Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:06 PM EST

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

This is a 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:

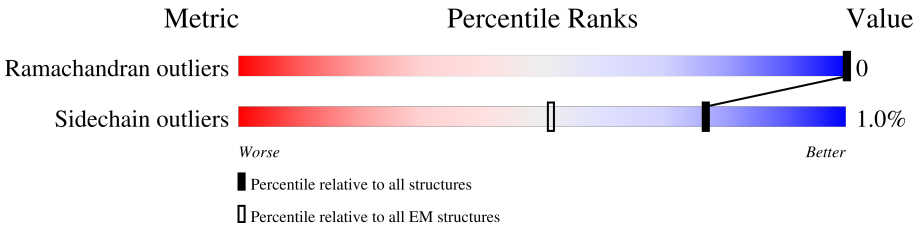
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	559	96%
1	B	559	72% 96%
1	E	559	72% 96%
1	F	559	96%
1	I	559	98% 96%
1	J	559	15% 96%
1	M	559	93% 96%
1	N	559	88% 96%
1	Q	559	10% 96%

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Mol	Chain	Length	Quality of chain
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
4	UTP	A	605	X	-	-	-
4	UTP	B	601	X	-	-	-
4	UTP	E	603	X	-	-	-
4	UTP	F	601	X	-	-	-
4	UTP	I	605	X	-	-	-
4	UTP	J	601	X	-	-	-
4	UTP	M	603	X	-	-	-
4	UTP	N	601	X	-	-	-
4	UTP	Q	605	X	-	-	-
4	UTP	R	605	X	-	-	-
4	UTP	S	601	X	-	-	-
4	UTP	T	601	X	-	-	-
4	UTP	Y	603	X	-	-	-
4	UTP	Z	603	X	-	-	-
4	UTP	a	601	X	-	-	-
4	UTP	b	601	X	-	-	-
4	UTP	g	605	X	-	-	-
4	UTP	h	601	X	-	-	-

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

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 177180 atoms, of which 88240 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CTP synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
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		

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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

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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

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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

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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

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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

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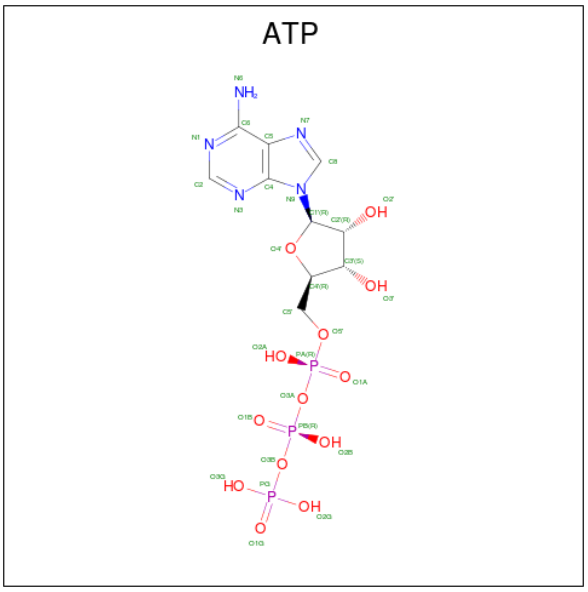
Chain	Residue	Modelled	Actual	Comment	Reference
g	?	-	HIS	deletion	UNP A0A6A5PYW3
g	?	-	MET	deletion	UNP A0A6A5PYW3
g	?	-	GLY	deletion	UNP A0A6A5PYW3
g	?	-	GLY	deletion	UNP A0A6A5PYW3
k	?	-	TYR	deletion	UNP A0A6A5PYW3
k	?	-	MET	deletion	UNP A0A6A5PYW3
k	?	-	PRO	deletion	UNP A0A6A5PYW3
k	?	-	GLU	deletion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

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



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

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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 (three-letter code: 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	

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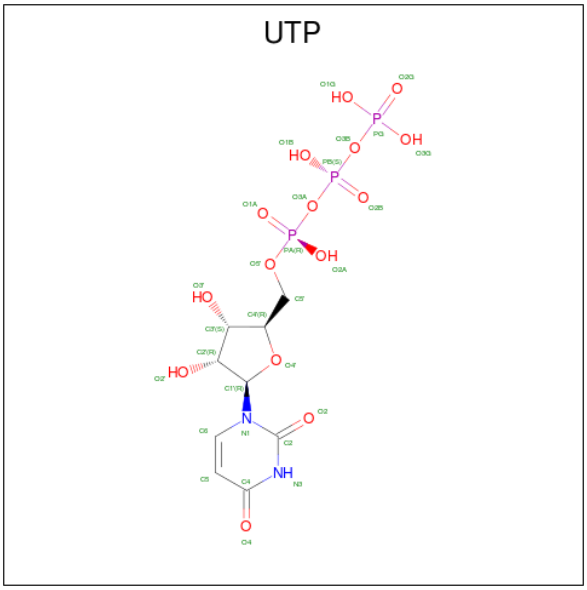
Mol	Chain	Residues	Atoms	AltConf
3	Z	1	Total Mg 1 1	0
3	T	3	Total Mg 3 3	0
3	b	1	Total Mg 1 1	0
3	g	3	Total Mg 3 3	0
3	k	1	Total Mg 1 1	0
3	h	3	Total Mg 3 3	0
3	l	1	Total Mg 1 1	0

- Molecule 4 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).



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

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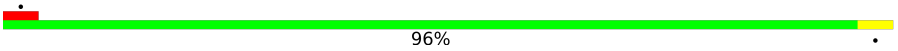
Mol	Chain	Residues	Atoms						AltConf
4	Q	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	Y	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	S	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	a	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	I	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	M	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	J	1	Total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

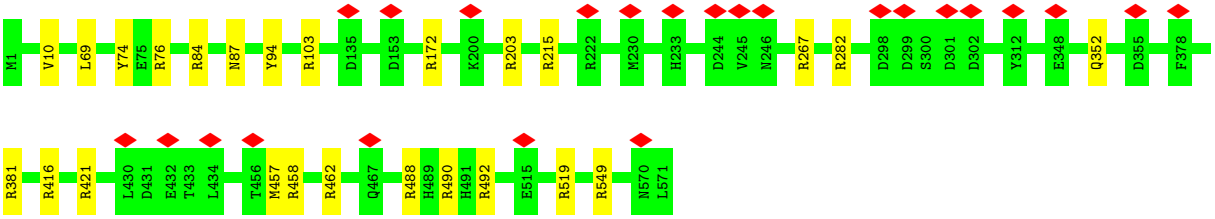
3 Residue-property plots (i)

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

- Molecule 1: CTP synthase

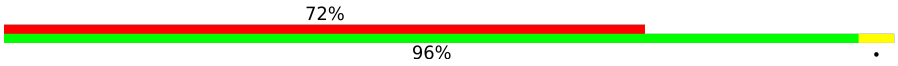
Chain A:

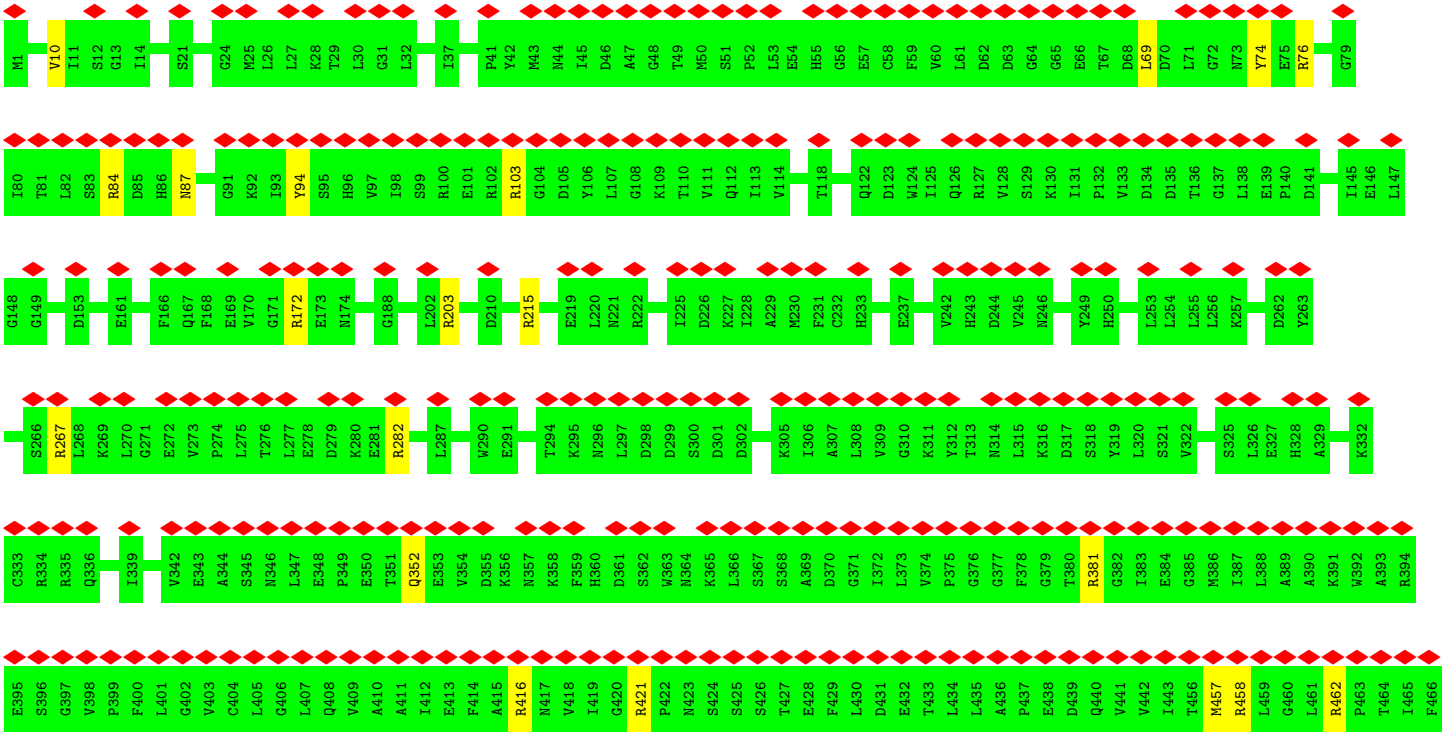


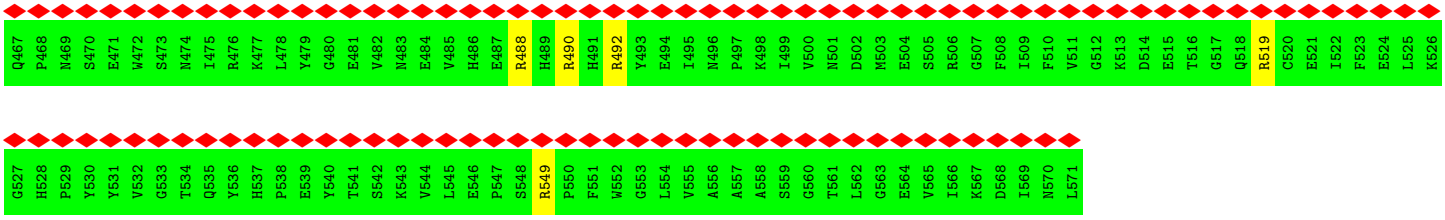


- Molecule 1: CTP synthase

Chain E:

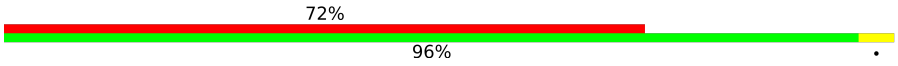


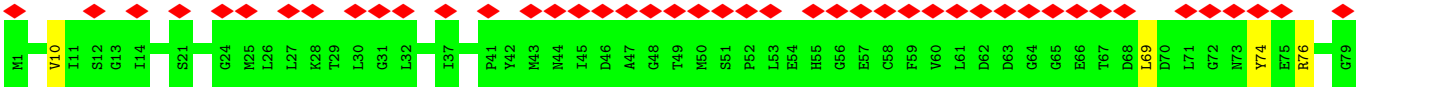




• Molecule 1: CTP synthase

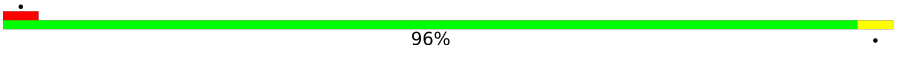
Chain B:

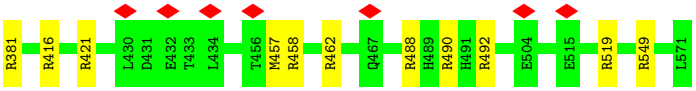




• Molecule 1: CTP synthase

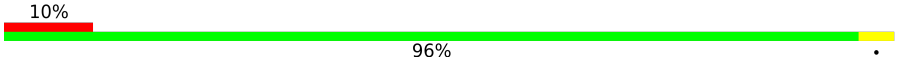
Chain F:

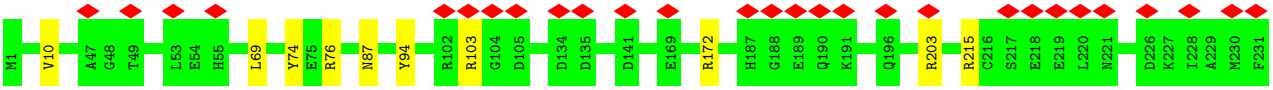


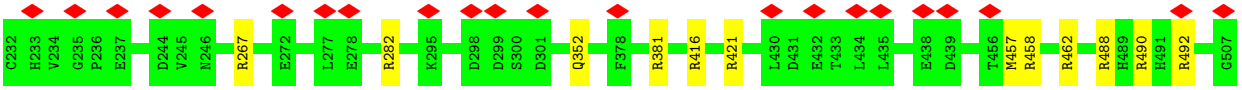


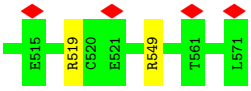
• Molecule 1: CTP synthase

Chain Q:



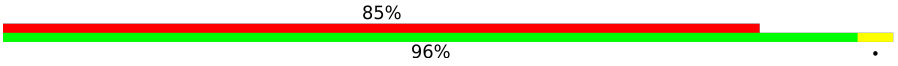


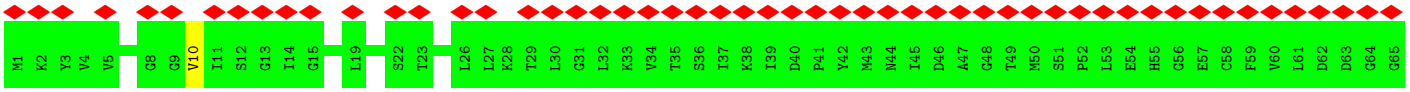


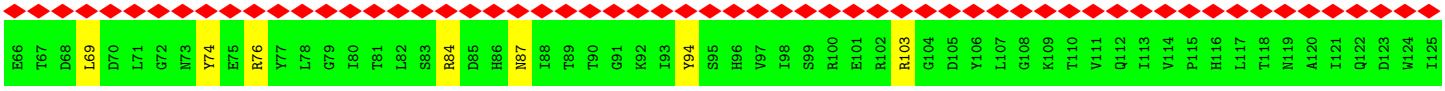


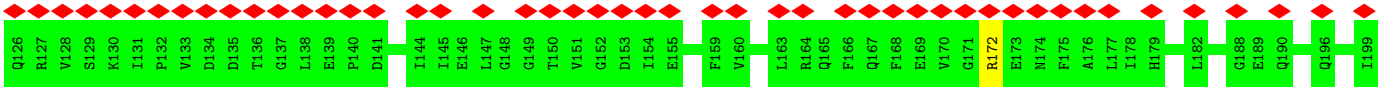
• Molecule 1: CTP synthase

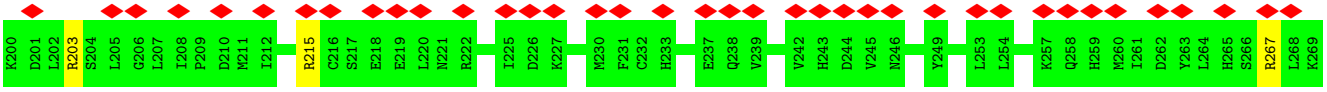
Chain Y:

