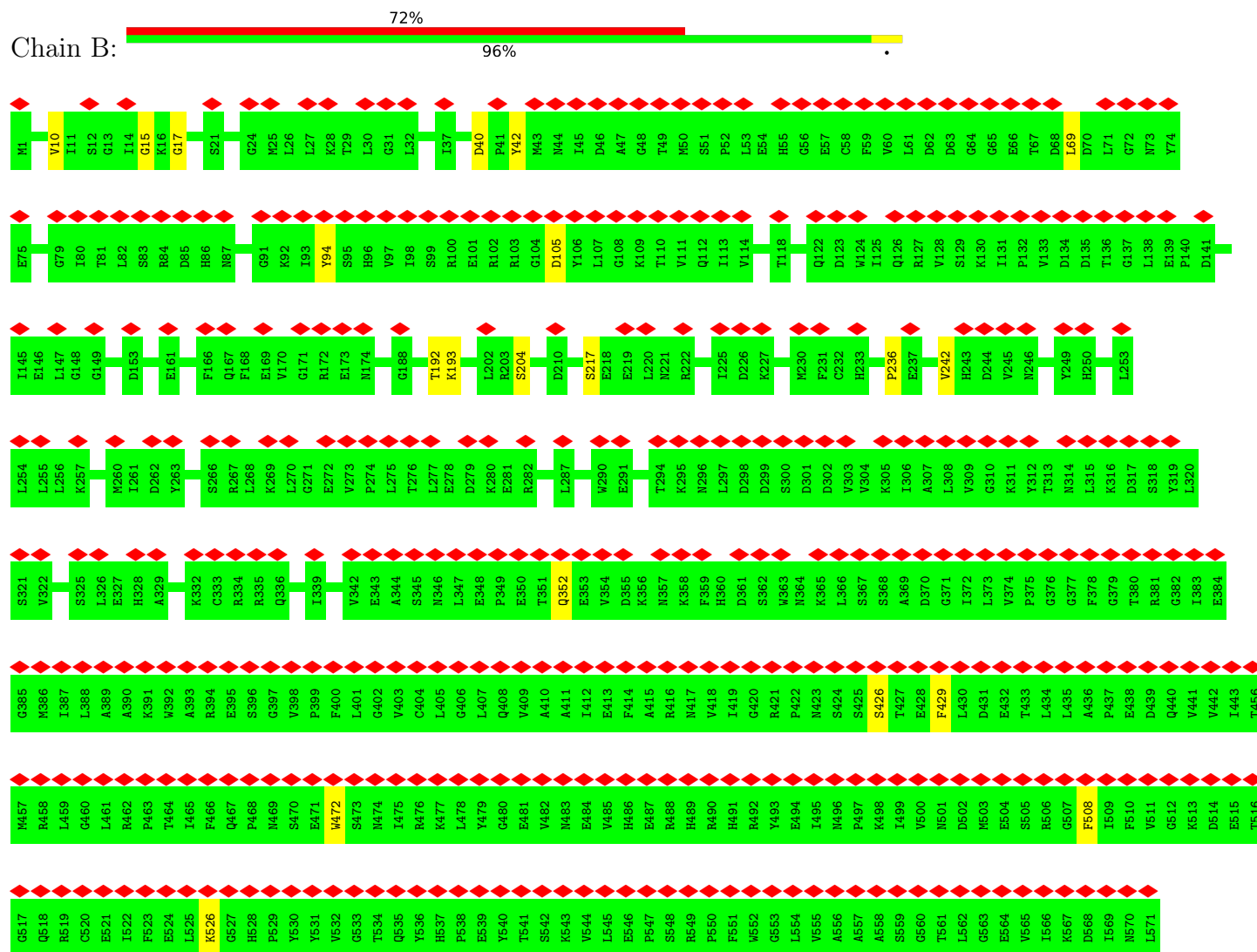


- Molecule 1: CTP synthase

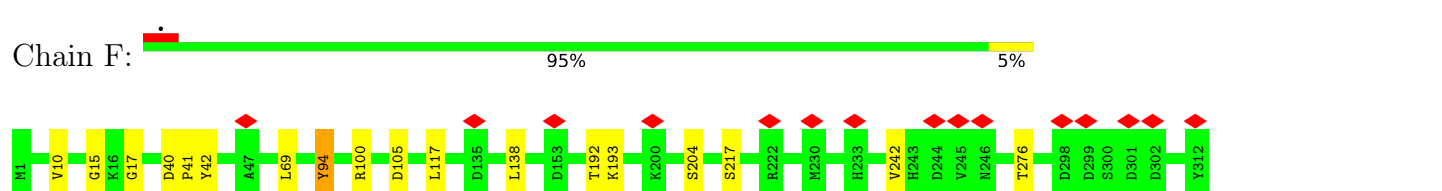


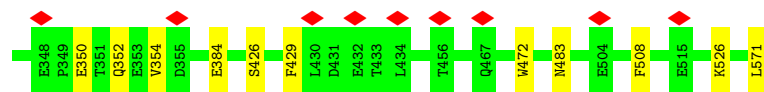


• Molecule 1: CTP synthase

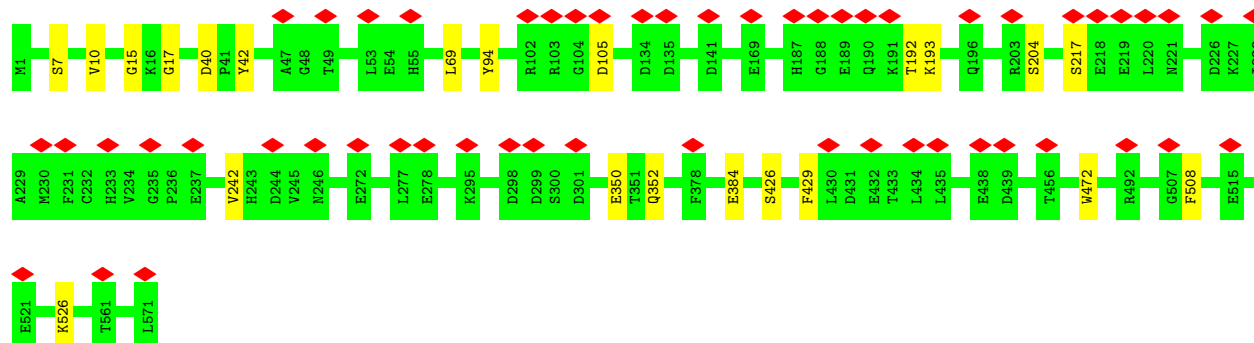


• Molecule 1: CTP synthase

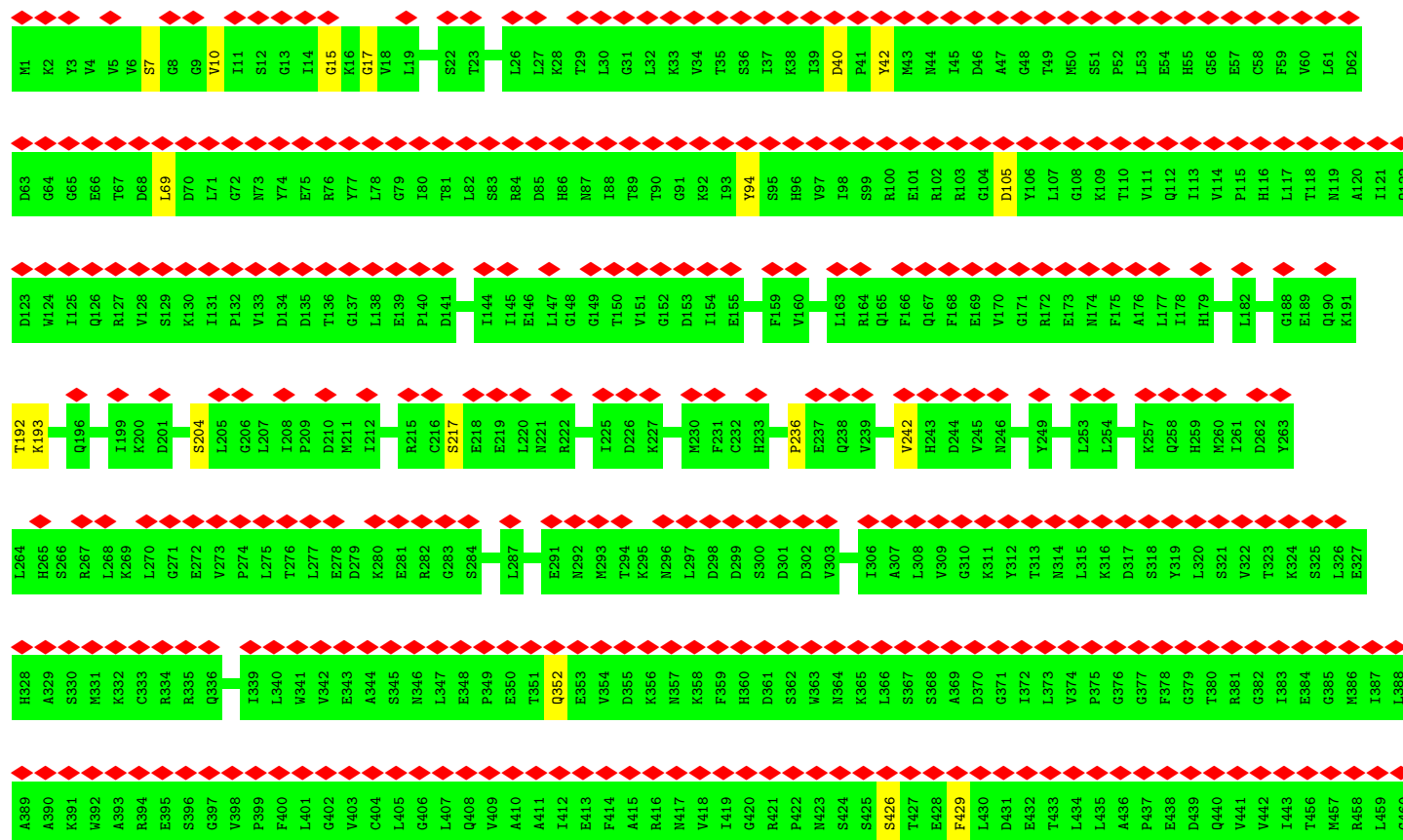
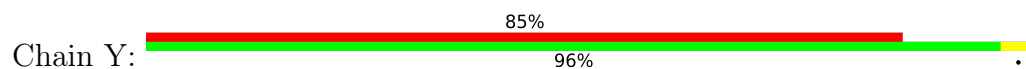


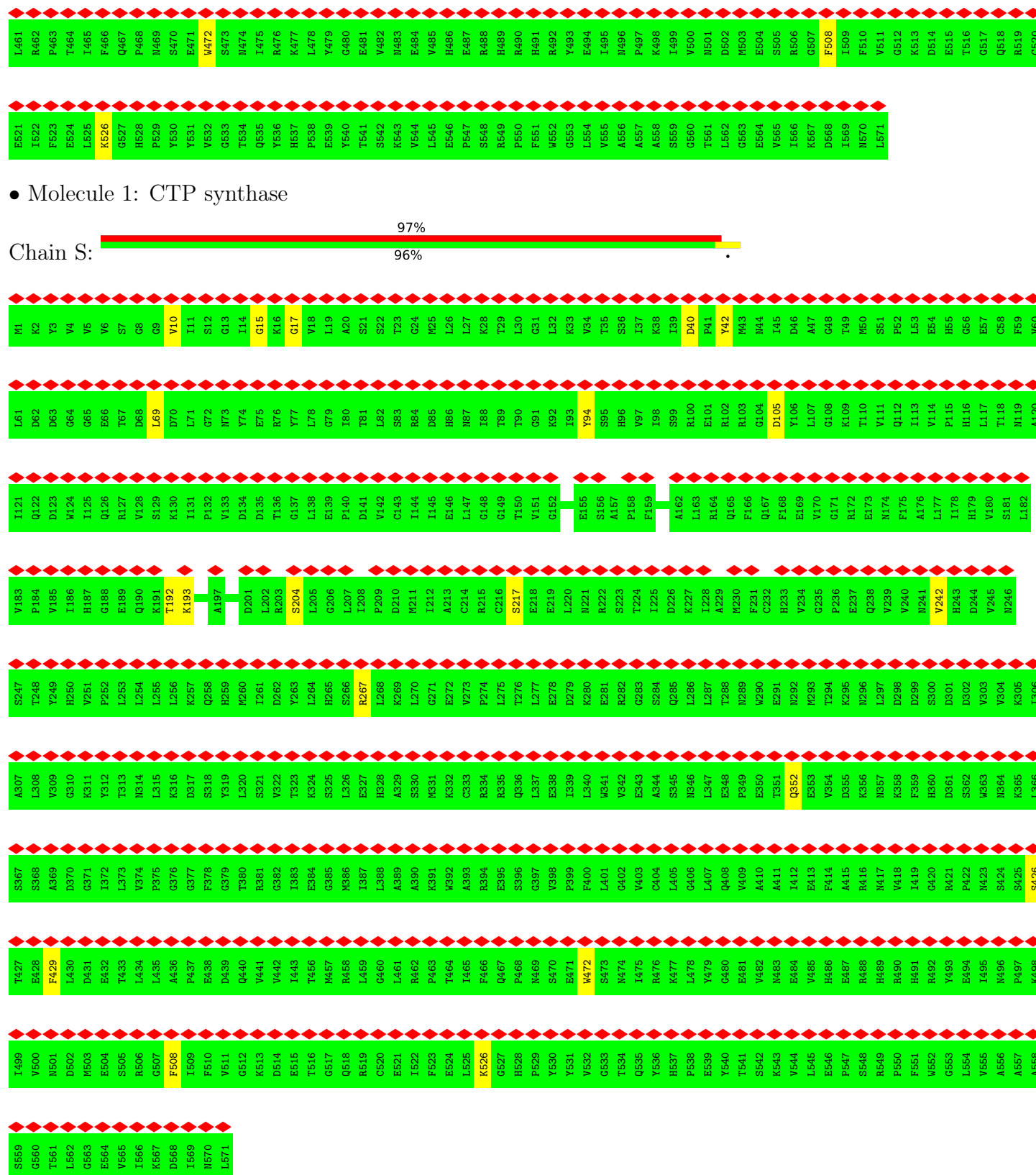


• Molecule 1: CTP synthase

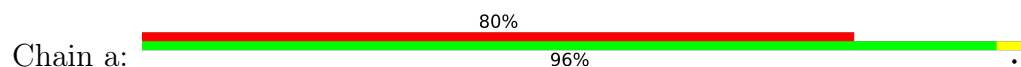


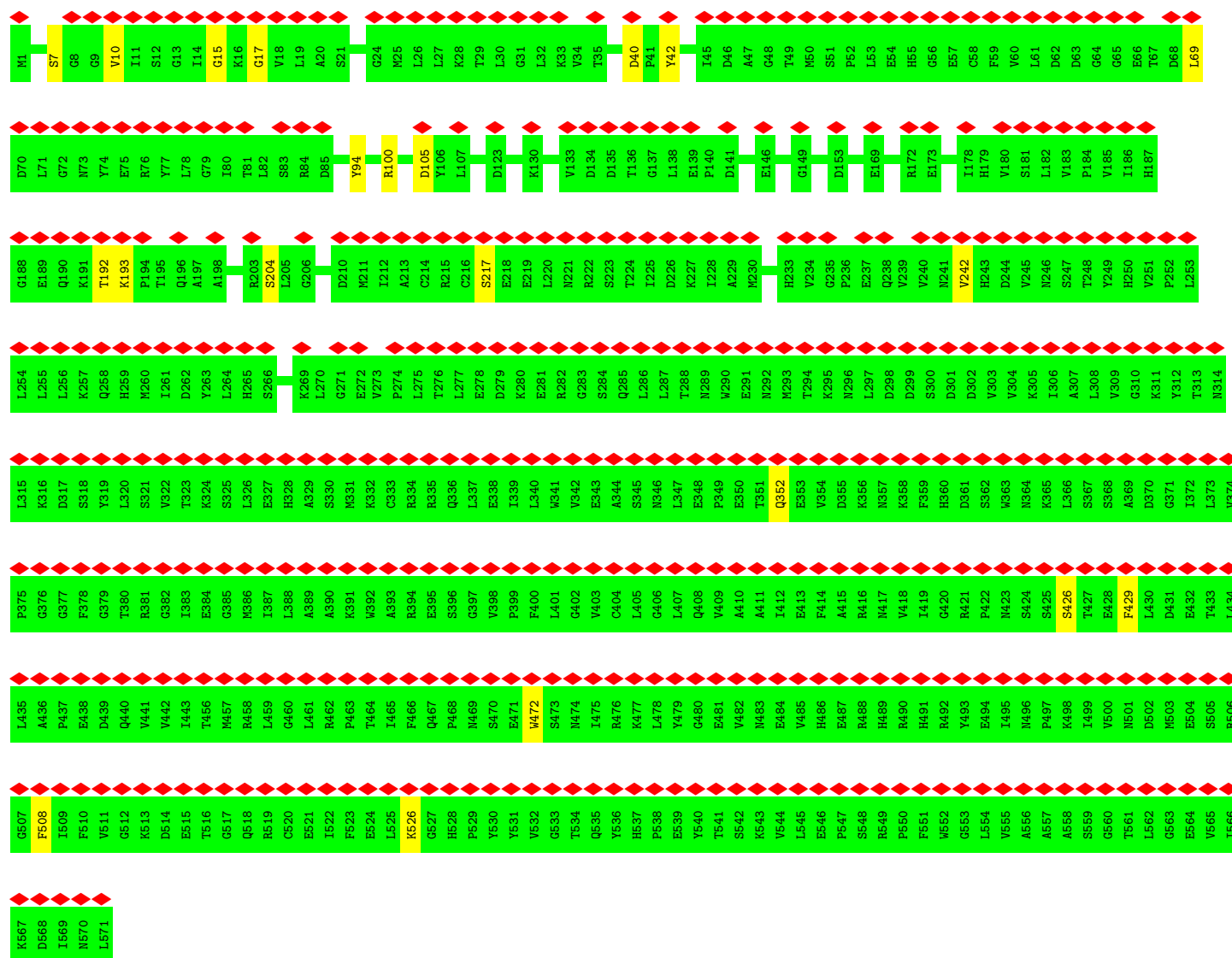
• Molecule 1: CTP synthase





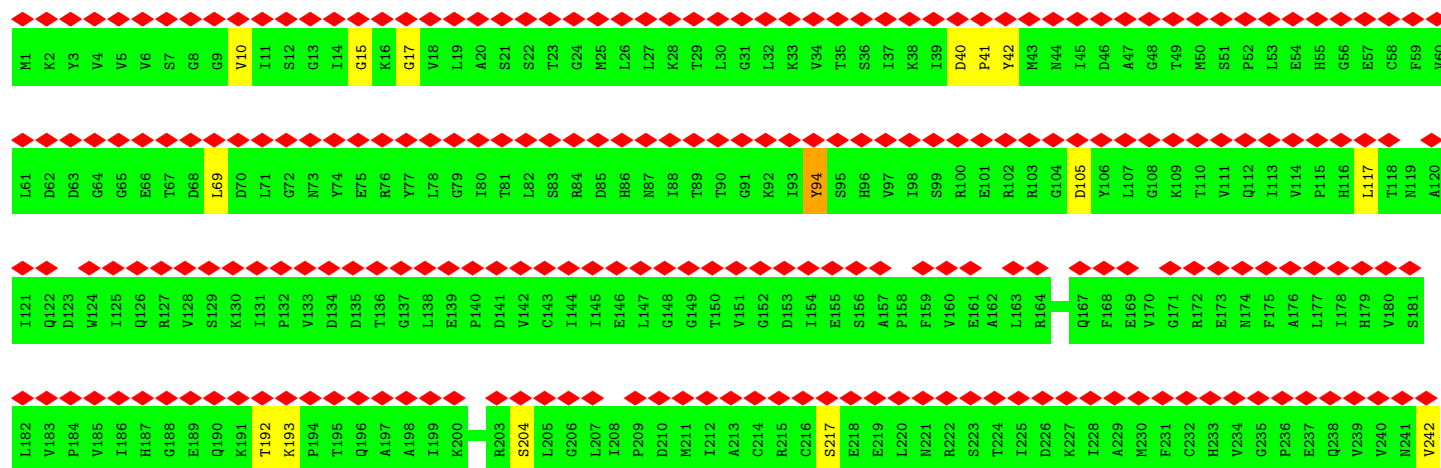
• Molecule 1: CTP synthase





• Molecule 1: CTP synthase

Chain I:

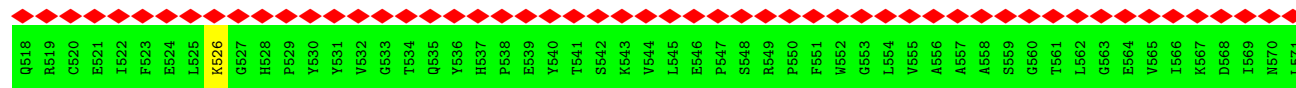
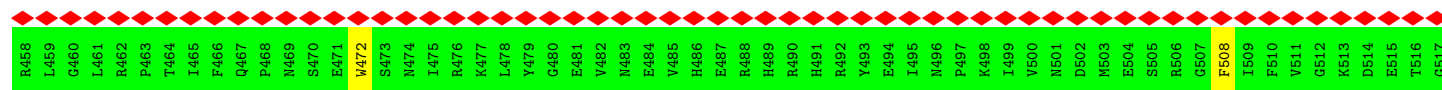


H243	V303	W363	M423	I496	V556
D244	V304	K364	S424	M496	A556
V245	K305	K365	S425	P497	A557
N246	I306	L366	S426	K498	A558
S247	A307	S367	T427	I499	S559
T248	L308	S368	E428	V500	G560
Y249	V309	A369	F429	N501	T561
H250	G310	D370	L430	D502	L562
V251	K311	G371	D431	M503	G563
P252	Y312	I372	E432	E504	E564
L253	T313	L373	T433	S505	V565
L254	N314	V374	L434	R506	I566
L255	L315	P375	L435	G507	K567
L256	K316	G376	A436	F508	D568
K257	D317	G377	P437	I509	I569
Q258	S318	F378	E438	F510	N570
H259	Y319	G379	D439	V511	L571
M260	L320	T380	Q440	G512	
I261	S321	R381	V441	K513	
D262	V322	G382	V442	D514	
Y263	T323	I383	I443	E515	
L264	K324	E384	T456	T516	
H265	S325	G385	M457	G517	
S266	L326	M386	R458	Q518	
R267	E327	I387	L459	R519	
L268	H328	L388	G460	C520	
K269	A329	A389	L461	E521	
L270	S330	A390	R462	I522	
G271	M331	K391	P463	F523	
E272	K332	W392	T464	E524	
V273	C333	A393	I465	L525	
P274	R334	R394	F466	K526	
L275	R335	E395	Q467	G527	
T276	Q336	S396	P468	H528	
L277	L337	G397	M469	F529	
E278	E338	V398	S470	Y530	
D279	I339	P399	E471	Y531	
K280	L340	F400	W472	V532	
E281	W401	L401	S473	G533	
R282	V342	G402	M474	T534	
G283	E343	V403	I475	Q535	
S284	A344	C404	R476	Y536	
Q285	S345	L405	K477	H537	
L286	N346	G406	L478	P538	
L287	L347	Q407	Y479	E539	
L288	E348	Q408	G480	Y540	
N289	P349	V409	E481	T541	
W290	E350	A410	V482	S542	
E291	T351	A411	M483	K543	
N292	Q352	I412	E484	V544	
M293	E353	E413	V485	L545	
T294	V354	F414	H486	E546	
K295	D355	A415	E487	P547	
N296	K356	R416	R488	S548	
L297	N357	N417	H489	R549	
D298	K358	V418	R490	P550	
D299	F359	I419	H491	F551	
S300	H360	G420	R492	N552	
D301	D361	R421	Y493	G553	
D302	S362	P422	E494	L554	

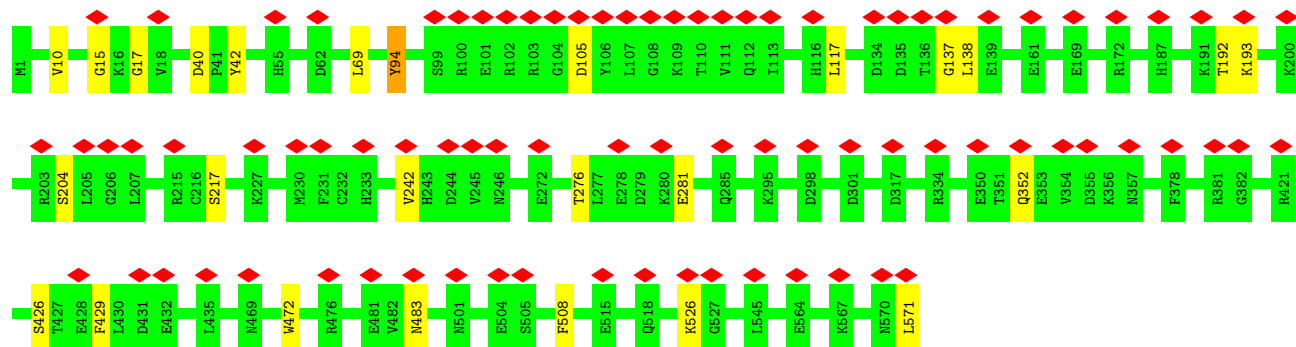
● Molecule 1: CTP synthase



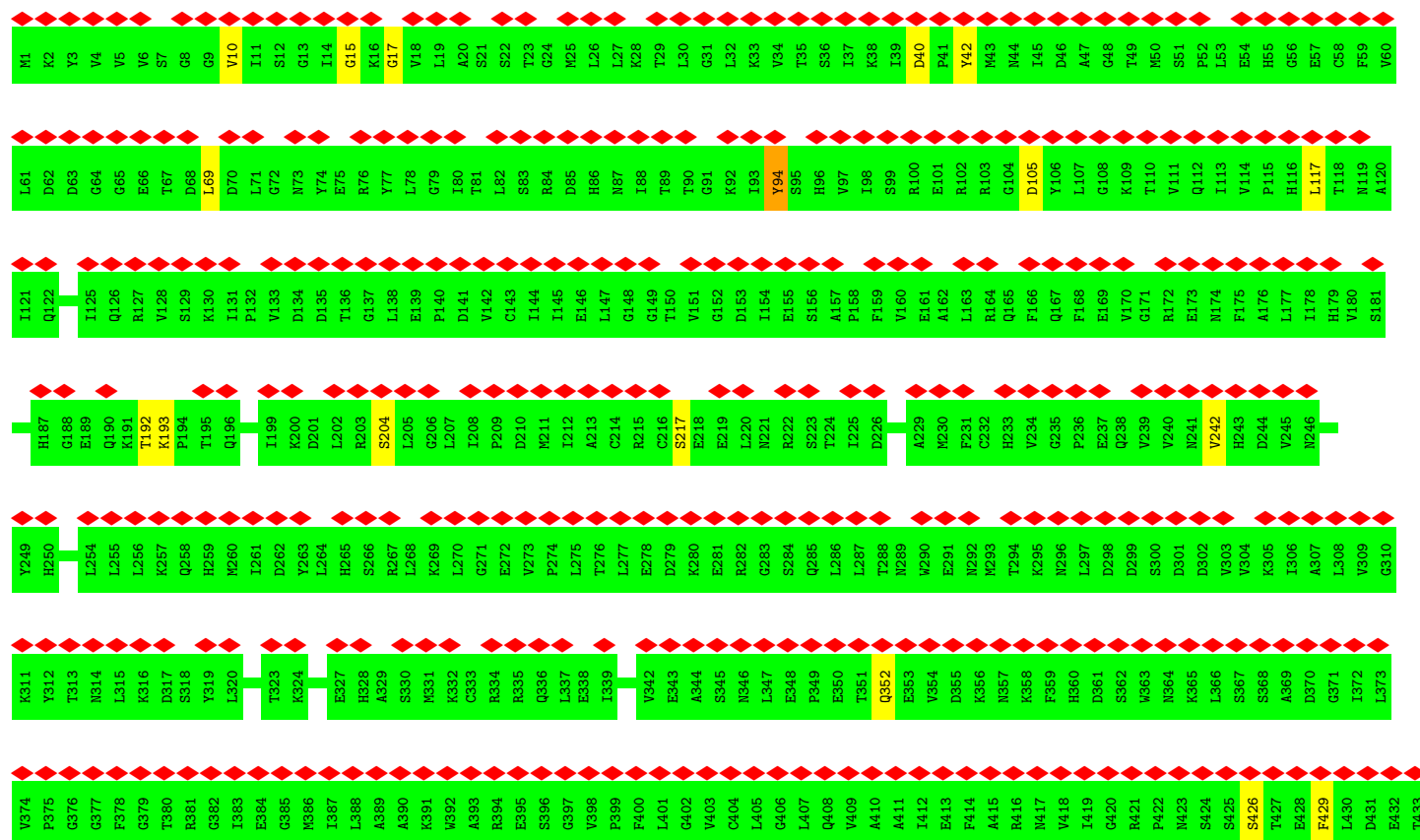
M1	L61	D141	G206	S266	L326	M366
K2	D62	V142	L207	R267	E327	I367
Y3	D63	C143	I208	L268	H328	L368
V4	G64	T144	P209	K269	A329	A369
V5	G65	T145	D210	L270	S330	A390
W6	E66	I146	M211	G271	M331	K391
S7	T67	L147	I212	E272	K332	W392
G8	D68	I148	A213	V273	C333	A393
G9	L69	G149	C214	P274	R394	R394
V10	D70	T150	R215	L275	R395	E395
I11	L71	V151	C216	T276	Q396	S396
S12	G72	G152	S217	L277	G397	G397
G13	M73	D153	E218	E278	V398	V398
I14	W74	I154	E219	D279	P399	P399
G15	E75	E155	L220	K280	F400	F400
K16	R76	S156	N221	E281	L401	L401
G17	Y77		A222	R282	G402	G402
V18	L78		S223	G283	V403	V403
L19	G79		T224	S284	A344	A344
A20	T80		I225	Q285	S345	S345
S21	T81		D226	L286	G406	G406
S22	L82		K227	L287	L407	L407
T23	S83		I228	T288	Q408	Q408
Q24	R84		A229	M289	V409	V409
M25	D85		M230	W290	A410	A410
K26	H86		F231	E291	T351	T351
L27	M87		C232	N292	Q352	Q352
K28	T88		H233	M293	E353	E353
T29	T89		V294	T294	V354	V354
L30	T90		Q235	K295	D355	D355
G31	C91		P236	N296	K356	K356
L32	R92		E237	L297	N357	N357
K33	I93		Q238	D298	K358	K358
V34	H179		V239	D299	F359	F359
T35	Y180		V240	S300	H360	H360
S36	G104		N241	D301	D361	D361
I37	Y106		V242	D302	S362	S362
K38	L107		H243	V303	W363	W363
I39	G108		D244	V304	N364	N364
D40			V245	K305	K365	K365
P41			N246	I306	L366	L366
Y42			S247	A307	S367	S367
M43			T248	L308	S368	S368
N44	Q126		Y249	V309	A369	A369
I45	R127		H250	G310	D370	D370
D46	V128		V251	K311	G371	G371
A47	S129		P252	Y312	E432	E432
O48	K130		L253	T313	T433	T433
T49	I131		L254	N314	V374	V374
M50	P132		L255	L315	P375	P375
S51	V133		L256	K316	G376	G376
P52	D134		K257	D317	G377	G377
L53	T135		Q258	S318	F378	F378
E54	P136		M259	Y319	D399	D399
H55	G137		M260	L320	T380	T380
O56	L138		T261	S321	R381	R381
E57	E139		D262	T322	G382	G382
F59	P140		L263	K324	I443	I443
V60			H265	S325	T456	T456

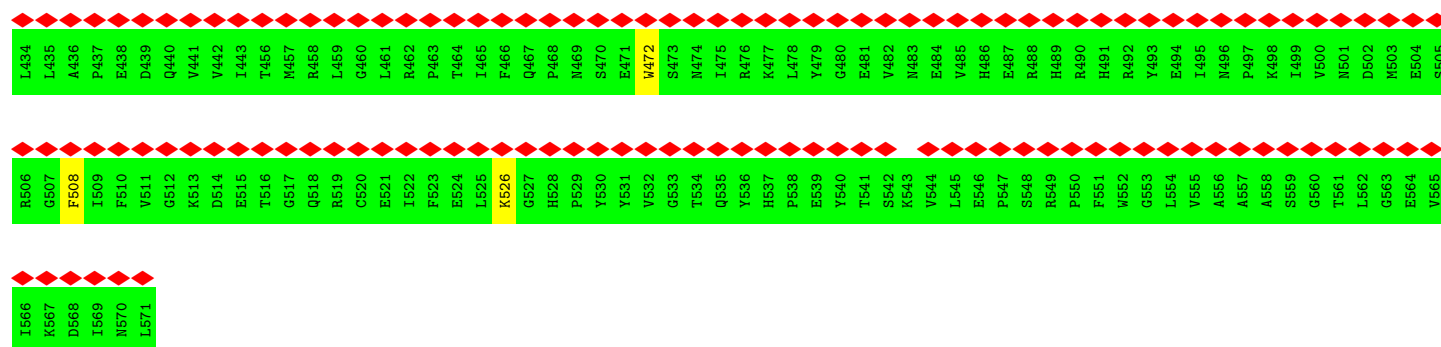


• Molecule 1: CTP synthase

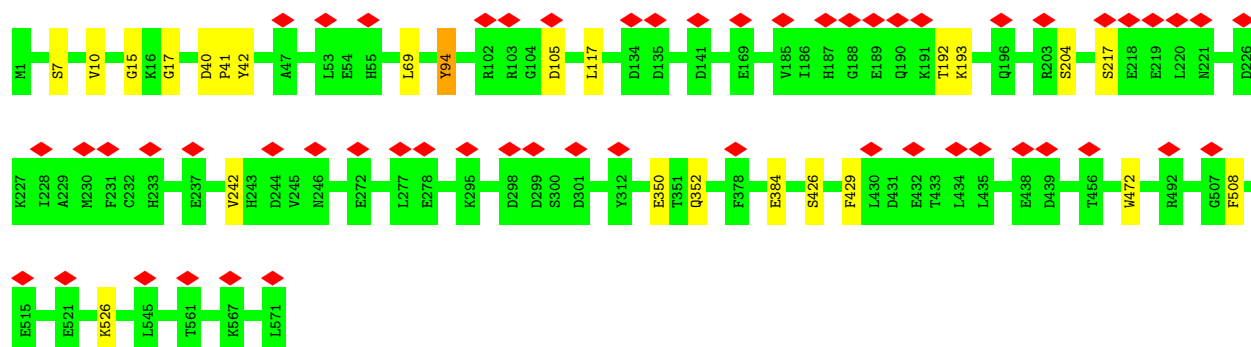


• Molecule 1: CTP synthase

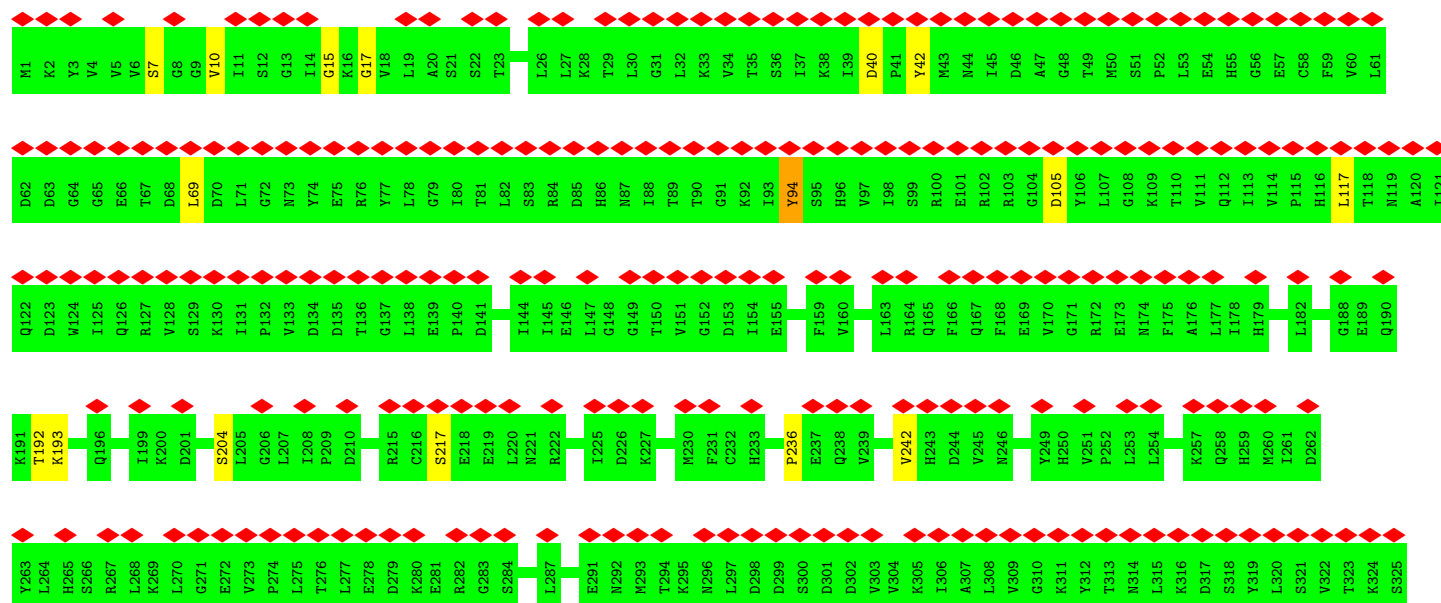
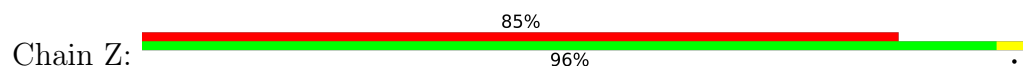