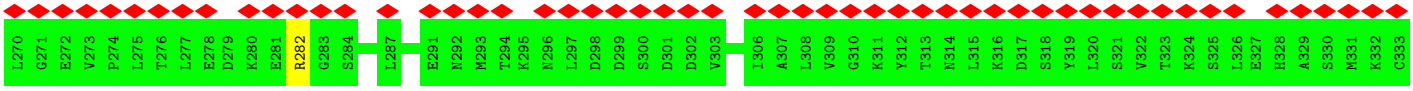


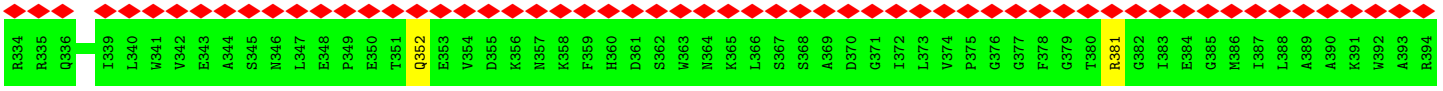


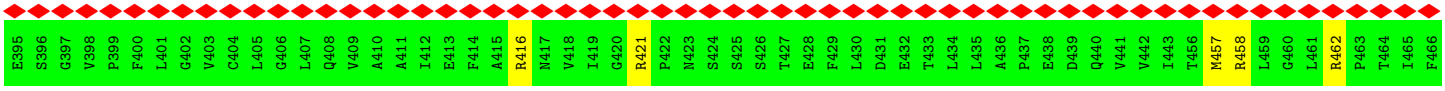












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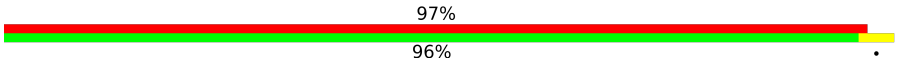
G527 H528 P529 Y530 Y531 V532 G533 T534 Q535 Y536 H537 P538 E539 Y540 T541 S542 K543 V544 L545 E546 P547 S548 R549 P550 F551 W552 G553 L554 V555 A556 A557 A558 S559 G560 T561 L562 G563 E564 V565 I566 K567 D568 I569 N570 L571

• Molecule 1: CTP synthase

Chain S:



M1 K2 Y3 V4 V5 V6 S7 G8 G9 V10 I11 S12 G13 I14 G15 K16 G17 V18 L19 A20 S21 S22 T23 G24 M25 L26 L27 K28 T29 L30 G31 L32 K33 V34 T35 S36 I37 K38 I39 D40 P41 Y42 M43 N44 I45 D46 A47 G48 T49 M50 S51 P52 L53 E54 H55 G56 E57 C58 F59 V60

L61 D62 D63 G64 G65 E66 T67 D68 L69 D70 L71 G72 N73 Y74 E75 R76 Y77 L78 G79 I80 T81 L82 S83 R84 D85 H86 N87 I88 T89 T90 G91 K92 I93 Y94 S95 H96 V97 I98 S99 R100 E101 R102 R103 G104 D105 Y106 L107 G108 K109 T110 V111 Q112 I113 V114 P115 H116 L117 T118 N119 A120

I121 Q122 D123 W124 I125 Q126 R127 V128 S129 K130 I131 P132 V133 D134 D135 T136 G137 L138 E139 P140 D141 V142 C143 I144 I145 E146 L147 G148 G149 T150 V151 G152 E155 S156 A157 P158 F159 A162 L163 R164 Q165 F166 Q167 F168 E169 V170 G171 R172 E173 N174 F175 A176 L177 I178 H179 V180 S181 L182

V183 P184 V185 I186 H187 G188 E189 Q190 K191 T192 K193 A197 D201 L202 R203 S204 L205 G206 L207 I208 P209 D210 M211 I212 A213 C214 R215 C216 S217 E218 E219 L220 N221 R222 S223 T224 I225 D226 K227 I228 A229 M230 F231 C232 H233 V234 G235 P236 E237 Q238 V239 V240 N241 V242 H243 D244 V245 N246

S247 T248 Y249 H250 V251 P252 L253 L254 L255 L256 K257 Q258 H259 M260 I261 D262 Y263 L264 H265 S266 R267 L268 K269 L270 G271 E272 V273 P274 L275 T276 L277 E278 D279 K280 E281 R282 G283 S284 Q285 L286 L287 T288 N289 W290 E291 N292 M293 T294 K295 N296 L297 D298 D299 S300 D301 D302 V303 V304 K305 I306

A307 L308 V309 G310 K311 Y312 T313 N314 L315 K316 D317 S318 Y319 L320 S321 V322 T323 K324 S325 L326 E327 H328 A329 S330 M331 K332 C333 R334 R335 Q336 L337 E338 I339 L340 W341 V342 E343 A344 S345 N346 L347 E348 P349 E350 T351 Q352 E353 V354 D355 K356 N357 K358 F359 H360 D361 S362 W363 N364 K365 L366

S367 S368 A369 D370 G371 I372 L373 V374 P375 G376 G377 F378 G379 T380 R381 G382 I383 E384 G385 M386 I387 L388 A389 A390 K391 W392 A393 R394 E395 S396 G397 V398 P399 F400 L401 G402 V403 C404 L405 G406 L407 Q408 V409 A410 A411 I412 E413 F414 A415 R416 N417 V418 I419 G420 R421 P422 N423 S424 S425 S426

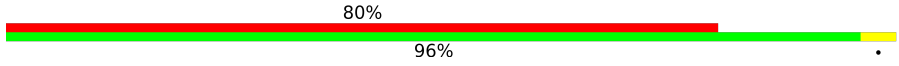
T427 E428 F429 L430 D431 E432 T433 L434 L435 A436 P437 E438 D439 Q440 V441 V442 I443 T456 M457 R458 L459 G460 L461 R462 P463 T464 I465 F466 Q467 P468 N469 S470 E471 W472 S473 N474 I475 R476 K477 L478 Y479 G480 E481 V482 N483 E484 V485 H486 E487 R488 H489 R490 H491 R492 Y493 E494 I495 N496 P497 K498

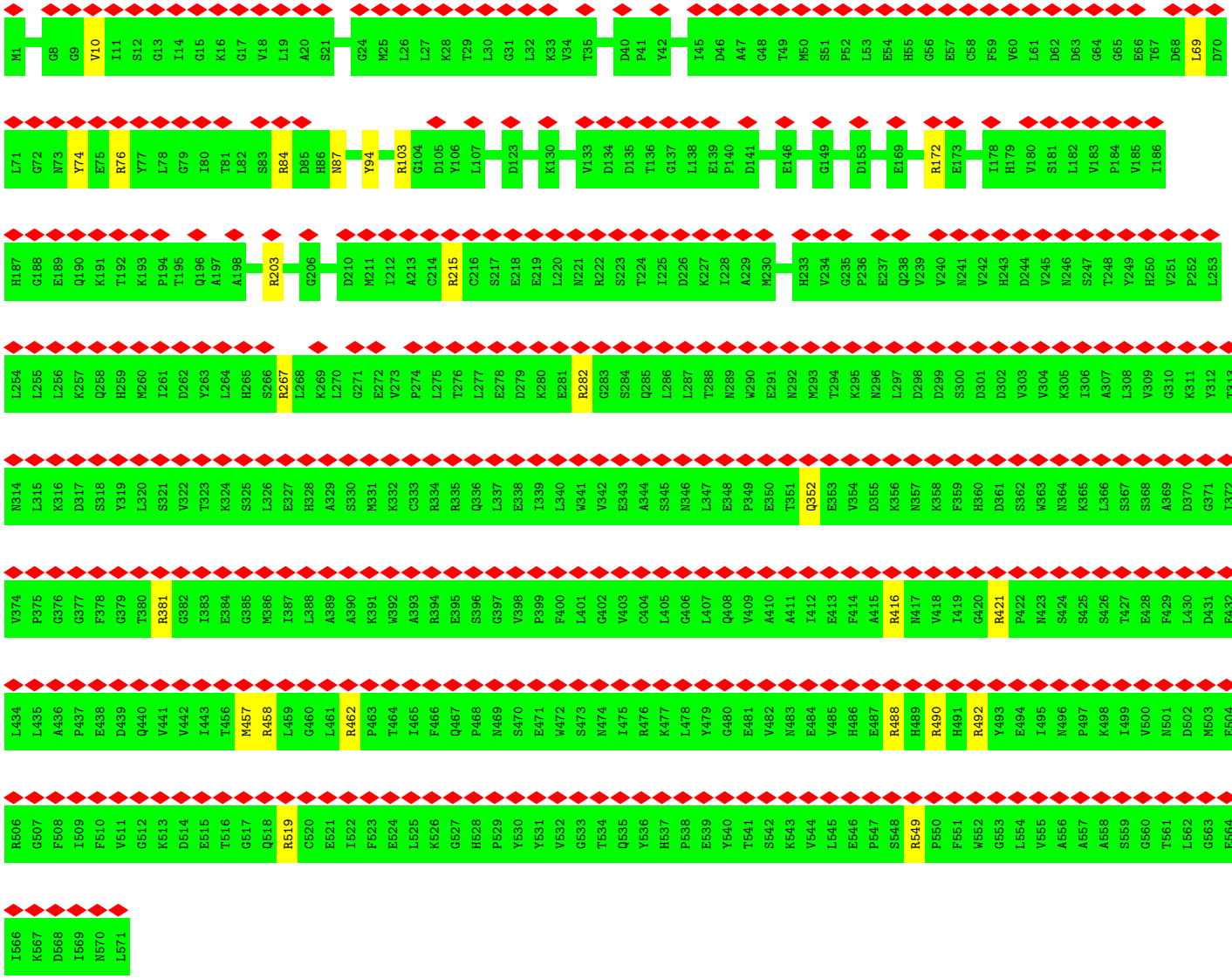
I499 V500 N501 D502 M503 E504 S505 R506 G507 F508 I509 F510 V511 G512 K513 D514 E515 T516 G517 Q518 R519 C520 E521 I522 F523 E524 L525 K526 G527 H528 P529 Y530 Y531 V532 G533 T534 Q535 Y536 H537 P538 E539 Y540 T541 S542 K543 V544 L545 E546 P547 S548 R549 P550 F551 W552 G553 L554 V555 A556 A557 A558

S559 G560 T561 L562 G563 E564 V565 I566 K567 D568 I569 N570 L571

• Molecule 1: CTP synthase

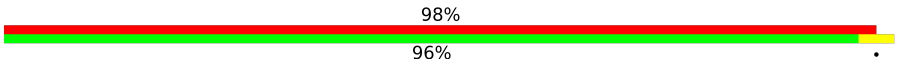
Chain a:

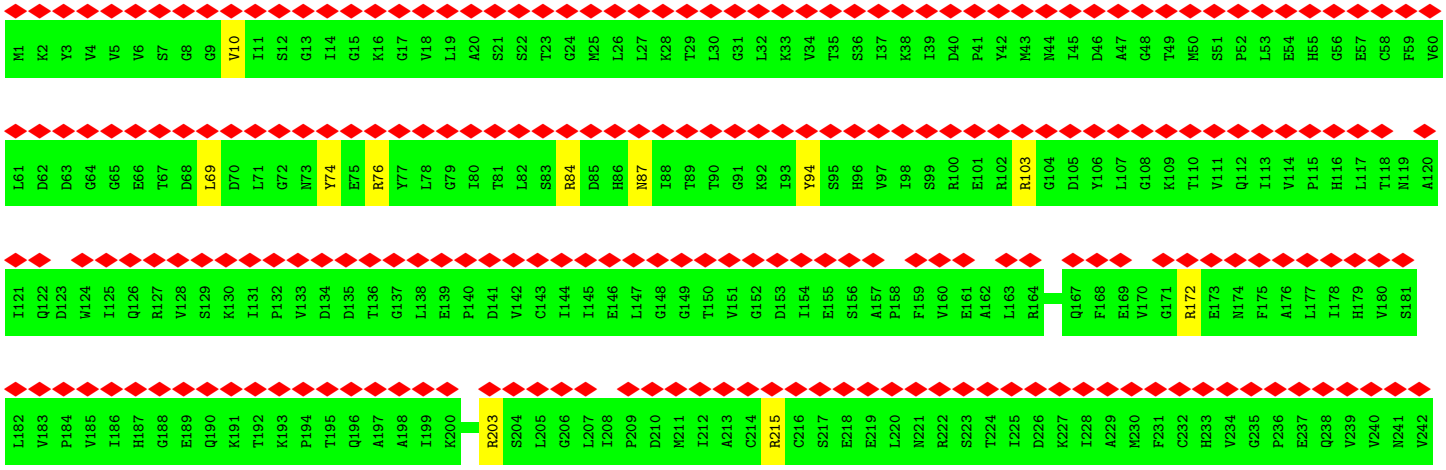




• Molecule 1: CTP synthase

Chain I:





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V303 V304 K305 I306 A307 L308 V309 G310 K311 Y312 T313 N314 L315 K316 D317 S318 Y319 L320 S321 V322 T323 K324 S325 L326 E327 H328 A329 S330 M331 K332 C333 R334 R335 Q336 L337 E338 I339 L340 W341 V342 E343 A344 S345 N346 L347 E348 P349 E350 T351 Q352 E353 V354 D355 K356 N357 K358 F359 H360 D361 S362

W363 N364 K365 L366 S367 S368 A369 D370 G371 I372 L373 V374 P375 G376 G377 F378 G379 T380 R381 G382 I383 E384 G385 M386 I387 L388 A389 A390 K391 W392 A393 R394 E395 S396 G397 V398 P399 F400 L401 G402 V403 C404 L405 G406 L407 Q408 V409 A410 A411 I412 E413 F414 A415 R416 N417 V418 I419 G420 R421 P422

N423 S424 S425 S426 T427 E428 F429 L430 D431 E432 T433 L434 L435 A436 P437 E438 D439 Q440 V441 V442 I443 T456 M457 R458 L459 G460 L461 R462 P463 T464 I465 F466 Q467 P468 N469 S470 E471 W472 S473 N474 I475 R476 K477 L478 Y479 G480 E481 V482 N483 E484 V485 H486 E487 R488 H489 R490 H491 R492 Y493 E494

I495 N496 P497 K498 I499 V500 N501 D502 M503 E504 S505 R506 G507 F508 I509 F510 V511 G512 K513 D514 E515 T516 G517 Q518 R519 C520 E521 I522 F523 E524 L525 K526 G527 H528 P529 Y530 Y531 V532 G533 T534 Q535 Y536 H537 P538 E539 Y540 T541 S542 K543 V544 L545 E546 P547 S548 R549 P550 F551 W552 G553 L554

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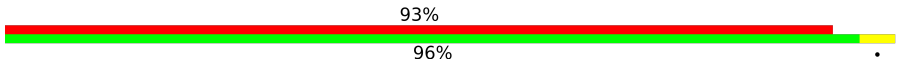
- Molecule 1: CTP synthase

Chain M:



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L61 D62 D63 G64 G65 E66 T67 D68 L69 D70 L71 G72 N73 Y74 E75 R76 Y77 L78 G79 I80 T81 L82 S83 R84 D85 H86 N87 I88 T89 T90 G91 K92 I93 Y94 R103 L107 G108 D123 W124 I125 Q126 R127 V128 S129 K130 I131 P132 V133 D134 D135 T136 G137 L138 E139 P140 D141 V142

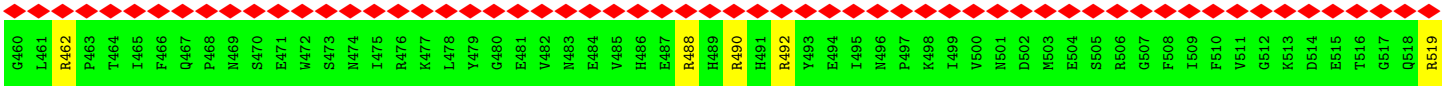
C143 I144 I145 E146 L147 G148 G149 T150 V151 G152 D153 I154 E155 S156 L163 R164 Q165 F166 Q167 F168 E169 V170 G171 R172 E173 N174 F175 A176 L177 I178 H179 V180 S181 L182 V183 P184 V185 I186 H187 G188 E189 Q190 K191 T192 K193 P194 T195 Q196 A197 A198 I199 K200 D201 L202 R203 S204 L205 G206 L207

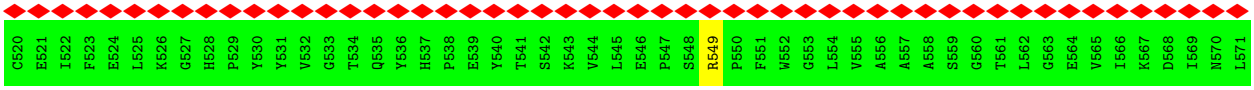
I208 P209 D210 M211 I212 A213 C214 R215 C216 S217 E218 E219 L220 N221 R222 S223 T224 I225 D226 K227 I228 A229 M230 F231 C232 H233 V234 G235 P236 E237 Q238 V239 Y240 N241 V242 H243 D244 V245 N246 S247 T248 Y249 H250 V251 P252 L253 L254 L255 L256 K257 Q258 H259 M260 I261 D262 Y263 L264 H265 S266 R267

L268 K269 L270 G271 E272 V273 P274 L275 T276 L277 E278 D279 K280 E281 R282 G283 S284 Q285 L286 L287 T288 N289 W290 E291 N292 M293 T294 K295 N296 L297 D298 D299 S300 D301 D302 V303 V304 K305 I306 A307 L308 V309 G310 K311 Y312 T313 N314 L315 K316 D317 S318 Y319 L320 S321 V322 T323 K324 S325 L326 E327