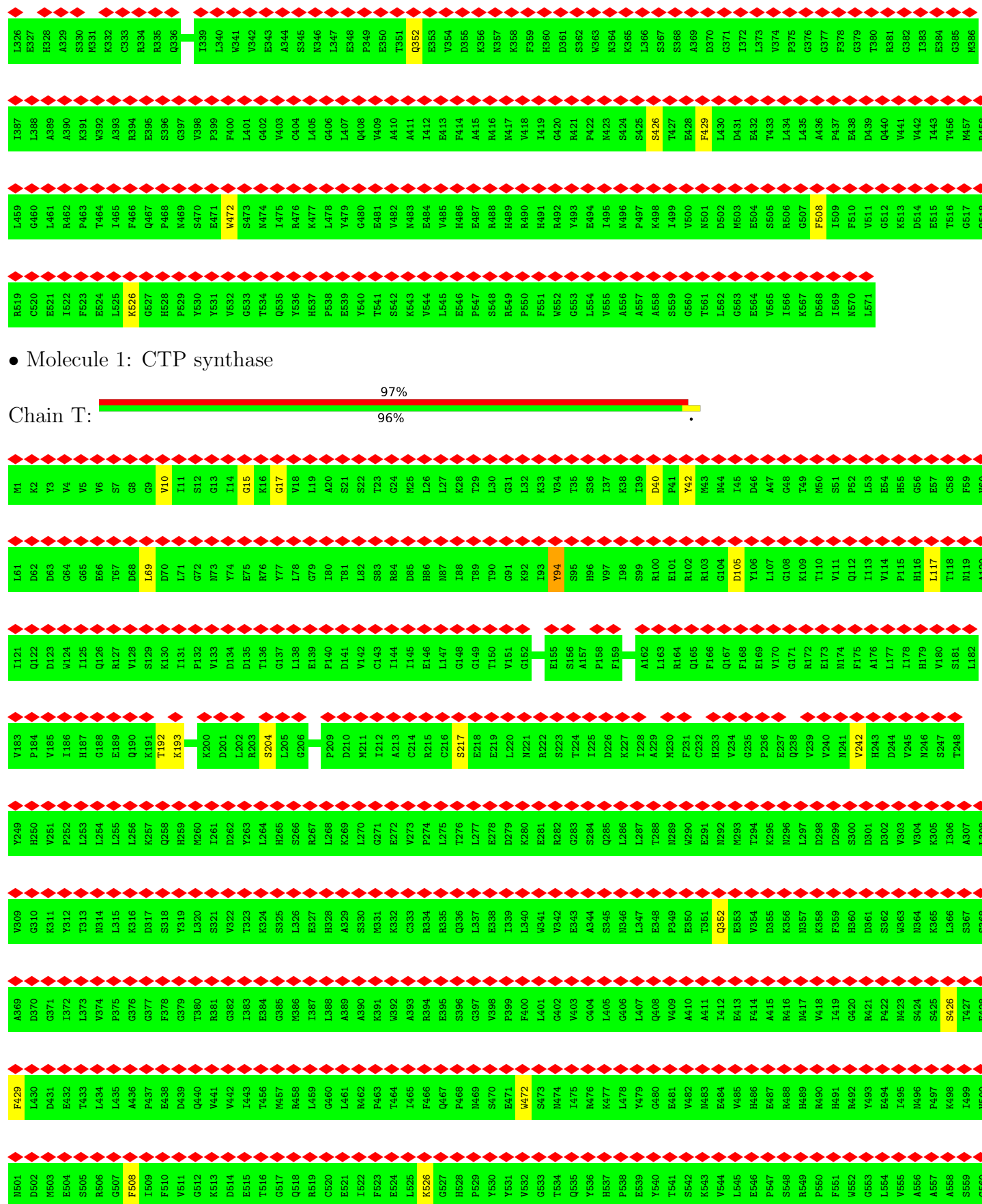


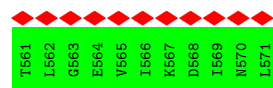
• Molecule 1: CTP synthase



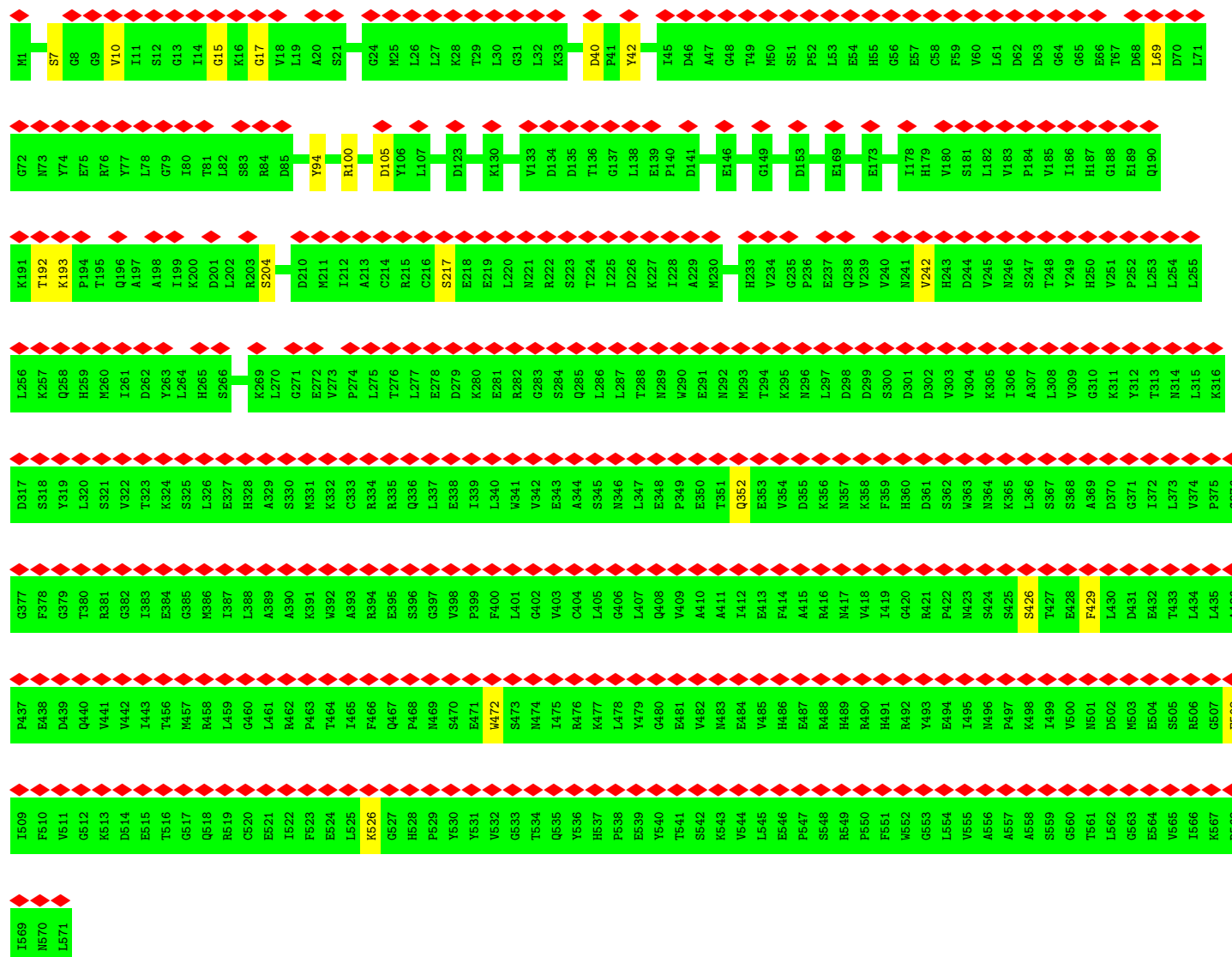
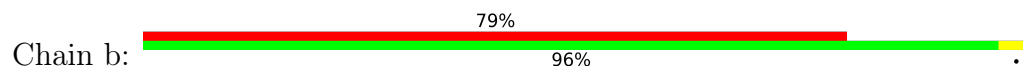
• Molecule 1: CTP synthase



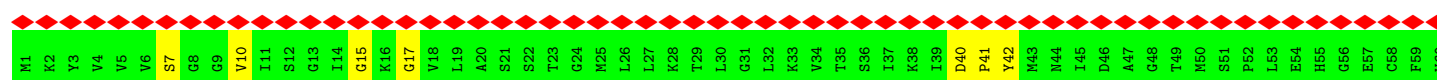


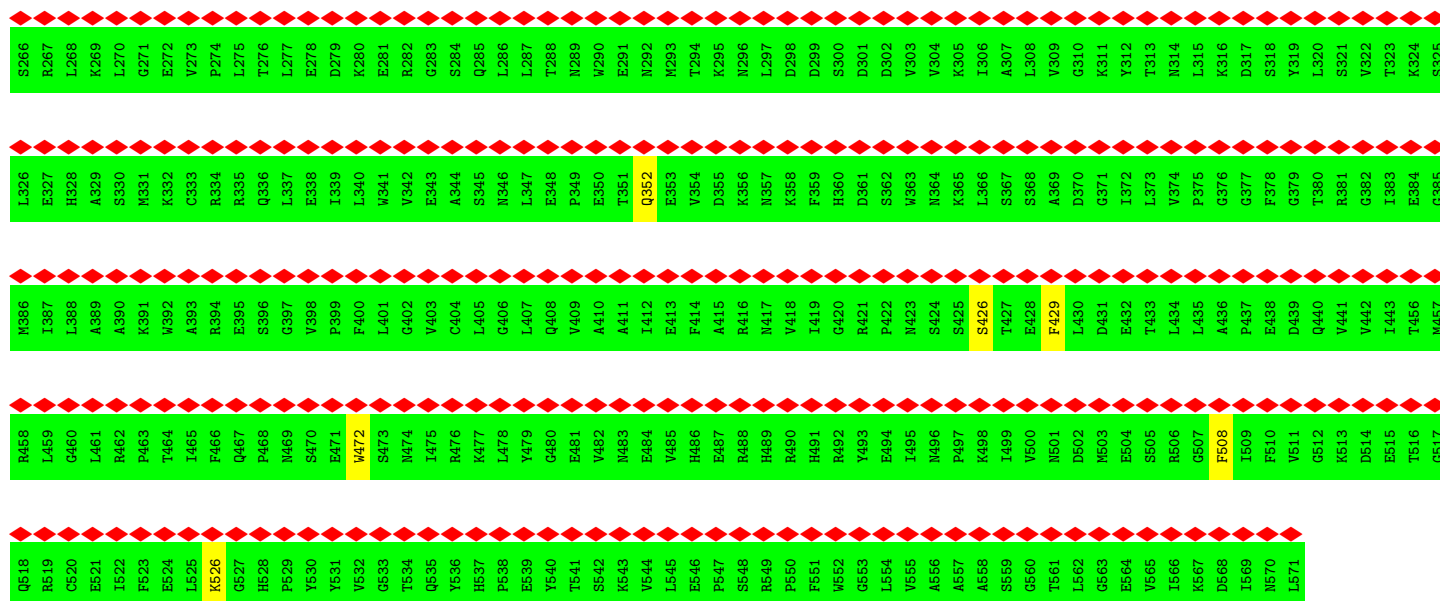


• Molecule 1: CTP synthase

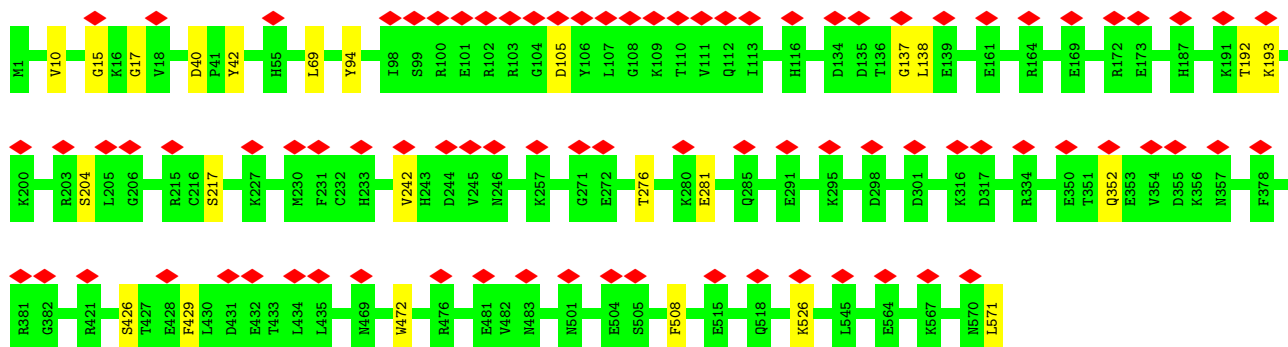


• Molecule 1: CTP synthase

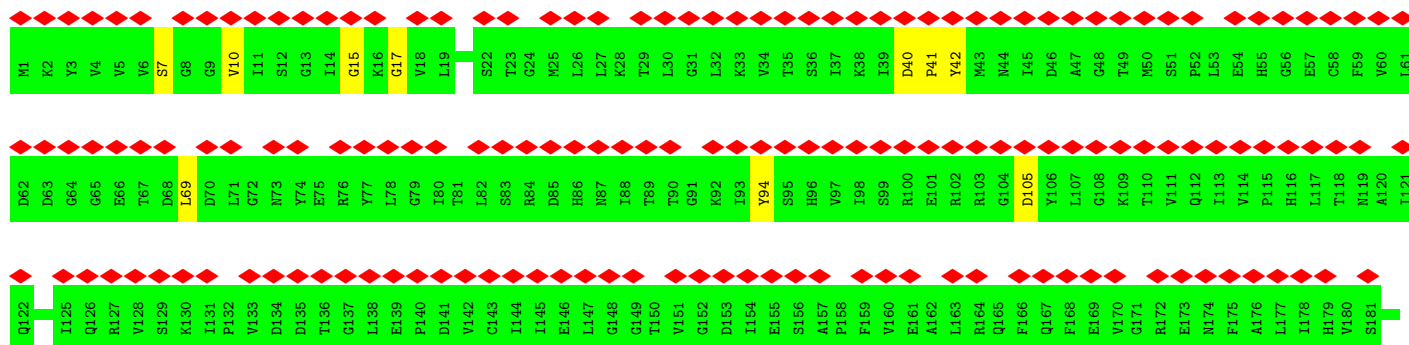
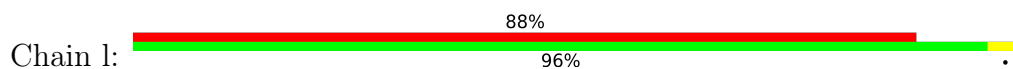




• Molecule 1: CTP synthase



• Molecule 1: CTP synthase





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 (Å)	537.6, 537.6, 537.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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	0.77	0/4471	1.32	4/6056 (0.1%)
1	B	0.77	0/4471	1.32	3/6056 (0.0%)
1	E	0.77	0/4471	1.32	4/6056 (0.1%)
1	F	0.77	0/4471	1.32	3/6056 (0.0%)
1	I	0.77	0/4471	1.32	4/6056 (0.1%)
1	J	0.77	0/4471	1.32	3/6056 (0.0%)
1	M	0.77	0/4471	1.32	4/6056 (0.1%)
1	N	0.77	0/4471	1.32	3/6056 (0.0%)
1	Q	0.77	0/4471	1.32	4/6056 (0.1%)
1	R	0.77	0/4471	1.32	4/6056 (0.1%)
1	S	0.77	0/4471	1.32	4/6056 (0.1%)
1	T	0.77	0/4471	1.32	3/6056 (0.0%)
1	Y	0.77	0/4471	1.32	4/6056 (0.1%)
1	Z	0.77	0/4471	1.32	4/6056 (0.1%)
1	a	0.77	0/4471	1.32	4/6056 (0.1%)
1	b	0.77	0/4471	1.32	4/6056 (0.1%)
1	g	0.77	0/4471	1.32	5/6056 (0.1%)
1	h	0.77	0/4471	1.32	3/6056 (0.0%)
1	k	0.77	0/4471	1.32	4/6056 (0.1%)
1	l	0.77	0/4471	1.32	4/6056 (0.1%)
All	All	0.77	0/89420	1.32	75/121120 (0.1%)

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.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	105	ASP	CA-CB-CG	6.65	119.25	112.60
1	F	105	ASP	CA-CB-CG	6.62	119.22	112.60
1	Q	105	ASP	CA-CB-CG	6.62	119.22	112.60
1	l	105	ASP	CA-CB-CG	6.62	119.22	112.60
1	N	105	ASP	CA-CB-CG	6.60	119.20	112.60
1	T	105	ASP	CA-CB-CG	6.59	119.19	112.60
1	B	105	ASP	CA-CB-CG	6.59	119.19	112.60
1	S	105	ASP	CA-CB-CG	6.58	119.18	112.60
1	M	105	ASP	CA-CB-CG	6.58	119.18	112.60
1	R	105	ASP	CA-CB-CG	6.57	119.17	112.60
1	Z	105	ASP	CA-CB-CG	6.57	119.17	112.60
1	a	105	ASP	CA-CB-CG	6.57	119.17	112.60
1	J	105	ASP	CA-CB-CG	6.57	119.17	112.60
1	k	105	ASP	CA-CB-CG	6.57	119.17	112.60
1	A	105	ASP	CA-CB-CG	6.56	119.16	112.60
1	E	105	ASP	CA-CB-CG	6.56	119.16	112.60
1	Y	105	ASP	CA-CB-CG	6.55	119.16	112.60
1	h	105	ASP	CA-CB-CG	6.55	119.15	112.60
1	I	105	ASP	CA-CB-CG	6.54	119.14	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	105	ASP	CA-CB-CG	6.53	119.13	112.60
1	T	217	SER	N-CA-C	6.10	121.78	113.37
1	J	217	SER	N-CA-C	6.10	121.78	113.37
1	R	217	SER	N-CA-C	6.08	121.76	113.37
1	B	217	SER	N-CA-C	6.08	121.75	113.37
1	b	217	SER	N-CA-C	6.08	121.75	113.37
1	l	217	SER	N-CA-C	6.08	121.75	113.37
1	A	217	SER	N-CA-C	6.07	121.75	113.37
1	F	217	SER	N-CA-C	6.07	121.75	113.37
1	N	217	SER	N-CA-C	6.07	121.75	113.37
1	Z	217	SER	N-CA-C	6.07	121.75	113.37
1	a	217	SER	N-CA-C	6.07	121.75	113.37
1	g	217	SER	N-CA-C	6.07	121.75	113.37
1	E	217	SER	N-CA-C	6.07	121.74	113.37
1	Y	217	SER	N-CA-C	6.07	121.74	113.37
1	S	217	SER	N-CA-C	6.07	121.74	113.37
1	Q	217	SER	N-CA-C	6.06	121.73	113.37
1	I	217	SER	N-CA-C	6.06	121.73	113.37
1	M	217	SER	N-CA-C	6.05	121.72	113.37
1	h	217	SER	N-CA-C	6.05	121.72	113.37
1	k	217	SER	N-CA-C	6.03	121.70	113.37
1	b	508	PHE	CA-CB-CG	5.38	119.19	113.80
1	N	508	PHE	CA-CB-CG	5.36	119.16	113.80
1	l	508	PHE	CA-CB-CG	5.36	119.16	113.80
1	a	508	PHE	CA-CB-CG	5.36	119.16	113.80
1	F	508	PHE	CA-CB-CG	5.35	119.15	113.80
1	Q	508	PHE	CA-CB-CG	5.34	119.14	113.80
1	Z	508	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	508	PHE	CA-CB-CG	5.33	119.12	113.80
1	S	508	PHE	CA-CB-CG	5.32	119.12	113.80
1	R	508	PHE	CA-CB-CG	5.32	119.12	113.80
1	E	508	PHE	CA-CB-CG	5.32	119.12	113.80
1	g	508	PHE	CA-CB-CG	5.31	119.11	113.80
1	M	508	PHE	CA-CB-CG	5.31	119.11	113.80
1	h	508	PHE	CA-CB-CG	5.31	119.11	113.80
1	Y	508	PHE	CA-CB-CG	5.30	119.10	113.80
1	I	508	PHE	CA-CB-CG	5.29	119.09	113.80
1	J	508	PHE	CA-CB-CG	5.29	119.09	113.80
1	B	508	PHE	CA-CB-CG	5.29	119.09	113.80
1	k	508	PHE	CA-CB-CG	5.28	119.08	113.80
1	T	508	PHE	CA-CB-CG	5.27	119.07	113.80
1	M	7	SER	N-CA-C	5.07	116.94	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	7	SER	N-CA-C	5.05	116.92	108.99
1	Y	7	SER	N-CA-C	5.04	116.91	108.99
1	S	267	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	E	7	SER	N-CA-C	5.03	116.89	108.99
1	k	7	SER	N-CA-C	5.03	116.89	108.99
1	Q	7	SER	N-CA-C	5.03	116.88	108.99
1	R	7	SER	N-CA-C	5.03	116.88	108.99
1	l	7	SER	N-CA-C	5.02	116.86	108.99
1	A	7	SER	N-CA-C	5.01	116.86	108.99
1	g	267	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	a	7	SER	N-CA-C	5.01	116.86	108.99
1	I	267	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	b	7	SER	N-CA-C	5.01	116.86	108.99
1	Z	7	SER	N-CA-C	5.00	116.84	108.99

There are no chirality outliers.

All (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	I	94	TYR	Sidechain
1	J	94	TYR	Sidechain
1	M	94	TYR	Sidechain
1	N	94	TYR	Sidechain
1	Q	94	TYR	Sidechain
1	R	94	TYR	Sidechain
1	S	94	TYR	Sidechain
1	T	94	TYR	Sidechain
1	Y	94	TYR	Sidechain
1	Z	94	TYR	Sidechain
1	a	94	TYR	Sidechain
1	b	94	TYR	Sidechain
1	g	94	TYR	Sidechain
1	h	94	TYR	Sidechain
1	k	94	TYR	Sidechain
1	l	94	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	4385	4393	4390	60	0
1	B	4385	4393	4390	36	0
1	E	4385	4393	4390	36	0
1	F	4385	4393	4390	56	0
1	I	4385	4393	4390	37	0
1	J	4385	4393	4390	49	0
1	M	4385	4393	4390	34	0
1	N	4385	4393	4390	35	0
1	Q	4385	4393	4390	36	0
1	R	4385	4393	4390	38	0
1	S	4385	4393	4390	36	0
1	T	4385	4393	4390	35	0
1	Y	4385	4393	4390	42	0
1	Z	4385	4393	4390	38	0
1	a	4385	4393	4390	36	0
1	b	4385	4393	4390	34	0
1	g	4385	4393	4390	35	0
1	h	4385	4393	4390	49	0
1	k	4385	4393	4390	36	0
1	l	4385	4393	4390	35	0
2	A	31	12	12	13	0
2	B	31	12	12	12	0
2	E	31	12	12	12	0
2	F	31	12	12	12	0
2	I	31	12	12	13	0
2	J	31	12	12	12	0
2	M	31	12	12	12	0
2	N	31	12	12	12	0
2	Q	31	12	12	12	0
2	R	31	12	12	12	0
2	S	31	12	12	13	0
2	T	31	12	12	12	0
2	Y	31	12	12	13	0
2	Z	31	12	12	12	0
2	a	31	12	12	13	0
2	b	31	12	12	12	0
2	g	31	12	12	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	h	31	12	12	13	0
2	k	31	12	12	12	0
2	l	31	12	12	12	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	Q	3	0	0	0	0
3	R	3	0	0	0	0
3	S	3	0	0	0	0
3	T	3	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
3	a	1	0	0	0	0
3	b	1	0	0	0	0
3	g	3	0	0	0	0
3	h	3	0	0	0	0
3	k	1	0	0	0	0
3	l	1	0	0	0	0
4	A	29	7	9	23	0
4	B	29	7	9	23	0
4	E	29	7	9	23	0
4	F	29	7	9	24	0
4	I	29	7	9	23	0
4	J	29	7	9	23	0
4	M	29	7	9	23	0
4	N	29	7	9	24	0
4	Q	29	7	9	23	0
4	R	29	7	9	21	0
4	S	29	7	9	23	0
4	T	29	7	9	22	0
4	Y	29	7	9	23	0
4	Z	29	7	9	23	0
4	a	29	7	9	24	0
4	b	29	7	9	24	0
4	g	29	7	9	24	0
4	h	29	7	9	24	0
4	k	29	7	9	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1	29	7	9	24	0
All	All	88940	88240	88220	776	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 4.