H328 A329 S330 M331 K332 C333 R334 R335 Q336 L337 E338 I339 L340 W341 V342 E343 A344 S345 N346 L347 E348 P349 E350 T351 Q352 E353 V354 D355 K356 N357 K358 F359 H360 D361 S362 W363 N364 K365 L366 S367 S368 A369 D370 G371 I372 L373 V374 P375 G376 G377 F378 G379 T380 R381 G382 I383 E384 G385 M386 I387

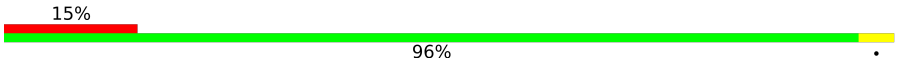
L388 A389 A390 K391 W392 A393 R394 E395 S396 G397 V398 P399 F400 L401 G402 V403 C404 L405 G406 L407 Q408 V409 A410 A411 I412 E413 F414 A415 R416 N417 V418 I419 G420 R421 P422 N423 S424 S425 S426 T427 E428 F429 L430 D431 E432 T433 L434 L435 A436 P437 E438 D439 Q440 V441 V442 I443 T456 M457 R458 L459

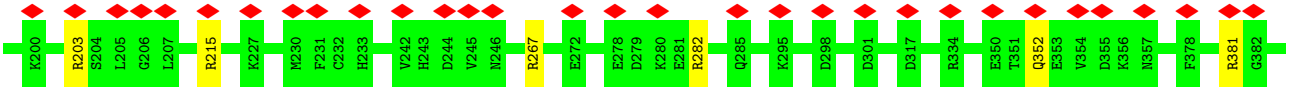


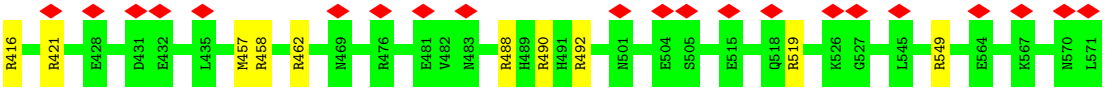


• Molecule 1: CTP synthase

Chain J:

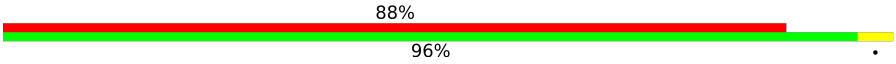


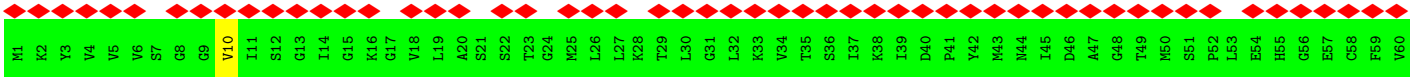


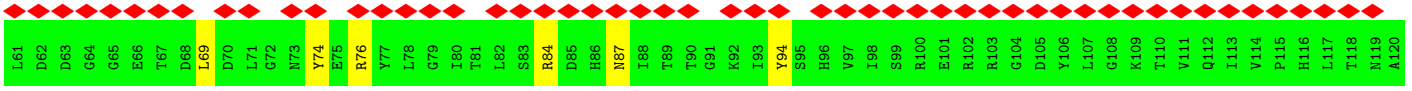


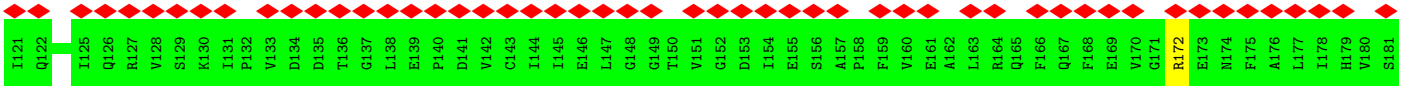
• Molecule 1: CTP synthase

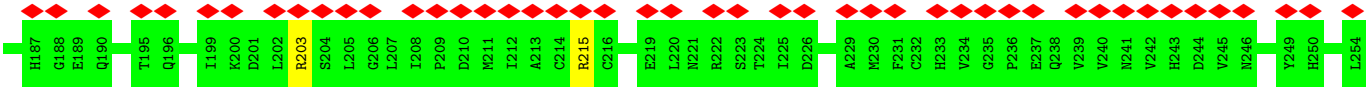
Chain N:

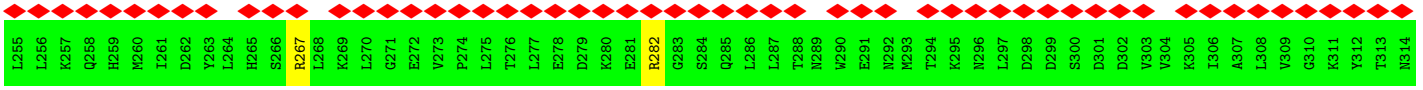


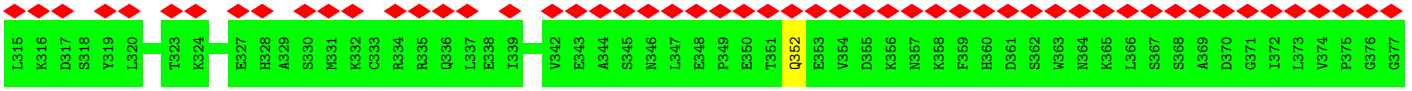


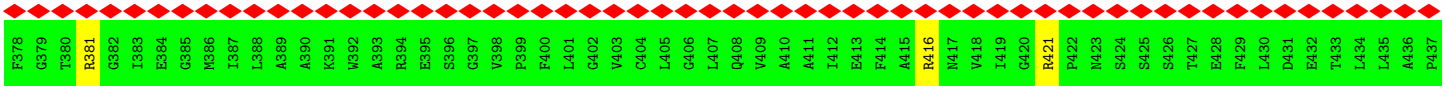


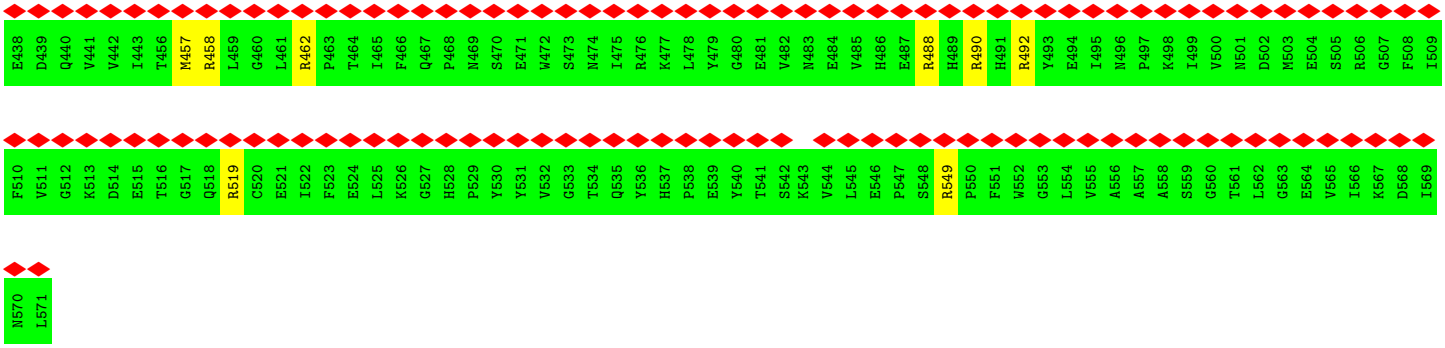






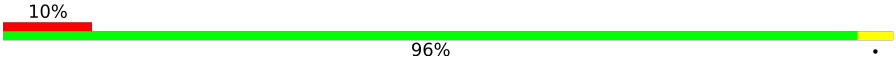


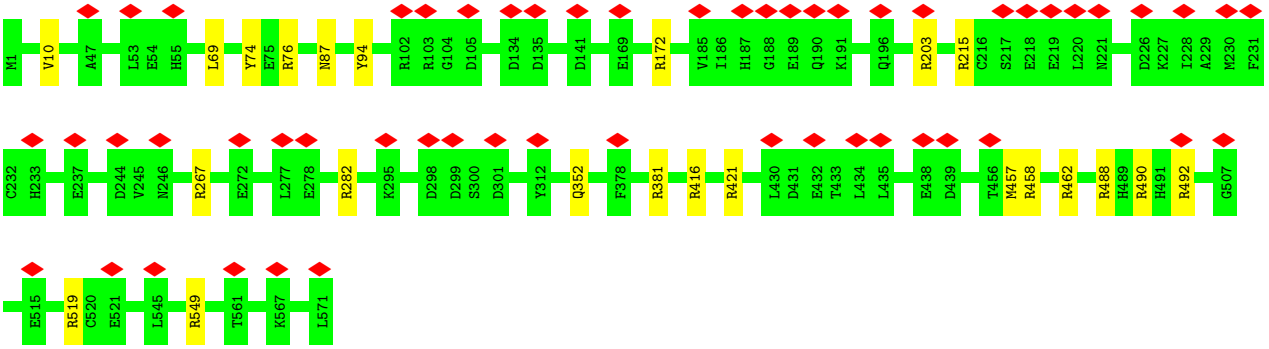




• Molecule 1: CTP synthase

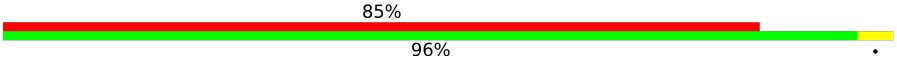
Chain R:

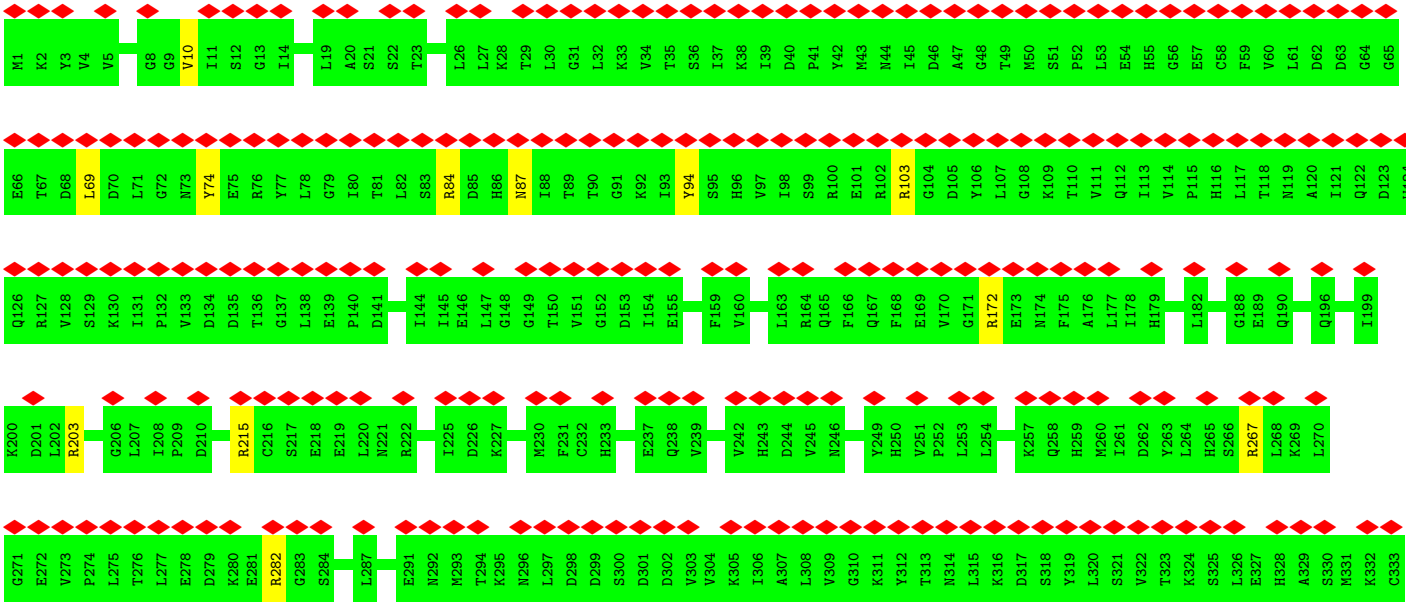


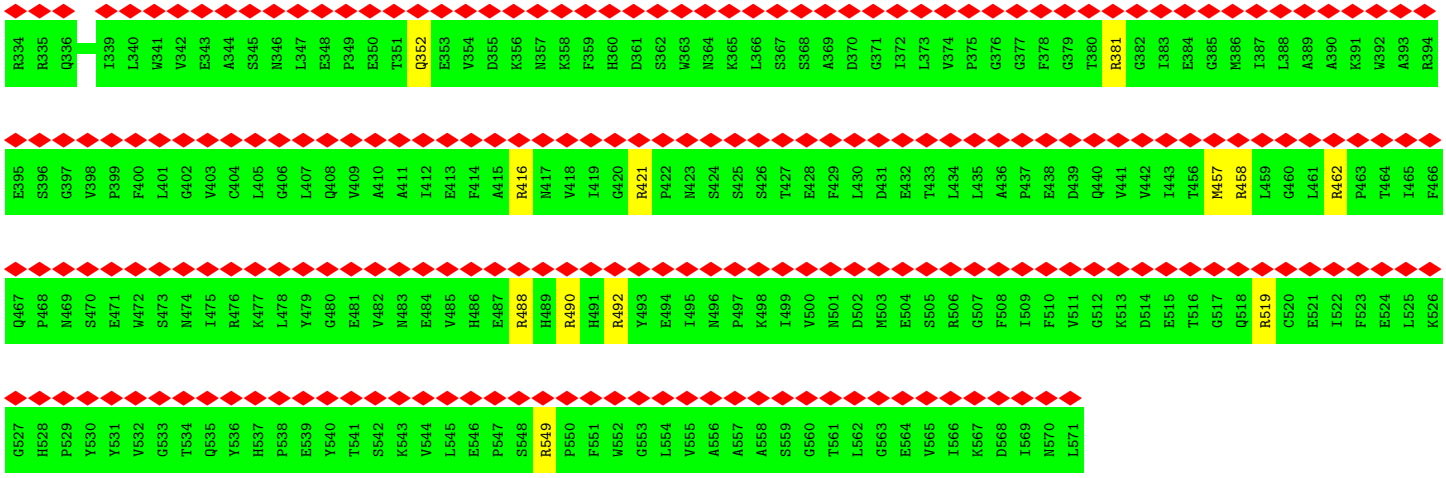


• Molecule 1: CTP synthase

Chain Z:

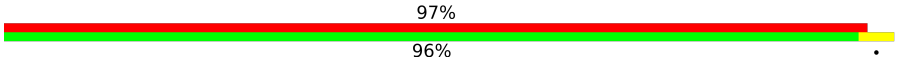


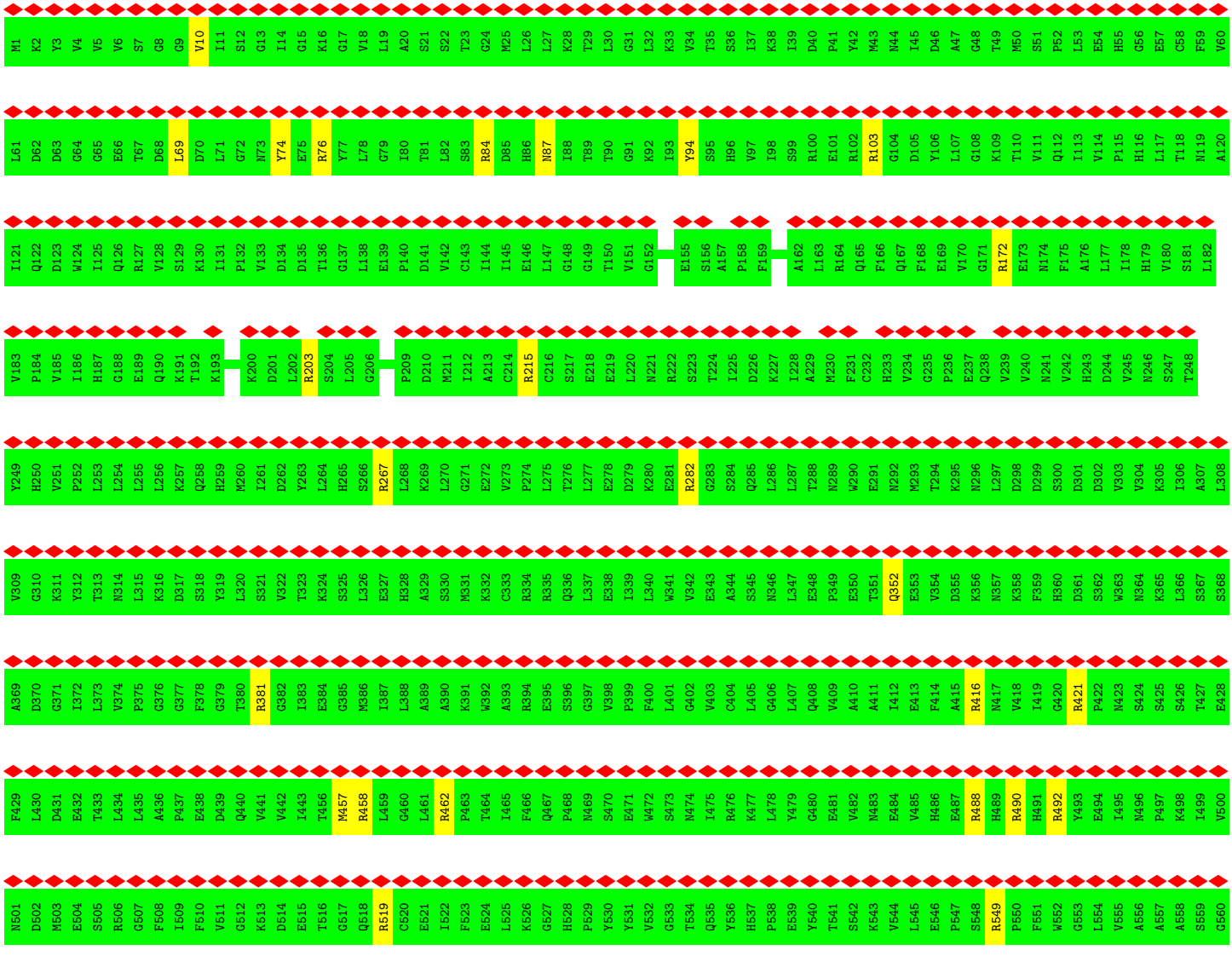


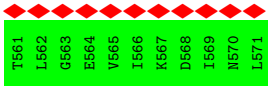


- Molecule 1: CTP synthase

Chain T:

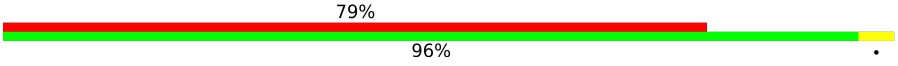


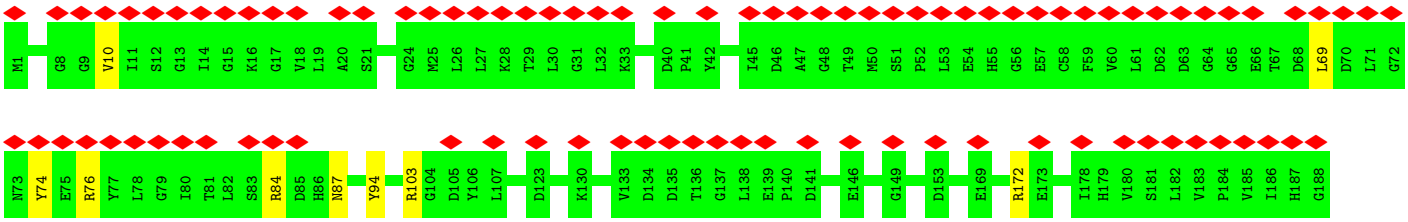




• Molecule 1: CTP synthase

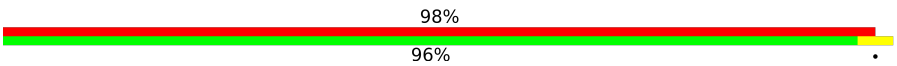
Chain b:

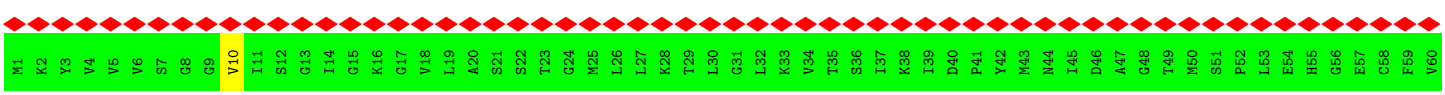


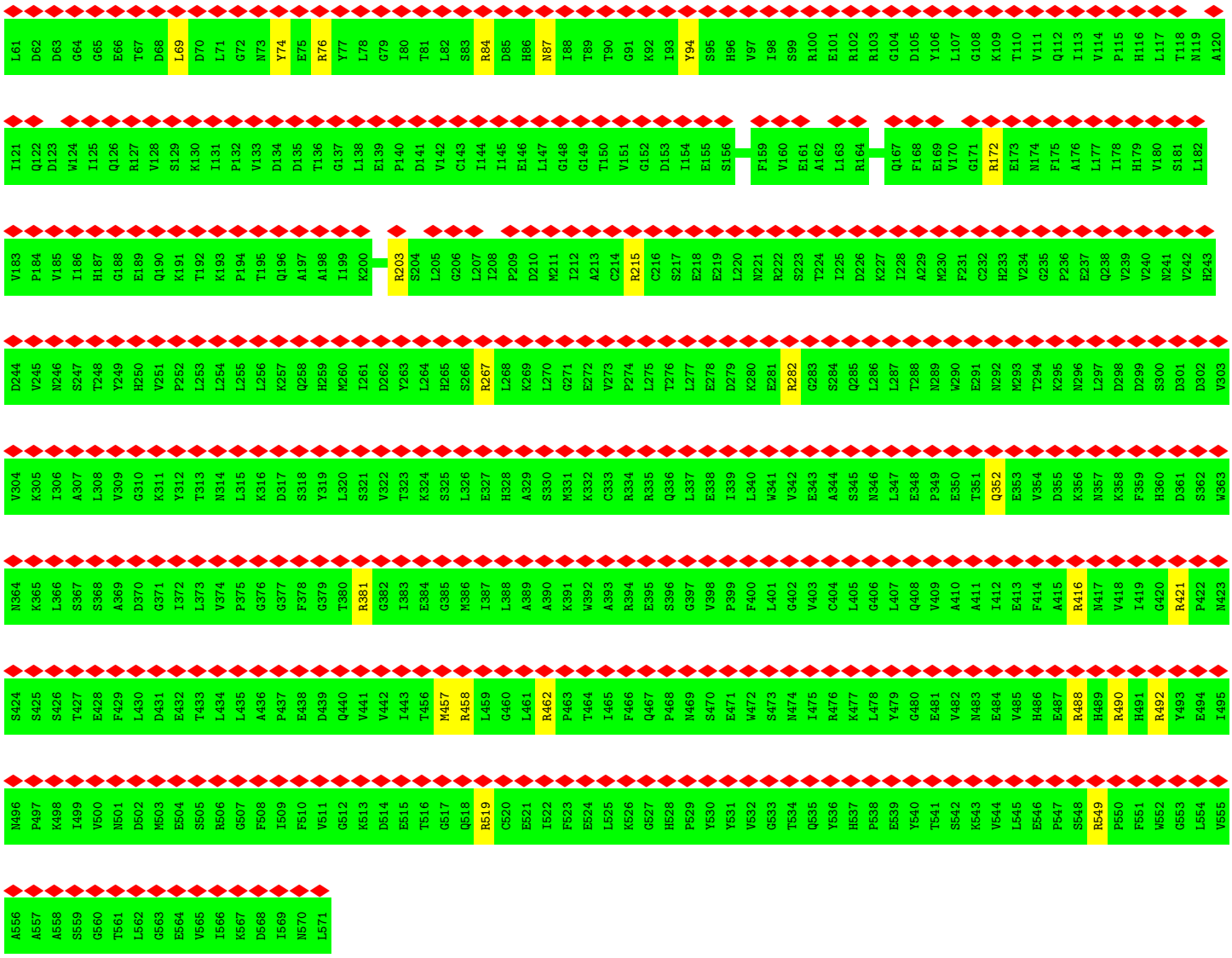


• Molecule 1: CTP synthase

Chain g:

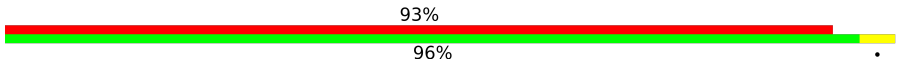


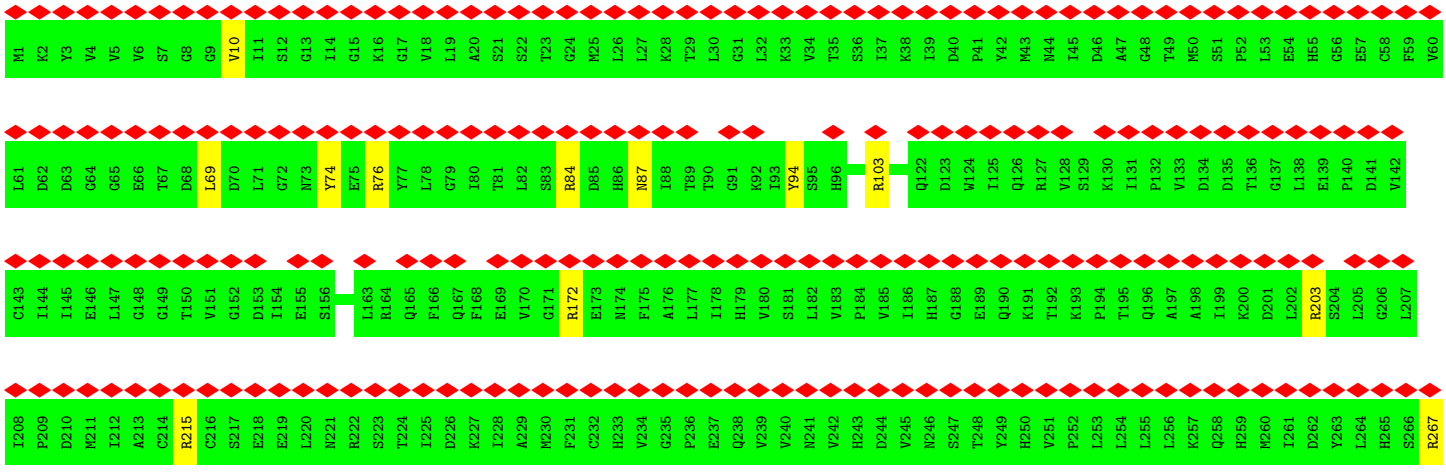


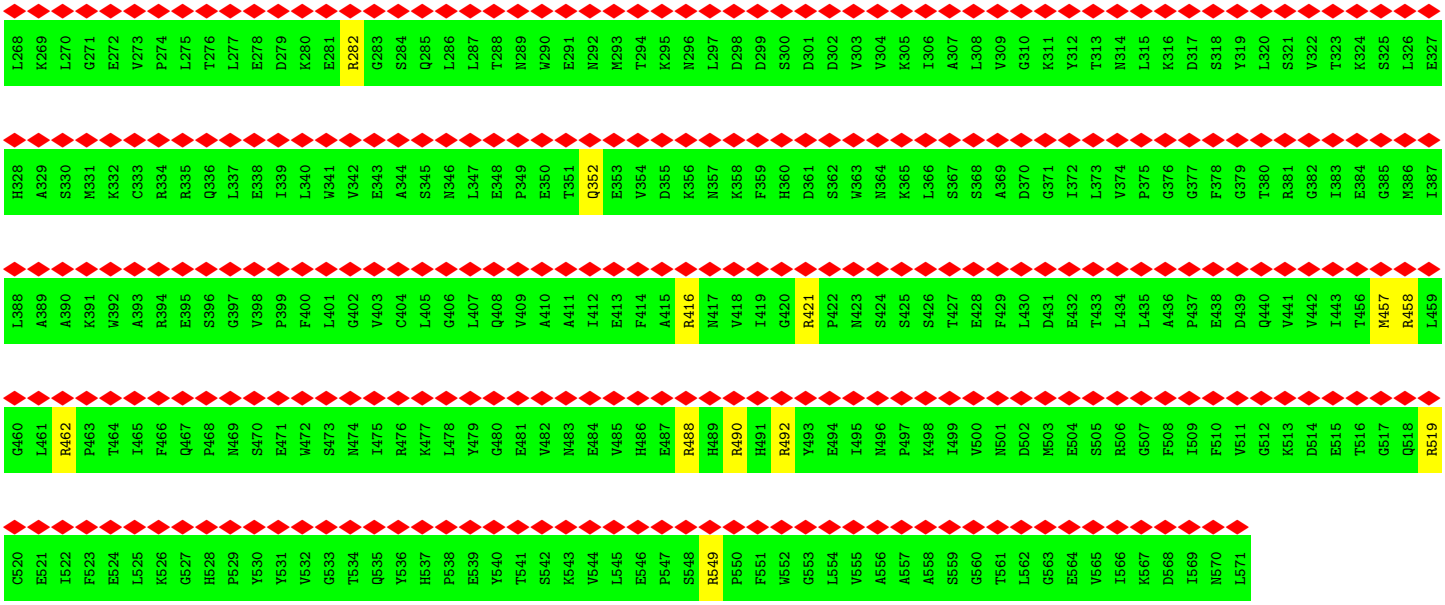


• Molecule 1: CTP synthase

Chain k:

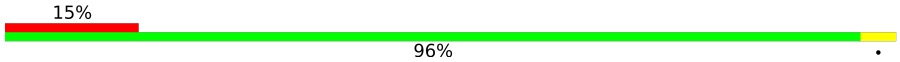


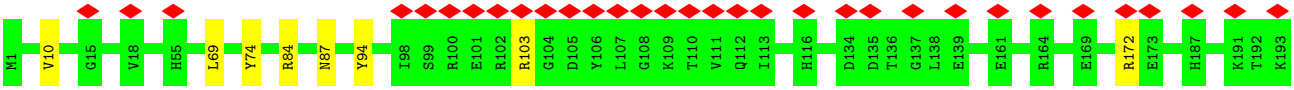


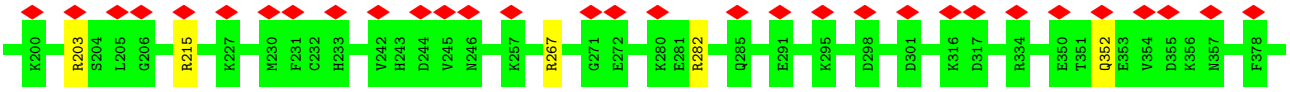


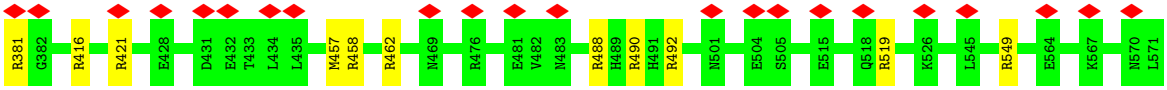
- Molecule 1: CTP synthase

Chain h:



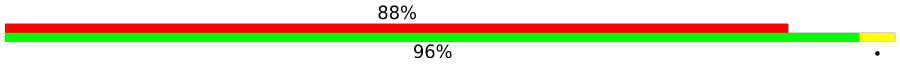


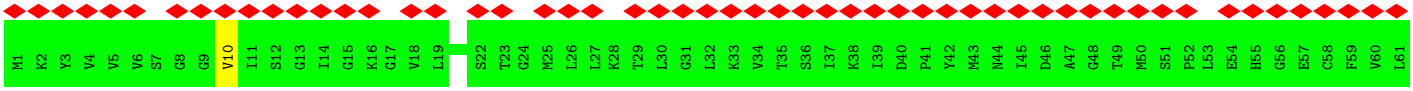


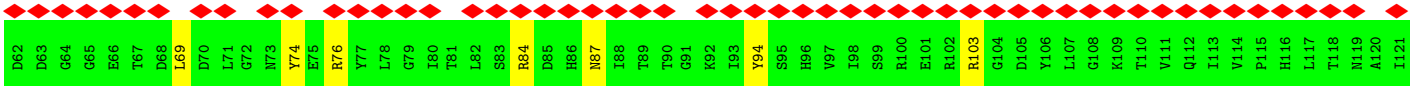


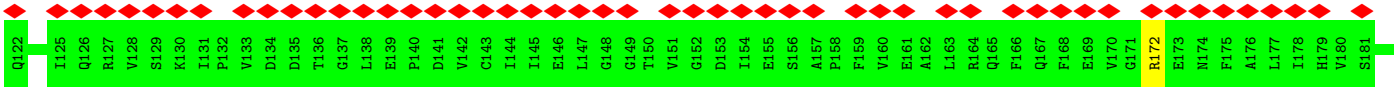
- Molecule 1: CTP synthase

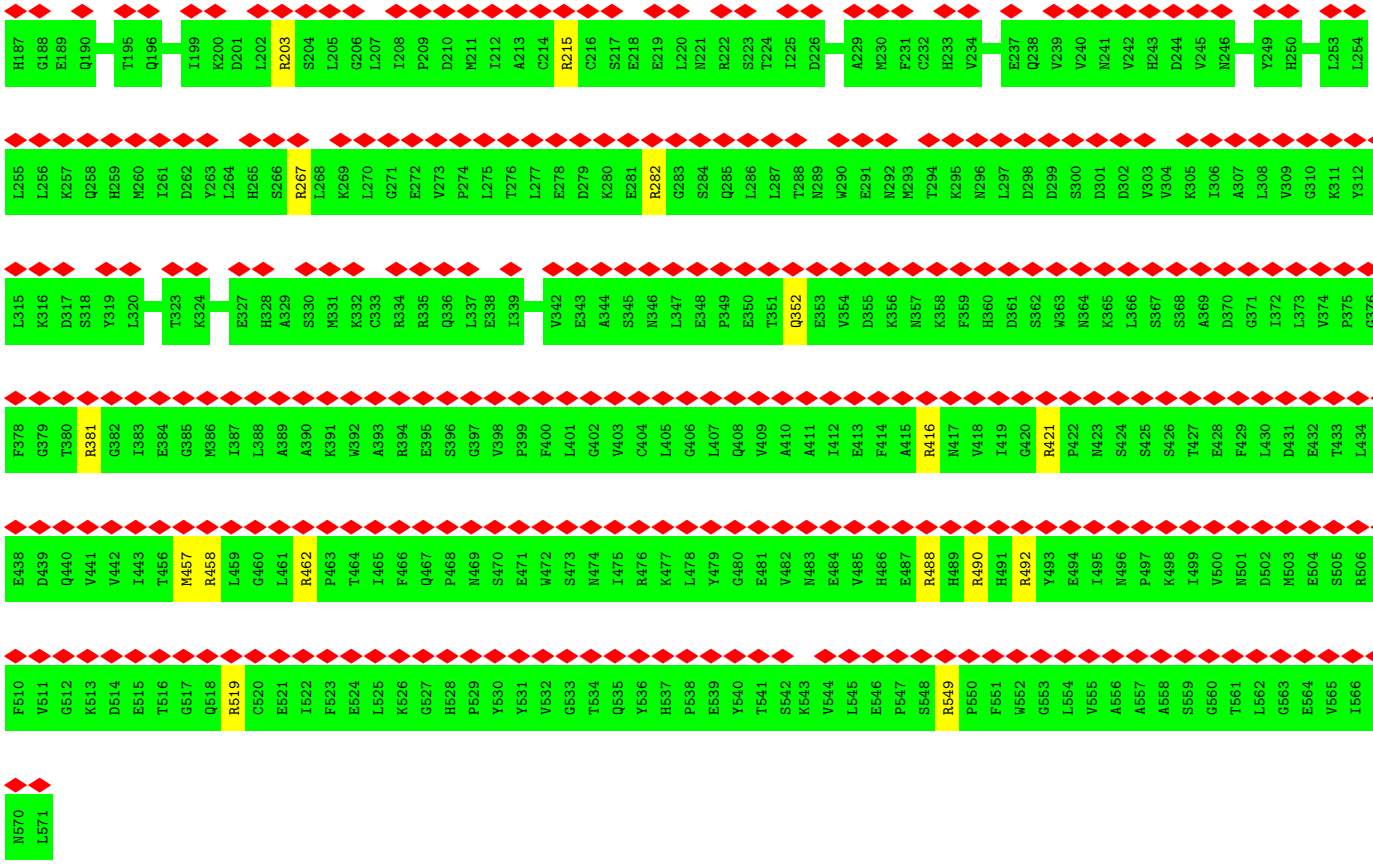
Chain l:







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L255 L256 K257 Q258 H259 M260 I261 D262 Y263 L264 H265 S266 R267 L268 K269 L270 G271 E272 V273 P274 L275 T276 L277 E278 D279 K280 E281 R282 G283 S284 Q285 L286 L287 T288 N289 W290 E291 N292 M293 T294 K295 N296 L297 D298 D299 S300 D301 D302 V303 V304 K305 I306 A307 L308 V309 G310 K311 Y312 T313 N314
L315 K316 D317 S318 Y319 L320 T323 K324 E327 H328 A329 S330 M331 K332 C333 R334 R335 Q336 L337 E338 I339 V342 E343 A344 S345 N346 L347 E348 P349 E350 T351 Q352 E353 V354 D355 K356 N357 K358 F359 H360 D361 S362 W363 N364 K365 L366 S367 S368 A369 D370 G371 I372 L373 V374 P375 G376 G377
F378 G379 T380 R381 G382 I383 E384 G385 M386 I387 L388 A389 A390 K391 W392 A393 R394 E395 S396 G397 V398 P399 F400 L401 G402 V403 C404 L405 G406 L407 Q408 V409 A410 A411 I412 E413 F414 A415 R416 N417 V418 I419 G420 R421 P422 N423 S424 S425 S426 T427 E428 F429 L430 D431 E432 T433 L434 L435 A436 P437
E438 D439 Q440 V441 V442 I443 T456 M457 R458 L459 G460 L461 R462 P463 T464 I465 F466 Q467 P468 N469 S470 E471 W472 S473 N474 I475 R476 K477 L478 Y479 G480 E481 V482 N483 E484 V485 H486 E487 R488 H489 R490 H491 R492 Y493 E494 I495 N496 P497 K498 I499 V500 N501 D502 M503 E504 S505 R506 G507 F508 I509
F510 V511 G512 K513 D514 E515 T516 G517 Q518 R519 C520 E521 I522 F523 E524 L525 K526 G527 H528 P529 Y530 Y531 V532 G533 T534 Q535 Y536 H537 P538 E539 Y540 T541 S542 K543 V544 L545 E546 P547 S548 R549 P550 F551 W552 G553 L554 V555 A556 A557 A558 S559 G560 T561 L562 G563 E564 V565 I566 K567 D568 I569
N570 L571

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UTP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.63	0/4471	1.04	19/6056 (0.3%)
1	B	0.63	0/4471	1.04	19/6056 (0.3%)
1	E	0.63	0/4471	1.04	19/6056 (0.3%)
1	F	0.63	0/4471	1.04	19/6056 (0.3%)
1	I	0.63	0/4471	1.04	20/6056 (0.3%)
1	J	0.63	0/4471	1.04	18/6056 (0.3%)
1	M	0.63	0/4471	1.04	18/6056 (0.3%)
1	N	0.63	0/4471	1.04	18/6056 (0.3%)
1	Q	0.63	0/4471	1.04	19/6056 (0.3%)
1	R	0.63	0/4471	1.04	17/6056 (0.3%)
1	S	0.63	0/4471	1.04	18/6056 (0.3%)
1	T	0.63	0/4471	1.04	19/6056 (0.3%)
1	Y	0.63	0/4471	1.04	19/6056 (0.3%)
1	Z	0.63	0/4471	1.04	18/6056 (0.3%)
1	a	0.63	0/4471	1.04	19/6056 (0.3%)
1	b	0.63	0/4471	1.04	19/6056 (0.3%)
1	g	0.63	0/4471	1.04	18/6056 (0.3%)
1	h	0.63	0/4471	1.04	18/6056 (0.3%)
1	k	0.63	0/4471	1.04	18/6056 (0.3%)
1	l	0.63	0/4471	1.04	19/6056 (0.3%)
All	All	0.63	0/89420	1.04	371/121120 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	E	0	1

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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 (371) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	549	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	T	549	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	a	549	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	S	549	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	k	549	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	h	549	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	g	549	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	F	549	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	B	549	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	N	549	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	b	549	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	E	549	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	I	549	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	M	549	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	Q	549	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	Y	549	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	549	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	Z	549	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	l	549	ARG	NE-CZ-NH1	7.93	124.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	549	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	Q	488	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	T	488	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	E	488	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	B	488	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	k	488	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	I	488	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	h	488	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	R	488	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	488	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	M	488	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	J	488	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	Z	488	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	S	488	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	N	488	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	Y	488	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	l	488	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	F	488	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	g	488	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	a	488	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	b	488	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	h	462	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	b	462	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	R	462	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	k	462	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	l	462	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	a	462	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	N	462	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	g	462	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	462	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	F	462	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	E	462	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	B	462	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	Q	462	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	T	462	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	S	462	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	Y	462	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	J	462	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	M	462	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	Z	462	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	I	462	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	S	267	ARG	NE-CZ-NH2	6.86	123.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	g	267	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	I	267	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	N	267	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	B	267	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	F	267	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	b	267	ARG	NE-CZ-NH2	6.77	123.69	120.30
1	A	267	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	R	267	ARG	NE-CZ-NH2	6.73	123.66	120.30
1	T	267	ARG	NE-CZ-NH2	6.73	123.66	120.30
1	l	267	ARG	NE-CZ-NH2	6.71	123.65	120.30
1	h	267	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	a	267	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	J	267	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	Z	267	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	Y	267	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	k	267	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	E	267	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	M	267	ARG	NE-CZ-NH2	6.63	123.62	120.30
1	Q	267	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	S	519	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	a	519	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	h	519	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	I	519	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	b	519	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	F	519	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	519	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	I	215	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	Z	519	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	N	519	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	T	519	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	J	519	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	R	519	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	Q	519	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	l	519	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	Z	215	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	519	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	h	215	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	E	519	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	k	519	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	Y	215	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	N	215	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	Y	519	ARG	NE-CZ-NH1	6.30	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	215	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	J	215	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	Q	215	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	215	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	g	519	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	E	215	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	k	215	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	l	492	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	S	492	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	b	215	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	J	492	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	M	215	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	F	215	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	k	492	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	M	519	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	215	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	I	492	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	R	215	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	S	215	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	g	215	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	l	215	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	b	492	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	E	492	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	492	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	T	215	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	N	492	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	T	492	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	F	492	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	R	492	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	Z	492	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	M	492	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	492	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	Y	492	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	g	492	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	Q	492	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	T	74	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	Y	74	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	Q	74	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	E	74	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	h	492	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	h	74	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	Z	74	TYR	CB-CG-CD2	-6.06	117.36	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	492	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	74	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	M	74	TYR	CB-CG-CD2	-6.06	117.37	121.00
1	B	74	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	S	74	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	a	74	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	l	416	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	I	74	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	g	74	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	R	74	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	N	74	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	k	74	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	J	74	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	M	416	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	F	74	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	b	74	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	Y	416	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	b	416	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	a	416	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	l	74	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	R	416	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	N	416	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	416	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	Z	416	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	F	416	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	I	416	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	k	416	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	Q	416	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	E	416	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	h	416	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	g	416	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	S	458	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	g	458	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	h	458	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	B	416	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	J	416	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	458	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	I	458	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	N	458	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	T	458	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	Q	458	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	A	458	ARG	NE-CZ-NH2	5.78	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	458	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	b	458	ARG	NE-CZ-NH2	5.77	123.18	120.30
1	l	458	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	Y	458	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	S	416	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	T	416	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	F	458	ARG	NE-CZ-NH2	5.73	123.16	120.30
1	J	458	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	a	458	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	k	458	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	M	458	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	E	458	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	Z	458	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	Q	490	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	k	203	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	R	490	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	I	490	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	Z	421	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	S	203	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	490	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	h	421	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	h	490	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	Z	203	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	J	203	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	g	490	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	k	490	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	Z	490	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	M	203	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	E	490	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	l	203	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	T	203	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	T	421	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	h	203	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	203	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	a	490	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	E	421	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	B	421	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	k	421	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	a	172	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	S	172	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	l	490	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	N	203	ARG	NE-CZ-NH1	5.39	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	g	203	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	203	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	h	172	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	Y	203	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	E	203	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	J	282	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	F	490	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	M	421	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	R	421	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	Y	421	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	S	421	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	Y	282	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	Y	490	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	J	421	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	b	172	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	Y	172	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	R	203	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	g	421	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	N	490	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	M	282	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	F	172	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	I	203	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	490	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	M	490	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	M	172	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	E	282	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	S	282	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	Z	172	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	Q	203	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	J	490	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	S	490	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	b	490	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	N	381	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	h	282	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	172	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	Q	172	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	Q	421	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	172	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	282	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	k	172	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	a	421	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	J	172	ARG	NE-CZ-NH1	5.29	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	172	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	l	172	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	172	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	F	203	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	g	76	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	I	421	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	421	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	k	282	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	F	421	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	T	490	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	b	203	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	l	421	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	T	282	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	I	282	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	g	172	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	l	282	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	R	282	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	a	203	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	N	421	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	b	381	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	M	103	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	Q	76	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	R	76	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	R	381	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	76	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	b	421	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	Z	282	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	b	282	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	I	76	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	N	282	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	I	172	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	R	172	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	282	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	F	282	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	N	172	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	a	76	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	h	103	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	a	381	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	A	381	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	F	381	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	b	76	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	g	381	ARG	NE-CZ-NH2	5.16	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	103	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	T	76	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	l	381	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	g	282	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	J	76	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	F	76	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	a	84	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	a	282	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	b	84	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	T	381	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	N	84	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	E	103	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	l	76	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	76	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	k	103	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	Q	381	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	I	381	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	a	103	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	g	84	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	Y	103	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	T	103	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	381	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	M	76	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	Z	84	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	l	84	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	103	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	Q	282	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	h	381	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	Y	76	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	J	84	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	Z	381	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	S	76	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	F	84	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	N	76	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	k	84	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	E	84	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	84	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	I	490	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	E	76	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	S	381	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	B	103	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	I	103	ARG	NE-CZ-NH1	5.03	122.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	490	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	I	84	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	h	84	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	l	103	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	Q	103	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	Y	84	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	T	84	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	k	76	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	J	381	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	A	84	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	M	381	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	A	103	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	E	381	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	S	103	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	Y	381	ARG	NE-CZ-NH2	5.00	122.80	120.30
1	b	103	ARG	NE-CZ-NH1	5.00	122.80	120.30

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 (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	B	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	E	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	F	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	I	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	J	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	M	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	N	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	Q	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	R	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	S	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	T	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	Y	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	Z	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	a	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	b	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	g	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	h	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	k	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
1	l	555/559 (99%)	541 (98%)	14 (2%)	0	100	100
All	All	11100/11180 (99%)	10820 (98%)	280 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	B	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	E	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	F	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	I	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	J	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	M	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	N	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	Q	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	R	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	S	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	T	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	Y	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	Z	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	a	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	b	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	g	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	h	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	k	488/488 (100%)	483 (99%)	5 (1%)	76	86
1	l	488/488 (100%)	483 (99%)	5 (1%)	76	86
All	All	9760/9760 (100%)	9660 (99%)	100 (1%)	77	86

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	69	LEU
1	A	87	ASN
1	A	352	GLN
1	A	457	MET
1	E	10	VAL
1	E	69	LEU
1	E	87	ASN
1	E	352	GLN
1	E	457	MET
1	B	10	VAL
1	B	69	LEU
1	B	87	ASN
1	B	352	GLN
1	B	457	MET
1	F	10	VAL
1	F	69	LEU
1	F	87	ASN
1	F	352	GLN
1	F	457	MET
1	Q	10	VAL
1	Q	69	LEU
1	Q	87	ASN
1	Q	352	GLN
1	Q	457	MET
1	Y	10	VAL
1	Y	69	LEU
1	Y	87	ASN
1	Y	352	GLN
1	Y	457	MET
1	S	10	VAL
1	S	69	LEU
1	S	87	ASN
1	S	352	GLN
1	S	457	MET
1	a	10	VAL
1	a	69	LEU
1	a	87	ASN
1	a	352	GLN
1	a	457	MET
1	I	10	VAL
1	I	69	LEU
1	I	87	ASN

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Mol	Chain	Res	Type
1	I	352	GLN
1	I	457	MET
1	M	10	VAL
1	M	69	LEU
1	M	87	ASN
1	M	352	GLN
1	M	457	MET
1	J	10	VAL
1	J	69	LEU
1	J	87	ASN
1	J	352	GLN
1	J	457	MET
1	N	10	VAL
1	N	69	LEU
1	N	87	ASN
1	N	352	GLN
1	N	457	MET
1	R	10	VAL
1	R	69	LEU
1	R	87	ASN
1	R	352	GLN
1	R	457	MET
1	Z	10	VAL
1	Z	69	LEU
1	Z	87	ASN
1	Z	352	GLN
1	Z	457	MET
1	T	10	VAL
1	T	69	LEU
1	T	87	ASN
1	T	352	GLN
1	T	457	MET
1	b	10	VAL
1	b	69	LEU
1	b	87	ASN
1	b	352	GLN
1	b	457	MET
1	g	10	VAL
1	g	69	LEU
1	g	87	ASN
1	g	352	GLN
1	g	457	MET

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Mol	Chain	Res	Type
1	k	10	VAL
1	k	69	LEU
1	k	87	ASN
1	k	352	GLN
1	k	457	MET
1	h	10	VAL
1	h	69	LEU
1	h	87	ASN
1	h	352	GLN
1	h	457	MET
1	l	10	VAL
1	l	69	LEU
1	l	87	ASN
1	l	352	GLN
1	l	457	MET