All (776) 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:E:15:GLY:HA3	2:E:601:ATP:C8	1.60	1.37
1:F:15:GLY:HA3	2:F:602:ATP:C8	1.60	1.37
1:M:15:GLY:HA3	2:M:601:ATP:C8	1.60	1.37
1:h:15:GLY:HA3	2:h:602:ATP:C8	1.60	1.37
1:a:15:GLY:HA3	2:a:602:ATP:C8	1.60	1.37
1:I:15:GLY:HA3	2:I:601:ATP:C8	1.60	1.36
1:N:15:GLY:HA3	2:N:602:ATP:C8	1.60	1.36
1:Z:15:GLY:HA3	2:Z:601:ATP:C8	1.59	1.36
1:S:15:GLY:HA3	2:S:602:ATP:C8	1.59	1.36
1:T:15:GLY:HA3	2:T:602:ATP:C8	1.60	1.36
1:b:15:GLY:HA3	2:b:602:ATP:C8	1.60	1.36
1:Y:15:GLY:HA3	2:Y:601:ATP:C8	1.60	1.35
1:Q:15:GLY:HA3	2:Q:601:ATP:C8	1.60	1.35
1:J:15:GLY:HA3	2:J:602:ATP:C8	1.60	1.35
1:R:15:GLY:HA3	2:R:601:ATP:C8	1.60	1.35
1:g:15:GLY:HA3	2:g:601:ATP:C8	1.60	1.35
1:l:15:GLY:HA3	2:l:602:ATP:C8	1.59	1.34
4:Y:603:UTP:O2'	1:S:42:TYR:HD1	1.11	1.34
1:k:15:GLY:HA3	2:k:601:ATP:C8	1.60	1.34
1:B:15:GLY:HA3	2:B:602:ATP:C8	1.60	1.33
4:I:605:UTP:O2'	1:N:42:TYR:HD1	1.11	1.33
1:A:15:GLY:HA3	2:A:601:ATP:C8	1.60	1.32
1:E:42:TYR:HD1	4:B:601:UTP:O2'	1.11	1.32
1:M:42:TYR:HD1	4:J:601:UTP:O2'	1.11	1.32
4:E:603:UTP:O2'	1:B:42:TYR:HD1	1.11	1.31
4:Z:603:UTP:O2'	1:T:42:TYR:HD1	1.11	1.30
1:R:42:TYR:HD1	4:b:601:UTP:O2'	1.11	1.30
4:A:605:UTP:O2'	1:F:42:TYR:HD1	1.11	1.30
4:g:605:UTP:O2'	1:l:42:TYR:HD1	1.11	1.29
1:A:42:TYR:HD1	4:F:601:UTP:O2'	1.11	1.29
1:k:42:TYR:HD1	4:h:601:UTP:O2'	1.11	1.29
1:Q:42:TYR:HD1	4:a:601:UTP:O2'	1.11	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:42:TYR:HD1	4:S:601:UTP:O2'	1.11	1.25
4:M:603:UTP:O2'	1:J:42:TYR:HD1	1.11	1.25
1:Z:42:TYR:HD1	4:T:601:UTP:O2'	1.11	1.25
4:Q:605:UTP:O2'	1:a:42:TYR:HD1	1.11	1.25
4:k:603:UTP:O2'	1:h:42:TYR:HD1	1.11	1.25
1:I:42:TYR:HD1	4:N:601:UTP:O2'	1.11	1.24
1:g:42:TYR:HD1	4:l:601:UTP:O2'	1.11	1.24
4:R:605:UTP:O2'	1:b:42:TYR:HD1	1.11	1.24
1:Y:40:ASP:OD1	4:S:601:UTP:H5	1.21	1.24
1:A:40:ASP:OD1	4:F:601:UTP:H5	1.21	1.23
4:Z:603:UTP:H5	1:T:40:ASP:OD1	1.21	1.23
4:M:603:UTP:H5	1:J:40:ASP:OD1	1.21	1.23
4:Q:605:UTP:H5	1:a:40:ASP:OD1	1.21	1.22
1:I:40:ASP:OD1	4:N:601:UTP:H5	1.21	1.22
4:Y:603:UTP:H5	1:S:40:ASP:OD1	1.21	1.22
4:g:605:UTP:H5	1:l:40:ASP:OD1	1.21	1.21
1:Y:40:ASP:OD1	4:S:601:UTP:C5	1.94	1.21
4:Y:603:UTP:C5	1:S:40:ASP:OD1	1.94	1.21
4:k:603:UTP:C5	1:h:40:ASP:OD1	1.94	1.21
4:A:605:UTP:H5	1:F:40:ASP:OD1	1.21	1.21
1:R:40:ASP:OD1	4:b:601:UTP:H5	1.21	1.21
1:g:40:ASP:OD1	4:l:601:UTP:H5	1.21	1.21
4:E:603:UTP:H5	1:B:40:ASP:OD1	1.21	1.20
1:Z:40:ASP:OD1	4:T:601:UTP:H5	1.21	1.20
4:g:605:UTP:C5	1:l:40:ASP:OD1	1.94	1.20
4:R:605:UTP:C5	1:b:40:ASP:OD1	1.94	1.20
1:g:40:ASP:OD1	4:l:601:UTP:C5	1.94	1.20
1:A:40:ASP:OD1	4:F:601:UTP:C5	1.94	1.19
4:I:605:UTP:C5	1:N:40:ASP:OD1	1.94	1.19
4:A:605:UTP:C5	1:F:40:ASP:OD1	1.94	1.19
1:E:40:ASP:OD1	4:B:601:UTP:C5	1.94	1.19
1:I:40:ASP:OD1	4:N:601:UTP:C5	1.94	1.19
4:Z:603:UTP:C5	1:T:40:ASP:OD1	1.94	1.19
1:k:40:ASP:OD1	4:h:601:UTP:C5	1.94	1.19
4:M:603:UTP:C5	1:J:40:ASP:OD1	1.94	1.19
1:Z:40:ASP:OD1	4:T:601:UTP:C5	1.94	1.19
1:Q:40:ASP:OD1	4:a:601:UTP:H5	1.21	1.19
1:Q:40:ASP:OD1	4:a:601:UTP:C5	1.94	1.19
1:M:40:ASP:OD1	4:J:601:UTP:C5	1.94	1.19
1:R:40:ASP:OD1	4:b:601:UTP:C5	1.94	1.19
4:R:605:UTP:H5	1:b:40:ASP:OD1	1.21	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:605:UTP:C5	1:a:40:ASP:OD1	1.94	1.19
4:I:605:UTP:H5	1:N:40:ASP:OD1	1.21	1.19
4:E:603:UTP:C5	1:B:40:ASP:OD1	1.94	1.18
1:k:40:ASP:OD1	4:h:601:UTP:H5	1.21	1.18
4:k:603:UTP:H5	1:h:40:ASP:OD1	1.21	1.18
1:E:40:ASP:OD1	4:B:601:UTP:H5	1.21	1.17
1:M:40:ASP:OD1	4:J:601:UTP:H5	1.21	1.16
4:R:605:UTP:O1G	1:T:193:LYS:HG3	1.53	1.08
4:g:605:UTP:O2G	1:h:193:LYS:HG3	1.53	1.08
1:g:193:LYS:HG3	4:h:601:UTP:O1G	1.54	1.08
1:Q:193:LYS:HG3	4:S:601:UTP:O2G	1.53	1.08
4:I:605:UTP:O2G	1:J:193:LYS:HG3	1.53	1.08
4:A:605:UTP:O2G	1:B:193:LYS:HG3	1.53	1.07
4:Q:605:UTP:O1G	1:S:193:LYS:HG3	1.53	1.07
1:I:193:LYS:HG3	4:J:601:UTP:O1G	1.54	1.07
4:M:603:UTP:O1G	1:N:193:LYS:HG3	1.55	1.06
1:Z:193:LYS:HG3	4:b:601:UTP:O1G	1.55	1.05
1:A:193:LYS:HG3	4:B:601:UTP:O1G	1.53	1.05
1:R:193:LYS:HG3	4:T:601:UTP:O2G	1.53	1.05
4:k:603:UTP:O1G	1:l:193:LYS:HG3	1.55	1.05
4:Y:603:UTP:O1G	1:a:193:LYS:HG3	1.55	1.05
1:M:193:LYS:HG3	4:N:601:UTP:O1G	1.55	1.05
4:E:603:UTP:O1G	1:F:193:LYS:HG3	1.55	1.04
4:Z:603:UTP:O1G	1:b:193:LYS:HG3	1.55	1.04
1:E:193:LYS:HG3	4:F:601:UTP:O2G	1.55	1.04
1:Y:193:LYS:HG3	4:a:601:UTP:O1G	1.55	1.04
1:k:193:LYS:HG3	4:l:601:UTP:O1G	1.55	1.03
1:M:15:GLY:CA	2:M:601:ATP:C8	2.42	1.03
1:A:15:GLY:CA	2:A:601:ATP:C8	2.42	1.03
1:B:15:GLY:CA	2:B:602:ATP:C8	2.42	1.03
1:h:15:GLY:CA	2:h:602:ATP:C8	2.42	1.03
1:Q:15:GLY:CA	2:Q:601:ATP:C8	2.42	1.03
1:Z:15:GLY:CA	2:Z:601:ATP:C8	2.42	1.03
1:b:15:GLY:CA	2:b:602:ATP:C8	2.42	1.03
1:Y:15:GLY:CA	2:Y:601:ATP:C8	2.42	1.02
1:l:15:GLY:CA	2:l:602:ATP:H8	1.73	1.02
1:Y:15:GLY:CA	2:Y:601:ATP:H8	1.73	1.02
1:S:15:GLY:CA	2:S:602:ATP:C8	2.42	1.02
1:a:15:GLY:CA	2:a:602:ATP:C8	2.42	1.02
1:N:15:GLY:CA	2:N:602:ATP:C8	2.42	1.02
1:g:15:GLY:CA	2:g:601:ATP:H8	1.73	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLY:CA	2:A:601:ATP:H8	1.73	1.02
1:E:15:GLY:CA	2:E:601:ATP:H8	1.73	1.02
1:M:15:GLY:CA	2:M:601:ATP:H8	1.73	1.01
1:R:15:GLY:CA	2:R:601:ATP:C8	2.42	1.01
1:R:15:GLY:CA	2:R:601:ATP:H8	1.73	1.01
1:T:15:GLY:CA	2:T:602:ATP:C8	2.42	1.01
1:g:15:GLY:CA	2:g:601:ATP:C8	2.42	1.01
1:k:15:GLY:CA	2:k:601:ATP:C8	2.42	1.01
1:E:15:GLY:CA	2:E:601:ATP:C8	2.42	1.01
1:F:15:GLY:CA	2:F:602:ATP:C8	2.42	1.01
1:F:15:GLY:CA	2:F:602:ATP:H8	1.73	1.01
1:Q:15:GLY:CA	2:Q:601:ATP:H8	1.73	1.01
1:l:15:GLY:CA	2:l:602:ATP:C8	2.42	1.01
1:I:15:GLY:CA	2:I:601:ATP:C8	2.42	1.01
1:S:15:GLY:CA	2:S:602:ATP:H8	1.73	1.01
1:a:15:GLY:HA3	2:a:602:ATP:H8	1.18	1.01
1:I:15:GLY:CA	2:I:601:ATP:H8	1.73	1.01
1:b:15:GLY:CA	2:b:602:ATP:H8	1.73	1.01
1:k:15:GLY:HA3	2:k:601:ATP:H8	1.18	1.01
1:h:15:GLY:CA	2:h:602:ATP:H8	1.73	1.01
1:J:15:GLY:CA	2:J:602:ATP:C8	2.42	1.00
1:N:15:GLY:CA	2:N:602:ATP:H8	1.73	1.00
1:T:15:GLY:CA	2:T:602:ATP:H8	1.73	1.00
1:k:15:GLY:CA	2:k:601:ATP:H8	1.73	1.00
1:Y:15:GLY:HA3	2:Y:601:ATP:H8	1.18	1.00
1:a:15:GLY:CA	2:a:602:ATP:H8	1.73	1.00
1:J:15:GLY:CA	2:J:602:ATP:H8	1.73	1.00
1:B:15:GLY:CA	2:B:602:ATP:H8	1.73	1.00
1:A:483:ASN:ND2	1:Y:236:PRO:HG3	1.77	0.99
1:l:15:GLY:HA3	2:l:602:ATP:H8	1.18	0.99
1:Z:15:GLY:CA	2:Z:601:ATP:H8	1.73	0.99
1:Z:15:GLY:HA3	2:Z:601:ATP:H8	1.18	0.98
1:M:15:GLY:HA3	2:M:601:ATP:H8	1.18	0.97
1:g:15:GLY:HA3	2:g:601:ATP:H8	1.18	0.96
1:Q:15:GLY:HA3	2:Q:601:ATP:H8	1.18	0.95
2:E:601:ATP:O1G	4:B:601:UTP:O4	1.85	0.95
4:g:605:UTP:O4	2:l:602:ATP:O1G	1.85	0.95
4:A:605:UTP:O4	2:F:602:ATP:O1G	1.85	0.94
2:R:601:ATP:O1G	4:b:601:UTP:O4	1.85	0.94
2:Z:601:ATP:O1G	4:T:601:UTP:O4	1.85	0.94
4:Y:603:UTP:O4	2:S:602:ATP:O1G	1.85	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:k:603:UTP:O4	2:h:602:ATP:O1G	1.85	0.94
4:Q:605:UTP:O4	2:a:602:ATP:O1G	1.85	0.94
2:M:601:ATP:O1G	4:J:601:UTP:O4	1.85	0.94
4:R:605:UTP:O4	2:b:602:ATP:O1G	1.85	0.93
2:Y:601:ATP:O1G	4:S:601:UTP:O4	1.85	0.93
2:I:601:ATP:O1G	4:N:601:UTP:O4	1.85	0.93
2:k:601:ATP:O1G	4:h:601:UTP:O4	1.85	0.93
4:M:603:UTP:O4	2:J:602:ATP:O1G	1.85	0.93
1:A:483:ASN:ND2	1:Y:236:PRO:CG	2.31	0.93
1:E:15:GLY:HA3	2:E:601:ATP:H8	1.18	0.93
2:Q:601:ATP:O1G	4:a:601:UTP:O4	1.85	0.93
1:I:15:GLY:HA3	2:I:601:ATP:H8	1.18	0.93
1:J:15:GLY:HA3	2:J:602:ATP:H8	1.18	0.93
4:E:603:UTP:O4	2:B:602:ATP:O1G	1.85	0.92
4:I:605:UTP:O4	2:N:602:ATP:O1G	1.85	0.92
2:g:601:ATP:O1G	4:l:601:UTP:O4	1.85	0.92
2:A:601:ATP:O1G	4:F:601:UTP:O4	1.85	0.92
1:F:15:GLY:HA3	2:F:602:ATP:H8	1.18	0.92
4:Z:603:UTP:O4	2:T:602:ATP:O1G	1.85	0.92
1:A:350:GLU:CD	1:h:138:LEU:HD11	1.95	0.92
1:R:15:GLY:HA3	2:R:601:ATP:H8	1.18	0.92
1:B:15:GLY:HA3	2:B:602:ATP:H8	1.18	0.91
1:A:15:GLY:HA3	2:A:601:ATP:H8	1.18	0.90
1:A:15:GLY:HA3	2:A:601:ATP:N7	1.87	0.90
1:B:15:GLY:HA3	2:B:602:ATP:N7	1.87	0.90
1:M:15:GLY:HA3	2:M:601:ATP:N7	1.87	0.90
1:Z:15:GLY:HA3	2:Z:601:ATP:N7	1.87	0.89
1:I:15:GLY:HA3	2:I:601:ATP:N7	1.87	0.89
1:l:15:GLY:HA3	2:l:602:ATP:N7	1.87	0.89
1:h:15:GLY:HA3	2:h:602:ATP:N7	1.87	0.89
1:b:15:GLY:HA3	2:b:602:ATP:H8	1.18	0.89
1:h:15:GLY:HA3	2:h:602:ATP:H8	1.18	0.89
1:g:15:GLY:HA3	2:g:601:ATP:N7	1.87	0.89
1:b:15:GLY:HA3	2:b:602:ATP:N7	1.87	0.89
1:A:354:VAL:HG22	1:h:137:GLY:HA3	1.54	0.89
1:S:15:GLY:HA3	2:S:602:ATP:N7	1.87	0.88
1:a:15:GLY:HA3	2:a:602:ATP:N7	1.87	0.88
1:k:15:GLY:HA3	2:k:601:ATP:N7	1.87	0.88
1:N:15:GLY:HA3	2:N:602:ATP:N7	1.87	0.88
1:T:15:GLY:HA3	2:T:602:ATP:N7	1.87	0.88
1:J:15:GLY:HA3	2:J:602:ATP:N7	1.87	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:15:GLY:HA3	2:R:601:ATP:N7	1.88	0.88
1:E:15:GLY:HA3	2:E:601:ATP:N7	1.87	0.87
1:F:483:ASN:ND2	1:Z:236:PRO:HG3	1.89	0.87
1:Y:15:GLY:HA3	2:Y:601:ATP:N7	1.87	0.87
1:N:15:GLY:HA3	2:N:602:ATP:H8	1.18	0.87
1:F:15:GLY:HA3	2:F:602:ATP:N7	1.87	0.87
1:F:350:GLU:CD	1:J:138:LEU:HD11	1.99	0.87
1:Q:15:GLY:HA3	2:Q:601:ATP:N7	1.87	0.87
1:A:483:ASN:CG	1:Y:236:PRO:HG3	2.01	0.85
1:F:354:VAL:HG22	1:J:137:GLY:HA3	1.58	0.84
1:T:15:GLY:HA3	2:T:602:ATP:H8	1.18	0.83
1:S:15:GLY:HA3	2:S:602:ATP:H8	1.18	0.83
4:g:605:UTP:H2'	1:l:42:TYR:HB3	1.62	0.82
1:k:42:TYR:HB3	4:h:601:UTP:H2'	1.62	0.82
4:Z:603:UTP:H2'	1:T:42:TYR:HB3	1.62	0.82
4:A:605:UTP:H2'	1:F:42:TYR:HB3	1.62	0.81
4:k:603:UTP:H2'	1:h:42:TYR:HB3	1.62	0.81
1:R:42:TYR:HB3	4:b:601:UTP:H2'	1.62	0.81
1:Z:42:TYR:HB3	4:T:601:UTP:H2'	1.62	0.81
1:g:42:TYR:HB3	4:l:601:UTP:H2'	1.62	0.81
4:I:605:UTP:H2'	1:N:42:TYR:HB3	1.62	0.81
1:F:483:ASN:ND2	1:Z:236:PRO:CG	2.44	0.81
4:Y:603:UTP:H2'	1:S:42:TYR:HB3	1.62	0.81
1:E:42:TYR:HB3	4:B:601:UTP:H2'	1.62	0.80
4:R:605:UTP:H2'	1:b:42:TYR:HB3	1.62	0.80
4:E:603:UTP:H2'	1:B:42:TYR:HB3	1.62	0.80
1:I:42:TYR:HB3	4:N:601:UTP:H2'	1.62	0.80
1:M:42:TYR:HB3	4:J:601:UTP:H2'	1.62	0.80
1:Y:42:TYR:HB3	4:S:601:UTP:H2'	1.62	0.80
1:Q:42:TYR:HB3	4:a:601:UTP:H2'	1.62	0.80
1:A:42:TYR:HB3	4:F:601:UTP:H2'	1.62	0.80
4:M:603:UTP:H2'	1:J:42:TYR:HB3	1.62	0.79
4:Q:605:UTP:H2'	1:a:42:TYR:HB3	1.62	0.78
1:Q:242:VAL:HG12	2:Q:601:ATP:HN62	1.49	0.78
1:T:242:VAL:HG12	2:T:602:ATP:HN62	1.49	0.78
1:E:242:VAL:HG12	2:E:601:ATP:HN62	1.49	0.77
1:a:242:VAL:HG12	2:a:602:ATP:HN62	1.49	0.77
1:M:242:VAL:HG12	2:M:601:ATP:HN62	1.50	0.77
1:B:242:VAL:HG12	2:B:602:ATP:HN62	1.49	0.77
1:F:483:ASN:CG	1:Z:236:PRO:HG3	2.10	0.77
1:b:242:VAL:HG12	2:b:602:ATP:HN62	1.50	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:242:VAL:HG12	2:Y:601:ATP:HN62	1.49	0.77
1:J:242:VAL:HG12	2:J:602:ATP:HN62	1.49	0.77
1:g:242:VAL:HG12	2:g:601:ATP:HN62	1.49	0.77
1:N:242:VAL:HG12	2:N:602:ATP:HN62	1.49	0.77
1:A:242:VAL:HG12	2:A:601:ATP:HN62	1.49	0.76
1:R:242:VAL:HG12	2:R:601:ATP:HN62	1.49	0.76
1:S:242:VAL:HG12	2:S:602:ATP:HN62	1.49	0.76
4:A:605:UTP:O2G	1:B:193:LYS:CG	2.34	0.76
1:h:242:VAL:HG12	2:h:602:ATP:HN62	1.49	0.76
1:l:242:VAL:HG12	2:l:602:ATP:HN62	1.50	0.76
4:A:605:UTP:O1A	1:B:193:LYS:NZ	2.19	0.76
1:F:350:GLU:HB3	1:J:138:LEU:HD21	1.67	0.76
1:k:15:GLY:HA2	2:k:601:ATP:PA	2.26	0.76
1:l:15:GLY:HA2	2:l:602:ATP:PA	2.26	0.76
1:F:15:GLY:HA2	2:F:602:ATP:PA	2.26	0.76
1:Y:15:GLY:HA2	2:Y:601:ATP:PA	2.26	0.76
1:Z:242:VAL:HG12	2:Z:601:ATP:HN62	1.49	0.76
1:g:15:GLY:HA2	2:g:601:ATP:PA	2.26	0.76
1:h:15:GLY:HA2	2:h:602:ATP:PA	2.26	0.76
1:B:15:GLY:HA2	2:B:602:ATP:PA	2.26	0.76
1:N:15:GLY:HA2	2:N:602:ATP:PA	2.26	0.76
1:b:15:GLY:HA2	2:b:602:ATP:PA	2.26	0.76
1:g:193:LYS:NZ	4:h:601:UTP:O2A	2.19	0.76
4:Q:605:UTP:O2A	1:S:193:LYS:NZ	2.19	0.76
1:a:15:GLY:HA2	2:a:602:ATP:PA	2.26	0.76
1:k:242:VAL:HG12	2:k:601:ATP:HN62	1.49	0.76
1:Q:193:LYS:NZ	4:S:601:UTP:O1A	2.19	0.75
4:I:605:UTP:O2G	1:J:193:LYS:CG	2.34	0.75
1:M:15:GLY:HA2	2:M:601:ATP:PA	2.26	0.75
1:Z:15:GLY:HA2	2:Z:601:ATP:PA	2.26	0.75
1:I:15:GLY:HA2	2:I:601:ATP:PA	2.26	0.75
1:T:15:GLY:HA2	2:T:602:ATP:PA	2.26	0.75
1:A:15:GLY:HA2	2:A:601:ATP:PA	2.26	0.75
1:I:193:LYS:NZ	4:J:601:UTP:O2A	2.19	0.75
1:E:15:GLY:HA2	2:E:601:ATP:PA	2.26	0.75
1:R:193:LYS:NZ	4:T:601:UTP:O1A	2.19	0.75
1:A:193:LYS:NZ	4:B:601:UTP:O2A	2.19	0.75
4:g:605:UTP:O1A	1:h:193:LYS:NZ	2.19	0.75
1:I:242:VAL:HG12	2:I:601:ATP:HN62	1.49	0.75
1:J:15:GLY:HA2	2:J:602:ATP:PA	2.26	0.75
1:F:242:VAL:HG12	2:F:602:ATP:HN62	1.50	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:15:GLY:HA2	2:Q:601:ATP:PA	2.26	0.75
1:g:193:LYS:CG	4:h:601:UTP:O1G	2.34	0.75
1:R:15:GLY:HA2	2:R:601:ATP:PA	2.26	0.75
1:S:15:GLY:HA2	2:S:602:ATP:PA	2.26	0.75
4:R:605:UTP:O1G	1:T:193:LYS:CG	2.34	0.75
4:I:605:UTP:O1A	1:J:193:LYS:NZ	2.19	0.74
4:Z:603:UTP:O1A	1:b:193:LYS:NZ	2.20	0.74
4:Y:603:UTP:O1A	1:a:193:LYS:NZ	2.20	0.74
4:R:605:UTP:O3A	1:T:193:LYS:HE3	1.88	0.74
4:M:603:UTP:O2A	1:N:193:LYS:NZ	2.20	0.74
4:R:605:UTP:O2A	1:T:193:LYS:NZ	2.19	0.74
1:A:193:LYS:HE3	4:B:601:UTP:O3A	1.88	0.74
1:R:193:LYS:CG	4:T:601:UTP:O2G	2.34	0.74
1:g:193:LYS:HE3	4:h:601:UTP:O3A	1.88	0.74
1:E:193:LYS:NZ	4:F:601:UTP:O1A	2.20	0.74
1:Y:193:LYS:HE3	4:a:601:UTP:O3A	1.88	0.74
4:k:603:UTP:O3A	1:l:193:LYS:HE3	1.88	0.74
1:M:193:LYS:NZ	4:N:601:UTP:O1A	2.20	0.74
1:k:193:LYS:HE3	4:l:601:UTP:O3A	1.88	0.74
4:Q:605:UTP:O3A	1:S:193:LYS:HE3	1.88	0.73
4:M:603:UTP:O3A	1:N:193:LYS:HE3	1.88	0.73
1:k:193:LYS:NZ	4:l:601:UTP:O1A	2.20	0.73
4:k:603:UTP:O2A	1:l:193:LYS:NZ	2.20	0.73
1:M:193:LYS:HE3	4:N:601:UTP:O3A	1.88	0.73
4:g:605:UTP:O2G	1:h:193:LYS:CG	2.34	0.73
4:E:603:UTP:O2A	1:F:193:LYS:NZ	2.20	0.73
4:g:605:UTP:O3A	1:h:193:LYS:HE3	1.88	0.73
4:Y:603:UTP:O1G	1:a:193:LYS:CG	2.36	0.73
4:I:605:UTP:O3A	1:J:193:LYS:HE3	1.87	0.73
4:A:605:UTP:O3A	1:B:193:LYS:HE3	1.88	0.73
1:Y:193:LYS:NZ	4:a:601:UTP:O2A	2.20	0.73
4:Z:603:UTP:O3A	1:b:193:LYS:HE3	1.88	0.73
4:M:603:UTP:O1G	1:N:193:LYS:CG	2.36	0.73
1:Z:193:LYS:NZ	4:b:601:UTP:O2A	2.20	0.73
1:Z:193:LYS:CG	4:b:601:UTP:O1G	2.36	0.72
1:E:193:LYS:HE3	4:F:601:UTP:O3A	1.88	0.72
4:Y:603:UTP:O3A	1:a:193:LYS:HE3	1.88	0.72
1:Q:193:LYS:HE3	4:S:601:UTP:O3A	1.88	0.72
1:I:193:LYS:HE3	4:J:601:UTP:O3A	1.88	0.72
1:E:193:LYS:CG	4:F:601:UTP:O2G	2.36	0.72
4:Q:605:UTP:O1G	1:S:193:LYS:CG	2.34	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:193:LYS:HE3	4:T:601:UTP:O3A	1.88	0.72
1:A:350:GLU:HB3	1:h:138:LEU:HD21	1.70	0.72
4:E:603:UTP:O3A	1:F:193:LYS:HE3	1.88	0.72
4:Q:605:UTP:C6	1:a:40:ASP:OD1	2.43	0.72
1:M:193:LYS:CG	4:N:601:UTP:O1G	2.36	0.72
4:E:603:UTP:C6	1:B:40:ASP:OD1	2.43	0.71
4:E:603:UTP:O1G	1:F:193:LYS:CG	2.36	0.71
1:Z:193:LYS:HE3	4:b:601:UTP:O3A	1.88	0.71
1:k:40:ASP:OD1	4:h:601:UTP:C6	2.43	0.71
4:R:605:UTP:C6	1:b:40:ASP:OD1	2.43	0.71
1:M:40:ASP:OD1	4:J:601:UTP:C6	2.43	0.71
1:Z:40:ASP:OD1	4:T:601:UTP:C6	2.43	0.71
1:A:193:LYS:CG	4:B:601:UTP:O1G	2.34	0.71
4:k:603:UTP:C6	1:h:40:ASP:OD1	2.43	0.71
1:A:40:ASP:OD1	4:F:601:UTP:C6	2.43	0.71
1:Q:193:LYS:CG	4:S:601:UTP:O2G	2.34	0.71
4:A:605:UTP:C6	1:F:40:ASP:OD1	2.43	0.71
1:I:193:LYS:CG	4:J:601:UTP:O1G	2.34	0.71
1:Y:193:LYS:CG	4:a:601:UTP:O1G	2.36	0.71
1:I:40:ASP:OD1	4:N:601:UTP:C6	2.43	0.71
1:E:40:ASP:OD1	4:B:601:UTP:C6	2.43	0.70
1:Q:40:ASP:OD1	4:a:601:UTP:C6	2.43	0.70
4:Y:603:UTP:C6	1:S:40:ASP:OD1	2.43	0.70
4:M:603:UTP:C6	1:J:40:ASP:OD1	2.43	0.70
4:Z:603:UTP:C6	1:T:40:ASP:OD1	2.43	0.70
1:A:483:ASN:ND2	1:Y:236:PRO:HG2	2.06	0.70
1:Y:40:ASP:OD1	4:S:601:UTP:C6	2.43	0.70
4:g:605:UTP:C6	1:l:40:ASP:OD1	2.43	0.70
1:R:40:ASP:OD1	4:b:601:UTP:C6	2.43	0.70
1:h:242:VAL:CG1	2:h:602:ATP:HN62	2.05	0.69
1:l:242:VAL:CG1	2:l:602:ATP:HN62	2.06	0.69
4:Z:603:UTP:O1G	1:b:193:LYS:CG	2.36	0.69
1:N:242:VAL:CG1	2:N:602:ATP:HN62	2.05	0.69
1:M:242:VAL:CG1	2:M:601:ATP:HN62	2.06	0.69
1:R:242:VAL:CG1	2:R:601:ATP:HN62	2.06	0.69
1:Z:242:VAL:CG1	2:Z:601:ATP:HN62	2.05	0.69
1:g:40:ASP:OD1	4:l:601:UTP:C6	2.43	0.69
1:A:242:VAL:CG1	2:A:601:ATP:HN62	2.05	0.69
4:I:605:UTP:C6	1:N:40:ASP:OD1	2.43	0.69
1:J:242:VAL:CG1	2:J:602:ATP:HN62	2.06	0.69
4:R:605:UTP:O3B	1:T:193:LYS:HE3	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:242:VAL:CG1	2:T:602:ATP:HN62	2.05	0.69
1:k:242:VAL:CG1	2:k:601:ATP:HN62	2.05	0.69
4:k:603:UTP:O1G	1:l:193:LYS:CG	2.36	0.69
1:F:242:VAL:CG1	2:F:602:ATP:HN62	2.05	0.69
1:Q:193:LYS:HE3	4:S:601:UTP:O3B	1.93	0.69
4:g:605:UTP:O3B	1:h:193:LYS:HE3	1.93	0.69
4:A:605:UTP:O3B	1:B:193:LYS:HE3	1.93	0.68
1:Y:242:VAL:CG1	2:Y:601:ATP:HN62	2.06	0.68
1:a:242:VAL:CG1	2:a:602:ATP:HN62	2.05	0.68
1:I:242:VAL:CG1	2:I:601:ATP:HN62	2.05	0.68
1:g:242:VAL:CG1	2:g:601:ATP:HN62	2.05	0.68
1:h:15:GLY:HA2	2:h:602:ATP:O5'	1.94	0.68
1:F:15:GLY:HA2	2:F:602:ATP:O5'	1.94	0.68
1:S:242:VAL:CG1	2:S:602:ATP:HN62	2.06	0.68
1:g:15:GLY:HA2	2:g:601:ATP:O5'	1.94	0.68
1:A:15:GLY:HA2	2:A:601:ATP:O5'	1.94	0.68
1:E:242:VAL:CG1	2:E:601:ATP:HN62	2.05	0.68
1:I:193:LYS:HE3	4:J:601:UTP:O3B	1.93	0.68
1:T:15:GLY:HA2	2:T:602:ATP:O5'	1.94	0.68
4:A:605:UTP:PG	1:B:193:LYS:HG3	2.34	0.68
1:F:354:VAL:HG22	1:J:137:GLY:CA	2.23	0.68
1:Q:242:VAL:CG1	2:Q:601:ATP:HN62	2.05	0.68
1:R:193:LYS:HE3	4:T:601:UTP:O3B	1.93	0.68
1:b:242:VAL:CG1	2:b:602:ATP:HN62	2.05	0.68
4:Q:605:UTP:PG	1:S:193:LYS:HG3	2.34	0.68
4:I:605:UTP:O3B	1:J:193:LYS:HE3	1.93	0.68
1:J:15:GLY:HA2	2:J:602:ATP:O5'	1.94	0.68
1:Y:15:GLY:HA2	2:Y:601:ATP:O5'	1.94	0.68
1:I:15:GLY:HA2	2:I:601:ATP:O5'	1.94	0.68
1:S:15:GLY:HA2	2:S:602:ATP:O5'	1.94	0.68
1:a:15:GLY:HA2	2:a:602:ATP:O5'	1.94	0.68
1:g:193:LYS:HE3	4:h:601:UTP:O3B	1.93	0.68
4:g:605:UTP:PG	1:h:193:LYS:HG3	2.34	0.68
1:E:15:GLY:HA2	2:E:601:ATP:O5'	1.94	0.68
4:Q:605:UTP:O3B	1:S:193:LYS:HE3	1.93	0.68
1:M:15:GLY:HA2	2:M:601:ATP:O5'	1.94	0.68
1:R:15:GLY:HA2	2:R:601:ATP:O5'	1.94	0.68
1:Q:15:GLY:HA2	2:Q:601:ATP:O5'	1.94	0.67
1:l:15:GLY:HA2	2:l:602:ATP:O5'	1.94	0.67
1:A:193:LYS:HE3	4:B:601:UTP:O3B	1.93	0.67
1:B:242:VAL:CG1	2:B:602:ATP:HN62	2.05	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:605:UTP:PG	1:J:193:LYS:HG3	2.34	0.67
1:N:15:GLY:HA2	2:N:602:ATP:O5'	1.94	0.67
1:A:193:LYS:HG3	4:B:601:UTP:PG	2.34	0.67
4:Y:603:UTP:O3B	1:a:193:LYS:HE3	1.95	0.67
1:Z:15:GLY:HA2	2:Z:601:ATP:O5'	1.94	0.67
4:Z:603:UTP:O3B	1:b:193:LYS:HE3	1.95	0.67
1:g:193:LYS:HG3	4:h:601:UTP:PG	2.34	0.67
4:E:603:UTP:O3B	1:F:193:LYS:HE3	1.95	0.67
1:k:193:LYS:CG	4:l:601:UTP:O1G	2.36	0.67
1:Y:193:LYS:HE3	4:a:601:UTP:O3B	1.95	0.67
1:B:15:GLY:HA2	2:B:602:ATP:O5'	1.94	0.67
1:M:193:LYS:HE3	4:N:601:UTP:O3B	1.95	0.67
1:R:193:LYS:HG3	4:T:601:UTP:PG	2.34	0.67
1:Z:193:LYS:HE3	4:b:601:UTP:O3B	1.95	0.67
1:b:15:GLY:HA2	2:b:602:ATP:O5'	1.94	0.67
1:Q:193:LYS:HG3	4:S:601:UTP:PG	2.34	0.66
1:k:15:GLY:HA2	2:k:601:ATP:O5'	1.94	0.66
1:E:193:LYS:HE3	4:F:601:UTP:O3B	1.95	0.66
4:k:603:UTP:O3B	1:l:193:LYS:HE3	1.95	0.66
1:I:193:LYS:HG3	4:J:601:UTP:PG	2.34	0.66
4:R:605:UTP:PG	1:T:193:LYS:HG3	2.34	0.66
4:k:603:UTP:PG	1:l:193:LYS:HG3	2.36	0.66
4:M:603:UTP:O3B	1:N:193:LYS:HE3	1.95	0.66
4:Z:603:UTP:PG	1:b:193:LYS:HG3	2.36	0.66
1:k:193:LYS:HE3	4:l:601:UTP:O3B	1.95	0.66
4:Y:603:UTP:PG	1:a:193:LYS:HG3	2.36	0.66
1:A:354:VAL:HG22	1:h:137:GLY:CA	2.25	0.65
4:E:603:UTP:PG	1:F:193:LYS:HG3	2.36	0.65
1:M:193:LYS:HG3	4:N:601:UTP:PG	2.36	0.65
1:R:193:LYS:HZ1	4:T:601:UTP:PA	2.18	0.65
1:Z:193:LYS:HG3	4:b:601:UTP:PG	2.36	0.65
1:E:193:LYS:HG3	4:F:601:UTP:PG	2.36	0.65
1:k:193:LYS:HG3	4:l:601:UTP:PG	2.36	0.65
4:M:603:UTP:PG	1:N:193:LYS:HG3	2.36	0.65
1:Y:193:LYS:HG3	4:a:601:UTP:PG	2.36	0.65
4:E:603:UTP:PA	1:F:193:LYS:HZ1	2.21	0.64
4:I:605:UTP:O3A	1:J:193:LYS:NZ	2.31	0.64
4:g:605:UTP:O3A	1:h:193:LYS:NZ	2.31	0.64
4:R:605:UTP:O3A	1:T:193:LYS:NZ	2.31	0.64
1:R:193:LYS:NZ	4:T:601:UTP:O3A	2.32	0.63
1:A:193:LYS:NZ	4:B:601:UTP:O3A	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:605:UTP:O3A	1:B:193:LYS:NZ	2.31	0.63
1:g:193:LYS:NZ	4:h:601:UTP:O3A	2.31	0.63
4:R:605:UTP:O3A	1:T:193:LYS:CE	2.47	0.63
4:R:605:UTP:PB	1:T:193:LYS:HE3	2.39	0.63
4:I:605:UTP:O3A	1:J:193:LYS:CE	2.47	0.63
1:Q:193:LYS:NZ	4:S:601:UTP:O3A	2.32	0.63
4:Q:605:UTP:O3A	1:S:193:LYS:NZ	2.31	0.63
1:Q:193:LYS:CE	4:S:601:UTP:O3A	2.47	0.62
4:A:605:UTP:PB	1:B:193:LYS:HE3	2.39	0.62
1:Q:193:LYS:HE3	4:S:601:UTP:PB	2.40	0.62
1:I:193:LYS:NZ	4:J:601:UTP:O3A	2.31	0.62
4:Y:603:UTP:O3A	1:a:193:LYS:NZ	2.33	0.62
1:I:193:LYS:HE3	4:J:601:UTP:PB	2.39	0.62
4:M:603:UTP:O3A	1:N:193:LYS:NZ	2.33	0.62
1:g:193:LYS:CE	4:h:601:UTP:O3A	2.47	0.62
4:A:605:UTP:O3A	1:B:193:LYS:CE	2.47	0.62
1:R:193:LYS:HE3	4:T:601:UTP:PB	2.40	0.62
4:g:605:UTP:O3A	1:h:193:LYS:CE	2.47	0.62
1:R:17:GLY:N	2:R:601:ATP:O1A	2.33	0.62
1:g:193:LYS:HE3	4:h:601:UTP:PB	2.39	0.62
1:A:384:GLU:OE1	1:h:276:THR:HG22	2.00	0.62
4:E:603:UTP:O3A	1:F:193:LYS:NZ	2.33	0.62
4:Q:605:UTP:O3A	1:S:193:LYS:CE	2.47	0.62
1:b:17:GLY:N	2:b:602:ATP:O1A	2.33	0.62
1:k:193:LYS:NZ	4:l:601:UTP:O3A	2.33	0.62
4:k:603:UTP:O3A	1:l:193:LYS:CE	2.48	0.62
1:h:17:GLY:N	2:h:602:ATP:O1A	2.33	0.62
1:I:193:LYS:CE	4:J:601:UTP:O3A	2.47	0.62
4:Z:603:UTP:O3A	1:b:193:LYS:CE	2.48	0.62
4:Z:603:UTP:O3A	1:b:193:LYS:NZ	2.33	0.62
1:A:193:LYS:HZ1	4:B:601:UTP:PA	2.23	0.61
1:A:193:LYS:CE	4:B:601:UTP:O3A	2.47	0.61
1:Y:193:LYS:NZ	4:a:601:UTP:O3A	2.33	0.61
4:Y:603:UTP:O3A	1:a:193:LYS:CE	2.48	0.61
4:I:605:UTP:PB	1:J:193:LYS:HE3	2.39	0.61
1:l:17:GLY:N	2:l:602:ATP:O1A	2.33	0.61
1:Z:193:LYS:CE	4:b:601:UTP:O3A	2.48	0.61
4:E:603:UTP:O3A	1:F:193:LYS:CE	2.48	0.61
1:R:193:LYS:CE	4:T:601:UTP:O3A	2.47	0.61
1:k:193:LYS:CE	4:l:601:UTP:O3A	2.48	0.61
1:k:193:LYS:HE3	4:l:601:UTP:PB	2.41	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:HE3	4:B:601:UTP:PB	2.40	0.61
4:E:603:UTP:PB	1:F:193:LYS:HE3	2.40	0.61
1:F:17:GLY:N	2:F:602:ATP:O1A	2.33	0.61
1:T:17:GLY:N	2:T:602:ATP:O1A	2.33	0.61
1:A:17:GLY:N	2:A:601:ATP:O1A	2.33	0.61
4:Q:605:UTP:PB	1:S:193:LYS:HE3	2.39	0.61
1:Y:193:LYS:CE	4:a:601:UTP:O3A	2.48	0.61
1:Z:17:GLY:N	2:Z:601:ATP:O1A	2.33	0.61
4:Z:603:UTP:PB	1:b:193:LYS:HE3	2.40	0.61
4:g:605:UTP:PB	1:h:193:LYS:HE3	2.39	0.61
1:B:17:GLY:N	2:B:602:ATP:O1A	2.33	0.61
1:Y:17:GLY:N	2:Y:601:ATP:O1A	2.33	0.61
4:Y:603:UTP:PB	1:a:193:LYS:HE3	2.40	0.61
1:g:17:GLY:N	2:g:601:ATP:O1A	2.33	0.61
1:k:17:GLY:N	2:k:601:ATP:O1A	2.33	0.61
1:E:17:GLY:N	2:E:601:ATP:O1A	2.33	0.61
1:E:193:LYS:HE3	4:F:601:UTP:PB	2.41	0.61
1:Z:193:LYS:NZ	4:b:601:UTP:O3A	2.33	0.61
4:k:603:UTP:O3A	1:l:193:LYS:NZ	2.33	0.61
1:A:571:LEU:HD21	1:a:100:ARG:HH12	1.66	0.61
1:E:193:LYS:CE	4:F:601:UTP:O3A	2.48	0.61
1:S:17:GLY:N	2:S:602:ATP:O1A	2.33	0.61
1:a:17:GLY:N	2:a:602:ATP:O1A	2.33	0.61
1:M:193:LYS:NZ	4:N:601:UTP:O3A	2.33	0.61
1:E:193:LYS:NZ	4:F:601:UTP:O3A	2.33	0.61
1:Q:17:GLY:N	2:Q:601:ATP:O1A	2.33	0.61
1:M:193:LYS:CE	4:N:601:UTP:O3A	2.48	0.61
4:M:603:UTP:PB	1:N:193:LYS:HE3	2.40	0.61
1:Z:193:LYS:HE3	4:b:601:UTP:PB	2.41	0.61
1:F:571:LEU:HD21	1:b:100:ARG:HH12	1.66	0.60
4:M:603:UTP:O3A	1:N:193:LYS:CE	2.48	0.60
4:k:603:UTP:PB	1:l:193:LYS:HE3	2.40	0.60
1:Y:193:LYS:HE3	4:a:601:UTP:PB	2.41	0.60
1:M:17:GLY:N	2:M:601:ATP:O1A	2.33	0.60
1:M:193:LYS:HE3	4:N:601:UTP:PB	2.41	0.60
1:I:17:GLY:N	2:I:601:ATP:O1A	2.33	0.60
1:F:483:ASN:ND2	1:Z:236:PRO:HG2	2.17	0.60
1:N:17:GLY:N	2:N:602:ATP:O1A	2.33	0.60
1:J:17:GLY:N	2:J:602:ATP:O1A	2.33	0.59
1:Y:192:THR:OG1	4:a:601:UTP:O3G	2.20	0.59
1:R:192:THR:OG1	4:T:601:UTP:O3G	2.21	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:603:UTP:O3G	1:F:192:THR:OG1	2.21	0.59
4:A:605:UTP:PA	1:B:193:LYS:NZ	2.76	0.59
4:M:603:UTP:O3G	1:N:192:THR:OG1	2.21	0.59
4:I:605:UTP:PA	1:J:193:LYS:NZ	2.76	0.59
4:R:605:UTP:PA	1:T:193:LYS:NZ	2.76	0.59
1:g:193:LYS:NZ	4:h:601:UTP:PA	2.76	0.59
4:g:605:UTP:O3G	1:h:192:THR:OG1	2.21	0.59
1:I:193:LYS:NZ	4:J:601:UTP:PA	2.76	0.58
1:R:193:LYS:NZ	4:T:601:UTP:PA	2.76	0.58
4:A:605:UTP:PA	1:B:193:LYS:HZ1	2.25	0.58
4:M:603:UTP:PA	1:N:193:LYS:HZ2	2.26	0.58
1:A:571:LEU:HD21	1:a:100:ARG:NH1	2.19	0.58
1:Q:193:LYS:NZ	4:S:601:UTP:PA	2.76	0.58
4:g:605:UTP:PA	1:h:193:LYS:NZ	2.76	0.58
4:Q:605:UTP:PA	1:S:193:LYS:NZ	2.76	0.58
1:A:193:LYS:NZ	4:B:601:UTP:PA	2.76	0.58
4:I:605:UTP:O3G	1:J:192:THR:OG1	2.21	0.58
4:g:605:UTP:PA	1:h:193:LYS:HZ1	2.27	0.58
4:E:603:UTP:PA	1:F:193:LYS:NZ	2.77	0.57
4:M:603:UTP:PA	1:N:193:LYS:NZ	2.77	0.57
4:R:605:UTP:PA	1:T:193:LYS:HZ1	2.25	0.57
4:Z:603:UTP:PA	1:b:193:LYS:HZ1	2.27	0.57
4:Y:603:UTP:PA	1:a:193:LYS:NZ	2.77	0.57
1:Z:193:LYS:NZ	4:b:601:UTP:PA	2.78	0.57
4:Z:603:UTP:PA	1:b:193:LYS:NZ	2.77	0.57
1:g:42:TYR:HD1	4:l:601:UTP:C2'	2.15	0.57
1:M:192:THR:OG1	4:N:601:UTP:O2G	2.20	0.57
1:M:193:LYS:NZ	4:N:601:UTP:PA	2.78	0.57
1:E:193:LYS:NZ	4:F:601:UTP:PA	2.78	0.57
4:k:603:UTP:PA	1:l:193:LYS:NZ	2.77	0.57
1:F:384:GLU:OE1	1:J:276:THR:HA	2.05	0.56
1:Y:193:LYS:NZ	4:a:601:UTP:PA	2.78	0.56
4:Y:603:UTP:C2'	1:S:42:TYR:HD1	2.15	0.56
1:M:42:TYR:HD1	4:J:601:UTP:C2'	2.15	0.56
4:R:605:UTP:O3G	1:T:192:THR:OG1	2.21	0.56
4:E:603:UTP:C2'	1:B:42:TYR:HD1	2.15	0.56
1:k:193:LYS:NZ	4:l:601:UTP:PA	2.78	0.56
1:Q:42:TYR:HD1	4:a:601:UTP:C2'	2.15	0.56
1:I:42:TYR:HD1	4:N:601:UTP:C2'	2.15	0.55
1:I:192:THR:OG1	4:J:601:UTP:O3G	2.21	0.55
1:g:192:THR:OG1	4:h:601:UTP:O3G	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:k:603:UTP:O3G	1:l:192:THR:OG1	2.21	0.55
1:F:571:LEU:HD21	1:b:100:ARG:NH1	2.21	0.55
4:k:603:UTP:C2'	1:h:42:TYR:HD1	2.15	0.55
1:A:42:TYR:HD1	4:F:601:UTP:C2'	2.15	0.55
1:Y:42:TYR:HD1	4:S:601:UTP:C2'	2.15	0.55
1:k:192:THR:OG1	4:l:601:UTP:O2G	2.20	0.55
4:Z:603:UTP:O2G	1:b:192:THR:OG1	2.21	0.55
4:A:605:UTP:C2'	1:F:42:TYR:HD1	2.15	0.54
1:F:384:GLU:OE1	1:J:276:THR:HG22	2.07	0.54
1:g:193:LYS:HZ1	4:h:601:UTP:PA	2.31	0.54
4:g:605:UTP:C2'	1:l:42:TYR:HD1	2.15	0.54
4:Q:605:UTP:O3G	1:S:192:THR:OG1	2.21	0.54
1:E:192:THR:OG1	4:F:601:UTP:O3G	2.20	0.53
1:F:350:GLU:OE1	1:J:138:LEU:HD11	2.08	0.53
1:I:193:LYS:HZ1	4:J:601:UTP:PA	2.31	0.53
4:R:605:UTP:O2'	1:b:42:TYR:CD1	2.03	0.53
1:A:350:GLU:OE1	1:h:138:LEU:HD11	2.06	0.53
1:A:138:LEU:HD21	1:Q:350:GLU:HB3	1.90	0.53
4:A:605:UTP:O3G	1:B:192:THR:OG1	2.21	0.53
4:Z:603:UTP:C2'	1:T:42:TYR:HD1	2.15	0.53
1:k:42:TYR:HD1	4:h:601:UTP:C2'	2.15	0.53
4:Y:603:UTP:O2G	1:a:192:THR:OG1	2.21	0.53
4:Y:603:UTP:PA	1:a:193:LYS:HZ1	2.31	0.53
4:I:605:UTP:C2'	1:N:42:TYR:HD1	2.15	0.53
1:Z:42:TYR:HD1	4:T:601:UTP:C2'	2.15	0.52
4:R:605:UTP:C2'	1:b:42:TYR:HD1	2.15	0.52
4:Q:605:UTP:C2'	1:a:42:TYR:HD1	2.15	0.52
1:Q:193:LYS:HZ1	4:S:601:UTP:PA	2.32	0.52
4:I:605:UTP:PA	1:J:193:LYS:HZ1	2.33	0.51
1:Q:192:THR:OG1	4:S:601:UTP:O3G	2.21	0.51
1:Z:192:THR:OG1	4:b:601:UTP:O3G	2.20	0.51
1:F:350:GLU:CB	1:J:138:LEU:HD21	2.40	0.51
4:g:605:UTP:C4	2:l:602:ATP:O1G	2.63	0.51
1:A:192:THR:OG1	4:B:601:UTP:O3G	2.21	0.50
2:Y:601:ATP:O1G	4:S:601:UTP:C4	2.63	0.50
2:M:601:ATP:O1G	4:J:601:UTP:C4	2.63	0.50
2:I:601:ATP:O1G	4:N:601:UTP:C4	2.63	0.50
4:k:603:UTP:C4	2:h:602:ATP:O1G	2.63	0.50
1:A:429:PHE:O	1:h:281:GLU:HG3	2.10	0.50
4:Q:605:UTP:C4	2:a:602:ATP:O1G	2.63	0.50
1:S:426:SER:HB2	1:S:429:PHE:CZ	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:426:SER:HB2	1:M:429:PHE:CZ	2.47	0.50
1:B:426:SER:HB2	1:B:429:PHE:CZ	2.47	0.50
1:A:276:THR:HA	1:Q:384:GLU:OE1	2.12	0.50
2:A:601:ATP:O1G	4:F:601:UTP:C4	2.63	0.50
1:I:426:SER:HB2	1:I:429:PHE:CZ	2.47	0.50
1:b:426:SER:HB2	1:b:429:PHE:CZ	2.47	0.50
1:A:426:SER:HB2	1:A:429:PHE:CZ	2.47	0.50
1:A:483:ASN:CG	1:Y:236:PRO:CG	2.77	0.50
4:E:603:UTP:C4	2:B:602:ATP:O1G	2.63	0.50
1:M:193:LYS:HZ1	4:N:601:UTP:PA	2.34	0.50
1:Z:426:SER:HB2	1:Z:429:PHE:CZ	2.47	0.50
1:h:426:SER:HB2	1:h:429:PHE:CZ	2.47	0.50
1:a:426:SER:HB2	1:a:429:PHE:CZ	2.47	0.49
1:F:426:SER:HB2	1:F:429:PHE:CZ	2.47	0.49
1:N:426:SER:HB2	1:N:429:PHE:CZ	2.47	0.49
4:Z:603:UTP:O2'	1:T:42:TYR:CD1	2.03	0.49
1:Q:426:SER:HB2	1:Q:429:PHE:CZ	2.47	0.49
1:l:426:SER:HB2	1:l:429:PHE:CZ	2.47	0.49
1:F:138:LEU:HD21	1:R:350:GLU:HB3	1.93	0.49
2:g:601:ATP:O1G	4:l:601:UTP:C4	2.63	0.49
1:k:426:SER:HB2	1:k:429:PHE:CZ	2.47	0.49
4:I:605:UTP:C4	2:N:602:ATP:O1G	2.64	0.49
1:J:426:SER:HB2	1:J:429:PHE:CZ	2.47	0.49
1:Y:426:SER:HB2	1:Y:429:PHE:CZ	2.47	0.49
1:T:426:SER:HB2	1:T:429:PHE:CZ	2.47	0.49
1:g:426:SER:HB2	1:g:429:PHE:CZ	2.47	0.49
4:M:603:UTP:C4	2:J:602:ATP:O1G	2.63	0.49
1:R:426:SER:HB2	1:R:429:PHE:CZ	2.47	0.49
1:A:350:GLU:CB	1:h:138:LEU:HD21	2.41	0.49
1:E:42:TYR:CD1	4:B:601:UTP:O2'	2.03	0.49
4:I:605:UTP:O2'	1:N:42:TYR:CD1	2.03	0.49
1:E:42:TYR:HD1	4:B:601:UTP:C2'	2.15	0.48
1:E:426:SER:HB2	1:E:429:PHE:CZ	2.47	0.48
4:Y:603:UTP:C4	2:S:602:ATP:O1G	2.63	0.48
2:k:601:ATP:O1G	4:h:601:UTP:C4	2.63	0.48
4:R:605:UTP:C4	2:b:602:ATP:O1G	2.64	0.48
4:Y:603:UTP:O2'	1:S:42:TYR:CD1	2.03	0.48
1:M:204:SER:HA	1:N:204:SER:HA	1.96	0.48
1:A:483:ASN:HD21	1:Y:236:PRO:HG2	1.75	0.48
1:Y:42:TYR:CB	4:S:601:UTP:H2'	2.41	0.48
1:M:42:TYR:CD1	4:J:601:UTP:O2'	2.03	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:204:SER:HA	1:a:204:SER:HA	1.96	0.48
1:E:193:LYS:HZ2	4:F:601:UTP:PA	2.36	0.48
2:R:601:ATP:O1G	4:b:601:UTP:C4	2.63	0.48
4:M:603:UTP:C2'	1:J:42:TYR:HD1	2.15	0.48
1:A:350:GLU:CD	1:h:138:LEU:CD1	2.80	0.47
1:A:350:GLU:OE2	1:h:138:LEU:HD11	2.13	0.47
2:E:601:ATP:O1G	4:B:601:UTP:C4	2.63	0.47
1:F:384:GLU:OE1	1:J:276:THR:CB	2.62	0.47
4:Q:605:UTP:O2'	1:a:42:TYR:CD1	2.03	0.47
4:Q:605:UTP:PA	1:S:193:LYS:HZ1	2.37	0.47
1:R:42:TYR:CB	4:b:601:UTP:H2'	2.41	0.47
1:k:204:SER:HA	1:l:204:SER:HA	1.96	0.47
2:Z:601:ATP:O1G	4:T:601:UTP:C4	2.63	0.47
1:R:204:SER:HA	1:T:204:SER:HA	1.97	0.47
4:M:603:UTP:H2'	1:J:42:TYR:CB	2.41	0.47
1:E:42:TYR:CB	4:B:601:UTP:H2'	2.41	0.47
1:E:204:SER:HA	1:F:204:SER:HA	1.96	0.47
1:R:42:TYR:HD1	4:b:601:UTP:C2'	2.15	0.47
1:Z:472:TRP:CE2	1:Z:526:LYS:HE3	2.50	0.47
1:b:472:TRP:CE2	1:b:526:LYS:HE3	2.50	0.47
4:g:605:UTP:C2'	1:l:42:TYR:HB3	2.41	0.47
1:k:472:TRP:CE2	1:k:526:LYS:HE3	2.50	0.47
1:F:100:ARG:HH12	1:h:571:LEU:HD21	1.80	0.47
1:a:472:TRP:CE2	1:a:526:LYS:HE3	2.50	0.47
4:M:603:UTP:O2'	1:J:42:TYR:CD1	2.03	0.47
1:g:42:TYR:CD1	4:l:601:UTP:O2'	2.03	0.47
1:l:472:TRP:CE2	1:l:526:LYS:HE3	2.50	0.47
1:A:42:TYR:CB	4:F:601:UTP:H2'	2.41	0.47
1:E:472:TRP:CE2	1:E:526:LYS:HE3	2.50	0.46
1:Q:42:TYR:CD1	4:a:601:UTP:O2'	2.03	0.46
1:A:204:SER:HA	1:B:204:SER:HA	1.97	0.46
4:E:603:UTP:H2'	1:B:42:TYR:CB	2.41	0.46
1:F:100:ARG:NH1	1:h:571:LEU:HD21	2.30	0.46
1:M:42:TYR:CB	4:J:601:UTP:H2'	2.41	0.46
4:A:605:UTP:C4	2:F:602:ATP:O1G	2.63	0.46
1:Q:204:SER:HA	1:S:204:SER:HA	1.97	0.46
2:Q:601:ATP:O1G	4:a:601:UTP:C4	2.63	0.46
4:I:605:UTP:H2'	1:N:42:TYR:CB	2.41	0.46
1:k:42:TYR:CD1	4:h:601:UTP:O2'	2.03	0.46
1:S:472:TRP:CE2	1:S:526:LYS:HE3	2.50	0.46
1:g:204:SER:HA	1:h:204:SER:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:472:TRP:CE2	1:h:526:LYS:HE3	2.50	0.46
1:F:472:TRP:CE2	1:F:526:LYS:HE3	2.50	0.46
1:R:472:TRP:CE2	1:R:526:LYS:HE3	2.50	0.46
1:Z:204:SER:HA	1:b:204:SER:HA	1.96	0.46
1:g:472:TRP:CE2	1:g:526:LYS:HE3	2.50	0.46
1:F:276:THR:HA	1:R:384:GLU:OE1	2.16	0.46
1:Y:472:TRP:CE2	1:Y:526:LYS:HE3	2.50	0.46
1:I:204:SER:HA	1:J:204:SER:HA	1.96	0.46
1:I:472:TRP:CE2	1:I:526:LYS:HE3	2.50	0.46
1:Z:193:LYS:HZ1	4:b:601:UTP:PA	2.38	0.46
1:T:472:TRP:CE2	1:T:526:LYS:HE3	2.50	0.46
1:B:472:TRP:CE2	1:B:526:LYS:HE3	2.50	0.46
1:M:472:TRP:CE2	1:M:526:LYS:HE3	2.50	0.46
1:J:472:TRP:CE2	1:J:526:LYS:HE3	2.50	0.46
1:Q:472:TRP:CE2	1:Q:526:LYS:HE3	2.50	0.46
1:N:472:TRP:CE2	1:N:526:LYS:HE3	2.50	0.46
1:A:472:TRP:CE2	1:A:526:LYS:HE3	2.50	0.45
1:B:236:PRO:HG3	1:J:483:ASN:ND2	2.31	0.45
4:Y:603:UTP:H2'	1:S:42:TYR:CB	2.41	0.45
1:B:236:PRO:HG3	1:J:483:ASN:CG	2.41	0.45
4:Y:603:UTP:C2'	1:S:42:TYR:HB3	2.41	0.45
4:g:605:UTP:O2'	1:l:42:TYR:CD1	2.03	0.45
4:g:605:UTP:H2'	1:l:42:TYR:CB	2.41	0.45
1:g:42:TYR:HB3	4:l:601:UTP:C2'	2.42	0.45
1:Z:42:TYR:CB	4:T:601:UTP:H2'	2.41	0.45
4:Z:603:UTP:H2'	1:T:42:TYR:CB	2.41	0.45
1:A:350:GLU:OE2	1:h:138:LEU:CD1	2.64	0.45
1:k:42:TYR:CB	4:h:601:UTP:H2'	2.41	0.45
1:I:42:TYR:HB3	4:N:601:UTP:C2'	2.42	0.45
4:E:603:UTP:O2'	1:B:42:TYR:CD1	2.03	0.45
4:Z:603:UTP:C4	2:T:602:ATP:O1G	2.63	0.45
1:F:350:GLU:CD	1:J:138:LEU:CD1	2.81	0.44
1:k:193:LYS:HZ1	4:l:601:UTP:PA	2.39	0.44
4:k:603:UTP:O2'	1:h:42:TYR:CD1	2.03	0.44
4:E:603:UTP:C2'	1:B:42:TYR:HB3	2.42	0.44
1:Y:42:TYR:HB3	4:S:601:UTP:C2'	2.41	0.44
1:I:42:TYR:CD1	4:N:601:UTP:O2'	2.03	0.44
1:A:384:GLU:OE1	1:h:276:THR:CB	2.66	0.44
1:A:42:TYR:CD1	4:F:601:UTP:O2'	2.03	0.44
1:R:42:TYR:CD1	4:b:601:UTP:O2'	2.03	0.44
1:Z:42:TYR:CD1	4:T:601:UTP:O2'	2.03	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:42:TYR:HB3	4:h:601:UTP:C2'	2.41	0.44
1:F:429:PHE:O	1:J:281:GLU:HG3	2.18	0.43
4:k:603:UTP:PA	1:l:193:LYS:HZ2	2.35	0.43
4:Q:605:UTP:H2'	1:a:42:TYR:CB	2.41	0.43
4:M:603:UTP:C2'	1:J:42:TYR:HB3	2.41	0.43
4:k:603:UTP:H2'	1:h:42:TYR:CB	2.41	0.43
4:I:605:UTP:C2'	1:N:42:TYR:HB3	2.41	0.43
1:k:193:LYS:HZ2	4:l:601:UTP:PA	2.40	0.43
1:A:384:GLU:OE1	1:h:276:THR:CG2	2.66	0.43
1:E:42:TYR:HB3	4:B:601:UTP:C2'	2.41	0.43
4:A:605:UTP:C2'	1:F:42:TYR:HB3	2.41	0.42
1:S:15:GLY:HA2	2:S:602:ATP:H8	1.76	0.42
1:R:42:TYR:HB3	4:b:601:UTP:C2'	2.42	0.42
1:Q:42:TYR:CB	4:a:601:UTP:H2'	2.41	0.42
1:Q:42:TYR:HB3	4:a:601:UTP:C2'	2.41	0.42
4:A:605:UTP:O2'	1:F:42:TYR:CD1	2.03	0.42
1:Y:193:LYS:HZ1	4:a:601:UTP:PA	2.42	0.42
1:A:100:ARG:HH12	1:J:571:LEU:HD21	1.85	0.42
1:I:42:TYR:CB	4:N:601:UTP:H2'	2.41	0.42
1:A:42:TYR:HB3	4:F:601:UTP:C2'	2.42	0.41
4:Z:603:UTP:C2'	1:T:42:TYR:HB3	2.41	0.41
4:Q:605:UTP:PA	1:S:193:LYS:HZ2	2.38	0.41
1:Y:42:TYR:CD1	4:S:601:UTP:O2'	2.03	0.41
1:M:42:TYR:HB3	4:J:601:UTP:C2'	2.41	0.41
1:Y:193:LYS:HZ2	4:a:601:UTP:PA	2.37	0.41
1:E:94:TYR:CE1	1:E:117:LEU:HD11	2.57	0.40
1:h:15:GLY:HA2	2:h:602:ATP:H8	1.76	0.40
1:A:242:VAL:CG1	2:A:601:ATP:N6	2.81	0.40
1:E:193:LYS:HZ1	4:F:601:UTP:PA	2.44	0.40
1:F:94:TYR:CE1	1:F:117:LEU:HD11	2.57	0.40
1:I:41:PRO:HD2	4:N:601:UTP:C6	2.57	0.40
1:J:94:TYR:CE1	1:J:117:LEU:HD11	2.57	0.40
1:Z:94:TYR:CE1	1:Z:117:LEU:HD11	2.57	0.40
1:T:94:TYR:CE1	1:T:117:LEU:HD11	2.57	0.40
1:I:15:GLY:HA2	2:I:601:ATP:H8	1.76	0.40
1:I:94:TYR:CE1	1:I:117:LEU:HD11	2.57	0.40
1:N:94:TYR:CE1	1:N:117:LEU:HD11	2.57	0.40
1:R:41:PRO:HD2	4:b:601:UTP:C6	2.57	0.40
1:R:94:TYR:CE1	1:R:117:LEU:HD11	2.57	0.40
1:g:94:TYR:CE1	1:g:117:LEU:HD11	2.57	0.40
1:a:242:VAL:CG1	2:a:602:ATP:N6	2.81	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:605:UTP:C6	1:l:41:PRO:HD2	2.57	0.40
1:k:41:PRO:HD2	4:h:601:UTP:C6	2.57	0.40
1:A:94:TYR:CE1	1:A:117:LEU:HD11	2.57	0.40
4:A:605:UTP:C6	1:F:41:PRO:HD2	2.57	0.40
1:Y:242:VAL:CG1	2:Y:601:ATP:N6	2.81	0.40
1:g:41:PRO:HD2	4:l:601:UTP:C6	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	485 (99%)	3 (1%)	78	81
1	B	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	E	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	F	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	I	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	J	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	M	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	N	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	Q	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	R	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	S	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	T	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	Y	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	Z	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	a	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	b	488/488 (100%)	485 (99%)	3 (1%)	78	81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	g	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	h	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	k	488/488 (100%)	485 (99%)	3 (1%)	78	81
1	l	488/488 (100%)	485 (99%)	3 (1%)	78	81
All	All	9760/9760 (100%)	9700 (99%)	60 (1%)	76	81