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

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 80 ligands modelled in this entry, 40 are monoatomic - leaving 40 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	UTP	T	601	3	22,30,30	1.08	1 (4%)	27,47,47	1.45	5 (18%)
2	ATP	E	601	3	26,33,33	1.13	2 (7%)	31,52,52	1.48	4 (12%)
2	ATP	R	601	3	26,33,33	1.15	2 (7%)	31,52,52	1.48	4 (12%)
2	ATP	Y	601	3	26,33,33	1.12	2 (7%)	31,52,52	1.47	4 (12%)
2	ATP	k	601	3	26,33,33	1.12	2 (7%)	31,52,52	1.47	4 (12%)
2	ATP	l	602	3	26,33,33	1.13	2 (7%)	31,52,52	1.48	4 (12%)
2	ATP	B	602	3	26,33,33	1.14	2 (7%)	31,52,52	1.48	4 (12%)
2	ATP	M	601	3	26,33,33	1.13	2 (7%)	31,52,52	1.48	4 (12%)
4	UTP	b	601	3	22,30,30	1.07	1 (4%)	27,47,47	1.44	5 (18%)
2	ATP	a	602	3	26,33,33	1.15	2 (7%)	31,52,52	1.48	4 (12%)
4	UTP	M	603	3	22,30,30	1.06	1 (4%)	27,47,47	1.44	5 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	h	602	3	-	0/18/38/38	0/3/3/3
4	UTP	a	601	3	2/2/7/7	6/20/38/38	0/2/2/2
4	UTP	I	605	3	2/2/7/7	11/20/38/38	0/2/2/2
4	UTP	F	601	3	2/2/7/7	11/20/38/38	0/2/2/2
4	UTP	g	605	3	2/2/7/7	11/20/38/38	0/2/2/2
2	ATP	Z	601	3	-	0/18/38/38	0/3/3/3
2	ATP	T	602	3	-	0/18/38/38	0/3/3/3
4	UTP	B	601	3	2/2/7/7	6/20/38/38	0/2/2/2
4	UTP	E	603	3	2/2/7/7	6/20/38/38	0/2/2/2
2	ATP	N	602	3	-	0/18/38/38	0/3/3/3
4	UTP	Z	603	3	2/2/7/7	10/20/38/38	0/2/2/2
4	UTP	A	605	3	2/2/7/7	11/20/38/38	0/2/2/2
4	UTP	S	601	3	2/2/7/7	8/20/38/38	0/2/2/2
4	UTP	h	601	3	2/2/7/7	6/20/38/38	0/2/2/2
4	UTP	Y	603	3	2/2/7/7	10/20/38/38	0/2/2/2
2	ATP	F	602	3	-	0/18/38/38	0/3/3/3
2	ATP	I	601	3	-	0/18/38/38	0/3/3/3
2	ATP	g	601	3	-	0/18/38/38	0/3/3/3
2	ATP	b	602	3	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UTP	R	605	3	2/2/7/7	6/20/38/38	0/2/2/2
4	UTP	J	601	3	2/2/7/7	6/20/38/38	0/2/2/2
4	UTP	Q	605	3	2/2/7/7	6/20/38/38	0/2/2/2
4	UTP	N	601	3	2/2/7/7	10/20/38/38	0/2/2/2
2	ATP	A	601	3	-	0/18/38/38	0/3/3/3
2	ATP	Q	601	3	-	0/18/38/38	0/3/3/3
4	UTP	l	601	3	2/2/7/7	10/20/38/38	0/2/2/2
2	ATP	J	602	3	-	0/18/38/38	0/3/3/3
2	ATP	S	602	3	-	0/18/38/38	0/3/3/3
4	UTP	k	603	3	2/2/7/7	9/20/38/38	0/2/2/2
4	UTP	T	601	3	2/2/7/7	8/20/38/38	0/2/2/2
2	ATP	E	601	3	-	0/18/38/38	0/3/3/3
2	ATP	R	601	3	-	0/18/38/38	0/3/3/3
2	ATP	Y	601	3	-	0/18/38/38	0/3/3/3
2	ATP	k	601	3	-	0/18/38/38	0/3/3/3
2	ATP	l	602	3	-	0/18/38/38	0/3/3/3
2	ATP	B	602	3	-	0/18/38/38	0/3/3/3
2	ATP	M	601	3	-	0/18/38/38	0/3/3/3
4	UTP	b	601	3	2/2/7/7	6/20/38/38	0/2/2/2
2	ATP	a	602	3	-	0/18/38/38	0/3/3/3
4	UTP	M	603	3	2/2/7/7	9/20/38/38	0/2/2/2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	601	UTP	C4-N3	3.02	1.38	1.33
2	I	601	ATP	O4'-C1'	3.00	1.45	1.41
4	h	601	UTP	C4-N3	3.00	1.38	1.33
4	k	603	UTP	C4-N3	3.00	1.38	1.33
4	Y	603	UTP	C4-N3	3.00	1.38	1.33
4	l	601	UTP	C4-N3	3.00	1.38	1.33
4	F	601	UTP	C4-N3	2.99	1.38	1.33
4	J	601	UTP	C4-N3	2.99	1.38	1.33
2	Q	601	ATP	O4'-C1'	2.98	1.45	1.41
4	E	603	UTP	C4-N3	2.98	1.38	1.33
4	B	601	UTP	C4-N3	2.98	1.38	1.33
4	S	601	UTP	C4-N3	2.98	1.38	1.33
2	R	601	ATP	O4'-C1'	2.98	1.45	1.41
4	M	603	UTP	C4-N3	2.98	1.38	1.33
4	T	601	UTP	C4-N3	2.97	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ATP	O4'-C1'	2.97	1.45	1.41
4	N	601	UTP	C4-N3	2.97	1.38	1.33
4	I	605	UTP	C4-N3	2.96	1.38	1.33
4	g	605	UTP	C4-N3	2.96	1.38	1.33
2	S	602	ATP	O4'-C1'	2.95	1.45	1.41
4	Z	603	UTP	C4-N3	2.95	1.38	1.33
4	a	601	UTP	C4-N3	2.95	1.38	1.33
2	g	601	ATP	O4'-C1'	2.95	1.45	1.41
2	N	602	ATP	O4'-C1'	2.95	1.45	1.41
4	A	605	UTP	C4-N3	2.94	1.38	1.33
2	a	602	ATP	O4'-C1'	2.94	1.45	1.41
2	J	602	ATP	O4'-C1'	2.93	1.45	1.41
4	Q	605	UTP	C4-N3	2.93	1.38	1.33
2	M	601	ATP	O4'-C1'	2.93	1.45	1.41
2	F	602	ATP	O4'-C1'	2.93	1.45	1.41
2	B	602	ATP	O4'-C1'	2.92	1.45	1.41
2	T	602	ATP	O4'-C1'	2.91	1.45	1.41
2	h	602	ATP	O4'-C1'	2.91	1.45	1.41
4	R	605	UTP	C4-N3	2.89	1.38	1.33
2	b	602	ATP	O4'-C1'	2.89	1.45	1.41
2	E	601	ATP	O4'-C1'	2.87	1.45	1.41
2	Z	601	ATP	O4'-C1'	2.86	1.45	1.41
2	l	602	ATP	O4'-C1'	2.86	1.45	1.41
2	k	601	ATP	O4'-C1'	2.83	1.45	1.41
2	Y	601	ATP	O4'-C1'	2.81	1.45	1.41
2	R	601	ATP	C5-C4	-2.06	1.35	1.40
2	J	602	ATP	C5-C4	-2.06	1.35	1.40
2	g	601	ATP	C5-C4	-2.05	1.35	1.40
2	M	601	ATP	C5-C4	-2.04	1.35	1.40
2	S	602	ATP	C5-C4	-2.04	1.35	1.40
2	B	602	ATP	C5-C4	-2.04	1.35	1.40
2	l	602	ATP	C5-C4	-2.04	1.35	1.40
2	A	601	ATP	C5-C4	-2.04	1.35	1.40
2	N	602	ATP	C5-C4	-2.03	1.35	1.40
2	h	602	ATP	C5-C4	-2.03	1.35	1.40
2	Z	601	ATP	C5-C4	-2.03	1.35	1.40
2	b	602	ATP	C5-C4	-2.03	1.35	1.40
2	a	602	ATP	C5-C4	-2.03	1.35	1.40
2	T	602	ATP	C5-C4	-2.02	1.35	1.40
2	k	601	ATP	C5-C4	-2.02	1.35	1.40
2	Y	601	ATP	C5-C4	-2.02	1.35	1.40
2	E	601	ATP	C5-C4	-2.02	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	601	ATP	C5-C4	-2.02	1.35	1.40
2	I	601	ATP	C5-C4	-2.02	1.35	1.40
2	F	602	ATP	C5-C4	-2.02	1.35	1.40

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	602	ATP	C4-C5-N7	4.18	113.75	109.40
2	I	601	ATP	C4-C5-N7	4.17	113.75	109.40
2	g	601	ATP	C4-C5-N7	4.17	113.74	109.40
2	Q	601	ATP	C4-C5-N7	4.17	113.74	109.40
2	Z	601	ATP	C4-C5-N7	4.17	113.74	109.40
2	h	602	ATP	C4-C5-N7	4.16	113.74	109.40
2	A	601	ATP	C4-C5-N7	4.16	113.73	109.40
2	M	601	ATP	C4-C5-N7	4.16	113.73	109.40
4	l	601	UTP	C5-C4-N3	-4.16	114.17	123.31
2	B	602	ATP	C4-C5-N7	4.15	113.72	109.40
2	N	602	ATP	C4-C5-N7	4.15	113.72	109.40
2	R	601	ATP	C4-C5-N7	4.14	113.72	109.40
2	T	602	ATP	C4-C5-N7	4.14	113.72	109.40
4	b	601	UTP	C5-C4-N3	-4.14	114.20	123.31
4	T	601	UTP	C5-C4-N3	-4.14	114.20	123.31
4	g	605	UTP	C5-C4-N3	-4.14	114.21	123.31
2	l	602	ATP	C4-C5-N7	4.14	113.71	109.40
2	E	601	ATP	C4-C5-N7	4.13	113.71	109.40
2	b	602	ATP	C4-C5-N7	4.13	113.71	109.40
2	J	602	ATP	C4-C5-N7	4.13	113.70	109.40
4	E	603	UTP	C5-C4-N3	-4.13	114.22	123.31
4	F	601	UTP	C5-C4-N3	-4.13	114.22	123.31
4	k	603	UTP	C5-C4-N3	-4.13	114.23	123.31
4	J	601	UTP	C5-C4-N3	-4.12	114.24	123.31
4	h	601	UTP	C5-C4-N3	-4.12	114.24	123.31
4	Y	603	UTP	C5-C4-N3	-4.12	114.24	123.31
4	B	601	UTP	C5-C4-N3	-4.12	114.24	123.31
4	N	601	UTP	C5-C4-N3	-4.12	114.24	123.31
2	F	602	ATP	C4-C5-N7	4.12	113.69	109.40
4	A	605	UTP	C5-C4-N3	-4.12	114.25	123.31
4	I	605	UTP	C5-C4-N3	-4.12	114.25	123.31
4	Q	605	UTP	C5-C4-N3	-4.12	114.25	123.31
4	M	603	UTP	C5-C4-N3	-4.12	114.25	123.31
4	Z	603	UTP	C5-C4-N3	-4.12	114.25	123.31
4	S	601	UTP	C5-C4-N3	-4.11	114.26	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	a	601	UTP	C5-C4-N3	-4.11	114.26	123.31
2	k	601	ATP	C4-C5-N7	4.11	113.68	109.40
4	R	605	UTP	C5-C4-N3	-4.10	114.29	123.31
2	S	602	ATP	C4-C5-N7	4.10	113.67	109.40
2	Y	601	ATP	C4-C5-N7	4.08	113.65	109.40
2	R	601	ATP	PB-O3B-PG	-3.91	119.40	132.83
2	Z	601	ATP	PB-O3B-PG	-3.91	119.40	132.83
2	Y	601	ATP	PB-O3B-PG	-3.91	119.40	132.83
2	M	601	ATP	PB-O3B-PG	-3.91	119.40	132.83
2	h	602	ATP	PB-O3B-PG	-3.91	119.40	132.83
2	l	602	ATP	PB-O3B-PG	-3.91	119.42	132.83
2	S	602	ATP	PB-O3B-PG	-3.91	119.42	132.83
2	E	601	ATP	PB-O3B-PG	-3.91	119.42	132.83
2	B	602	ATP	PB-O3B-PG	-3.91	119.42	132.83
2	A	601	ATP	PB-O3B-PG	-3.90	119.43	132.83
2	g	601	ATP	PB-O3B-PG	-3.90	119.43	132.83
2	b	602	ATP	PB-O3B-PG	-3.90	119.44	132.83
2	I	601	ATP	PB-O3B-PG	-3.90	119.44	132.83
2	N	602	ATP	PB-O3B-PG	-3.90	119.45	132.83
2	T	602	ATP	PB-O3B-PG	-3.90	119.45	132.83
2	k	601	ATP	PB-O3B-PG	-3.90	119.45	132.83
2	Q	601	ATP	PB-O3B-PG	-3.90	119.46	132.83
2	F	602	ATP	PB-O3B-PG	-3.90	119.46	132.83
2	J	602	ATP	PB-O3B-PG	-3.89	119.47	132.83
2	a	602	ATP	PB-O3B-PG	-3.88	119.51	132.83
2	M	601	ATP	PA-O3A-PB	-3.29	121.52	132.83
2	E	601	ATP	PA-O3A-PB	-3.29	121.55	132.83
2	Z	601	ATP	PA-O3A-PB	-3.29	121.55	132.83
2	Y	601	ATP	PA-O3A-PB	-3.28	121.56	132.83
2	a	602	ATP	PA-O3A-PB	-3.28	121.56	132.83
2	k	601	ATP	PA-O3A-PB	-3.28	121.57	132.83
2	R	601	ATP	PA-O3A-PB	-3.28	121.58	132.83
2	T	602	ATP	PA-O3A-PB	-3.27	121.59	132.83
2	b	602	ATP	PA-O3A-PB	-3.27	121.59	132.83
2	A	601	ATP	PA-O3A-PB	-3.27	121.59	132.83
2	F	602	ATP	PA-O3A-PB	-3.27	121.59	132.83
2	N	602	ATP	PA-O3A-PB	-3.27	121.60	132.83
2	B	602	ATP	PA-O3A-PB	-3.27	121.60	132.83
2	h	602	ATP	PA-O3A-PB	-3.27	121.60	132.83
2	I	601	ATP	PA-O3A-PB	-3.27	121.61	132.83
2	l	602	ATP	PA-O3A-PB	-3.27	121.61	132.83
2	S	602	ATP	PA-O3A-PB	-3.27	121.62	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	601	ATP	PA-O3A-PB	-3.26	121.62	132.83
2	g	601	ATP	PA-O3A-PB	-3.26	121.64	132.83
2	J	602	ATP	PA-O3A-PB	-3.26	121.65	132.83
4	g	605	UTP	O4'-C1'-C2'	3.02	111.34	106.93
4	Z	603	UTP	O4'-C1'-C2'	3.01	111.33	106.93
4	Q	605	UTP	O4'-C1'-C2'	3.00	111.31	106.93
4	I	605	UTP	O4'-C1'-C2'	3.00	111.31	106.93
4	b	601	UTP	O4'-C1'-C2'	3.00	111.31	106.93
4	M	603	UTP	O4'-C1'-C2'	2.99	111.30	106.93
4	Y	603	UTP	O4'-C1'-C2'	2.98	111.29	106.93
4	A	605	UTP	O4'-C1'-C2'	2.97	111.27	106.93
4	h	601	UTP	O4'-C1'-C2'	2.97	111.27	106.93
4	E	603	UTP	O4'-C1'-C2'	2.97	111.26	106.93
4	l	601	UTP	O4'-C1'-C2'	2.97	111.26	106.93
4	F	601	UTP	O4'-C1'-C2'	2.96	111.26	106.93
4	B	601	UTP	O4'-C1'-C2'	2.96	111.25	106.93
4	k	603	UTP	O4'-C1'-C2'	2.96	111.25	106.93
4	N	601	UTP	O4'-C1'-C2'	2.96	111.25	106.93
4	R	605	UTP	O4'-C1'-C2'	2.95	111.24	106.93
4	J	601	UTP	O4'-C1'-C2'	2.95	111.23	106.93
4	S	601	UTP	O4'-C1'-C2'	2.94	111.22	106.93
4	a	601	UTP	O4'-C1'-C2'	2.93	111.21	106.93
4	T	601	UTP	O4'-C1'-C2'	2.93	111.20	106.93
4	R	605	UTP	O4'-C4'-C5'	2.57	117.84	109.37
4	A	605	UTP	O4'-C4'-C5'	2.56	117.78	109.37
4	I	605	UTP	O4'-C4'-C5'	2.56	117.78	109.37
4	a	601	UTP	O4'-C4'-C5'	2.55	117.76	109.37
4	h	601	UTP	O4'-C4'-C5'	2.55	117.75	109.37
4	g	605	UTP	O4'-C4'-C5'	2.55	117.75	109.37
4	Q	605	UTP	O4'-C4'-C5'	2.54	117.74	109.37
4	k	603	UTP	O4'-C4'-C5'	2.54	117.74	109.37
4	J	601	UTP	O4'-C4'-C5'	2.54	117.73	109.37
4	Y	603	UTP	O4'-C4'-C5'	2.54	117.73	109.37
4	T	601	UTP	O4'-C4'-C5'	2.54	117.72	109.37
4	b	601	UTP	O4'-C4'-C5'	2.54	117.72	109.37
4	F	601	UTP	O4'-C4'-C5'	2.54	117.72	109.37
4	B	601	UTP	O4'-C4'-C5'	2.54	117.71	109.37
4	Z	603	UTP	O4'-C4'-C5'	2.53	117.71	109.37
4	E	603	UTP	O4'-C4'-C5'	2.53	117.71	109.37
4	M	603	UTP	O4'-C4'-C5'	2.53	117.70	109.37
4	S	601	UTP	O4'-C4'-C5'	2.53	117.70	109.37
4	l	601	UTP	O4'-C4'-C5'	2.53	117.70	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	601	UTP	O4'-C4'-C5'	2.52	117.68	109.37
4	l	601	UTP	C5'-C4'-C3'	2.43	124.30	115.18
4	N	601	UTP	C5'-C4'-C3'	2.43	124.30	115.18
4	B	601	UTP	C5'-C4'-C3'	2.43	124.28	115.18
4	J	601	UTP	C5'-C4'-C3'	2.43	124.28	115.18
4	T	601	UTP	C5'-C4'-C3'	2.43	124.28	115.18
4	b	601	UTP	C5'-C4'-C3'	2.43	124.27	115.18
4	F	601	UTP	C5'-C4'-C3'	2.43	124.27	115.18
4	h	601	UTP	C5'-C4'-C3'	2.43	124.27	115.18
4	M	603	UTP	C5'-C4'-C3'	2.42	124.27	115.18
4	Q	605	UTP	C5'-C4'-C3'	2.42	124.25	115.18
4	a	601	UTP	C5'-C4'-C3'	2.42	124.25	115.18
4	S	601	UTP	C5'-C4'-C3'	2.42	124.25	115.18
4	E	603	UTP	C5'-C4'-C3'	2.41	124.23	115.18
4	g	605	UTP	C5'-C4'-C3'	2.41	124.23	115.18
4	A	605	UTP	C5'-C4'-C3'	2.41	124.22	115.18
4	k	603	UTP	C5'-C4'-C3'	2.41	124.22	115.18
4	Z	603	UTP	C5'-C4'-C3'	2.41	124.22	115.18
4	I	605	UTP	C5'-C4'-C3'	2.41	124.22	115.18
4	Y	603	UTP	C5'-C4'-C3'	2.41	124.21	115.18
4	R	605	UTP	C5'-C4'-C3'	2.40	124.19	115.18
4	Z	603	UTP	O4'-C4'-C3'	2.31	109.68	105.11
4	Y	603	UTP	O4'-C4'-C3'	2.31	109.68	105.11
4	M	603	UTP	O4'-C4'-C3'	2.30	109.67	105.11
4	S	601	UTP	O4'-C4'-C3'	2.30	109.67	105.11
4	E	603	UTP	O4'-C4'-C3'	2.30	109.67	105.11
4	b	601	UTP	O4'-C4'-C3'	2.30	109.66	105.11
4	B	601	UTP	O4'-C4'-C3'	2.29	109.65	105.11
4	g	605	UTP	O4'-C4'-C3'	2.29	109.65	105.11
4	k	603	UTP	O4'-C4'-C3'	2.29	109.65	105.11
4	T	601	UTP	O4'-C4'-C3'	2.29	109.64	105.11
4	J	601	UTP	O4'-C4'-C3'	2.29	109.64	105.11
4	F	601	UTP	O4'-C4'-C3'	2.29	109.64	105.11
4	N	601	UTP	O4'-C4'-C3'	2.29	109.64	105.11
4	h	601	UTP	O4'-C4'-C3'	2.29	109.64	105.11
4	R	605	UTP	O4'-C4'-C3'	2.29	109.64	105.11
4	A	605	UTP	O4'-C4'-C3'	2.28	109.63	105.11
4	I	605	UTP	O4'-C4'-C3'	2.28	109.63	105.11
4	Q	605	UTP	O4'-C4'-C3'	2.28	109.62	105.11
4	a	601	UTP	O4'-C4'-C3'	2.28	109.62	105.11
4	l	601	UTP	O4'-C4'-C3'	2.27	109.61	105.11
2	N	602	ATP	N6-C6-N1	-2.11	114.20	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	601	ATP	N6-C6-N1	-2.09	114.24	118.57
2	l	602	ATP	N6-C6-N1	-2.09	114.24	118.57
2	Q	601	ATP	N6-C6-N1	-2.09	114.25	118.57
2	Y	601	ATP	N6-C6-N1	-2.09	114.25	118.57
2	g	601	ATP	N6-C6-N1	-2.08	114.25	118.57
2	A	601	ATP	N6-C6-N1	-2.08	114.25	118.57
2	F	602	ATP	N6-C6-N1	-2.08	114.25	118.57
2	I	601	ATP	N6-C6-N1	-2.07	114.27	118.57
2	b	602	ATP	N6-C6-N1	-2.07	114.27	118.57
2	k	601	ATP	N6-C6-N1	-2.07	114.28	118.57
2	a	602	ATP	N6-C6-N1	-2.07	114.28	118.57
2	E	601	ATP	N6-C6-N1	-2.06	114.29	118.57
2	M	601	ATP	N6-C6-N1	-2.06	114.30	118.57
2	S	602	ATP	N6-C6-N1	-2.06	114.31	118.57
2	T	602	ATP	N6-C6-N1	-2.06	114.31	118.57
2	J	602	ATP	N6-C6-N1	-2.05	114.31	118.57
2	Z	601	ATP	N6-C6-N1	-2.05	114.31	118.57
2	B	602	ATP	N6-C6-N1	-2.05	114.33	118.57
2	h	602	ATP	N6-C6-N1	-2.05	114.33	118.57

All (40) chirality outliers are listed below:

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

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

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	UTP	C5’-O5’-PA-O1A
4	A	605	UTP	PB-O3B-PG-O1G
4	E	603	UTP	C5’-O5’-PA-O2A
4	B	601	UTP	C5’-O5’-PA-O2A
4	F	601	UTP	C5’-O5’-PA-O1A
4	F	601	UTP	PB-O3B-PG-O1G
4	Q	605	UTP	C5’-O5’-PA-O2A
4	Y	603	UTP	C5’-O5’-PA-O1A
4	Y	603	UTP	PB-O3B-PG-O3G
4	S	601	UTP	C5’-O5’-PA-O1A
4	S	601	UTP	PB-O3B-PG-O1G
4	a	601	UTP	C5’-O5’-PA-O2A
4	I	605	UTP	C5’-O5’-PA-O1A
4	I	605	UTP	PB-O3B-PG-O1G
4	M	603	UTP	C5’-O5’-PA-O2A
4	J	601	UTP	C5’-O5’-PA-O2A
4	N	601	UTP	C5’-O5’-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	N	601	UTP	PB-O3B-PG-O3G
4	R	605	UTP	C5'-O5'-PA-O2A
4	Z	603	UTP	C5'-O5'-PA-O1A
4	Z	603	UTP	PB-O3B-PG-O3G
4	T	601	UTP	C5'-O5'-PA-O1A
4	T	601	UTP	PB-O3B-PG-O1G
4	b	601	UTP	C5'-O5'-PA-O2A
4	g	605	UTP	C5'-O5'-PA-O1A
4	g	605	UTP	PB-O3B-PG-O1G
4	k	603	UTP	C5'-O5'-PA-O2A
4	h	601	UTP	C5'-O5'-PA-O2A
4	l	601	UTP	C5'-O5'-PA-O1A
4	l	601	UTP	PB-O3B-PG-O3G
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
4	h	601	UTP	PB-O3B-PG-O3G

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

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Mol	Chain	Res	Type	Atoms
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	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	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
4	M	603	UTP	PB-O3B-PG-O3G

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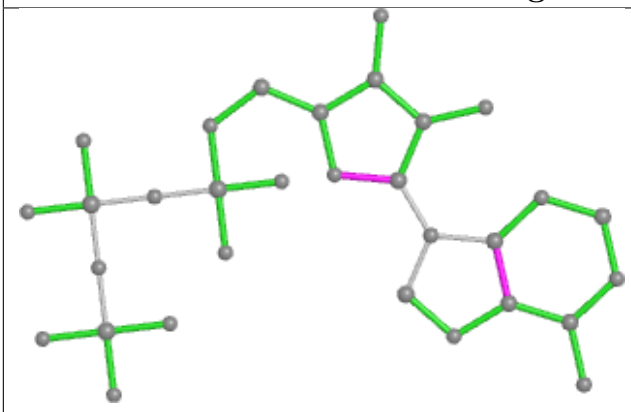
Mol	Chain	Res	Type	Atoms
4	R	605	UTP	PB-O3B-PG-O3G
4	T	601	UTP	PB-O3B-PG-O3G
4	k	603	UTP	PB-O3B-PG-O3G
4	A	605	UTP	PA-O3A-PB-O2B
4	A	605	UTP	PG-O3B-PB-O1B
4	F	601	UTP	PA-O3A-PB-O2B
4	F	601	UTP	PG-O3B-PB-O1B
4	Y	603	UTP	PA-O3A-PB-O2B
4	Y	603	UTP	PG-O3B-PB-O1B
4	I	605	UTP	PA-O3A-PB-O2B
4	I	605	UTP	PG-O3B-PB-O1B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

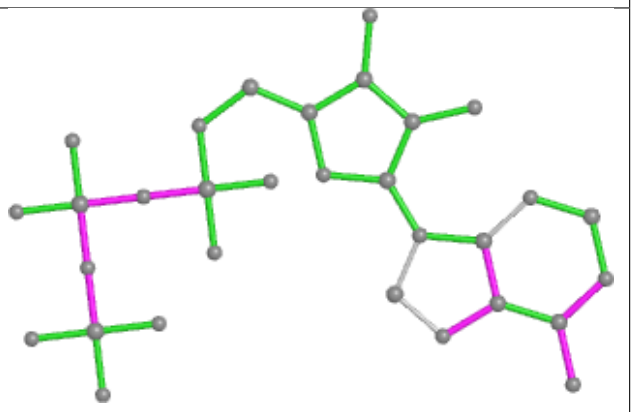
No monomer is involved in short contacts.

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

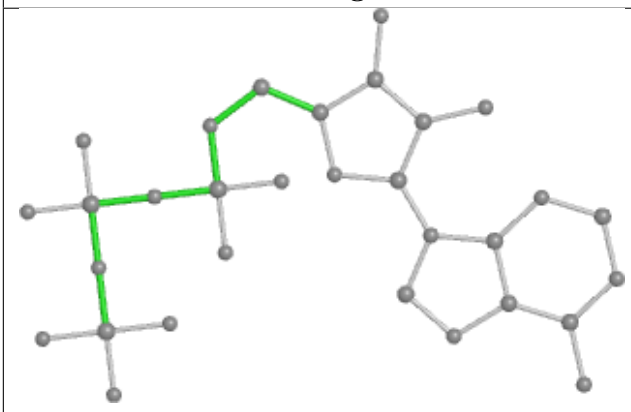
Ligand ATP h 602



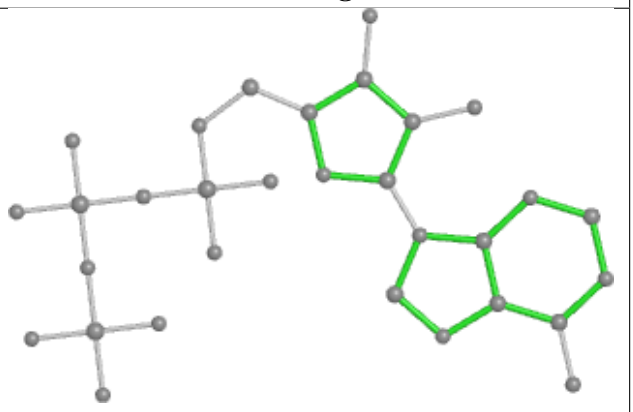
Bond lengths



Bond angles

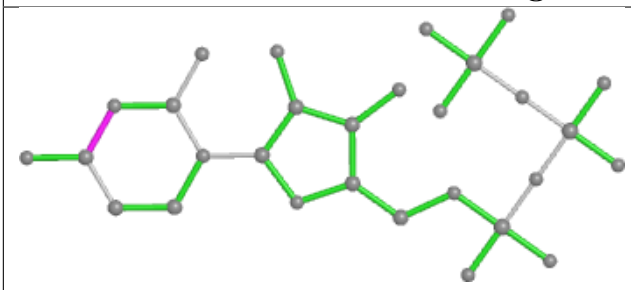


Torsions

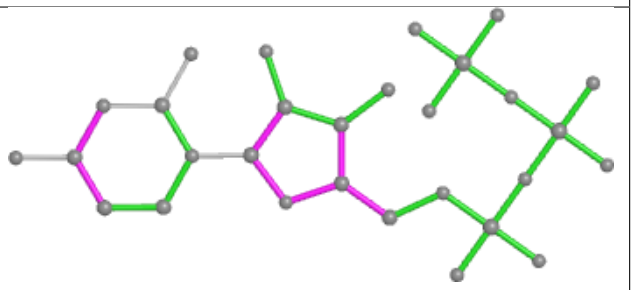


Rings

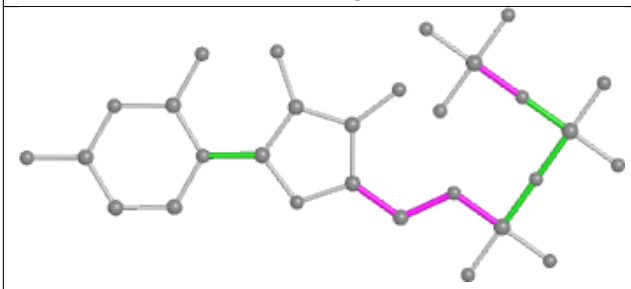
Ligand UTP a 601



Bond lengths



Bond angles



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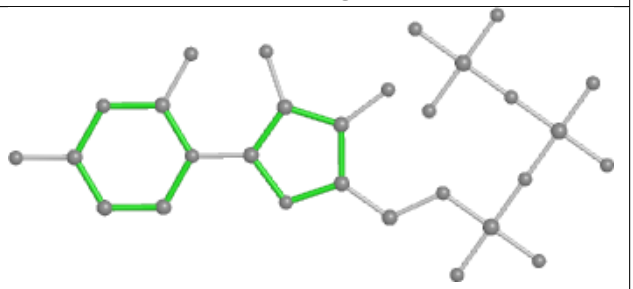
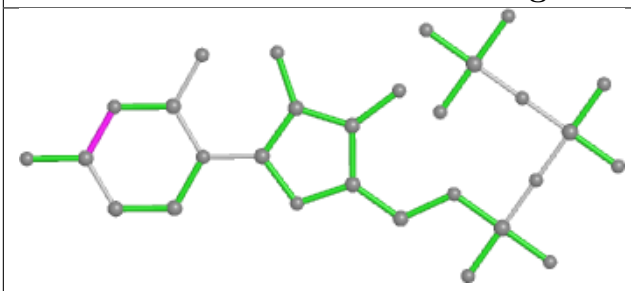
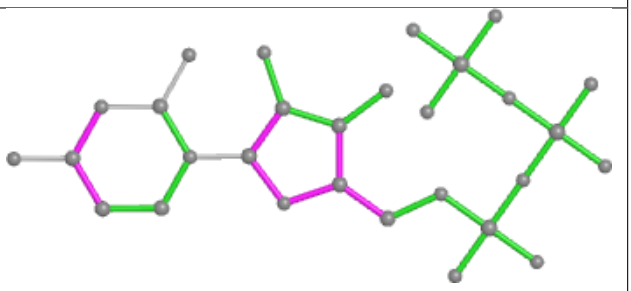


Rings

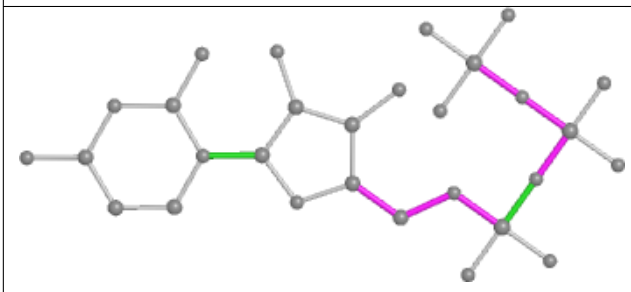
Ligand UTP I 605



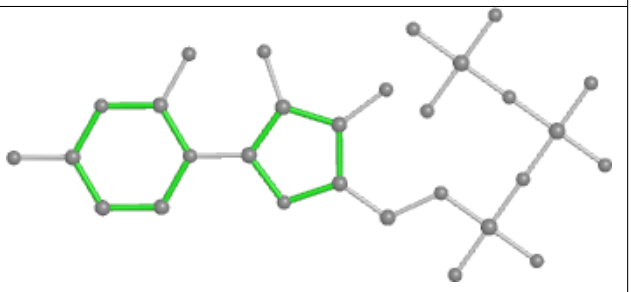
Bond lengths



Bond angles

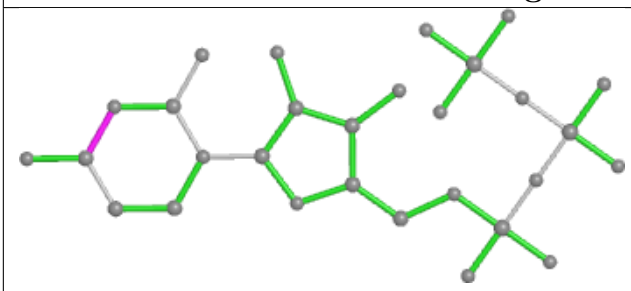


Torsions



Rings

Ligand UTP F 601



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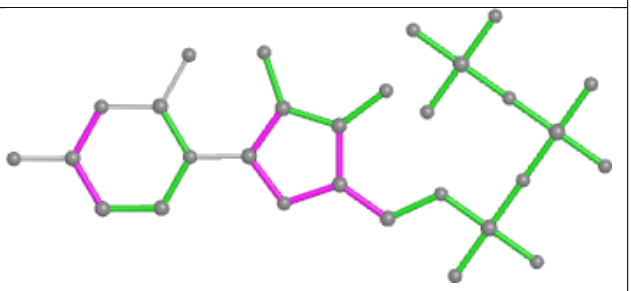