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

Mol	Chain	Res	Type
1	A	10	VAL
1	A	69	LEU
1	A	352	GLN
1	E	10	VAL
1	E	69	LEU
1	E	352	GLN
1	B	10	VAL
1	B	69	LEU
1	B	352	GLN
1	F	10	VAL
1	F	69	LEU
1	F	352	GLN
1	Q	10	VAL
1	Q	69	LEU
1	Q	352	GLN
1	Y	10	VAL
1	Y	69	LEU
1	Y	352	GLN
1	S	10	VAL
1	S	69	LEU
1	S	352	GLN
1	a	10	VAL
1	a	69	LEU
1	a	352	GLN
1	I	10	VAL
1	I	69	LEU
1	I	352	GLN
1	M	10	VAL
1	M	69	LEU
1	M	352	GLN
1	J	10	VAL
1	J	69	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	352	GLN
1	N	10	VAL
1	N	69	LEU
1	N	352	GLN
1	R	10	VAL
1	R	69	LEU
1	R	352	GLN
1	Z	10	VAL
1	Z	69	LEU
1	Z	352	GLN
1	T	10	VAL
1	T	69	LEU
1	T	352	GLN
1	b	10	VAL
1	b	69	LEU
1	b	352	GLN
1	g	10	VAL
1	g	69	LEU
1	g	352	GLN
1	k	10	VAL
1	k	69	LEU
1	k	352	GLN
1	h	10	VAL
1	h	69	LEU
1	h	352	GLN
1	l	10	VAL
1	l	69	LEU
1	l	352	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	165	GLN
1	A	221	ASN
1	A	483	ASN
1	E	119	ASN
1	E	165	GLN
1	E	221	ASN
1	B	119	ASN
1	B	165	GLN
1	B	221	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	119	ASN
1	F	165	GLN
1	F	221	ASN
1	F	483	ASN
1	Q	119	ASN
1	Q	165	GLN
1	Q	221	ASN
1	Y	119	ASN
1	Y	165	GLN
1	Y	221	ASN
1	Y	328	HIS
1	S	119	ASN
1	S	165	GLN
1	S	221	ASN
1	a	119	ASN
1	a	165	GLN
1	a	221	ASN
1	a	328	HIS
1	I	119	ASN
1	I	165	GLN
1	M	119	ASN
1	M	165	GLN
1	J	119	ASN
1	J	165	GLN
1	J	221	ASN
1	J	483	ASN
1	N	119	ASN
1	N	165	GLN
1	N	221	ASN
1	R	119	ASN
1	R	165	GLN
1	R	221	ASN
1	Z	119	ASN
1	Z	165	GLN
1	Z	221	ASN
1	Z	328	HIS
1	T	119	ASN
1	T	165	GLN
1	T	221	ASN
1	b	119	ASN
1	b	165	GLN
1	b	221	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	b	328	HIS
1	g	119	ASN
1	g	165	GLN
1	g	221	ASN
1	g	328	HIS
1	k	119	ASN
1	k	165	GLN
1	k	221	ASN
1	k	328	HIS
1	h	119	ASN
1	h	165	GLN
1	h	221	ASN
1	h	328	HIS
1	h	483	ASN
1	l	119	ASN
1	l	165	GLN
1	l	221	ASN
1	l	328	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 oligosaccharides 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	$\# Z > 2$
4	UTP	Z	603	3	29,30,30	0.59	0	43,47,47	1.26	6 (13%)
4	UTP	Y	603	3	29,30,30	0.60	0	43,47,47	1.26	6 (13%)
4	UTP	E	603	3	29,30,30	0.60	0	43,47,47	1.23	6 (13%)
4	UTP	l	601	3	29,30,30	0.59	0	43,47,47	1.26	6 (13%)
2	ATP	F	602	3	32,33,33	1.14	1 (3%)	48,52,52	1.16	3 (6%)
2	ATP	S	602	3	32,33,33	1.14	2 (6%)	48,52,52	1.16	3 (6%)
2	ATP	a	602	3	32,33,33	1.14	1 (3%)	48,52,52	1.16	3 (6%)
2	ATP	l	602	3	32,33,33	1.14	1 (3%)	48,52,52	1.16	3 (6%)
4	UTP	N	601	3	29,30,30	0.60	0	43,47,47	1.26	6 (13%)
2	ATP	g	601	3	32,33,33	1.14	2 (6%)	48,52,52	1.17	3 (6%)
4	UTP	Q	605	3	29,30,30	0.60	0	43,47,47	1.23	6 (13%)
4	UTP	g	605	3	29,30,30	0.60	0	43,47,47	1.25	6 (13%)
2	ATP	E	601	3	32,33,33	1.13	2 (6%)	48,52,52	1.16	3 (6%)
4	UTP	I	605	3	29,30,30	0.60	0	43,47,47	1.25	6 (13%)
4	UTP	A	605	3	29,30,30	0.60	0	43,47,47	1.25	6 (13%)
2	ATP	M	601	3	32,33,33	1.12	1 (3%)	48,52,52	1.16	3 (6%)
4	UTP	b	601	3	29,30,30	0.60	0	43,47,47	1.23	6 (13%)
2	ATP	R	601	3	32,33,33	1.14	2 (6%)	48,52,52	1.16	3 (6%)
2	ATP	b	602	3	32,33,33	1.14	1 (3%)	48,52,52	1.16	3 (6%)
2	ATP	I	601	3	32,33,33	1.14	2 (6%)	48,52,52	1.16	3 (6%)
2	ATP	A	601	3	32,33,33	1.14	1 (3%)	48,52,52	1.16	3 (6%)
4	UTP	F	601	3	29,30,30	0.60	0	43,47,47	1.25	6 (13%)
4	UTP	a	601	3	29,30,30	0.60	0	43,47,47	1.23	6 (13%)
4	UTP	T	601	3	29,30,30	0.61	0	43,47,47	1.24	6 (13%)
2	ATP	J	602	3	32,33,33	1.14	2 (6%)	48,52,52	1.16	3 (6%)
4	UTP	h	601	3	29,30,30	0.60	0	43,47,47	1.23	6 (13%)
2	ATP	Q	601	3	32,33,33	1.14	1 (3%)	48,52,52	1.16	3 (6%)
2	ATP	T	602	3	32,33,33	1.13	2 (6%)	48,52,52	1.16	3 (6%)
4	UTP	B	601	3	29,30,30	0.60	0	43,47,47	1.23	6 (13%)
4	UTP	J	601	3	29,30,30	0.59	0	43,47,47	1.23	6 (13%)
4	UTP	R	605	3	29,30,30	0.60	0	43,47,47	1.23	6 (13%)
2	ATP	Z	601	3	32,33,33	1.13	1 (3%)	48,52,52	1.16	3 (6%)
4	UTP	k	603	3	29,30,30	0.59	0	43,47,47	1.24	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	B	602	3	32,33,33	1.13	1 (3%)	48,52,52	1.16	3 (6%)
2	ATP	k	601	3	32,33,33	1.13	1 (3%)	48,52,52	1.16	3 (6%)
4	UTP	M	603	3	29,30,30	0.59	0	43,47,47	1.24	6 (13%)
2	ATP	N	602	3	32,33,33	1.14	1 (3%)	48,52,52	1.16	3 (6%)
2	ATP	h	602	3	32,33,33	1.13	1 (3%)	48,52,52	1.16	3 (6%)
4	UTP	S	601	3	29,30,30	0.61	0	43,47,47	1.24	6 (13%)
2	ATP	Y	601	3	32,33,33	1.12	1 (3%)	48,52,52	1.16	3 (6%)

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
4	UTP	Z	603	3	2/2/7/7	12/22/38/38	0/2/2/2
4	UTP	Y	603	3	2/2/7/7	12/22/38/38	0/2/2/2
4	UTP	E	603	3	2/2/7/7	8/22/38/38	0/2/2/2
4	UTP	l	601	3	2/2/7/7	12/22/38/38	0/2/2/2
2	ATP	F	602	3	-	0/22/38/38	0/3/3/3
2	ATP	S	602	3	-	0/22/38/38	0/3/3/3
2	ATP	a	602	3	-	0/22/38/38	0/3/3/3
2	ATP	l	602	3	-	0/22/38/38	0/3/3/3
4	UTP	N	601	3	2/2/7/7	12/22/38/38	0/2/2/2
2	ATP	g	601	3	-	0/22/38/38	0/3/3/3
4	UTP	Q	605	3	2/2/7/7	8/22/38/38	0/2/2/2
4	UTP	g	605	3	2/2/7/7	13/22/38/38	0/2/2/2
2	ATP	E	601	3	-	0/22/38/38	0/3/3/3
4	UTP	I	605	3	2/2/7/7	13/22/38/38	0/2/2/2
4	UTP	A	605	3	2/2/7/7	13/22/38/38	0/2/2/2
4	UTP	b	601	3	2/2/7/7	8/22/38/38	0/2/2/2
2	ATP	M	601	3	-	0/22/38/38	0/3/3/3
2	ATP	R	601	3	-	0/22/38/38	0/3/3/3
2	ATP	b	602	3	-	0/22/38/38	0/3/3/3
2	ATP	I	601	3	-	0/22/38/38	0/3/3/3
2	ATP	A	601	3	-	0/22/38/38	0/3/3/3
4	UTP	T	601	3	2/2/7/7	10/22/38/38	0/2/2/2
4	UTP	F	601	3	2/2/7/7	13/22/38/38	0/2/2/2
4	UTP	a	601	3	2/2/7/7	8/22/38/38	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	J	602	3	-	0/22/38/38	0/3/3/3
4	UTP	h	601	3	2/2/7/7	8/22/38/38	0/2/2/2
2	ATP	Q	601	3	-	0/22/38/38	0/3/3/3
2	ATP	T	602	3	-	0/22/38/38	0/3/3/3
4	UTP	B	601	3	2/2/7/7	8/22/38/38	0/2/2/2
4	UTP	J	601	3	2/2/7/7	8/22/38/38	0/2/2/2
4	UTP	R	605	3	2/2/7/7	8/22/38/38	0/2/2/2
2	ATP	Z	601	3	-	0/22/38/38	0/3/3/3
4	UTP	k	603	3	2/2/7/7	11/22/38/38	0/2/2/2
2	ATP	B	602	3	-	0/22/38/38	0/3/3/3
2	ATP	k	601	3	-	0/22/38/38	0/3/3/3
4	UTP	M	603	3	2/2/7/7	11/22/38/38	0/2/2/2
2	ATP	N	602	3	-	0/22/38/38	0/3/3/3
2	ATP	h	602	3	-	0/22/38/38	0/3/3/3
4	UTP	S	601	3	2/2/7/7	10/22/38/38	0/2/2/2
2	ATP	Y	601	3	-	0/22/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	g	601	ATP	PA-O3A	-2.19	1.57	1.59
2	a	602	ATP	PA-O3A	-2.17	1.57	1.59
2	I	601	ATP	PA-O3A	-2.17	1.57	1.59
2	R	601	ATP	PA-O3A	-2.16	1.57	1.59
2	Q	601	ATP	PA-O3A	-2.16	1.57	1.59
2	J	602	ATP	PA-O3A	-2.16	1.57	1.59
2	B	602	ATP	PA-O3A	-2.15	1.57	1.59
2	A	601	ATP	PA-O3A	-2.15	1.57	1.59
2	F	602	ATP	PA-O3A	-2.15	1.57	1.59
2	h	602	ATP	PA-O3A	-2.15	1.57	1.59
2	b	602	ATP	PA-O3A	-2.13	1.57	1.59
2	l	602	ATP	PA-O3A	-2.12	1.57	1.59
2	S	602	ATP	PA-O3A	-2.10	1.57	1.59
2	T	602	ATP	PA-O3A	-2.09	1.57	1.59
2	k	601	ATP	PB-O3A	-2.08	1.57	1.59
2	N	602	ATP	PA-O3A	-2.08	1.57	1.59
2	Y	601	ATP	PA-O3A	-2.07	1.57	1.59
2	S	602	ATP	PB-O3A	-2.06	1.57	1.59
2	Z	601	ATP	PB-O3A	-2.05	1.57	1.59
2	E	601	ATP	PB-O3A	-2.03	1.57	1.59
2	E	601	ATP	PA-O3A	-2.03	1.57	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	601	ATP	C5-C4	-2.02	1.35	1.39
2	J	602	ATP	C5-C4	-2.01	1.35	1.39
2	M	601	ATP	PB-O3A	-2.01	1.57	1.59
2	g	601	ATP	C5-C4	-2.01	1.35	1.39
2	T	602	ATP	PB-O3A	-2.00	1.57	1.59
2	I	601	ATP	PB-O3A	-2.00	1.57	1.59

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	601	UTP	O4'-C1'-N1	4.05	117.54	108.36
4	h	601	UTP	O4'-C1'-N1	4.04	117.50	108.36
4	S	601	UTP	O4'-C1'-N1	4.03	117.50	108.36
4	T	601	UTP	O4'-C1'-N1	4.03	117.48	108.36
4	l	601	UTP	O4'-C1'-N1	4.03	117.48	108.36
4	B	601	UTP	O4'-C1'-N1	4.02	117.47	108.36
4	I	605	UTP	O4'-C1'-N1	4.02	117.46	108.36
4	F	601	UTP	O4'-C1'-N1	4.01	117.46	108.36
4	N	601	UTP	O4'-C1'-N1	4.01	117.45	108.36
4	Q	605	UTP	O4'-C1'-N1	4.01	117.44	108.36
4	A	605	UTP	O4'-C1'-N1	4.01	117.44	108.36
4	R	605	UTP	O4'-C1'-N1	4.00	117.43	108.36
4	b	601	UTP	O4'-C1'-N1	4.00	117.43	108.36
4	a	601	UTP	O4'-C1'-N1	4.00	117.42	108.36
4	E	603	UTP	O4'-C1'-N1	4.00	117.42	108.36
4	Y	603	UTP	O4'-C1'-N1	4.00	117.42	108.36
4	k	603	UTP	O4'-C1'-N1	3.99	117.41	108.36
4	g	605	UTP	O4'-C1'-N1	3.99	117.40	108.36
4	M	603	UTP	O4'-C1'-N1	3.99	117.39	108.36
4	Z	603	UTP	O4'-C1'-N1	3.97	117.36	108.36
2	a	602	ATP	O2A-PA-O3A	3.17	115.83	107.27
2	b	602	ATP	O2A-PA-O3A	3.16	115.82	107.27
2	R	601	ATP	O2A-PA-O3A	3.16	115.82	107.27
2	E	601	ATP	O2A-PA-O3A	3.15	115.78	107.27
2	Y	601	ATP	O2A-PA-O3A	3.15	115.78	107.27
2	A	601	ATP	O2A-PA-O3A	3.15	115.78	107.27
2	F	602	ATP	O2A-PA-O3A	3.15	115.78	107.27
2	k	601	ATP	O2A-PA-O3A	3.14	115.77	107.27
2	I	601	ATP	O2A-PA-O3A	3.14	115.77	107.27
2	M	601	ATP	O2A-PA-O3A	3.14	115.77	107.27
2	h	602	ATP	O2A-PA-O3A	3.14	115.76	107.27
2	Q	601	ATP	O2A-PA-O3A	3.14	115.75	107.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	602	ATP	O2A-PA-O3A	3.14	115.75	107.27
2	B	602	ATP	O2A-PA-O3A	3.14	115.75	107.27
2	Z	601	ATP	O2A-PA-O3A	3.14	115.75	107.27
2	g	601	ATP	O2A-PA-O3A	3.14	115.75	107.27
2	J	602	ATP	O2A-PA-O3A	3.13	115.74	107.27
4	a	601	UTP	C2'-C1'-N1	3.13	121.96	113.25
2	T	602	ATP	O2A-PA-O3A	3.13	115.73	107.27
2	l	602	ATP	O2A-PA-O3A	3.13	115.73	107.27
4	R	605	UTP	C2'-C1'-N1	3.12	121.95	113.25
2	S	602	ATP	O2A-PA-O3A	3.12	115.72	107.27
4	b	601	UTP	C2'-C1'-N1	3.12	121.94	113.25
4	k	603	UTP	C2'-C1'-N1	3.12	121.93	113.25
4	F	601	UTP	C2'-C1'-N1	3.11	121.92	113.25
4	A	605	UTP	C2'-C1'-N1	3.11	121.91	113.25
4	N	601	UTP	C2'-C1'-N1	3.11	121.91	113.25
4	l	601	UTP	C2'-C1'-N1	3.11	121.90	113.25
4	S	601	UTP	C2'-C1'-N1	3.11	121.90	113.25
4	M	603	UTP	C2'-C1'-N1	3.10	121.89	113.25
4	T	601	UTP	C2'-C1'-N1	3.10	121.89	113.25
4	g	605	UTP	C2'-C1'-N1	3.10	121.89	113.25
4	Q	605	UTP	C2'-C1'-N1	3.10	121.88	113.25
4	I	605	UTP	C2'-C1'-N1	3.10	121.88	113.25
4	B	601	UTP	C2'-C1'-N1	3.10	121.88	113.25
4	E	603	UTP	C2'-C1'-N1	3.10	121.88	113.25
4	Z	603	UTP	C2'-C1'-N1	3.09	121.85	113.25
4	Y	603	UTP	C2'-C1'-N1	3.09	121.84	113.25
4	J	601	UTP	C2'-C1'-N1	3.08	121.83	113.25
4	h	601	UTP	C2'-C1'-N1	3.07	121.80	113.25
2	a	602	ATP	C4-C5-N7	2.77	113.75	110.58
2	I	601	ATP	C4-C5-N7	2.77	113.75	110.58
2	g	601	ATP	C4-C5-N7	2.76	113.74	110.58
2	Q	601	ATP	C4-C5-N7	2.76	113.74	110.58
2	Z	601	ATP	C4-C5-N7	2.76	113.74	110.58
2	h	602	ATP	C4-C5-N7	2.76	113.74	110.58
2	A	601	ATP	C4-C5-N7	2.76	113.73	110.58
2	M	601	ATP	C4-C5-N7	2.75	113.73	110.58
2	B	602	ATP	C4-C5-N7	2.74	113.72	110.58
2	N	602	ATP	C4-C5-N7	2.74	113.72	110.58
2	R	601	ATP	C4-C5-N7	2.74	113.72	110.58
2	T	602	ATP	C4-C5-N7	2.74	113.72	110.58
2	l	602	ATP	C4-C5-N7	2.74	113.71	110.58
2	E	601	ATP	C4-C5-N7	2.73	113.71	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	602	ATP	C4-C5-N7	2.73	113.71	110.58
2	J	602	ATP	C4-C5-N7	2.73	113.70	110.58
2	F	602	ATP	C4-C5-N7	2.72	113.69	110.58
2	k	601	ATP	C4-C5-N7	2.71	113.68	110.58
2	S	602	ATP	C4-C5-N7	2.70	113.67	110.58
2	Y	601	ATP	C4-C5-N7	2.68	113.65	110.58
2	g	601	ATP	C5-C4-N3	-2.67	123.04	126.72
4	R	605	UTP	O4'-C4'-C5'	2.65	117.84	109.33
2	Y	601	ATP	C5-C4-N3	-2.65	123.06	126.72
2	Q	601	ATP	C5-C4-N3	-2.65	123.06	126.72
2	E	601	ATP	C5-C4-N3	-2.65	123.07	126.72
2	b	602	ATP	C5-C4-N3	-2.64	123.08	126.72
2	k	601	ATP	C5-C4-N3	-2.64	123.08	126.72
4	A	605	UTP	O4'-C4'-C5'	2.64	117.78	109.33
4	I	605	UTP	O4'-C4'-C5'	2.64	117.78	109.33
2	F	602	ATP	C5-C4-N3	-2.63	123.09	126.72
2	M	601	ATP	C5-C4-N3	-2.63	123.09	126.72
2	R	601	ATP	C5-C4-N3	-2.63	123.09	126.72
4	a	601	UTP	O4'-C4'-C5'	2.63	117.76	109.33
4	h	601	UTP	O4'-C4'-C5'	2.63	117.75	109.33
4	g	605	UTP	O4'-C4'-C5'	2.63	117.75	109.33
2	N	602	ATP	C5-C4-N3	-2.63	123.10	126.72
4	Q	605	UTP	O4'-C4'-C5'	2.62	117.74	109.33
4	k	603	UTP	O4'-C4'-C5'	2.62	117.74	109.33
2	A	601	ATP	C5-C4-N3	-2.62	123.11	126.72
4	J	601	UTP	O4'-C4'-C5'	2.62	117.73	109.33
4	Y	603	UTP	O4'-C4'-C5'	2.62	117.73	109.33
2	l	602	ATP	C5-C4-N3	-2.62	123.11	126.72
4	T	601	UTP	O4'-C4'-C5'	2.62	117.72	109.33
4	b	601	UTP	O4'-C4'-C5'	2.62	117.72	109.33
2	S	602	ATP	C5-C4-N3	-2.62	123.11	126.72
4	F	601	UTP	O4'-C4'-C5'	2.62	117.72	109.33
4	B	601	UTP	O4'-C4'-C5'	2.62	117.71	109.33
4	Z	603	UTP	O4'-C4'-C5'	2.61	117.71	109.33
4	E	603	UTP	O4'-C4'-C5'	2.61	117.71	109.33
4	M	603	UTP	O4'-C4'-C5'	2.61	117.70	109.33
4	S	601	UTP	O4'-C4'-C5'	2.61	117.70	109.33
4	l	601	UTP	O4'-C4'-C5'	2.61	117.70	109.33
4	N	601	UTP	O4'-C4'-C5'	2.60	117.68	109.33
2	Z	601	ATP	C5-C4-N3	-2.60	123.13	126.72
2	J	602	ATP	C5-C4-N3	-2.60	123.13	126.72
2	a	602	ATP	C5-C4-N3	-2.60	123.14	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	601	ATP	C5-C4-N3	-2.59	123.15	126.72
2	B	602	ATP	C5-C4-N3	-2.59	123.15	126.72
2	h	602	ATP	C5-C4-N3	-2.58	123.17	126.72
2	T	602	ATP	C5-C4-N3	-2.58	123.17	126.72
4	l	601	UTP	C5'-C4'-C3'	2.52	124.30	115.21
4	N	601	UTP	C5'-C4'-C3'	2.52	124.30	115.21
4	B	601	UTP	C5'-C4'-C3'	2.52	124.28	115.21
4	J	601	UTP	C5'-C4'-C3'	2.52	124.28	115.21
4	T	601	UTP	C5'-C4'-C3'	2.52	124.28	115.21
4	b	601	UTP	C5'-C4'-C3'	2.52	124.27	115.21
4	F	601	UTP	C5'-C4'-C3'	2.52	124.27	115.21
4	h	601	UTP	C5'-C4'-C3'	2.52	124.27	115.21
4	M	603	UTP	C5'-C4'-C3'	2.52	124.27	115.21
4	Q	605	UTP	C5'-C4'-C3'	2.51	124.25	115.21
4	a	601	UTP	C5'-C4'-C3'	2.51	124.25	115.21
4	S	601	UTP	C5'-C4'-C3'	2.51	124.25	115.21
4	E	603	UTP	C5'-C4'-C3'	2.51	124.23	115.21
4	g	605	UTP	C5'-C4'-C3'	2.50	124.23	115.21
4	A	605	UTP	C5'-C4'-C3'	2.50	124.22	115.21
4	k	603	UTP	C5'-C4'-C3'	2.50	124.22	115.21
4	Z	603	UTP	C5'-C4'-C3'	2.50	124.22	115.21
4	I	605	UTP	C5'-C4'-C3'	2.50	124.22	115.21
4	Y	603	UTP	C5'-C4'-C3'	2.50	124.21	115.21
4	R	605	UTP	C5'-C4'-C3'	2.49	124.19	115.21
4	Z	603	UTP	O4'-C4'-C3'	2.28	109.68	105.15
4	Y	603	UTP	O4'-C4'-C3'	2.28	109.68	105.15
4	M	603	UTP	O4'-C4'-C3'	2.28	109.67	105.15
4	S	601	UTP	O4'-C4'-C3'	2.28	109.67	105.15
4	E	603	UTP	O4'-C4'-C3'	2.27	109.67	105.15
4	b	601	UTP	O4'-C4'-C3'	2.27	109.66	105.15
4	B	601	UTP	O4'-C4'-C3'	2.27	109.65	105.15
4	g	605	UTP	O4'-C4'-C3'	2.26	109.65	105.15
4	k	603	UTP	O4'-C4'-C3'	2.26	109.65	105.15
4	T	601	UTP	O4'-C4'-C3'	2.26	109.64	105.15
4	J	601	UTP	O4'-C4'-C3'	2.26	109.64	105.15
4	F	601	UTP	O4'-C4'-C3'	2.26	109.64	105.15
4	N	601	UTP	O4'-C4'-C3'	2.26	109.64	105.15
4	h	601	UTP	O4'-C4'-C3'	2.26	109.64	105.15
4	R	605	UTP	O4'-C4'-C3'	2.26	109.64	105.15
4	A	605	UTP	O4'-C4'-C3'	2.26	109.63	105.15
4	I	605	UTP	O4'-C4'-C3'	2.25	109.63	105.15
4	Q	605	UTP	O4'-C4'-C3'	2.25	109.62	105.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	601	UTP	O4'-C4'-C3'	2.25	109.62	105.15
4	l	601	UTP	O4'-C4'-C3'	2.24	109.61	105.15
4	g	605	UTP	O4'-C1'-C2'	2.21	111.34	106.62
4	Z	603	UTP	O4'-C1'-C2'	2.20	111.33	106.62
4	Q	605	UTP	O4'-C1'-C2'	2.19	111.31	106.62
4	I	605	UTP	O4'-C1'-C2'	2.19	111.31	106.62
4	b	601	UTP	O4'-C1'-C2'	2.19	111.31	106.62
4	M	603	UTP	O4'-C1'-C2'	2.19	111.30	106.62
4	Y	603	UTP	O4'-C1'-C2'	2.18	111.29	106.62
4	A	605	UTP	O4'-C1'-C2'	2.17	111.27	106.62
4	h	601	UTP	O4'-C1'-C2'	2.17	111.27	106.62
4	E	603	UTP	O4'-C1'-C2'	2.17	111.26	106.62
4	l	601	UTP	O4'-C1'-C2'	2.17	111.26	106.62
4	F	601	UTP	O4'-C1'-C2'	2.17	111.26	106.62
4	B	601	UTP	O4'-C1'-C2'	2.17	111.25	106.62
4	k	603	UTP	O4'-C1'-C2'	2.17	111.25	106.62
4	N	601	UTP	O4'-C1'-C2'	2.16	111.25	106.62
4	R	605	UTP	O4'-C1'-C2'	2.16	111.24	106.62
4	J	601	UTP	O4'-C1'-C2'	2.16	111.23	106.62
4	S	601	UTP	O4'-C1'-C2'	2.15	111.22	106.62
4	a	601	UTP	O4'-C1'-C2'	2.15	111.21	106.62
4	T	601	UTP	O4'-C1'-C2'	2.14	111.20	106.62

All (40) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	605	UTP	C4'
4	A	605	UTP	C1'
4	E	603	UTP	C4'
4	E	603	UTP	C1'
4	B	601	UTP	C4'
4	B	601	UTP	C1'
4	F	601	UTP	C4'
4	F	601	UTP	C1'
4	Q	605	UTP	C4'
4	Q	605	UTP	C1'
4	Y	603	UTP	C4'
4	Y	603	UTP	C1'
4	S	601	UTP	C4'
4	S	601	UTP	C1'
4	a	601	UTP	C4'
4	a	601	UTP	C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
4	I	605	UTP	C4'
4	I	605	UTP	C1'
4	M	603	UTP	C4'
4	M	603	UTP	C1'
4	J	601	UTP	C4'
4	J	601	UTP	C1'
4	N	601	UTP	C4'
4	N	601	UTP	C1'
4	R	605	UTP	C4'
4	R	605	UTP	C1'
4	Z	603	UTP	C4'
4	Z	603	UTP	C1'
4	T	601	UTP	C4'
4	T	601	UTP	C1'
4	b	601	UTP	C4'
4	b	601	UTP	C1'
4	g	605	UTP	C4'
4	g	605	UTP	C1'
4	k	603	UTP	C4'
4	k	603	UTP	C1'
4	h	601	UTP	C4'
4	h	601	UTP	C1'
4	l	601	UTP	C4'
4	l	601	UTP	C1'

All (206) 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	A	605	UTP	O4'-C1'-N1-C6
4	A	605	UTP	O4'-C1'-N1-C2
4	E	603	UTP	C5'-O5'-PA-O2A
4	E	603	UTP	O4'-C1'-N1-C6
4	E	603	UTP	O4'-C1'-N1-C2
4	B	601	UTP	C5'-O5'-PA-O2A
4	B	601	UTP	O4'-C1'-N1-C6
4	B	601	UTP	O4'-C1'-N1-C2
4	F	601	UTP	C5'-O5'-PA-O1A
4	F	601	UTP	PB-O3B-PG-O1G
4	F	601	UTP	O4'-C1'-N1-C6
4	F	601	UTP	O4'-C1'-N1-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	Q	605	UTP	C5'-O5'-PA-O2A
4	Q	605	UTP	O4'-C1'-N1-C6
4	Q	605	UTP	O4'-C1'-N1-C2
4	Y	603	UTP	C5'-O5'-PA-O1A
4	Y	603	UTP	PB-O3B-PG-O3G
4	Y	603	UTP	O4'-C1'-N1-C6
4	Y	603	UTP	O4'-C1'-N1-C2
4	S	601	UTP	C5'-O5'-PA-O1A
4	S	601	UTP	PB-O3B-PG-O1G
4	S	601	UTP	O4'-C1'-N1-C6
4	S	601	UTP	O4'-C1'-N1-C2
4	a	601	UTP	C5'-O5'-PA-O2A
4	a	601	UTP	O4'-C1'-N1-C6
4	a	601	UTP	O4'-C1'-N1-C2
4	I	605	UTP	C5'-O5'-PA-O1A
4	I	605	UTP	PB-O3B-PG-O1G
4	I	605	UTP	O4'-C1'-N1-C6
4	I	605	UTP	O4'-C1'-N1-C2
4	M	603	UTP	C5'-O5'-PA-O2A
4	M	603	UTP	O4'-C1'-N1-C6
4	M	603	UTP	O4'-C1'-N1-C2
4	J	601	UTP	C5'-O5'-PA-O2A
4	J	601	UTP	O4'-C1'-N1-C6
4	J	601	UTP	O4'-C1'-N1-C2
4	N	601	UTP	C5'-O5'-PA-O1A
4	N	601	UTP	PB-O3B-PG-O3G
4	N	601	UTP	O4'-C1'-N1-C6
4	N	601	UTP	O4'-C1'-N1-C2
4	R	605	UTP	C5'-O5'-PA-O2A
4	R	605	UTP	O4'-C1'-N1-C6
4	R	605	UTP	O4'-C1'-N1-C2
4	Z	603	UTP	C5'-O5'-PA-O1A
4	Z	603	UTP	PB-O3B-PG-O3G
4	Z	603	UTP	O4'-C1'-N1-C6
4	Z	603	UTP	O4'-C1'-N1-C2
4	T	601	UTP	C5'-O5'-PA-O1A
4	T	601	UTP	PB-O3B-PG-O1G
4	T	601	UTP	O4'-C1'-N1-C6
4	T	601	UTP	O4'-C1'-N1-C2
4	b	601	UTP	C5'-O5'-PA-O2A
4	b	601	UTP	O4'-C1'-N1-C6
4	b	601	UTP	O4'-C1'-N1-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	g	605	UTP	C5'-O5'-PA-O1A
4	g	605	UTP	PB-O3B-PG-O1G
4	g	605	UTP	O4'-C1'-N1-C6
4	g	605	UTP	O4'-C1'-N1-C2
4	k	603	UTP	C5'-O5'-PA-O2A
4	k	603	UTP	O4'-C1'-N1-C6
4	k	603	UTP	O4'-C1'-N1-C2
4	h	601	UTP	C5'-O5'-PA-O2A
4	h	601	UTP	O4'-C1'-N1-C6
4	h	601	UTP	O4'-C1'-N1-C2
4	l	601	UTP	C5'-O5'-PA-O1A
4	l	601	UTP	PB-O3B-PG-O3G
4	l	601	UTP	O4'-C1'-N1-C6
4	l	601	UTP	O4'-C1'-N1-C2
4	A	605	UTP	O4'-C4'-C5'-O5'
4	E	603	UTP	O4'-C4'-C5'-O5'
4	B	601	UTP	O4'-C4'-C5'-O5'
4	F	601	UTP	O4'-C4'-C5'-O5'
4	Q	605	UTP	O4'-C4'-C5'-O5'
4	Y	603	UTP	O4'-C4'-C5'-O5'
4	S	601	UTP	O4'-C4'-C5'-O5'
4	a	601	UTP	O4'-C4'-C5'-O5'
4	I	605	UTP	O4'-C4'-C5'-O5'
4	M	603	UTP	O4'-C4'-C5'-O5'
4	J	601	UTP	O4'-C4'-C5'-O5'
4	N	601	UTP	O4'-C4'-C5'-O5'
4	R	605	UTP	O4'-C4'-C5'-O5'
4	Z	603	UTP	O4'-C4'-C5'-O5'
4	T	601	UTP	O4'-C4'-C5'-O5'
4	b	601	UTP	O4'-C4'-C5'-O5'
4	g	605	UTP	O4'-C4'-C5'-O5'
4	k	603	UTP	O4'-C4'-C5'-O5'
4	h	601	UTP	O4'-C4'-C5'-O5'
4	l	601	UTP	O4'-C4'-C5'-O5'
4	A	605	UTP	PB-O3B-PG-O3G
4	B	601	UTP	PB-O3B-PG-O3G
4	F	601	UTP	PB-O3B-PG-O3G
4	S	601	UTP	PB-O3B-PG-O3G
4	a	601	UTP	PB-O3B-PG-O3G
4	J	601	UTP	PB-O3B-PG-O3G
4	b	601	UTP	PB-O3B-PG-O3G
4	g	605	UTP	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	h	601	UTP	PB-O3B-PG-O3G
4	A	605	UTP	C5'-O5'-PA-O2A
4	A	605	UTP	C5'-O5'-PA-O3A
4	E	603	UTP	C5'-O5'-PA-O1A
4	E	603	UTP	C5'-O5'-PA-O3A
4	B	601	UTP	C5'-O5'-PA-O1A
4	B	601	UTP	C5'-O5'-PA-O3A
4	F	601	UTP	C5'-O5'-PA-O2A
4	F	601	UTP	C5'-O5'-PA-O3A
4	Q	605	UTP	C5'-O5'-PA-O1A
4	Q	605	UTP	C5'-O5'-PA-O3A
4	Y	603	UTP	C5'-O5'-PA-O2A
4	Y	603	UTP	C5'-O5'-PA-O3A
4	S	601	UTP	C5'-O5'-PA-O2A
4	S	601	UTP	C5'-O5'-PA-O3A
4	a	601	UTP	C5'-O5'-PA-O1A
4	a	601	UTP	C5'-O5'-PA-O3A
4	I	605	UTP	C5'-O5'-PA-O2A
4	I	605	UTP	C5'-O5'-PA-O3A
4	M	603	UTP	C5'-O5'-PA-O1A
4	M	603	UTP	C5'-O5'-PA-O3A
4	J	601	UTP	C5'-O5'-PA-O1A
4	J	601	UTP	C5'-O5'-PA-O3A
4	N	601	UTP	C5'-O5'-PA-O2A
4	N	601	UTP	C5'-O5'-PA-O3A
4	R	605	UTP	C5'-O5'-PA-O1A
4	R	605	UTP	C5'-O5'-PA-O3A
4	Z	603	UTP	C5'-O5'-PA-O2A
4	Z	603	UTP	C5'-O5'-PA-O3A
4	T	601	UTP	C5'-O5'-PA-O2A
4	T	601	UTP	C5'-O5'-PA-O3A
4	b	601	UTP	C5'-O5'-PA-O1A
4	b	601	UTP	C5'-O5'-PA-O3A
4	g	605	UTP	C5'-O5'-PA-O2A
4	g	605	UTP	C5'-O5'-PA-O3A
4	k	603	UTP	C5'-O5'-PA-O1A
4	k	603	UTP	C5'-O5'-PA-O3A
4	h	601	UTP	C5'-O5'-PA-O1A
4	h	601	UTP	C5'-O5'-PA-O3A
4	l	601	UTP	C5'-O5'-PA-O2A
4	l	601	UTP	C5'-O5'-PA-O3A
4	Y	603	UTP	PG-O3B-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	k	603	UTP	PG-O3B-PB-O2B
4	A	605	UTP	PG-O3B-PB-O2B
4	F	601	UTP	PG-O3B-PB-O2B
4	I	605	UTP	PG-O3B-PB-O2B
4	M	603	UTP	PG-O3B-PB-O2B
4	N	601	UTP	PG-O3B-PB-O2B
4	Z	603	UTP	PG-O3B-PB-O2B
4	g	605	UTP	PG-O3B-PB-O2B
4	l	601	UTP	PG-O3B-PB-O2B
4	A	605	UTP	C4'-C5'-O5'-PA
4	E	603	UTP	C4'-C5'-O5'-PA
4	B	601	UTP	C4'-C5'-O5'-PA
4	F	601	UTP	C4'-C5'-O5'-PA
4	Q	605	UTP	C4'-C5'-O5'-PA
4	Y	603	UTP	C4'-C5'-O5'-PA
4	S	601	UTP	C4'-C5'-O5'-PA
4	a	601	UTP	C4'-C5'-O5'-PA
4	I	605	UTP	C4'-C5'-O5'-PA
4	M	603	UTP	C4'-C5'-O5'-PA
4	J	601	UTP	C4'-C5'-O5'-PA
4	N	601	UTP	C4'-C5'-O5'-PA
4	R	605	UTP	C4'-C5'-O5'-PA
4	Z	603	UTP	C4'-C5'-O5'-PA
4	T	601	UTP	C4'-C5'-O5'-PA
4	b	601	UTP	C4'-C5'-O5'-PA
4	g	605	UTP	C4'-C5'-O5'-PA
4	k	603	UTP	C4'-C5'-O5'-PA
4	h	601	UTP	C4'-C5'-O5'-PA
4	l	601	UTP	C4'-C5'-O5'-PA
4	A	605	UTP	PB-O3B-PG-O2G
4	F	601	UTP	PB-O3B-PG-O2G
4	Y	603	UTP	PB-O3B-PG-O2G
4	S	601	UTP	PB-O3B-PG-O2G
4	I	605	UTP	PB-O3B-PG-O2G
4	N	601	UTP	PB-O3B-PG-O2G
4	Z	603	UTP	PB-O3B-PG-O2G
4	T	601	UTP	PB-O3B-PG-O2G
4	g	605	UTP	PB-O3B-PG-O2G
4	l	601	UTP	PB-O3B-PG-O2G
4	E	603	UTP	PB-O3B-PG-O3G
4	Q	605	UTP	PB-O3B-PG-O3G
4	I	605	UTP	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	M	603	UTP	PB-O3B-PG-O3G
4	R	605	UTP	PB-O3B-PG-O3G
4	T	601	UTP	PB-O3B-PG-O3G
4	k	603	UTP	PB-O3B-PG-O3G
4	A	605	UTP	PA-O3A-PB-O2B
4	A	605	UTP	PG-O3B-PB-O1B
4	F	601	UTP	PA-O3A-PB-O2B
4	F	601	UTP	PG-O3B-PB-O1B
4	Y	603	UTP	PA-O3A-PB-O2B
4	Y	603	UTP	PG-O3B-PB-O1B
4	I	605	UTP	PA-O3A-PB-O2B
4	I	605	UTP	PG-O3B-PB-O1B
4	M	603	UTP	PA-O3A-PB-O2B
4	M	603	UTP	PG-O3B-PB-O1B
4	N	601	UTP	PA-O3A-PB-O2B
4	N	601	UTP	PG-O3B-PB-O1B
4	Z	603	UTP	PA-O3A-PB-O2B
4	Z	603	UTP	PG-O3B-PB-O1B
4	g	605	UTP	PA-O3A-PB-O2B
4	g	605	UTP	PG-O3B-PB-O1B
4	k	603	UTP	PA-O3A-PB-O2B
4	k	603	UTP	PG-O3B-PB-O1B
4	l	601	UTP	PA-O3A-PB-O2B
4	l	601	UTP	PG-O3B-PB-O1B

There are no ring outliers.

40 monomers are involved in 669 short contacts:

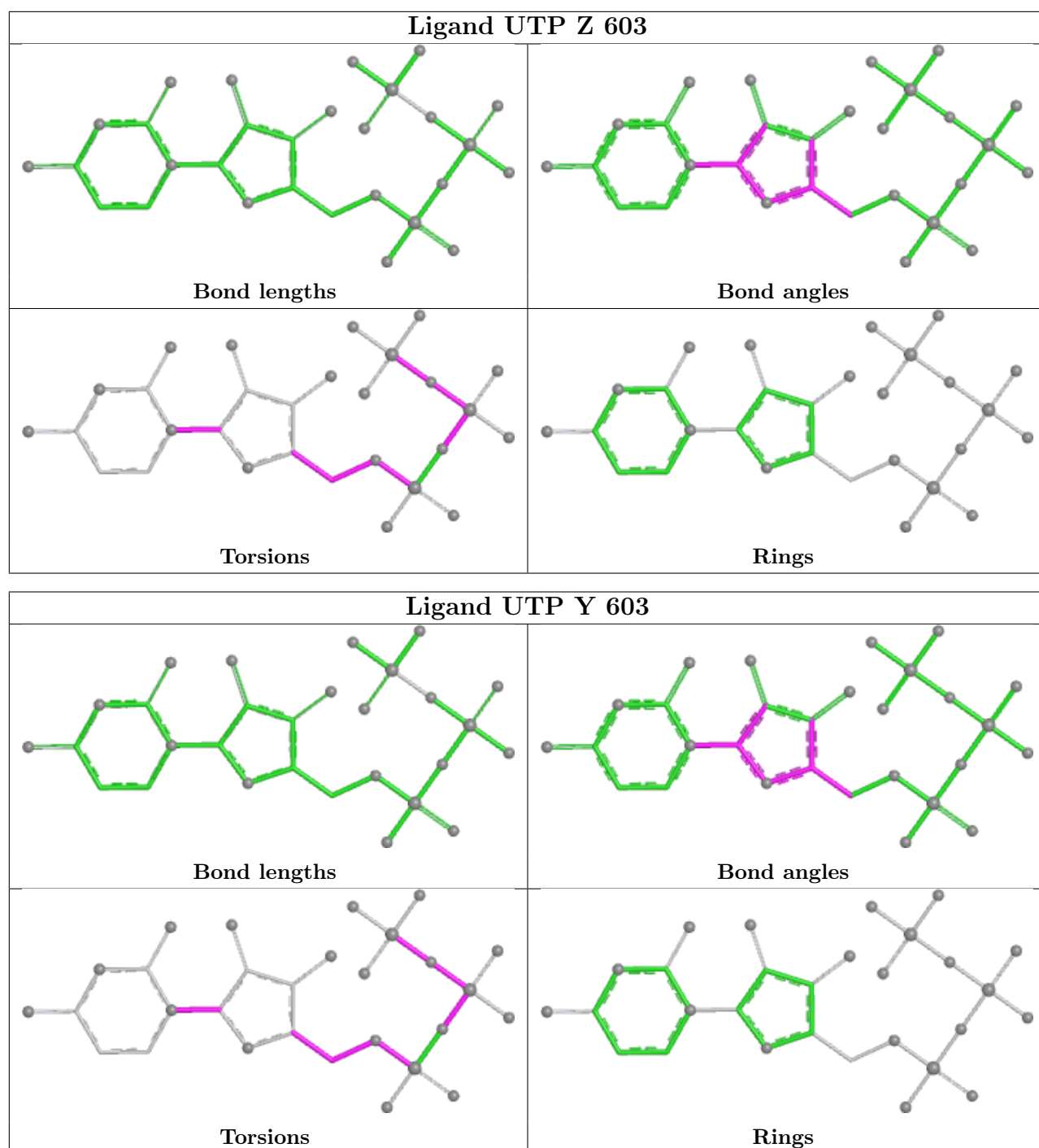
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	603	UTP	23	0
4	Y	603	UTP	23	0
4	E	603	UTP	23	0
4	l	601	UTP	24	0
2	F	602	ATP	12	0
2	S	602	ATP	13	0
2	a	602	ATP	13	0
2	l	602	ATP	12	0
4	N	601	UTP	24	0
2	g	601	ATP	12	0
4	Q	605	UTP	23	0
4	g	605	UTP	24	0
2	E	601	ATP	12	0

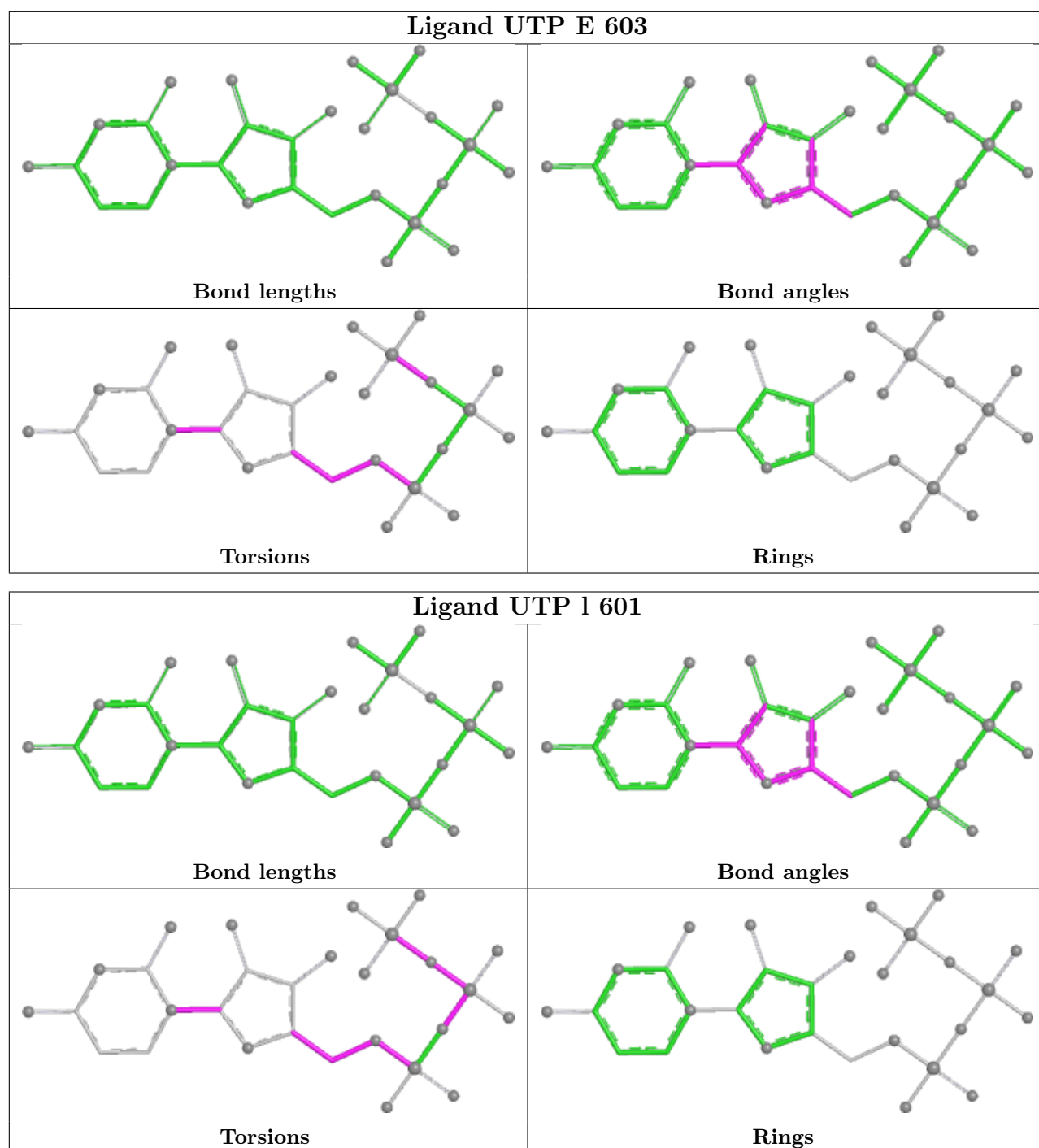
Continued on next page...

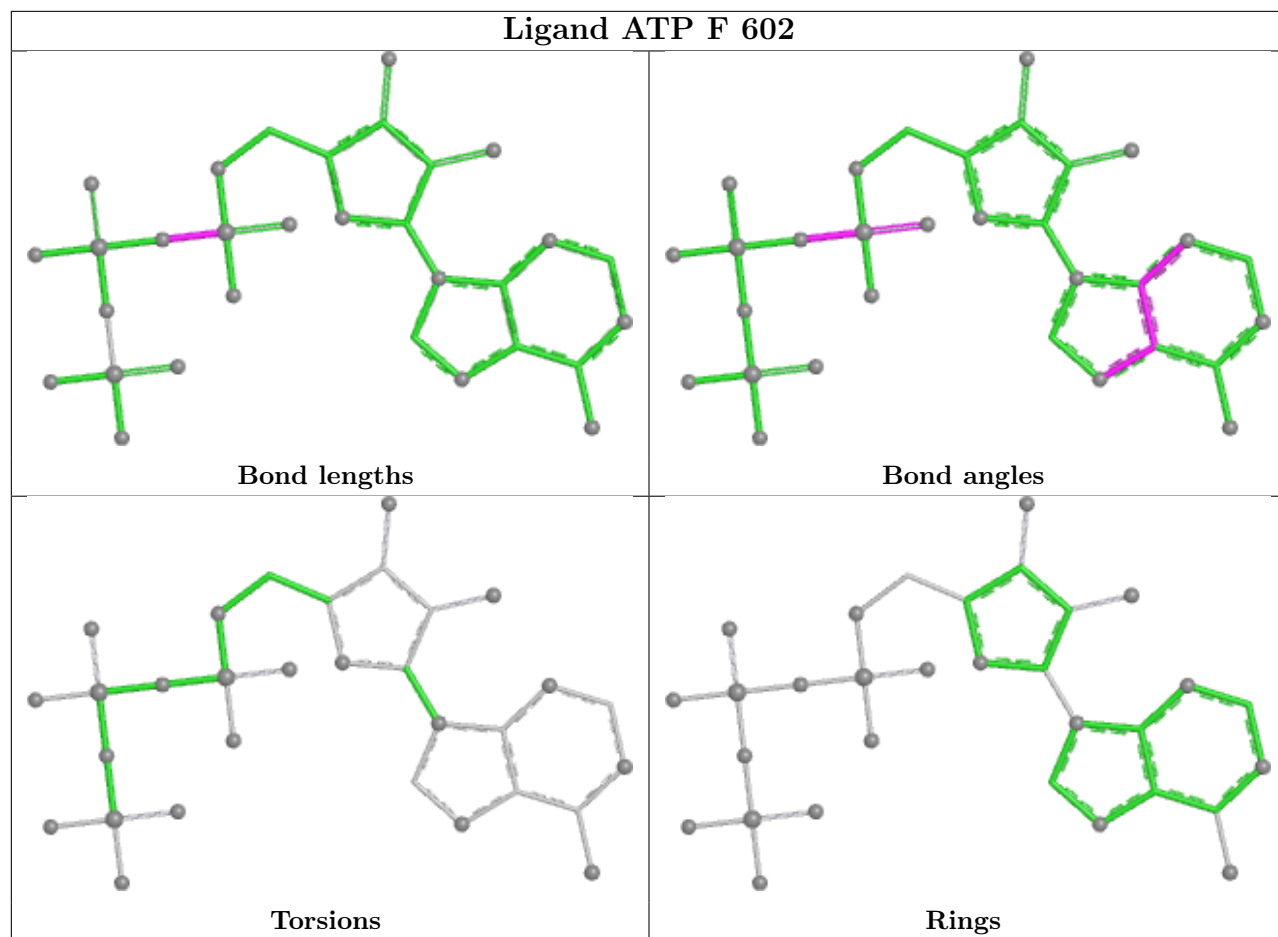
Continued from previous page...

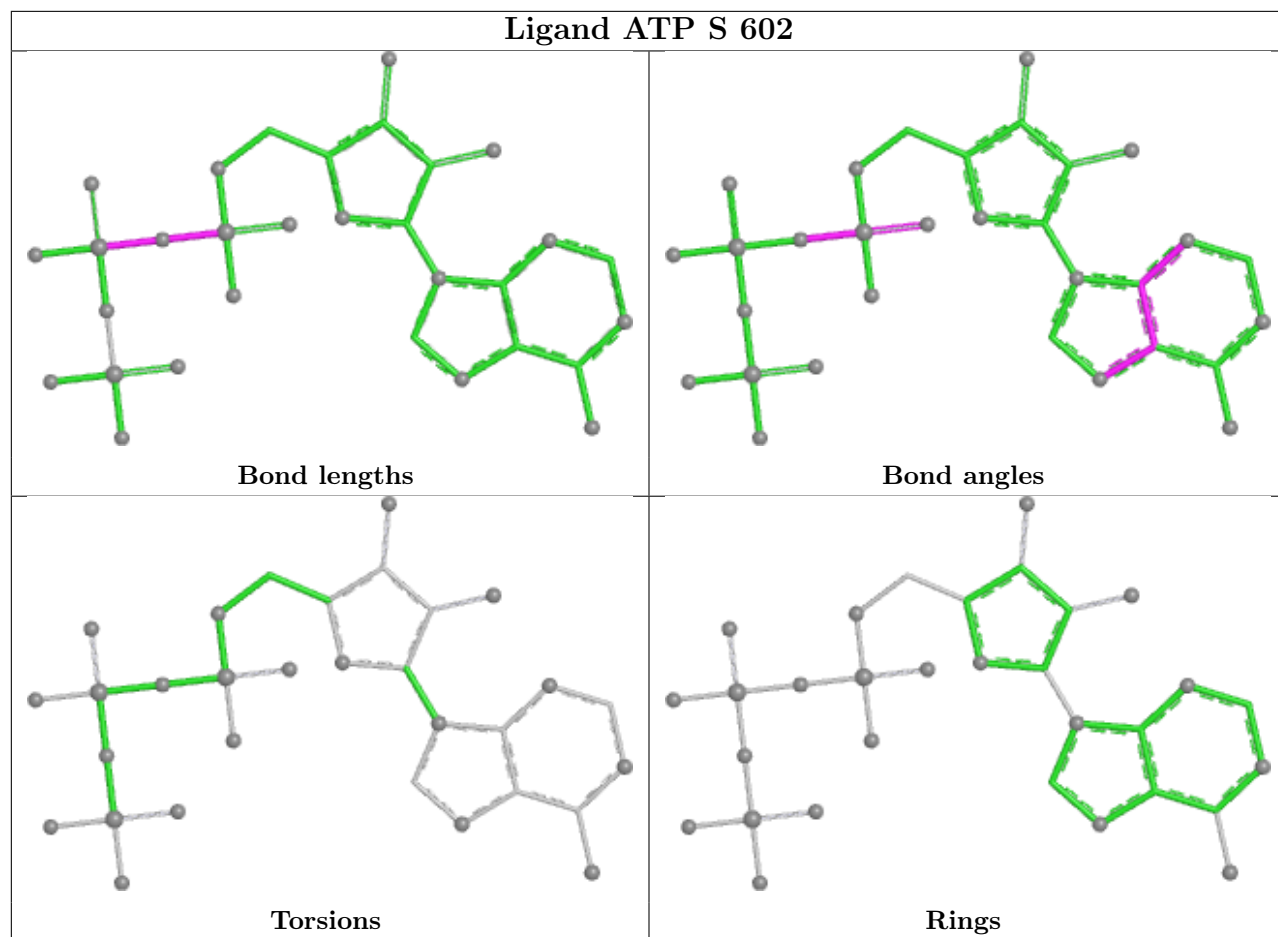
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	605	UTP	23	0
4	A	605	UTP	23	0
2	M	601	ATP	12	0
4	b	601	UTP	24	0
2	R	601	ATP	12	0
2	b	602	ATP	12	0
2	I	601	ATP	13	0
2	A	601	ATP	13	0
4	F	601	UTP	24	0
4	a	601	UTP	24	0
4	T	601	UTP	22	0
2	J	602	ATP	12	0
4	h	601	UTP	24	0
2	Q	601	ATP	12	0
2	T	602	ATP	12	0
4	B	601	UTP	23	0
4	J	601	UTP	23	0
4	R	605	UTP	21	0
2	Z	601	ATP	12	0
4	k	603	UTP	22	0
2	B	602	ATP	12	0
2	k	601	ATP	12	0
4	M	603	UTP	23	0
2	N	602	ATP	12	0
2	h	602	ATP	13	0
4	S	601	UTP	23	0
2	Y	601	ATP	13	0

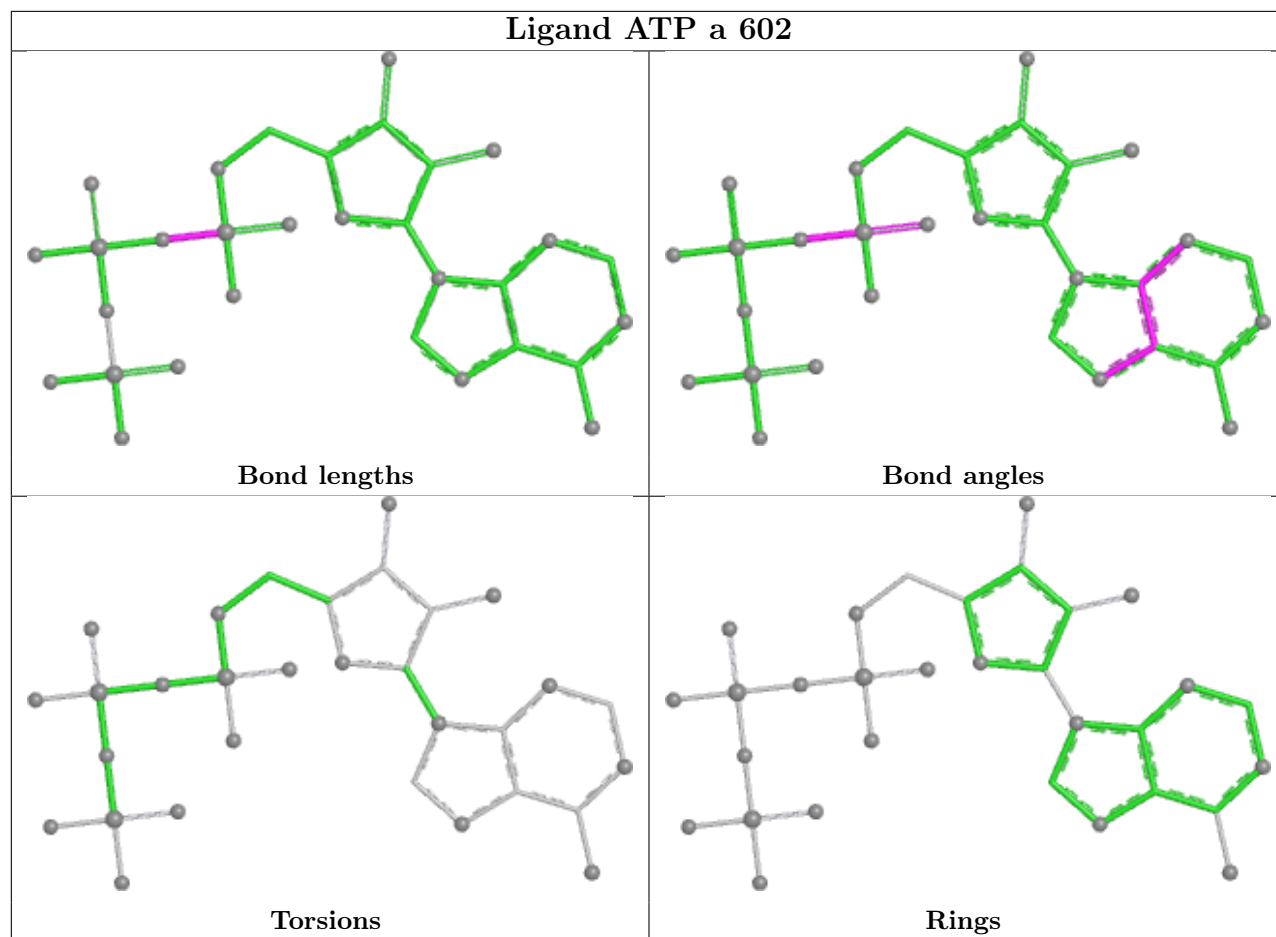
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



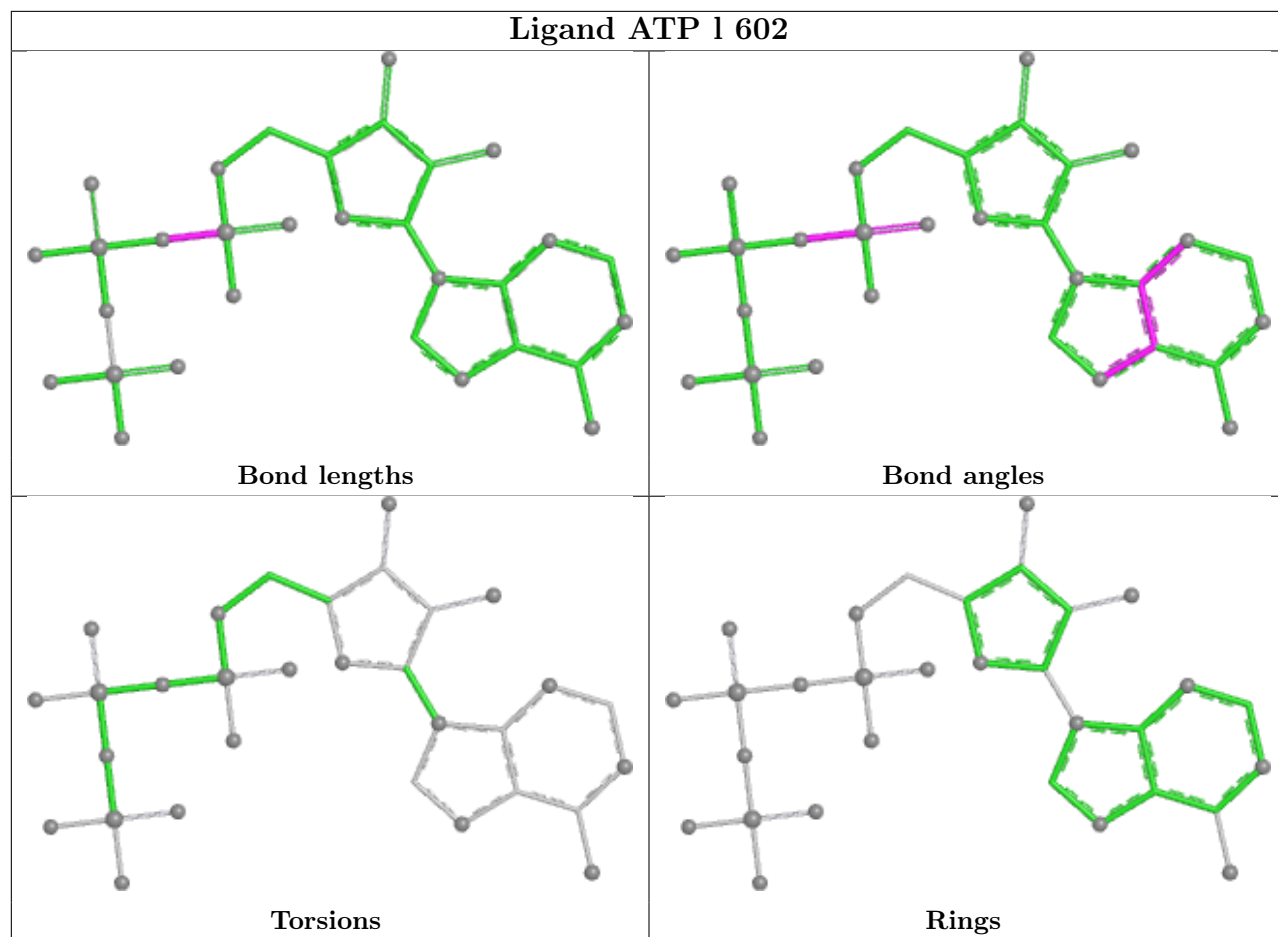




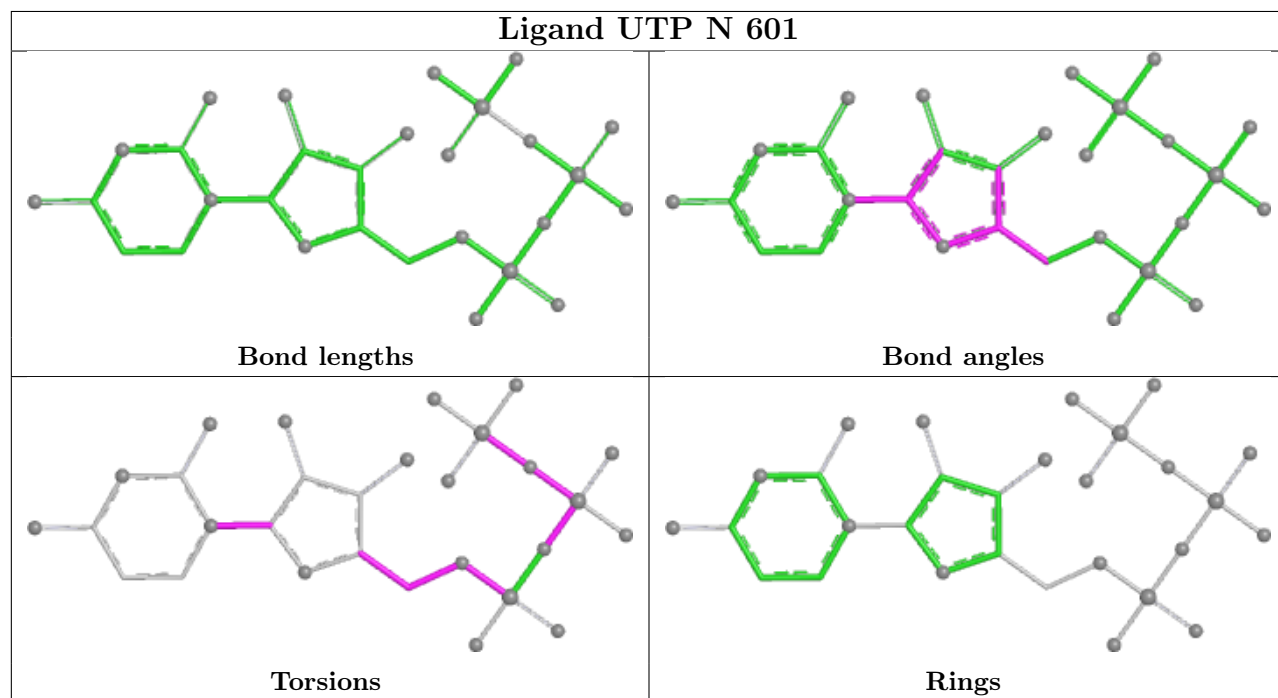


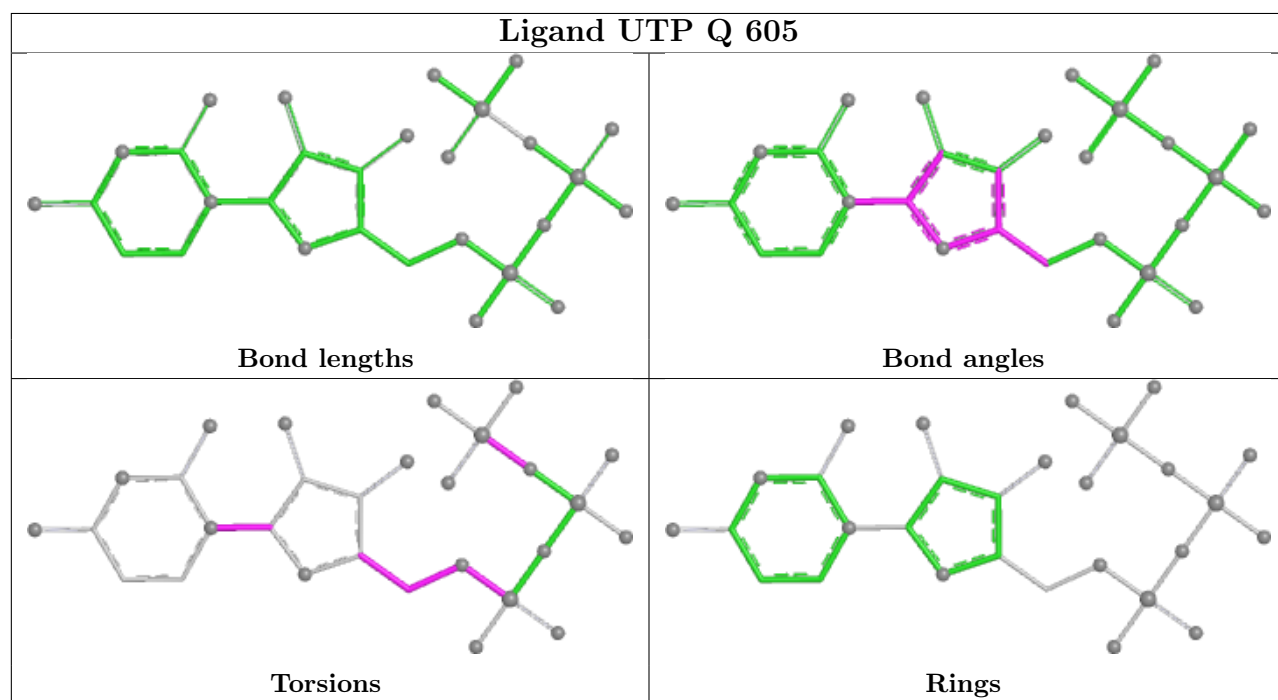
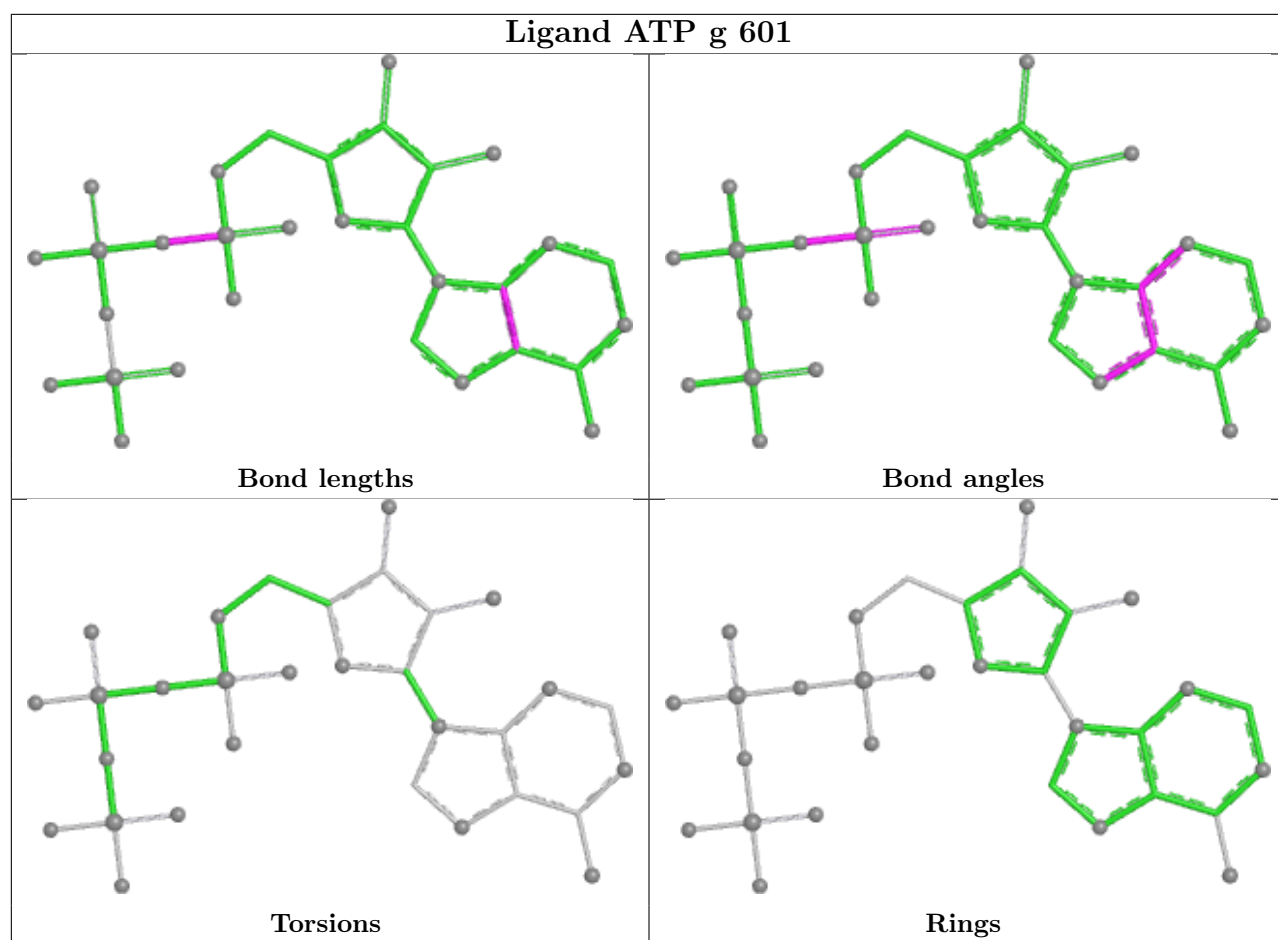


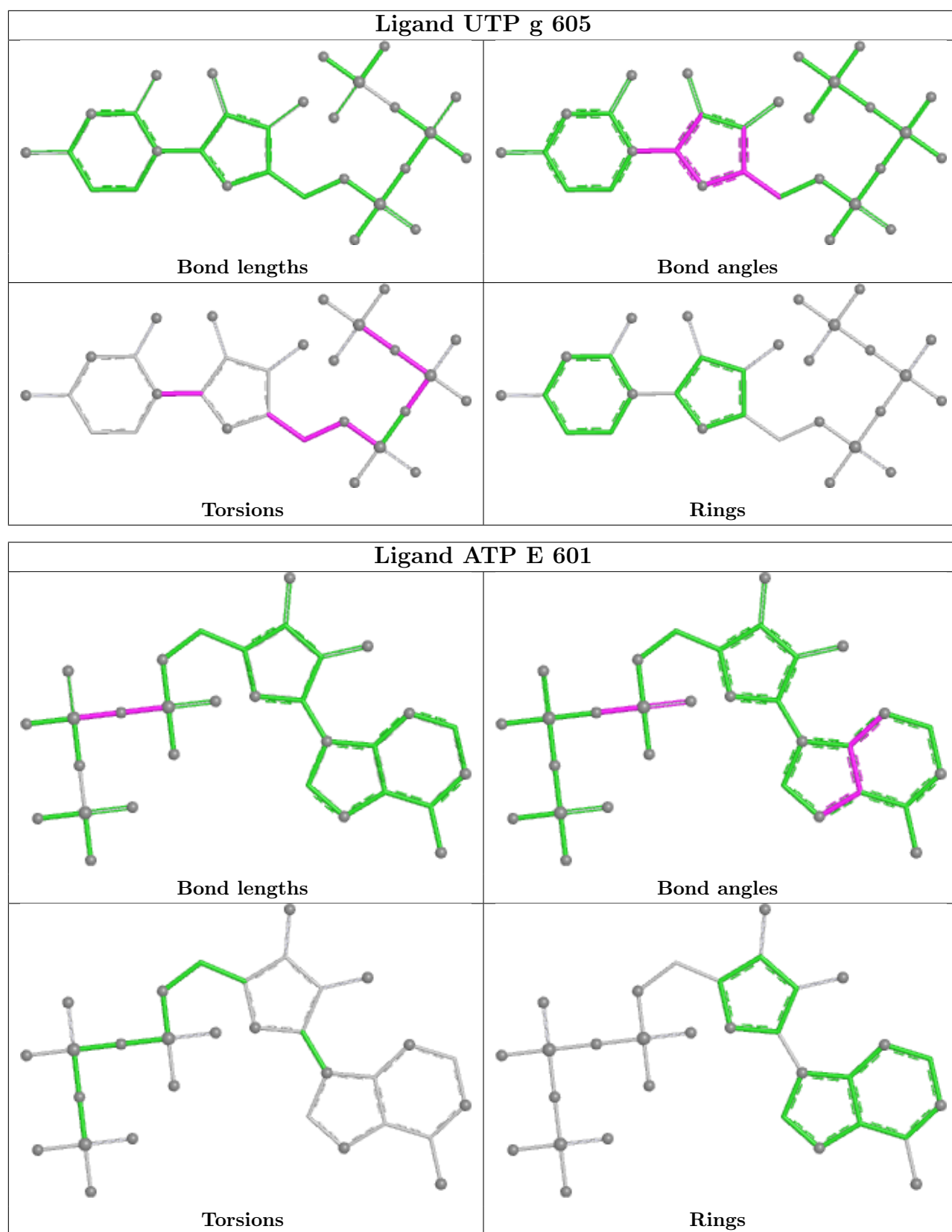
Ligand ATP 1 602

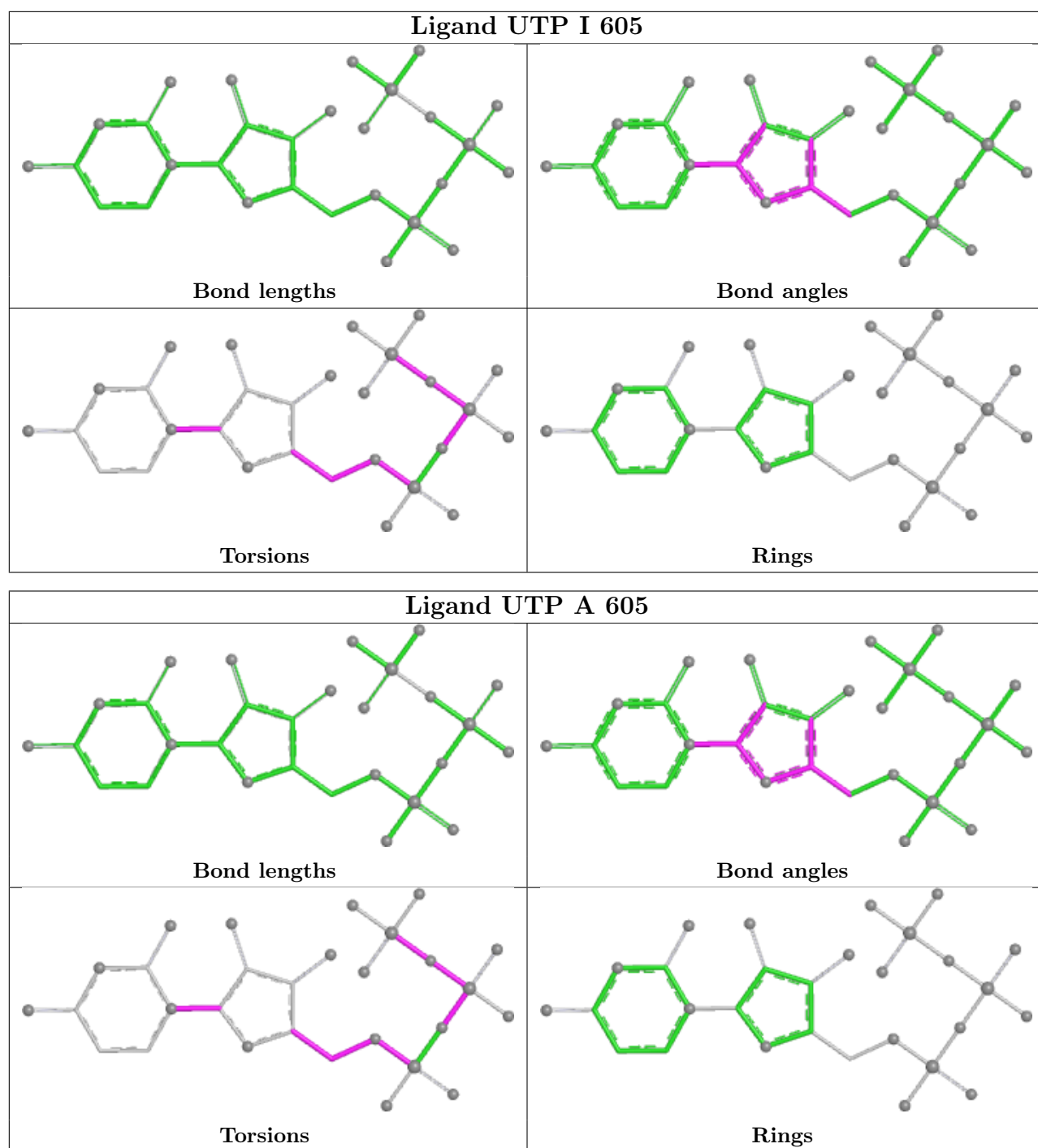


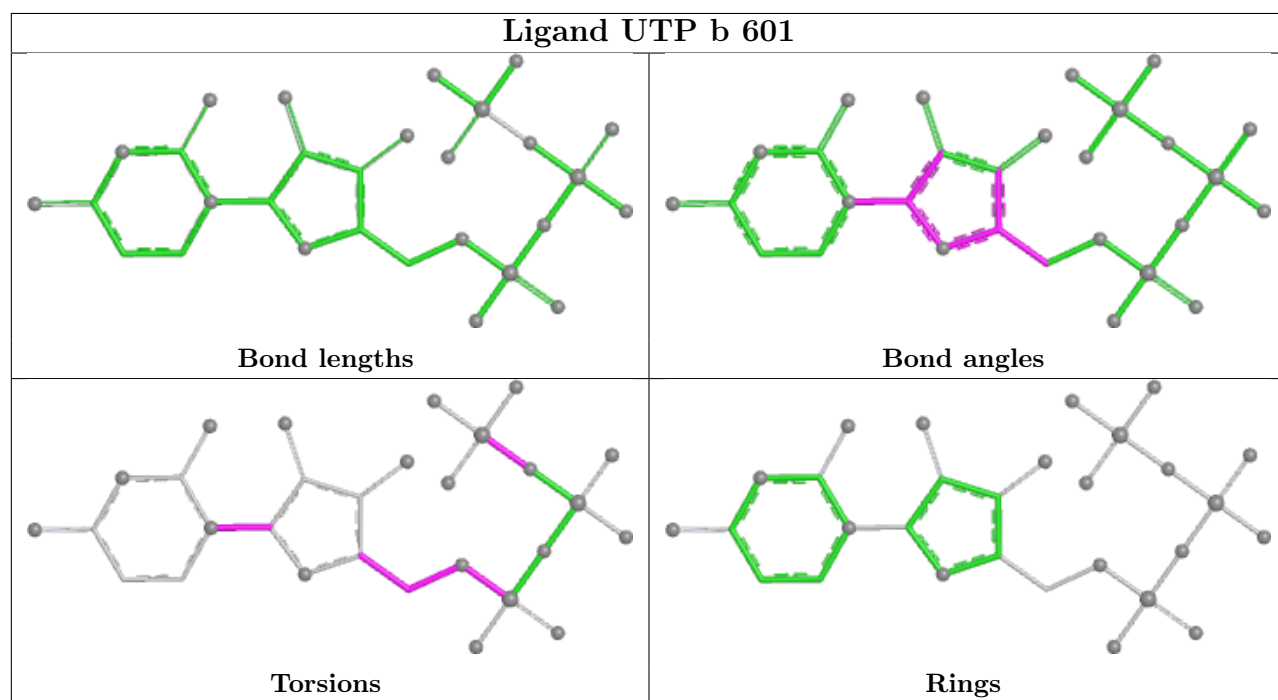
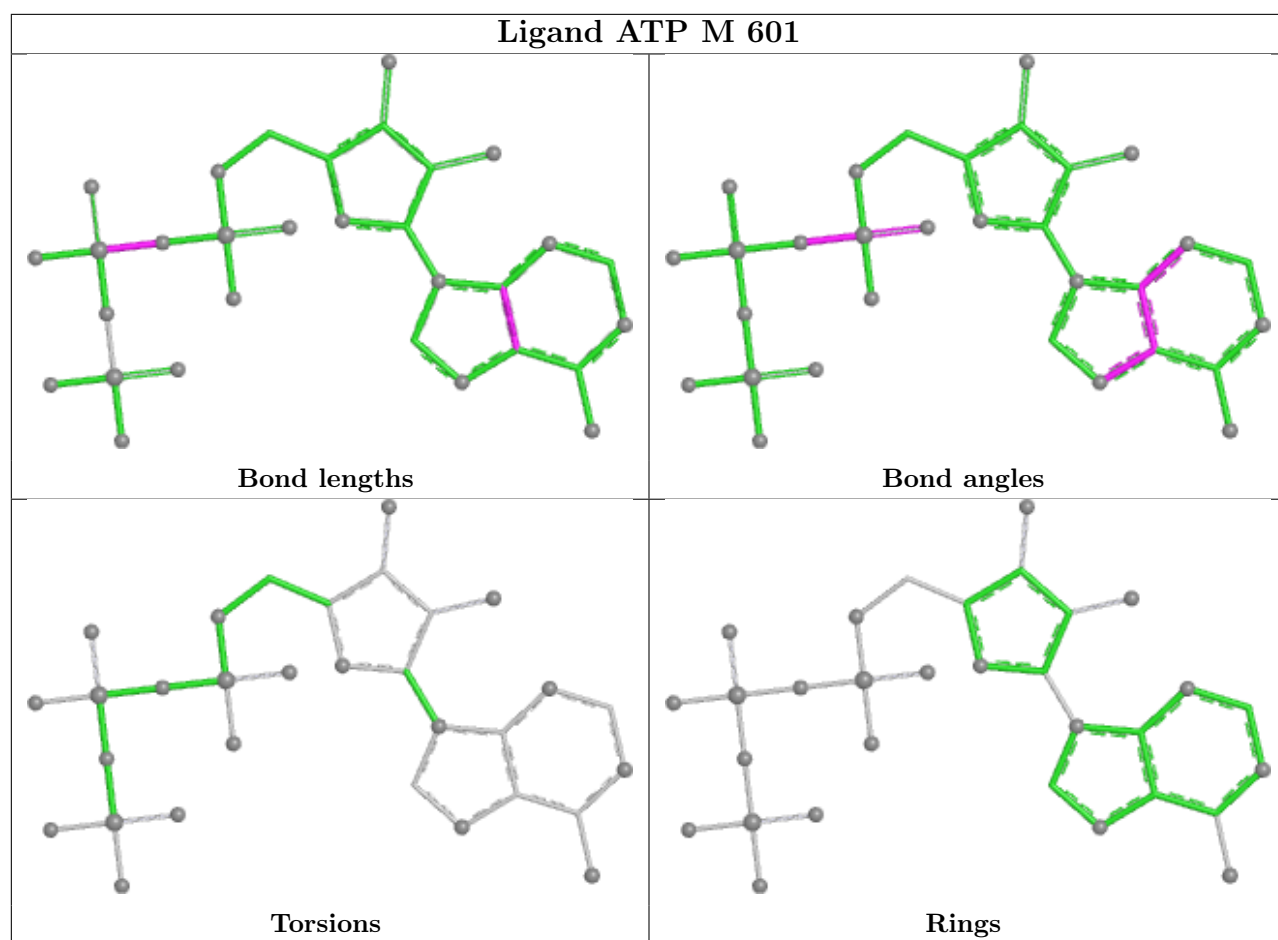
Ligand UTP N 601

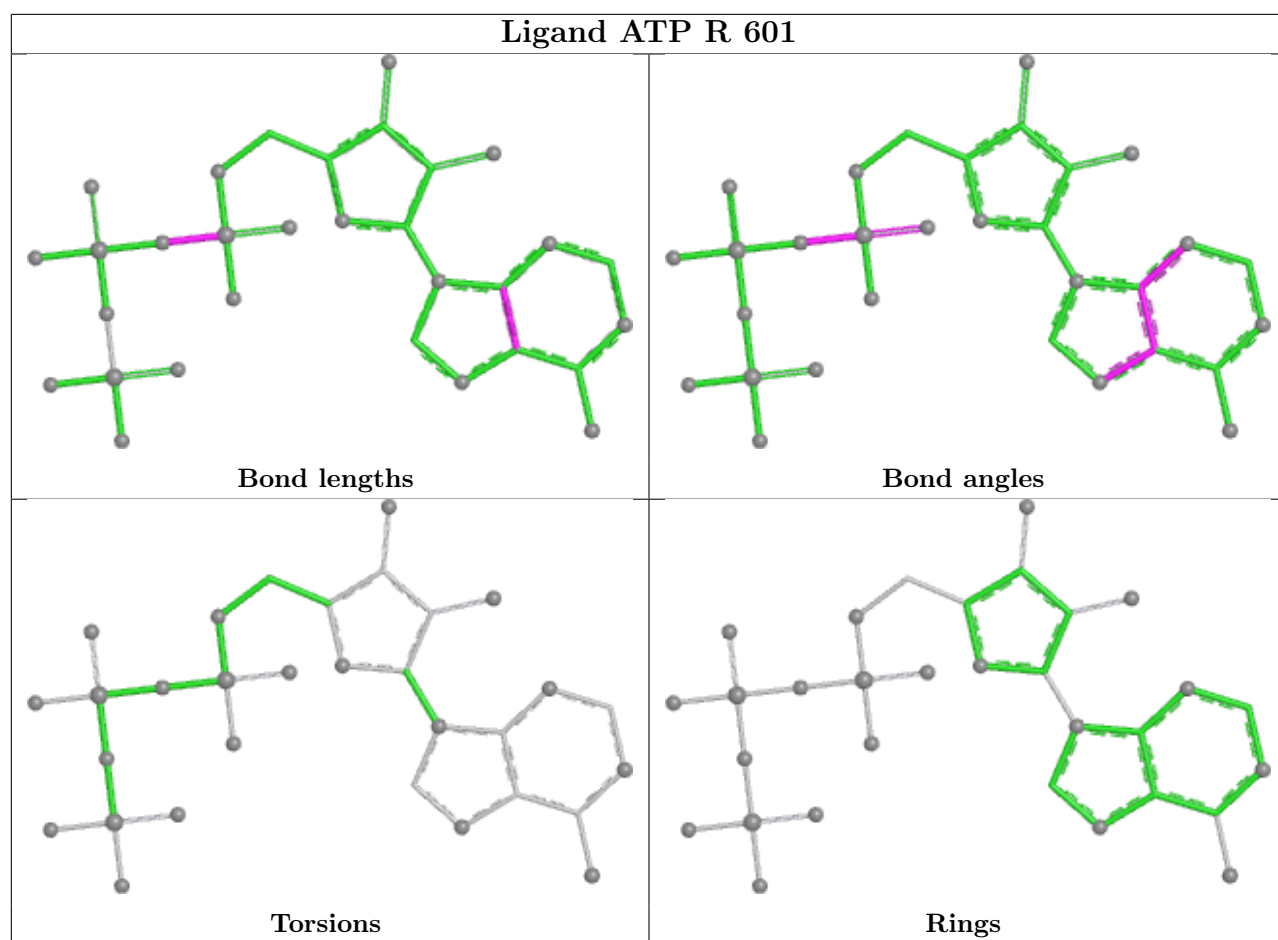


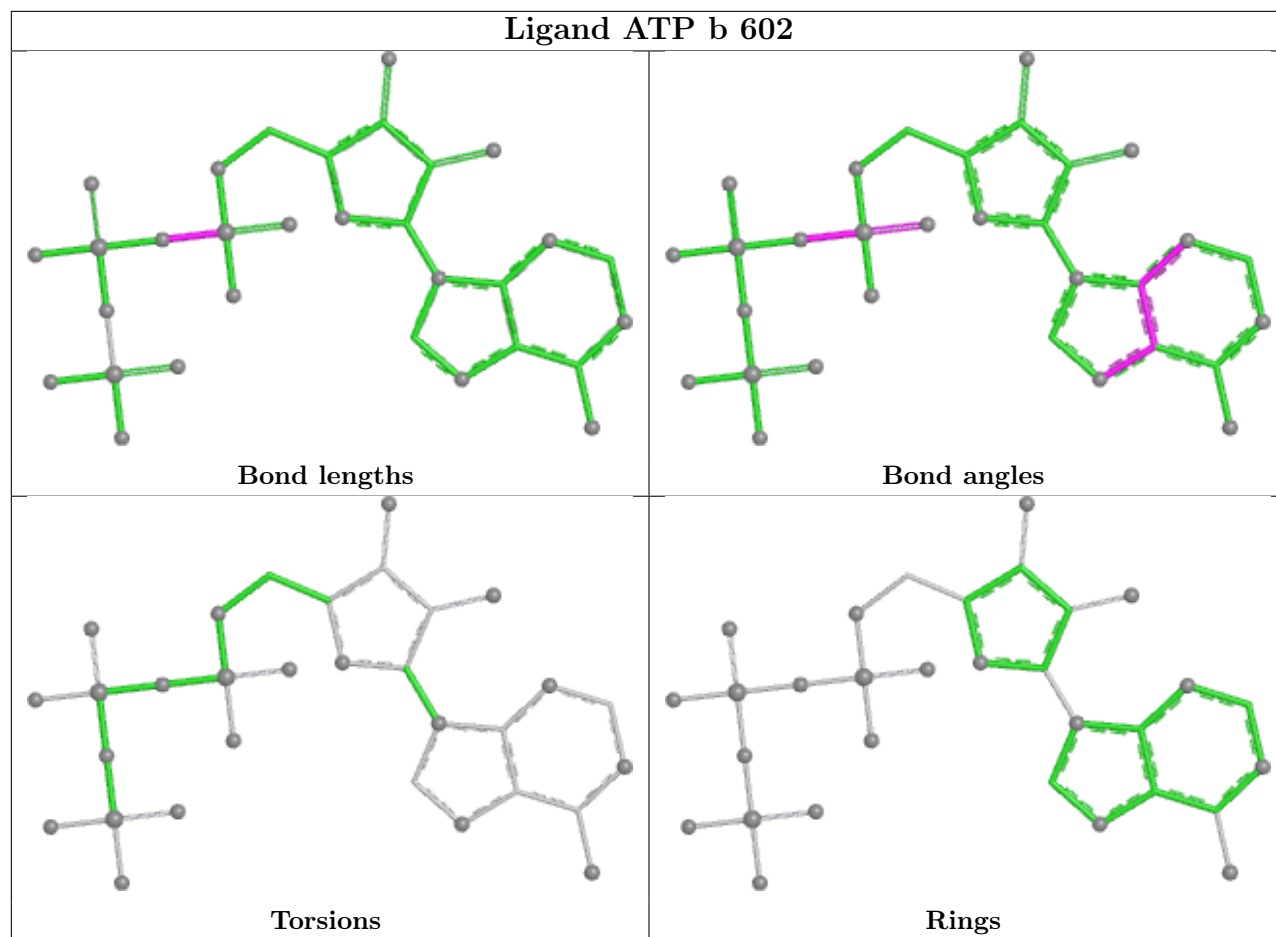


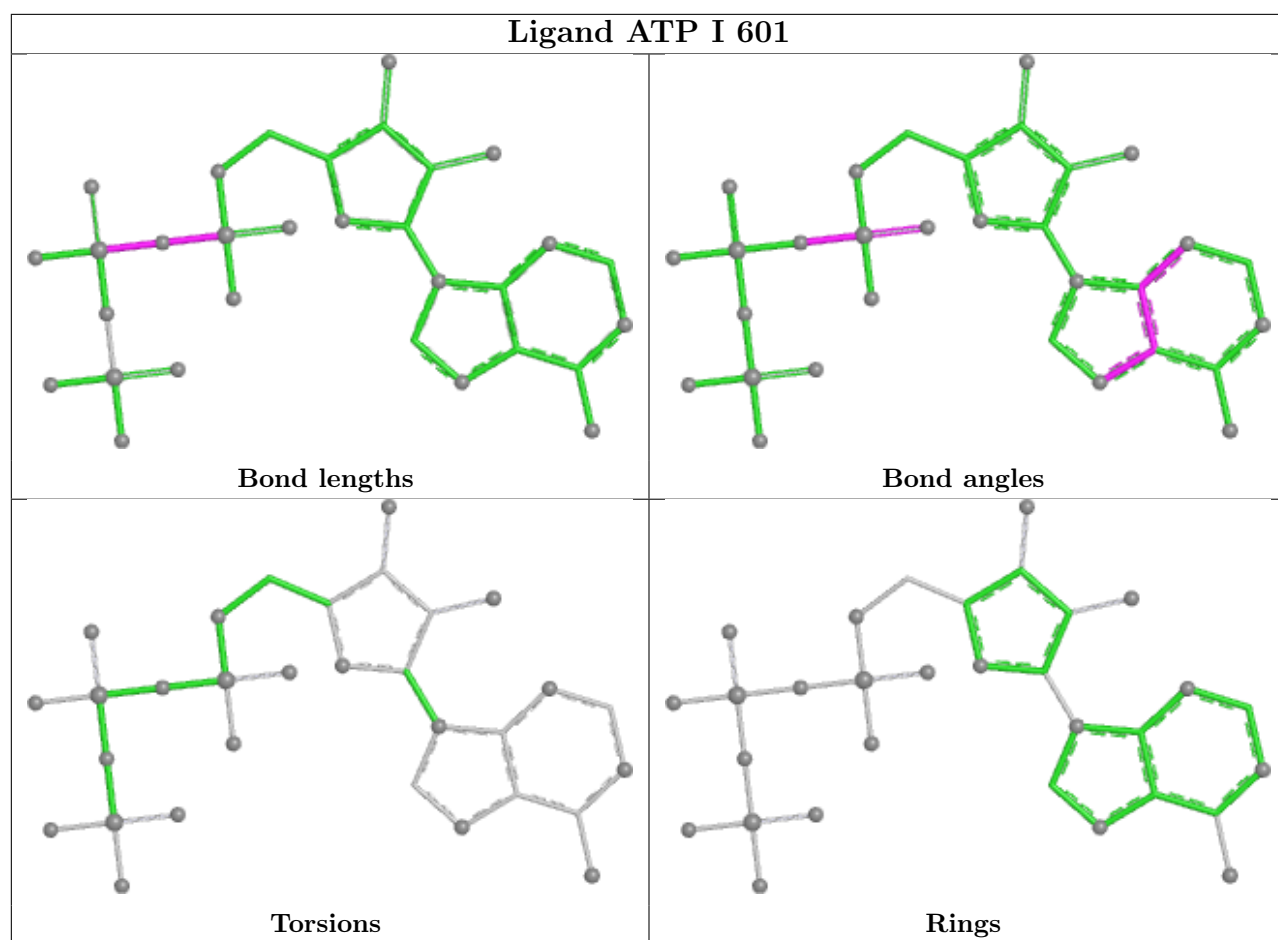


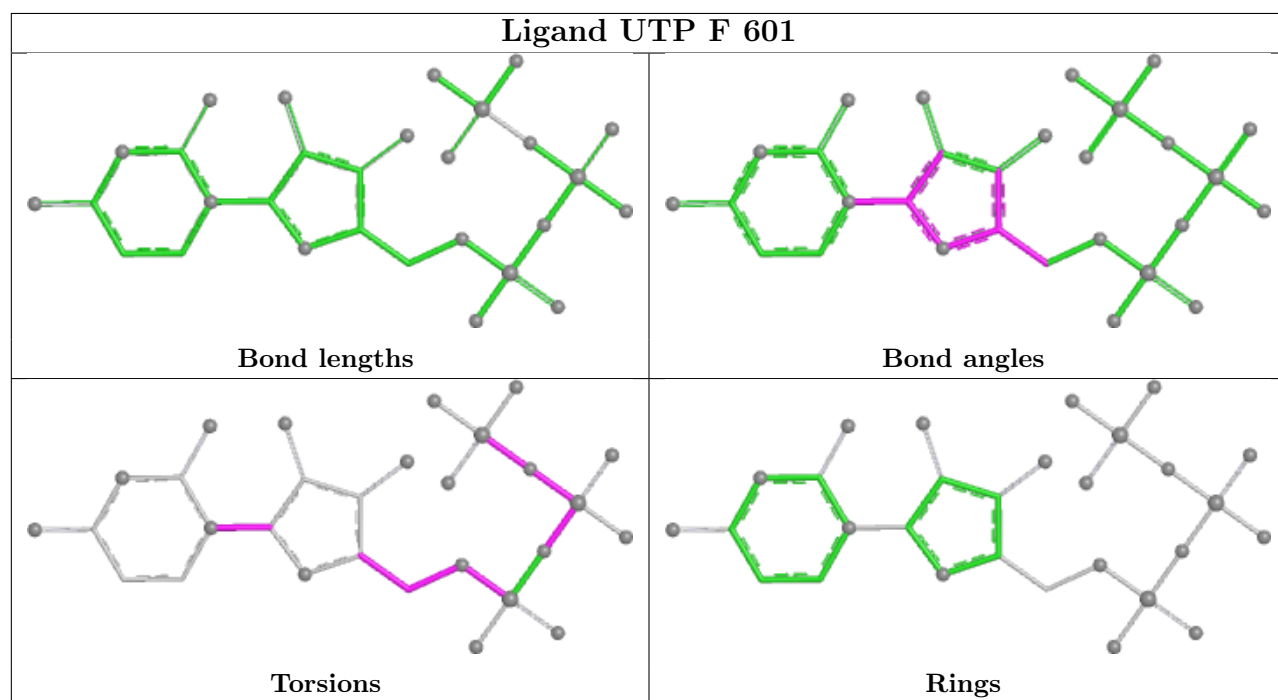
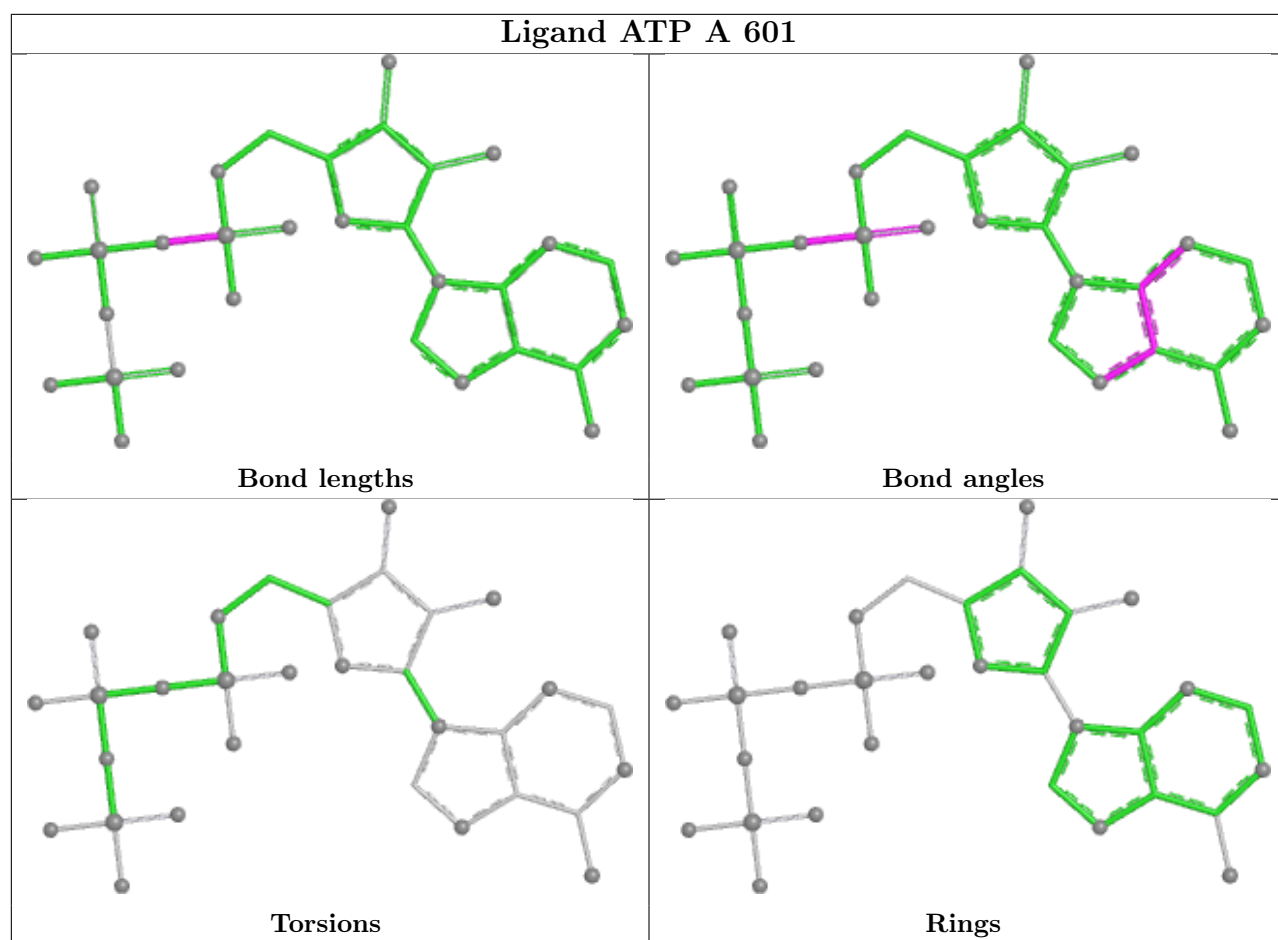


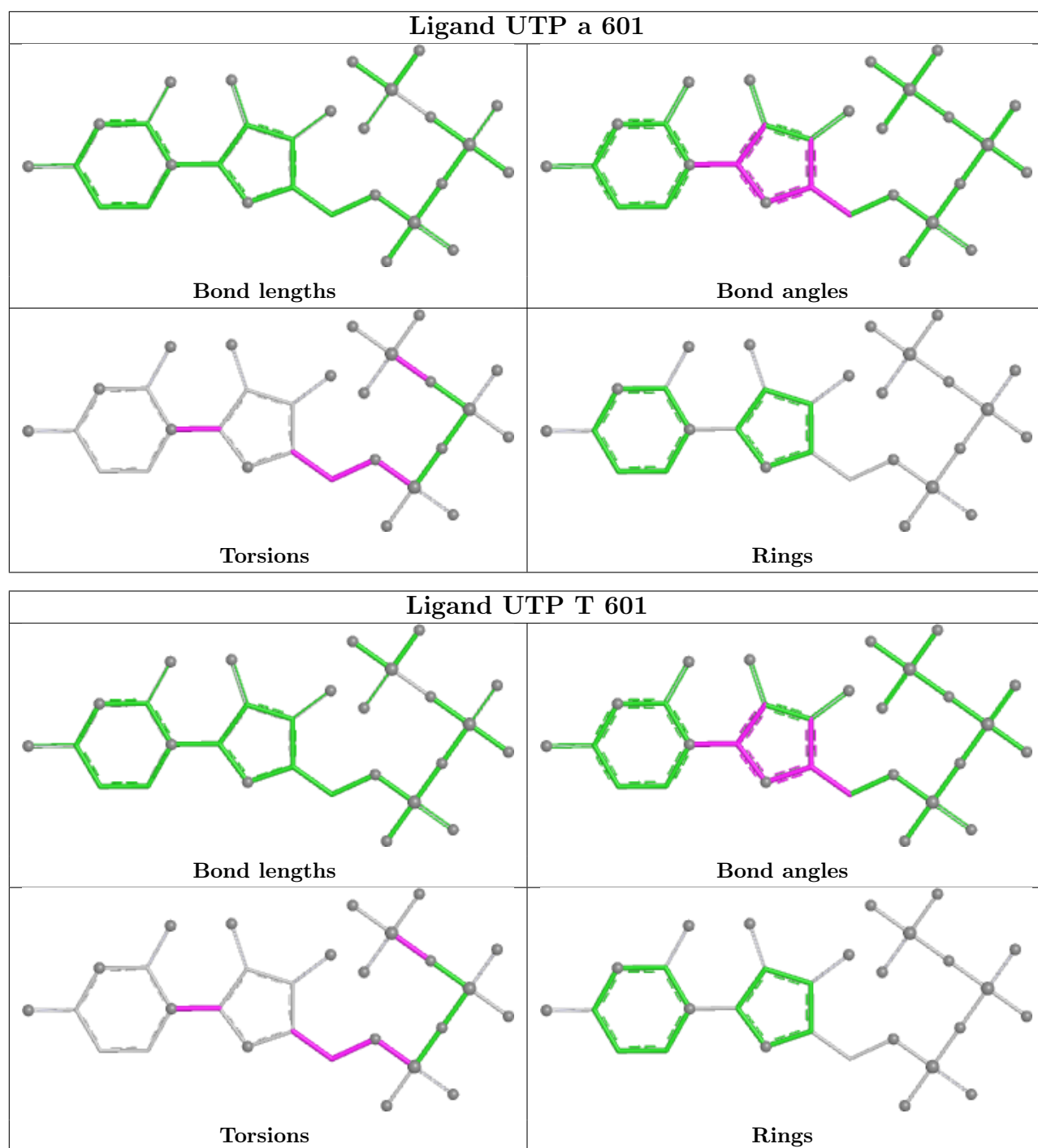




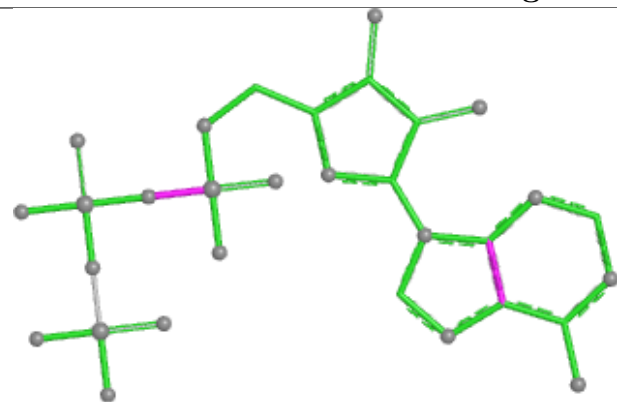




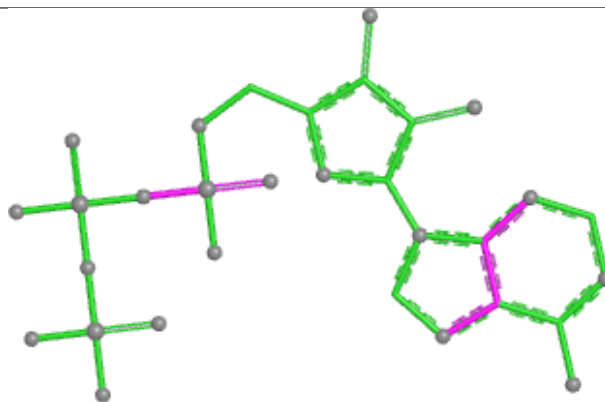




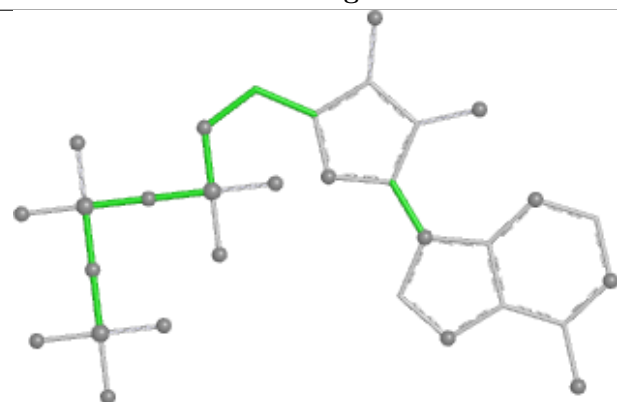
Ligand ATP J 602



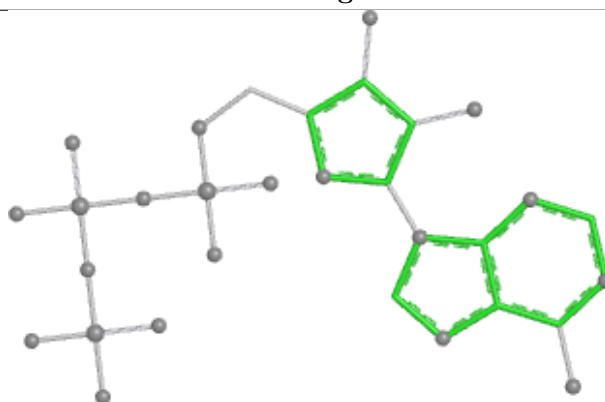
Bond lengths



Bond angles

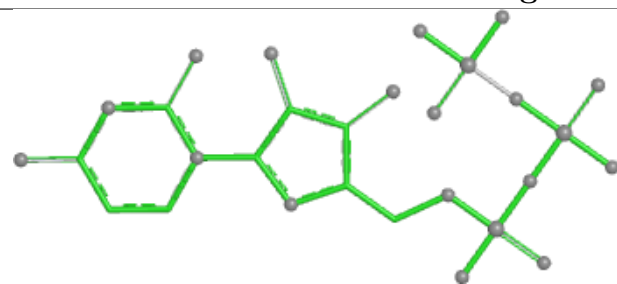


Torsions

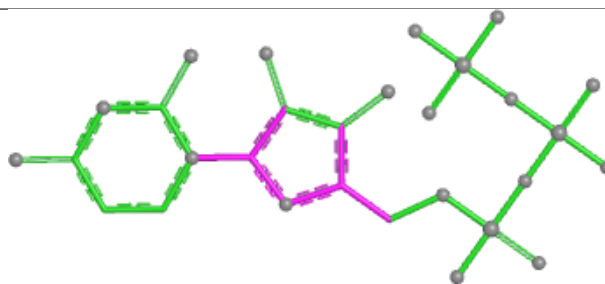


Rings

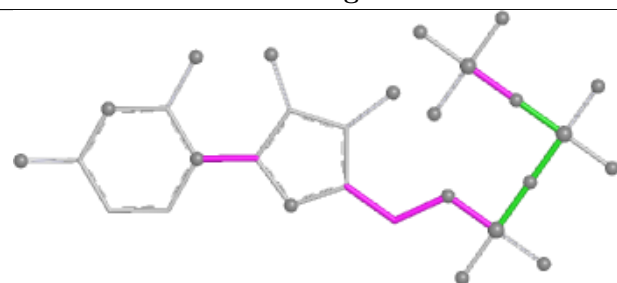
Ligand UTP h 601



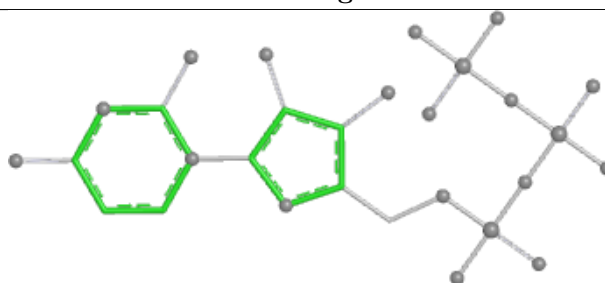
Bond lengths



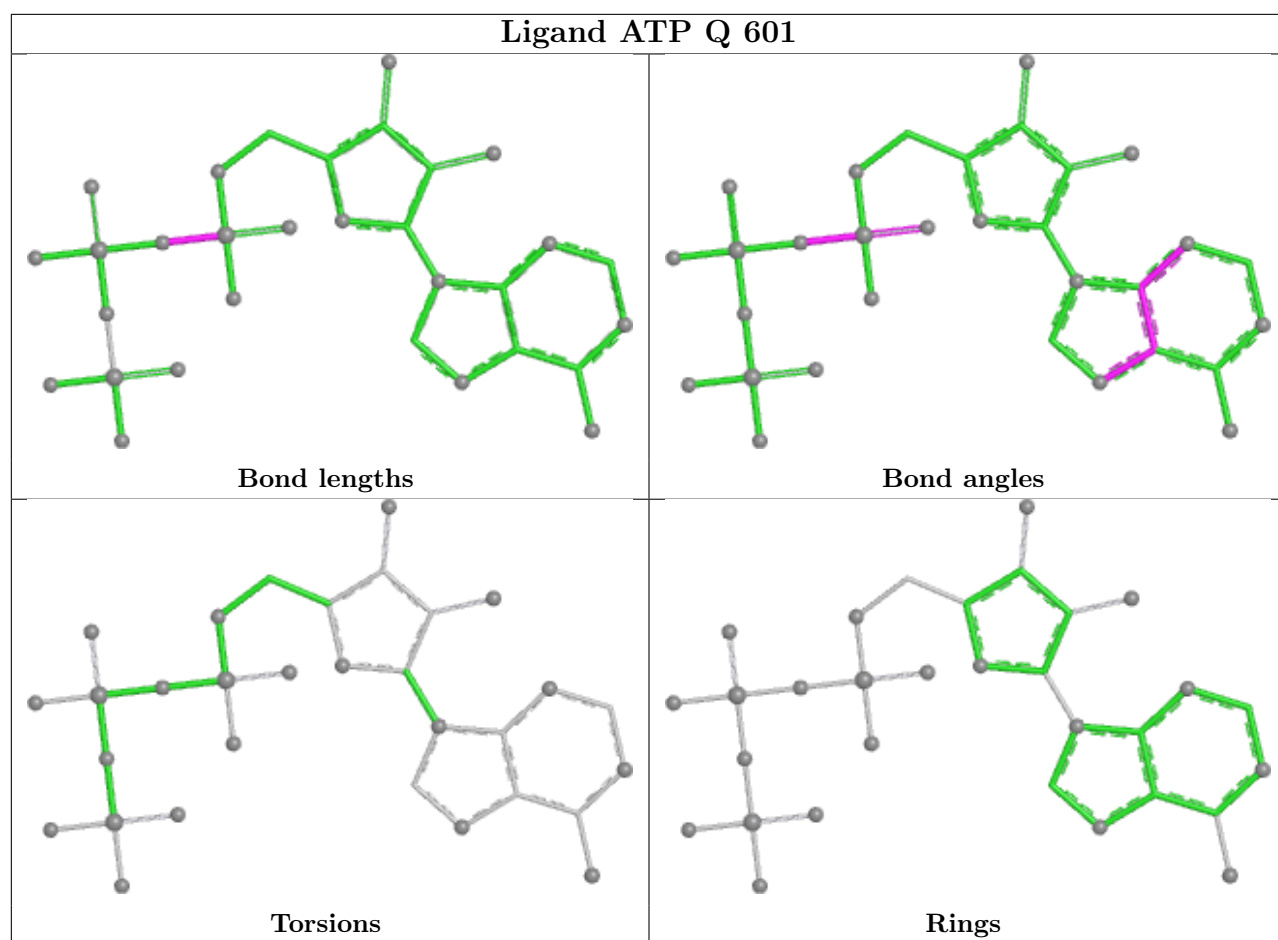
Bond angles



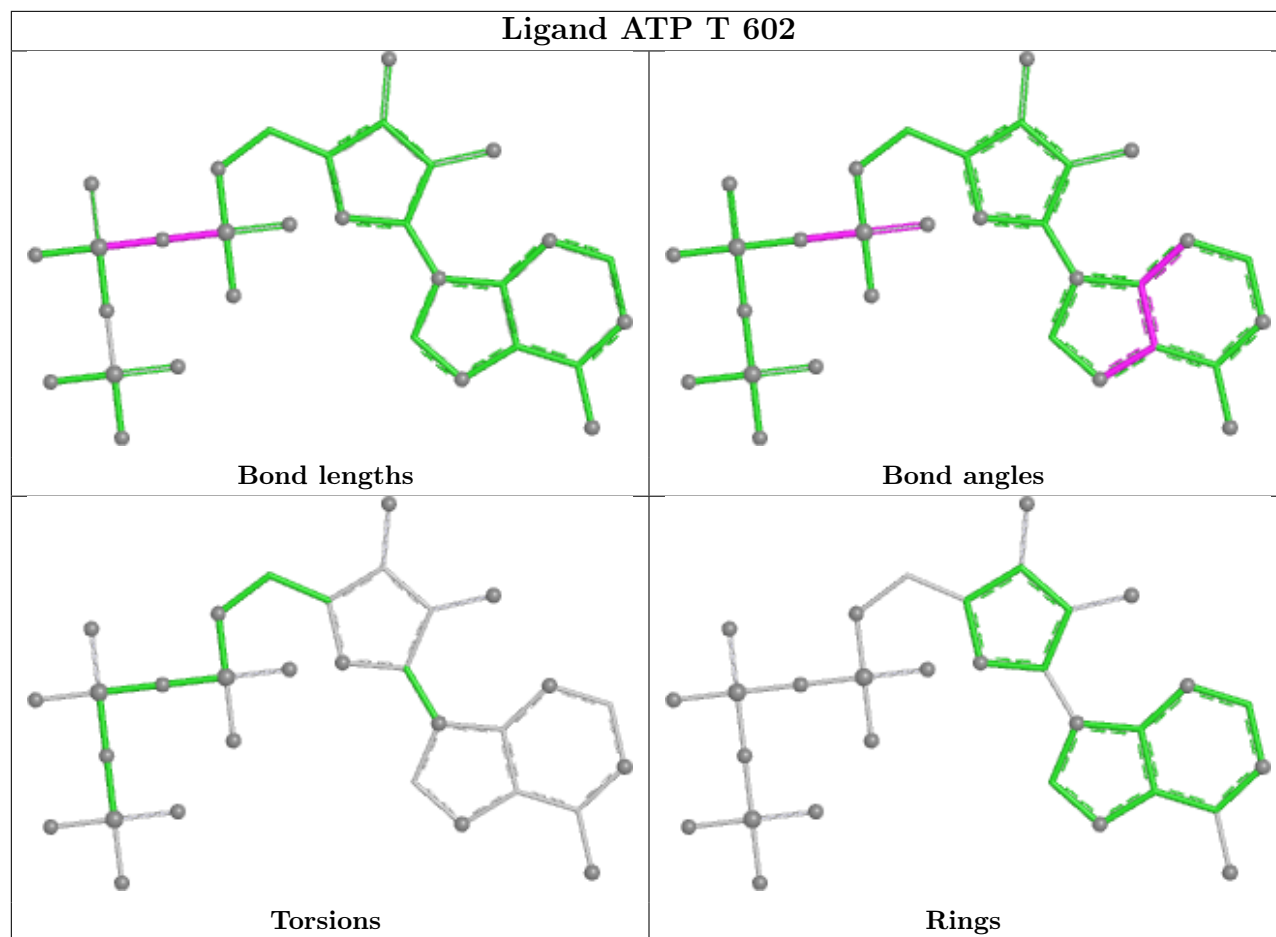
Torsions



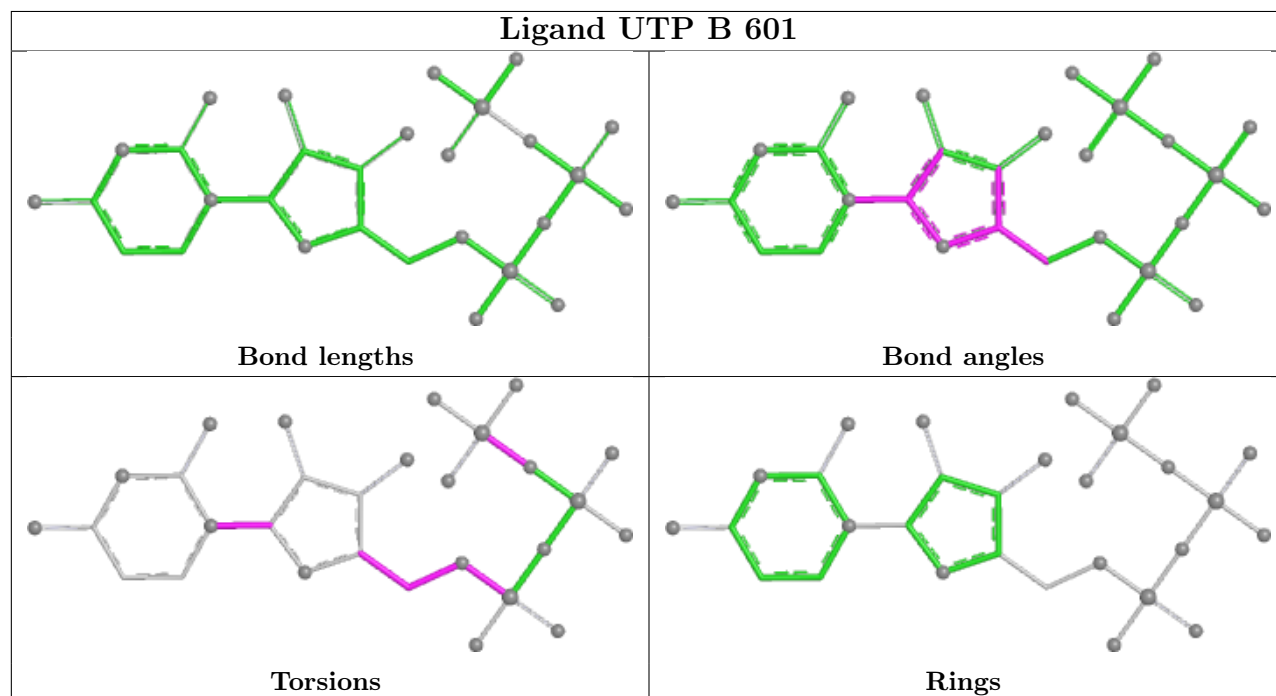
Rings

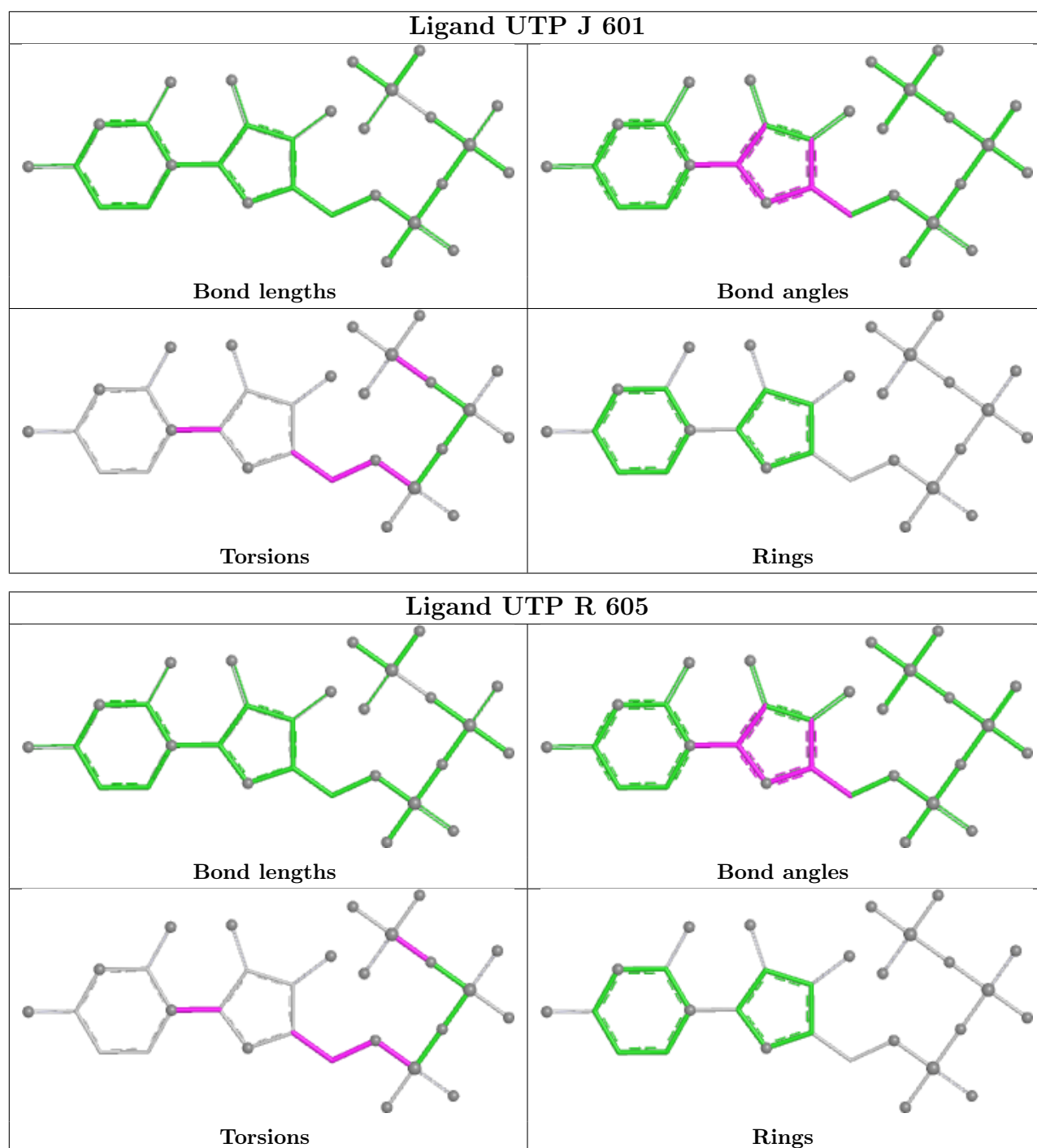


Ligand ATP T 602

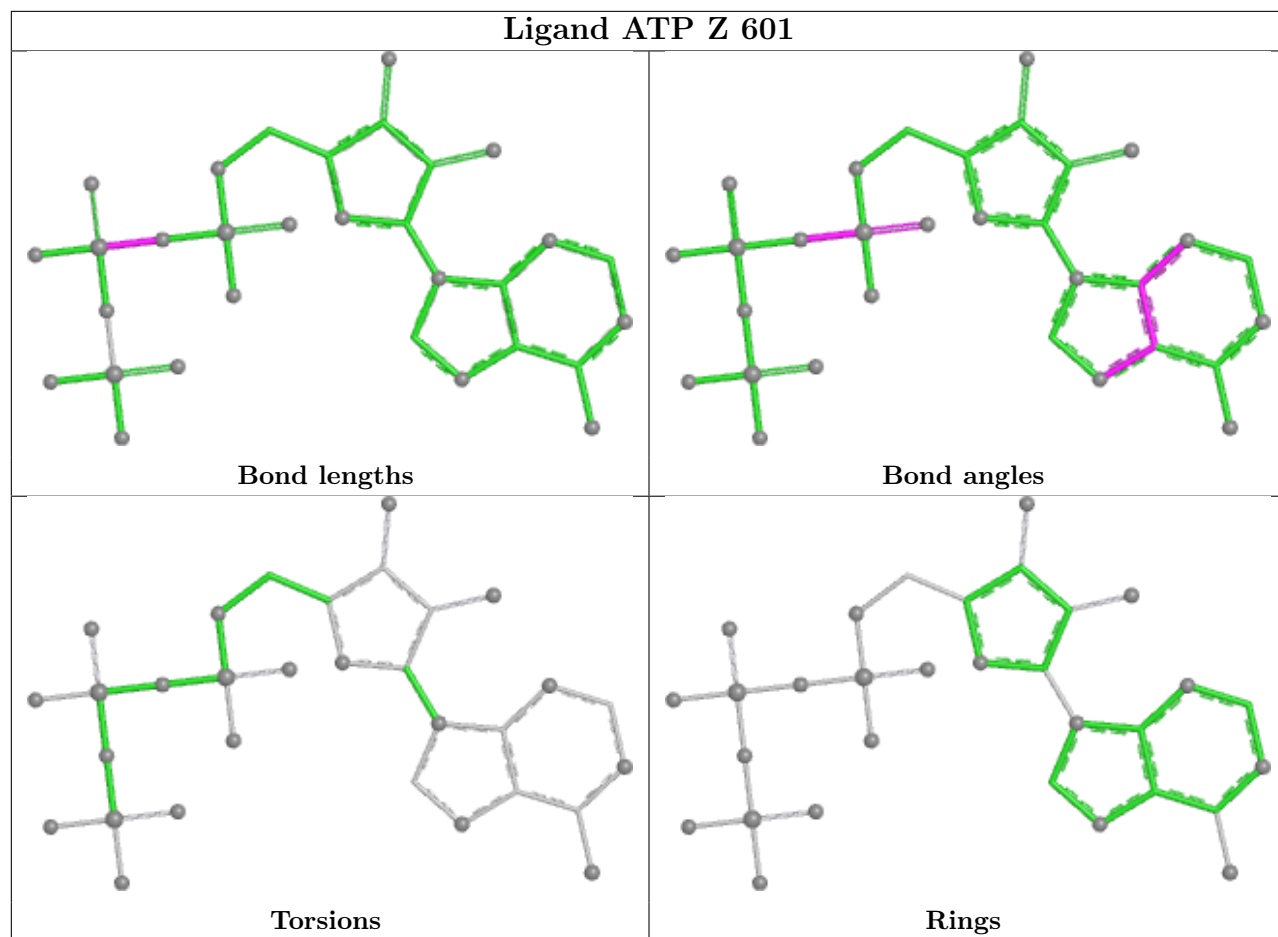


Ligand UTP B 601

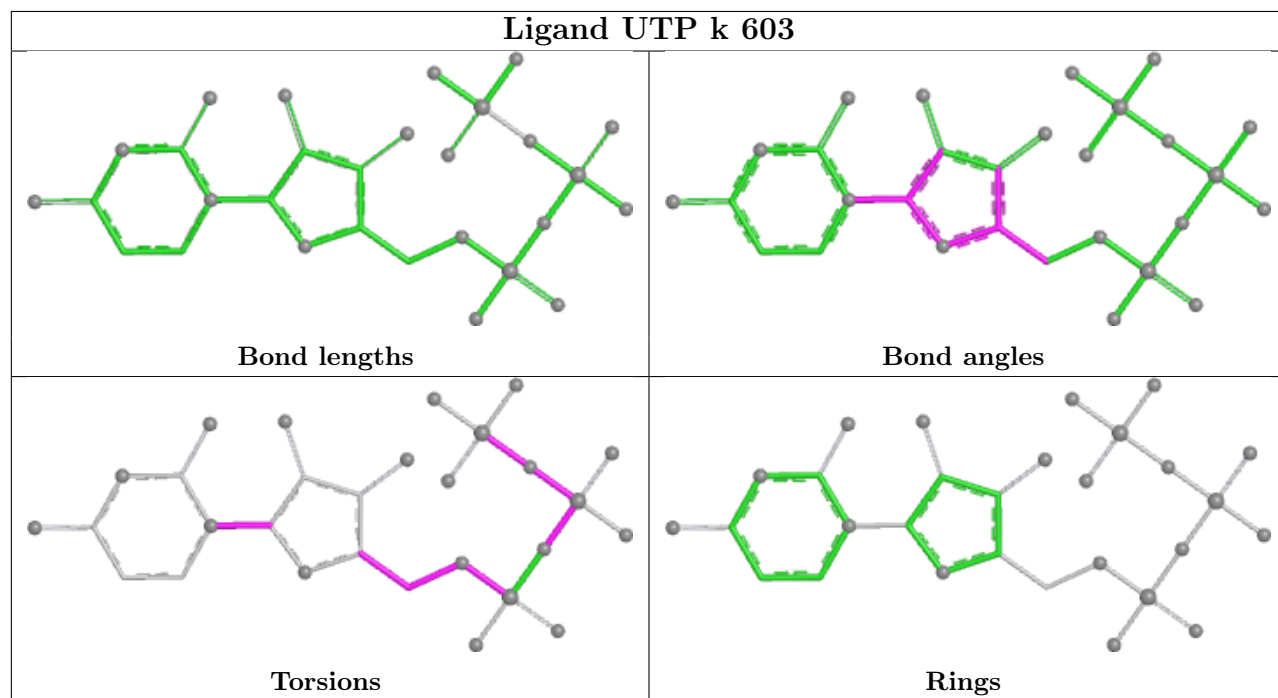


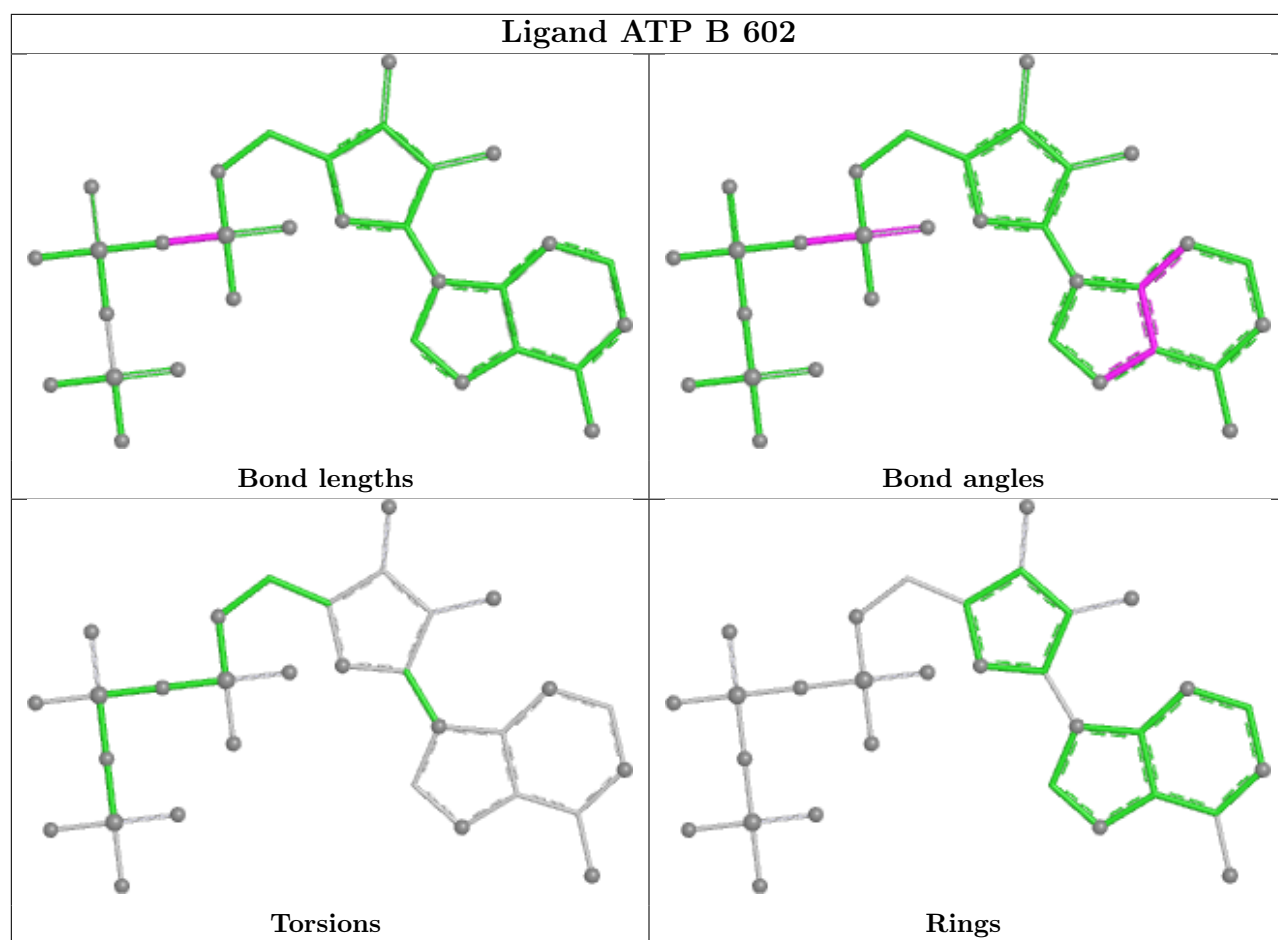


Ligand ATP Z 601

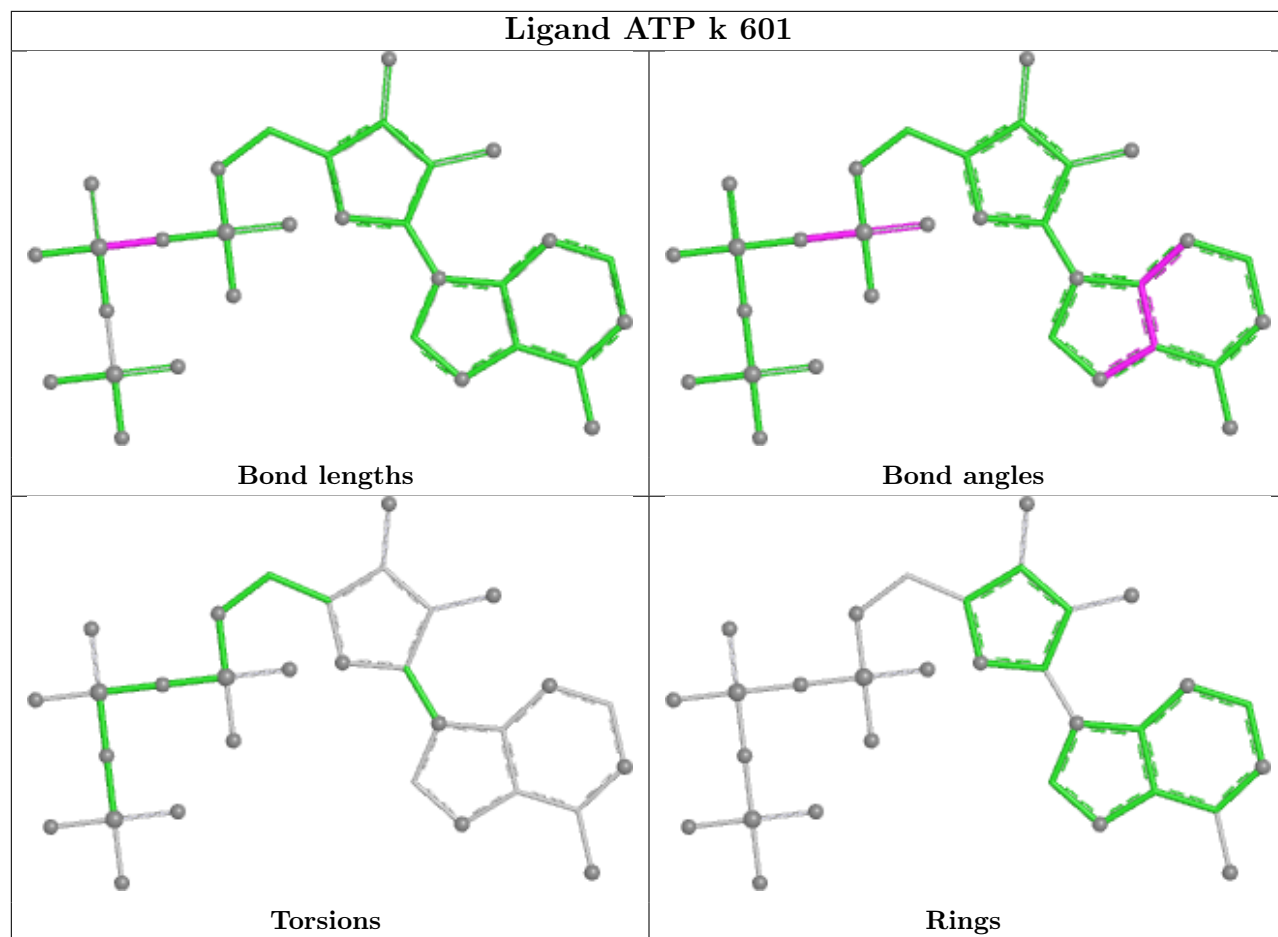


Ligand UTP k 603

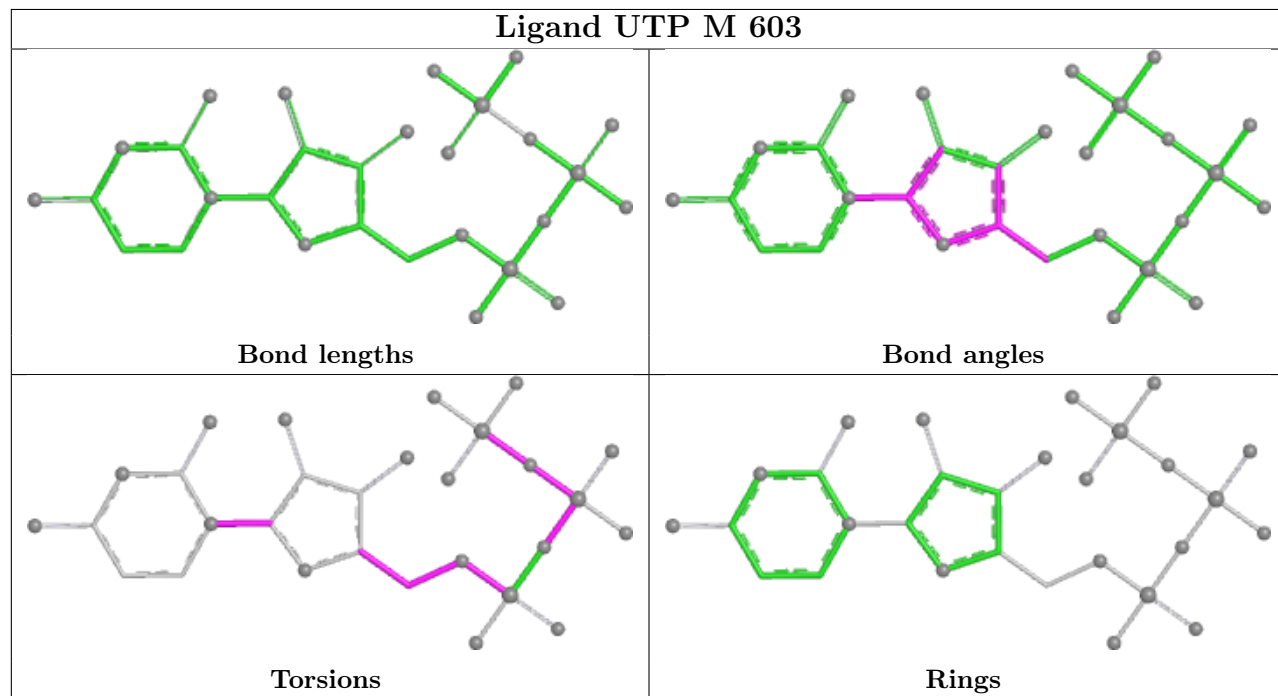


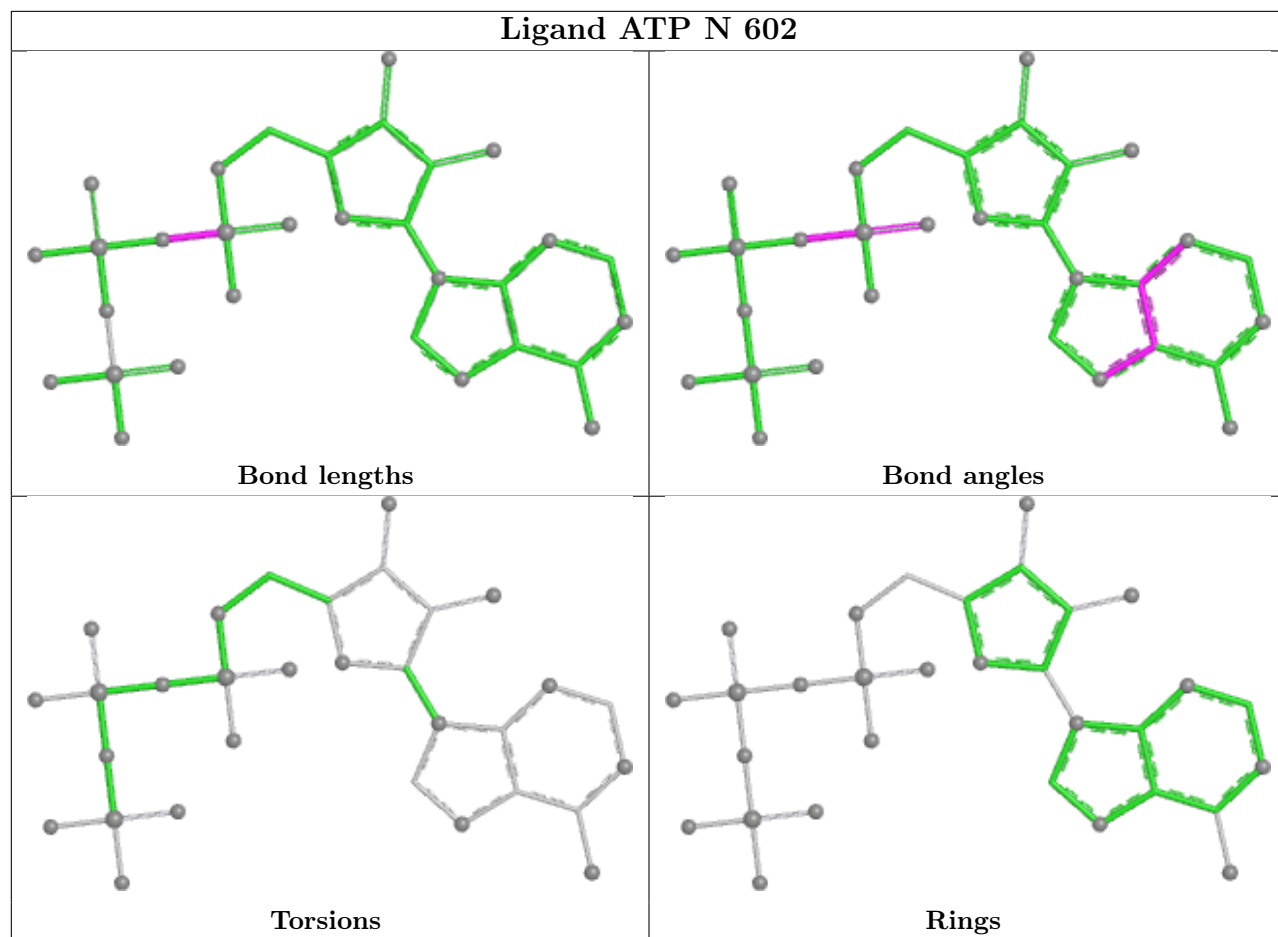


Ligand ATP k 601

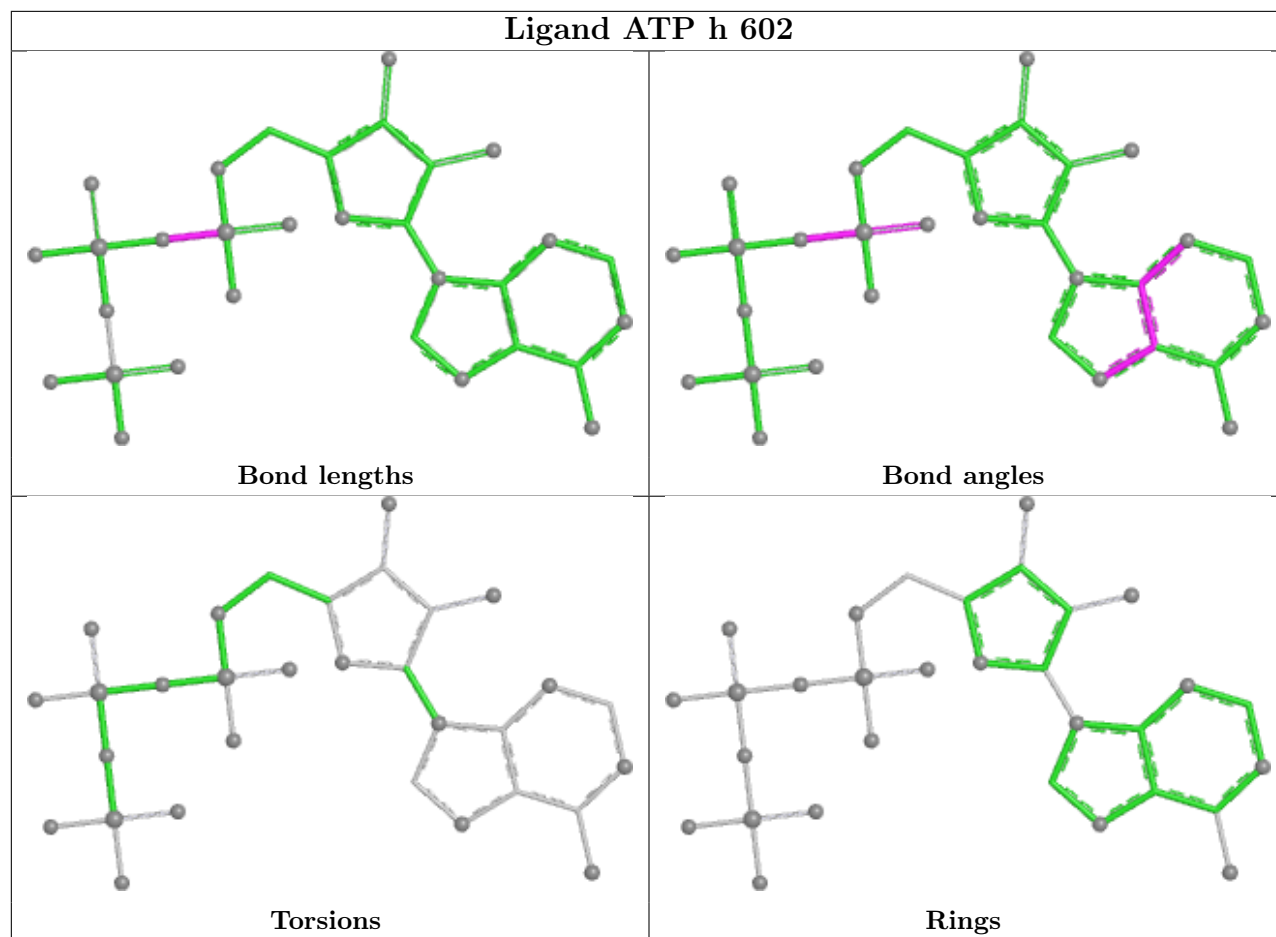


Ligand UTP M 603

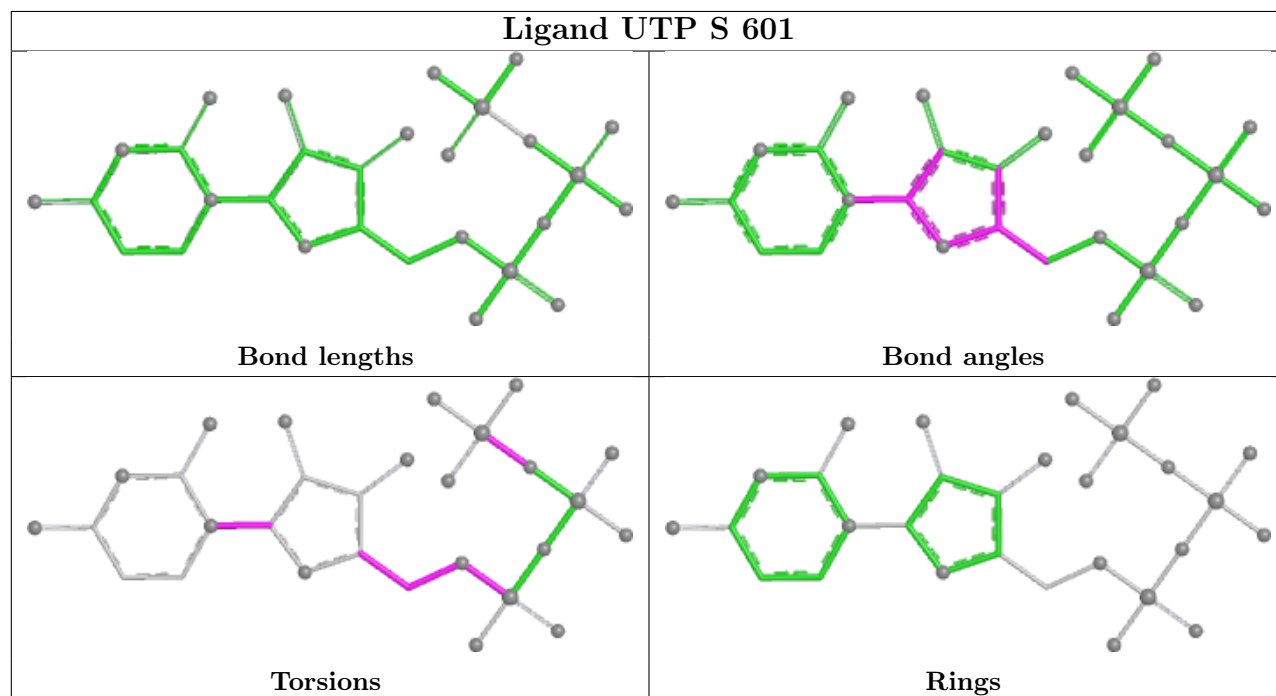


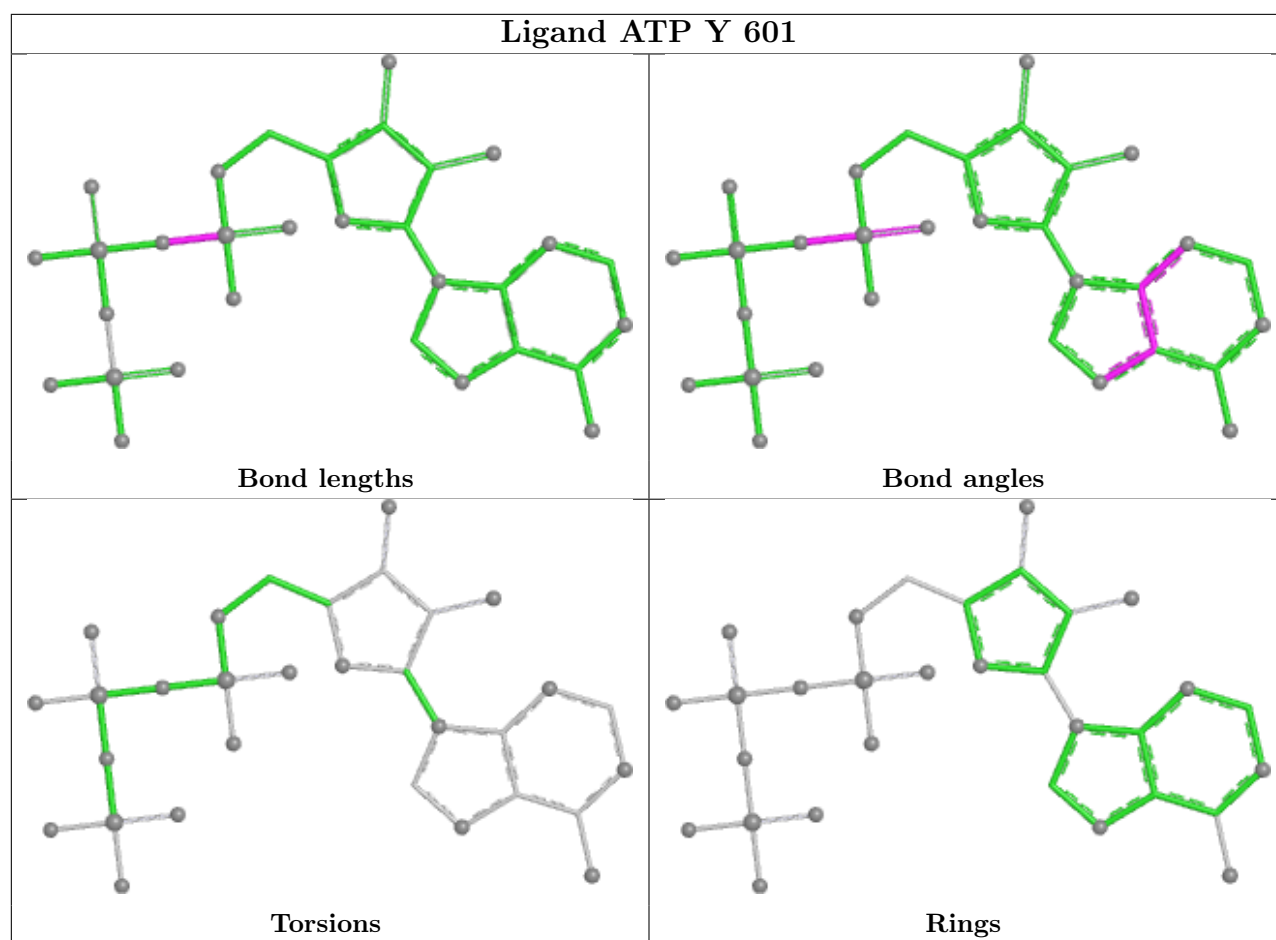


Ligand ATP h 602



Ligand UTP S 601





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

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
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

All 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
1	Y	443:ILE	C	456:THR	N	7.07
1	S	443:ILE	C	456:THR	N	7.07
1	a	443:ILE	C	456:THR	N	7.07
1	I	443:ILE	C	456:THR	N	7.07
1	M	443:ILE	C	456:THR	N	7.07
1	J	443:ILE	C	456:THR	N	7.07
1	N	443:ILE	C	456:THR	N	7.07
1	R	443:ILE	C	456:THR	N	7.07
1	Z	443:ILE	C	456:THR	N	7.07
1	T	443:ILE	C	456:THR	N	7.07
1	b	443:ILE	C	456:THR	N	7.07
1	g	443:ILE	C	456:THR	N	7.07
1	k	443:ILE	C	456:THR	N	7.07
1	h	443:ILE	C	456:THR	N	7.07
1	l	443:ILE	C	456:THR	N	7.07

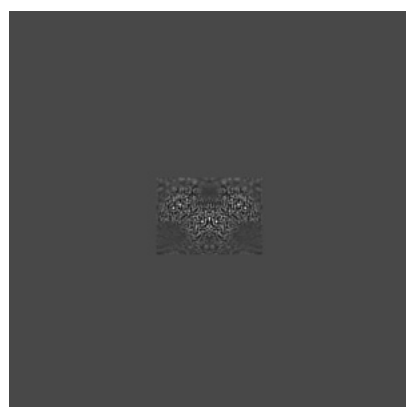
6 Map visualisation [i](#)

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.

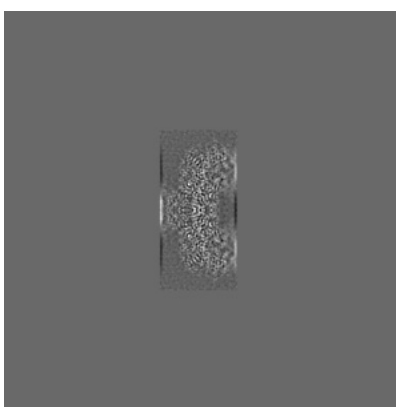
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

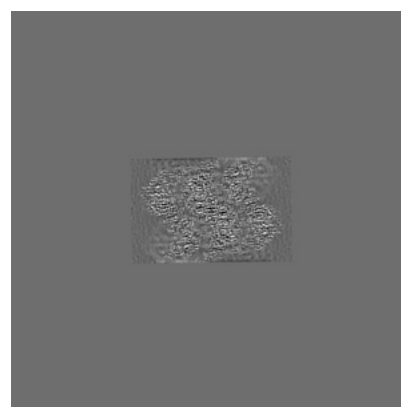
6.1.1 Primary map



X



Y



Z

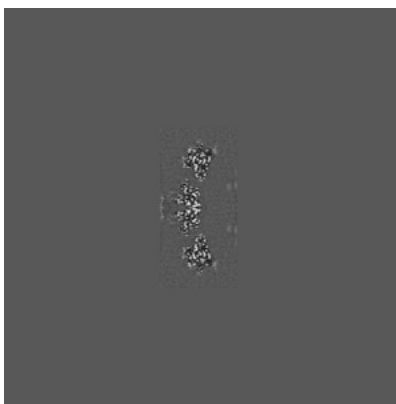
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

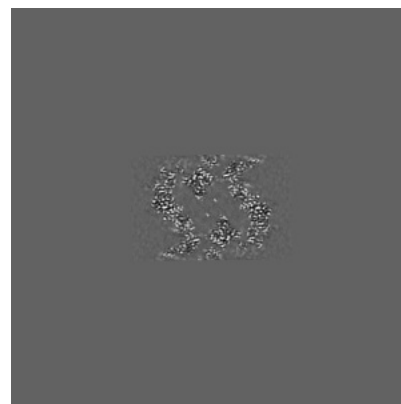
6.2.1 Primary map



X Index: 256



Y Index: 256

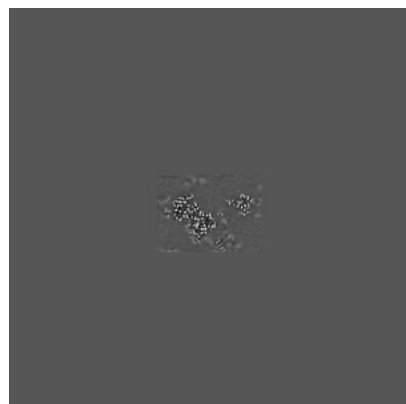


Z Index: 256

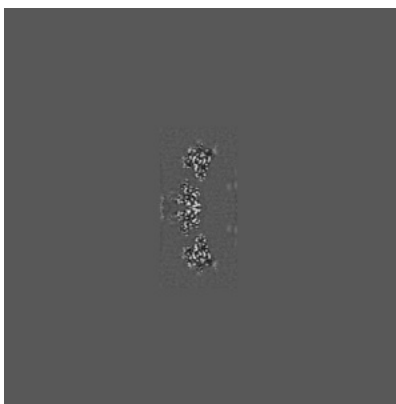
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

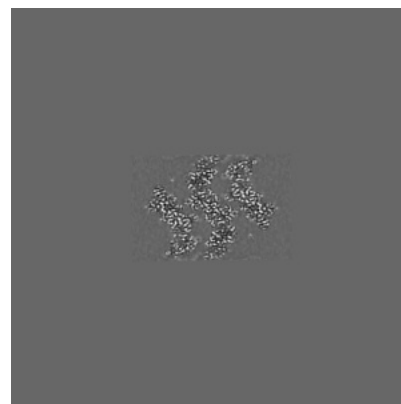
6.3.1 Primary map



X Index: 275



Y Index: 256

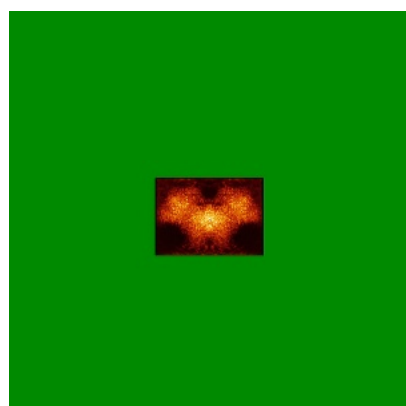


Z Index: 248

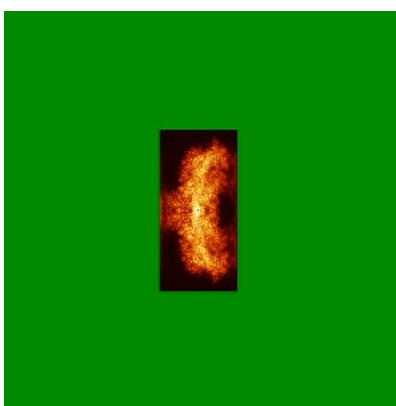
The images above show the largest variance slices of the map in three orthogonal directions.

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

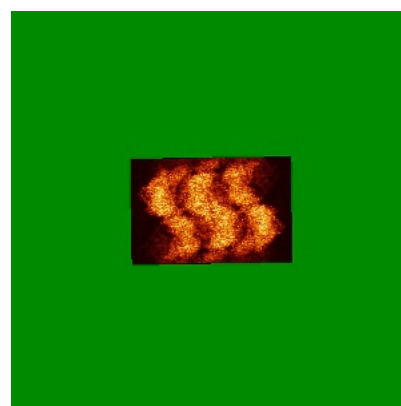
6.4.1 Primary map



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 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

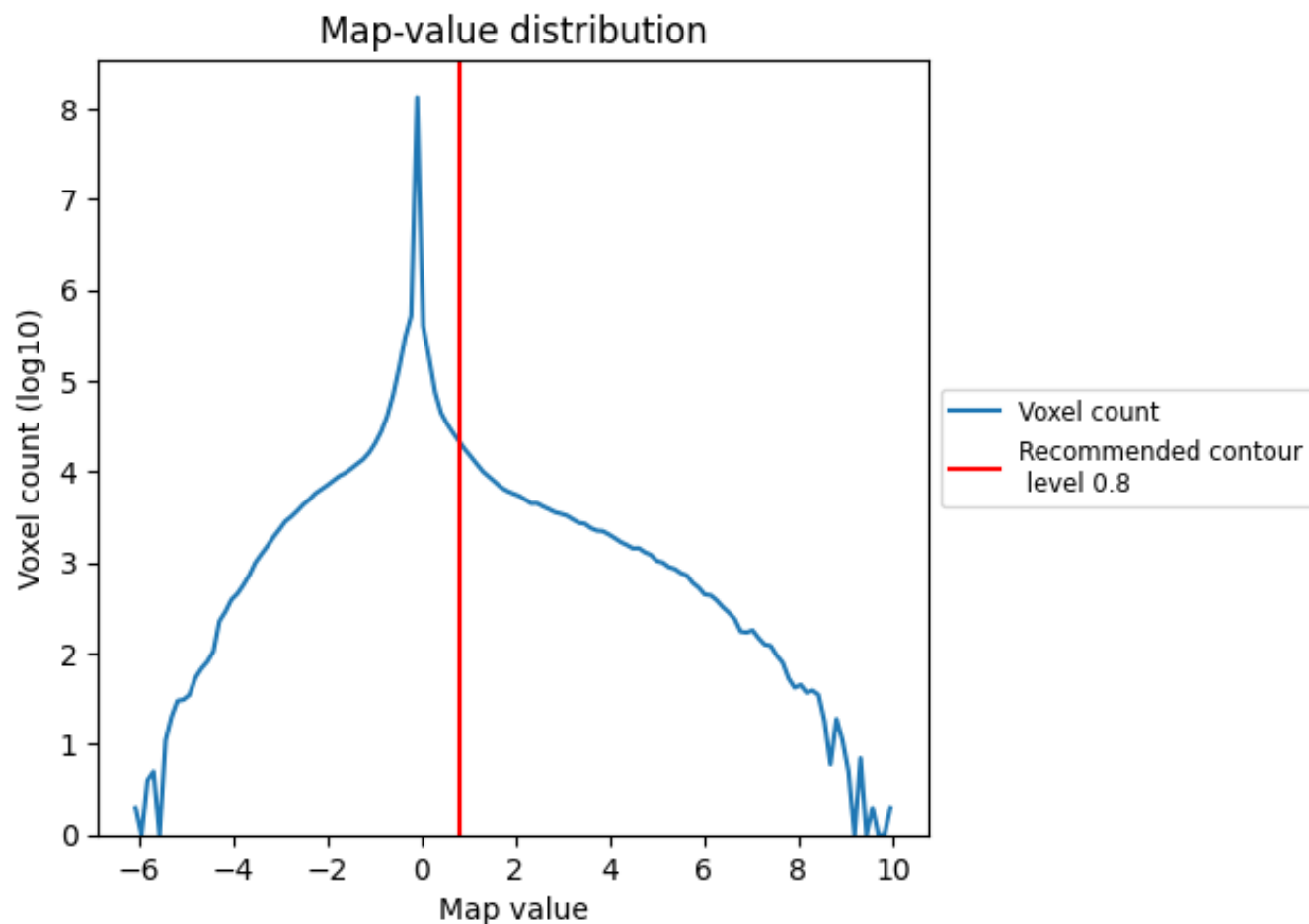
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

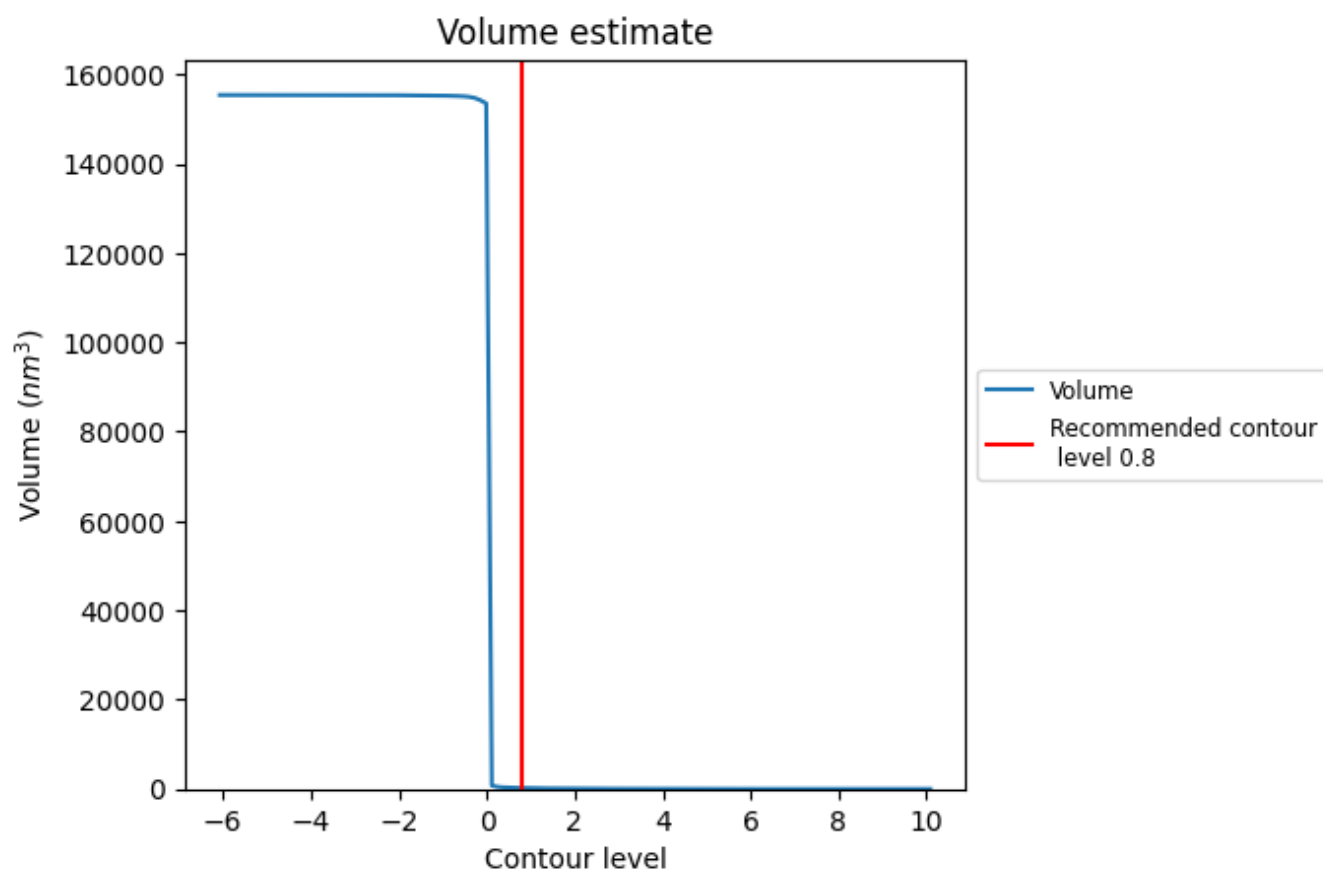
This section contains the results of statistical analysis of the map.

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.

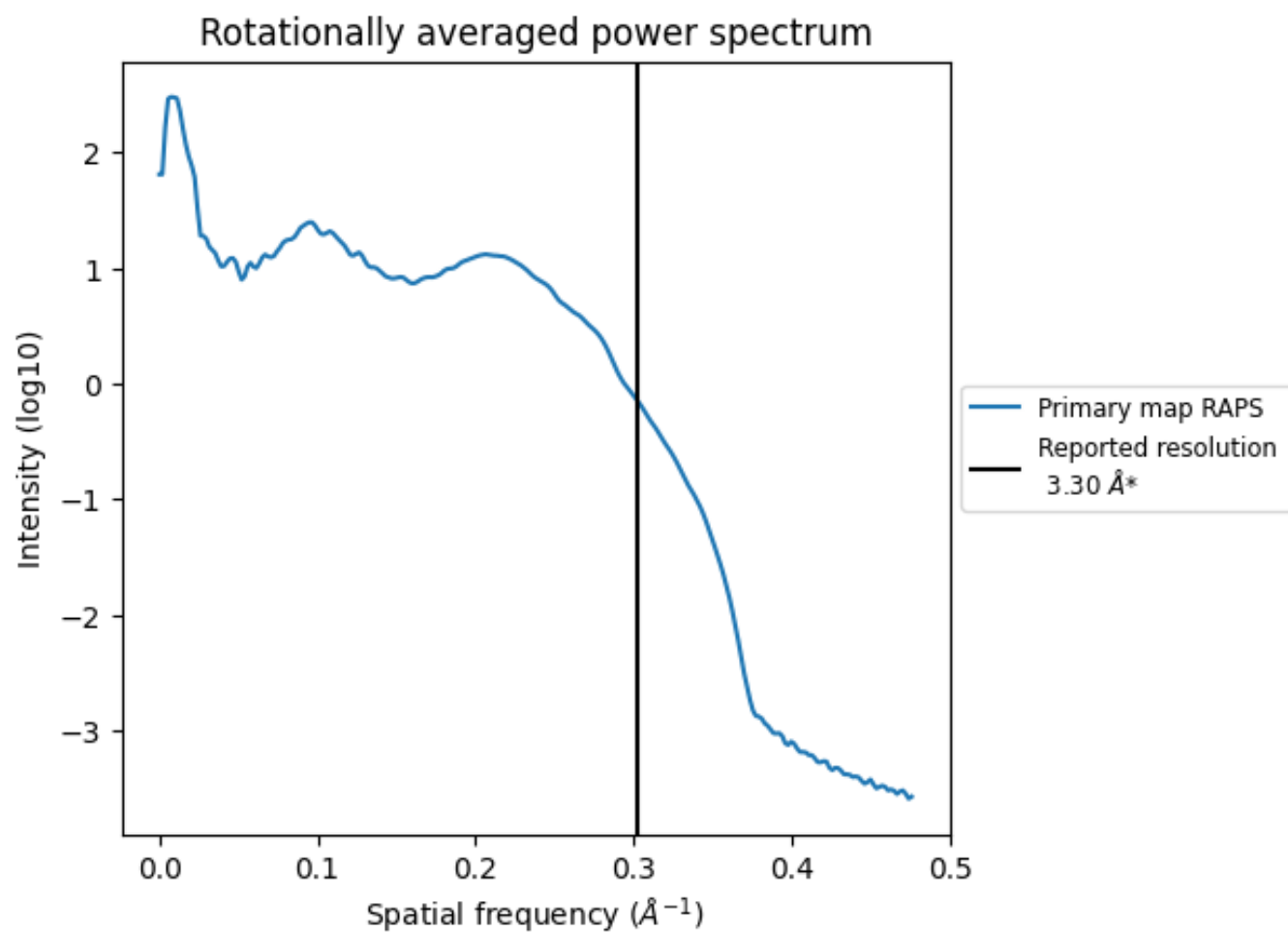
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



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

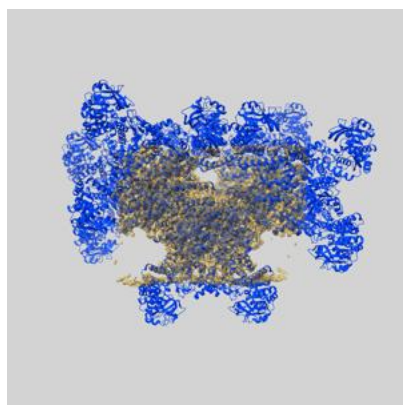
8 Fourier-Shell correlation ⓘ

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

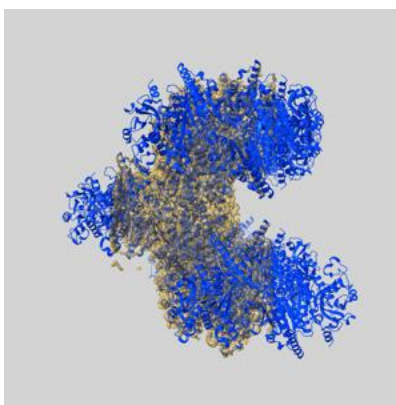
9 Map-model fit [i](#)

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](#).

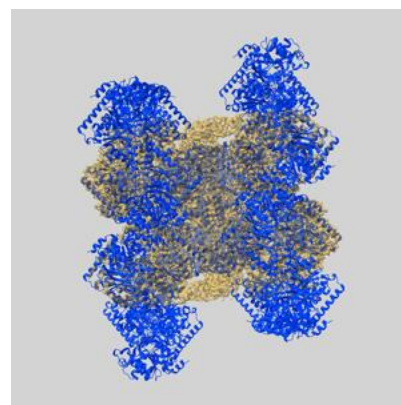
9.1 Map-model overlay [i](#)



X



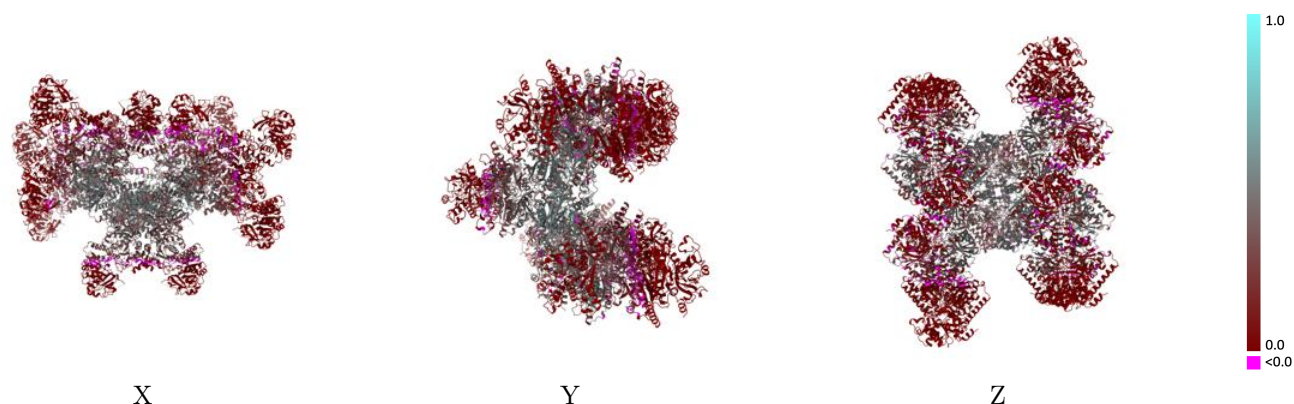
Y



Z

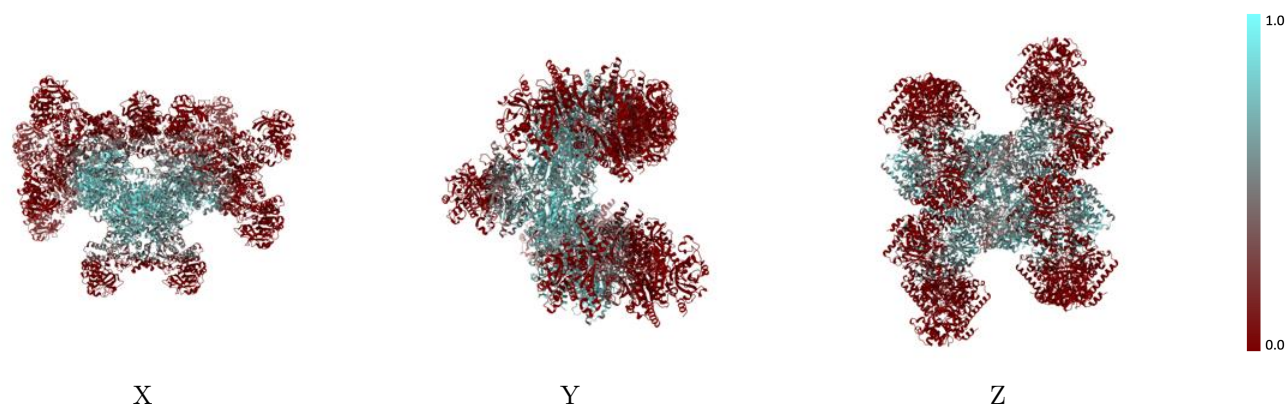
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



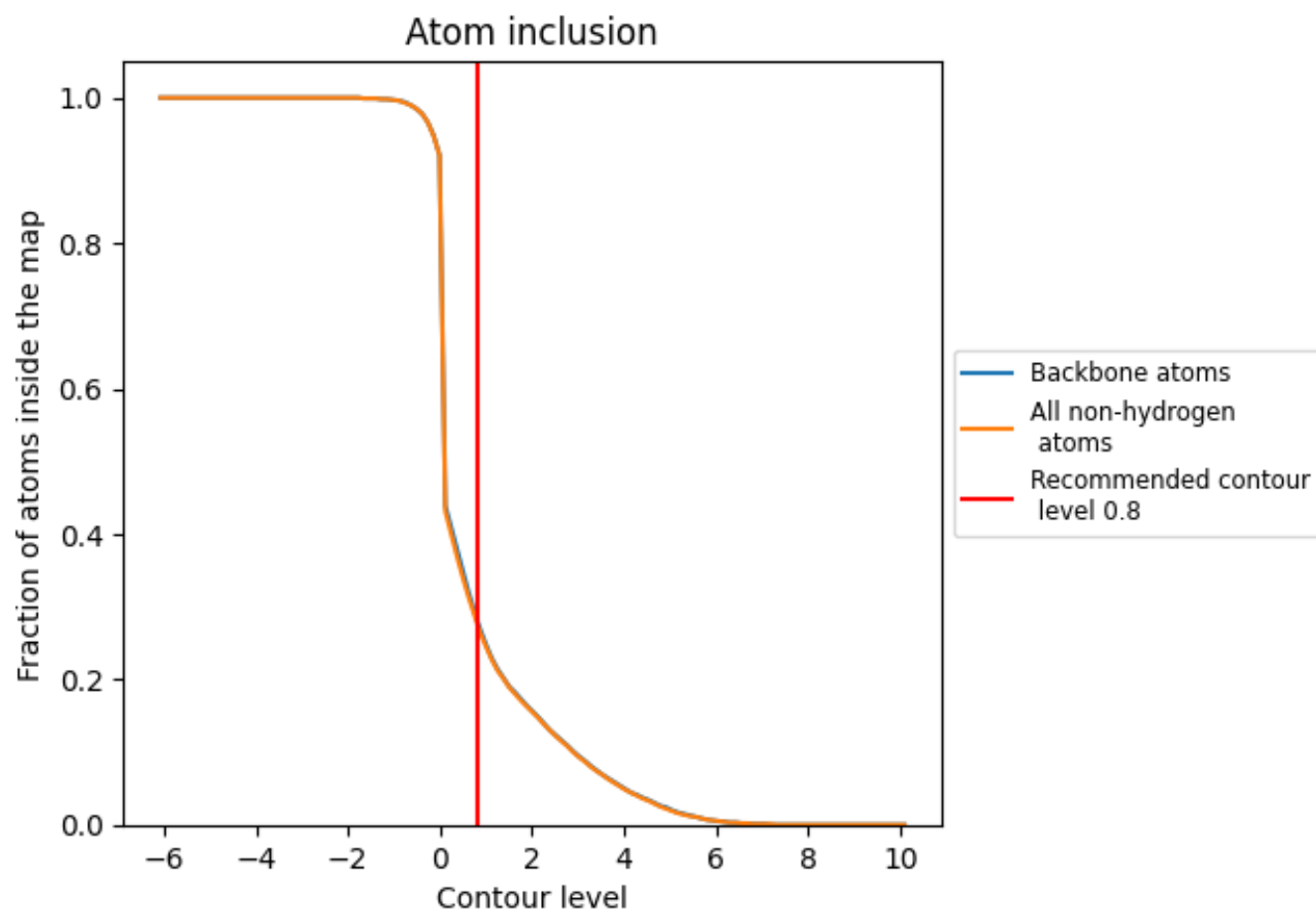
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	 0.2780	 0.1870
A	 0.7480	 0.4730
B	 0.2240	 0.1400
E	 0.2230	 0.1390
F	 0.7500	 0.4710
I	 0.0240	 0.0160
J	 0.6420	 0.3830
M	 0.0590	 0.0470
N	 0.1120	 0.0970
Q	 0.6910	 0.4150
R	 0.6910	 0.4130
S	 0.0320	 0.0420
T	 0.0310	 0.0420
Y	 0.1290	 0.0930
Z	 0.1320	 0.0930
a	 0.1700	 0.1610
b	 0.1740	 0.1640
g	 0.0250	 0.0160
h	 0.6430	 0.3870
k	 0.0600	 0.0490
l	 0.1140	 0.0970