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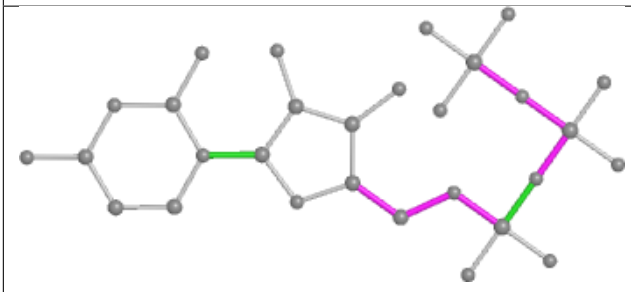
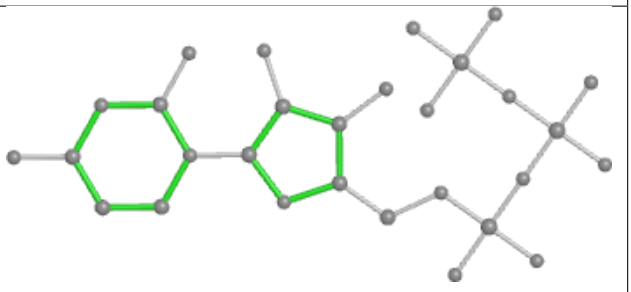
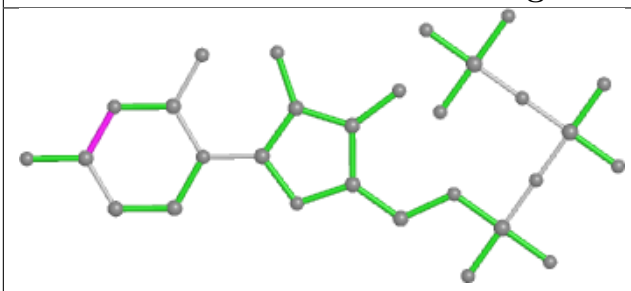


Torsions



Rings

Ligand UTP g 605



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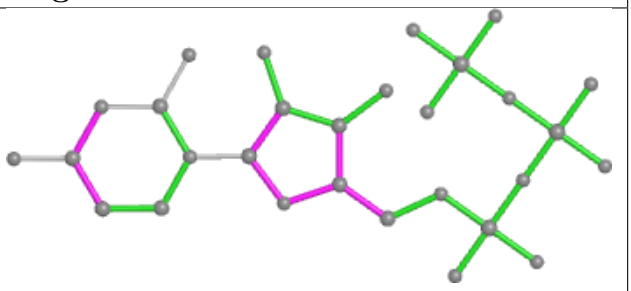

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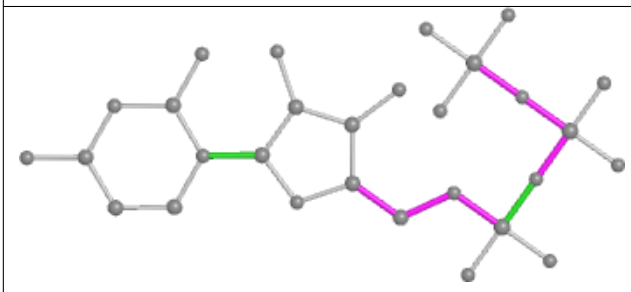

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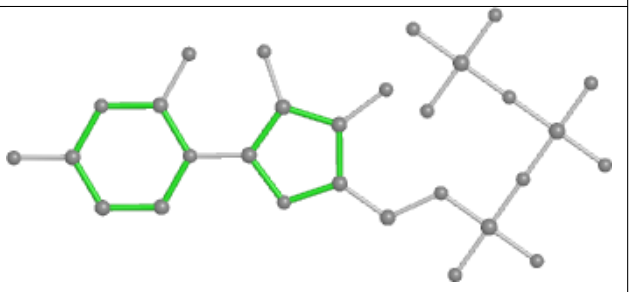
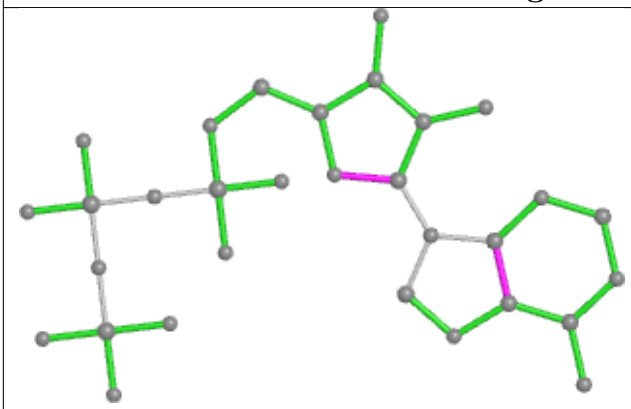


Rings

Ligand ATP Z 601



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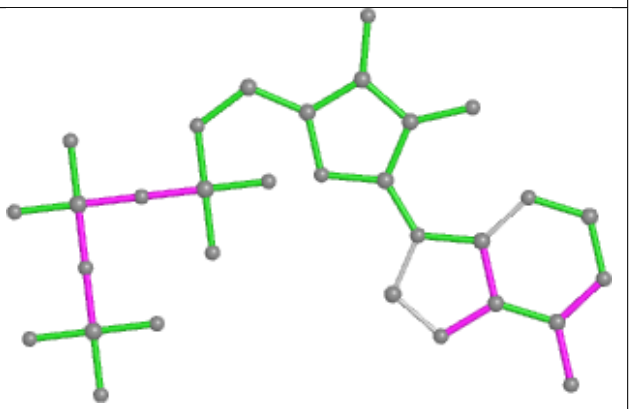

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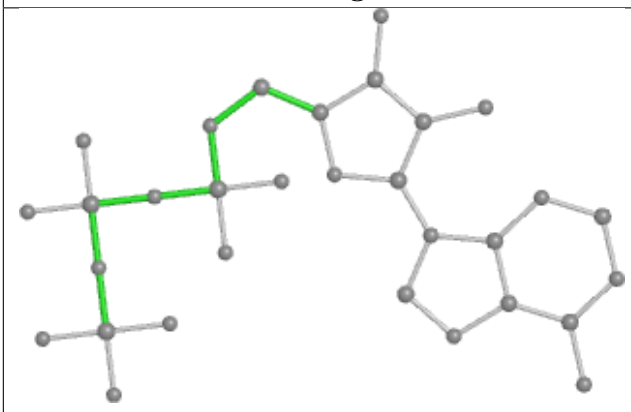

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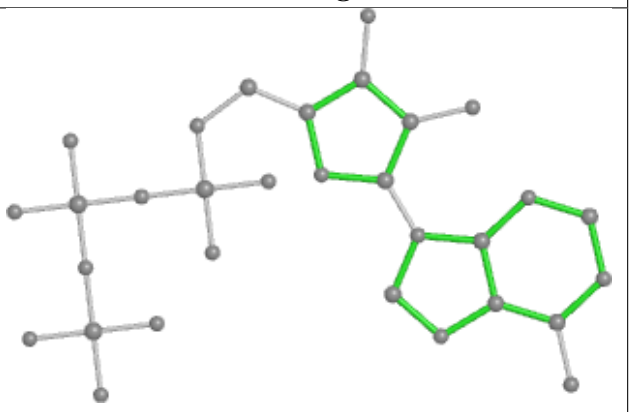

Rings

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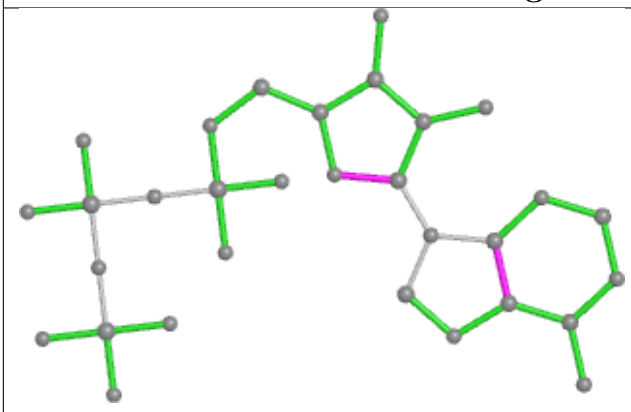

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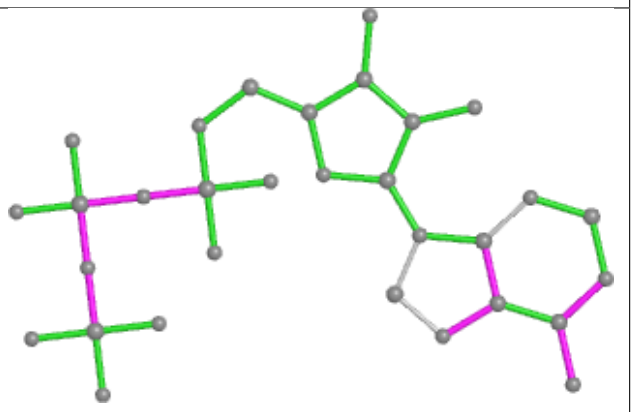

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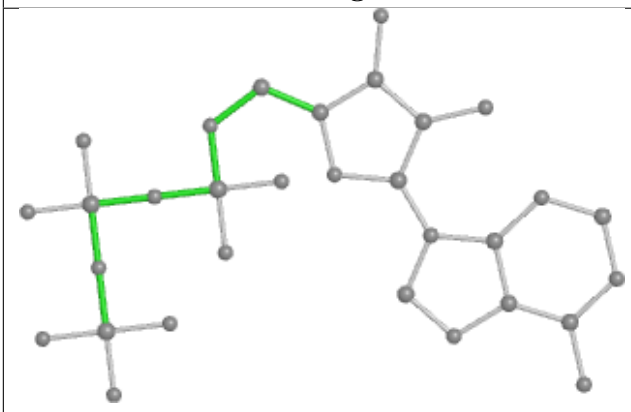

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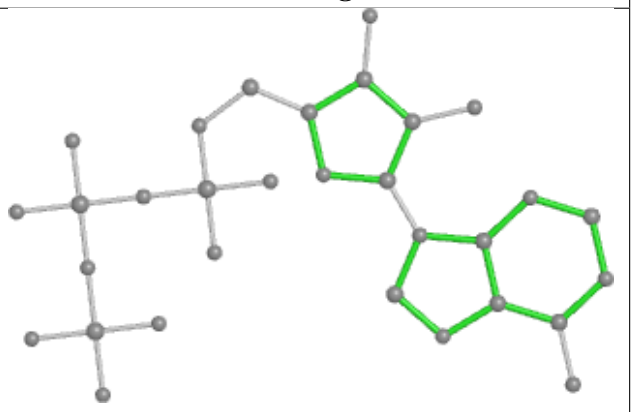
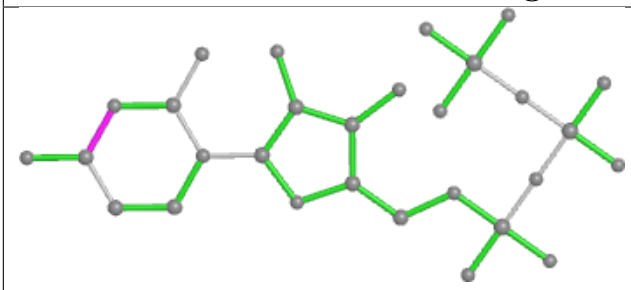


Rings

Ligand UTP B 601



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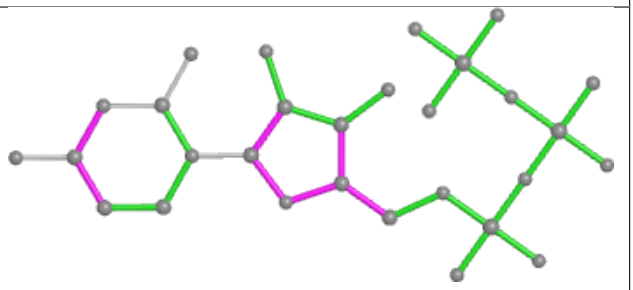

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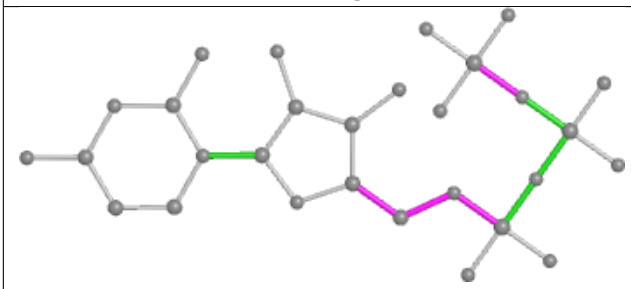

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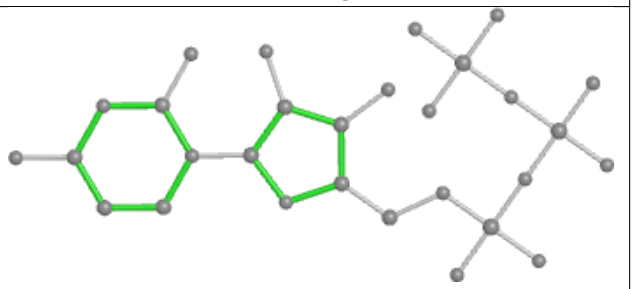
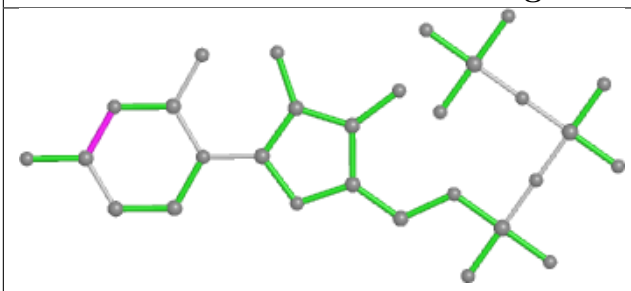


Rings

Ligand UTP E 603



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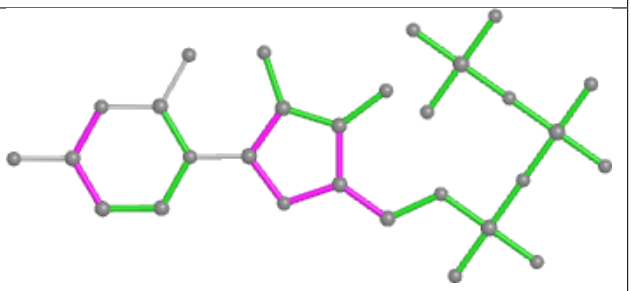

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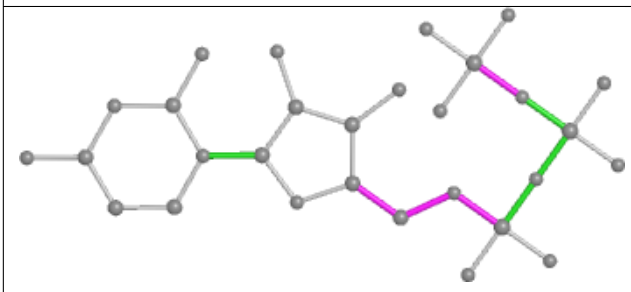

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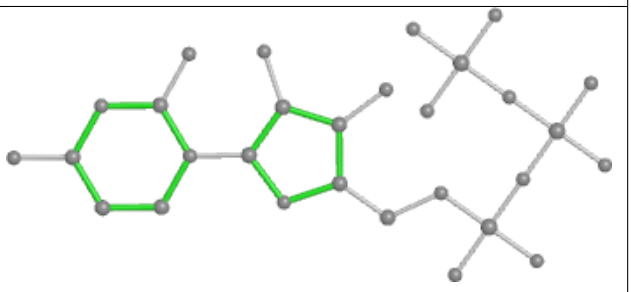
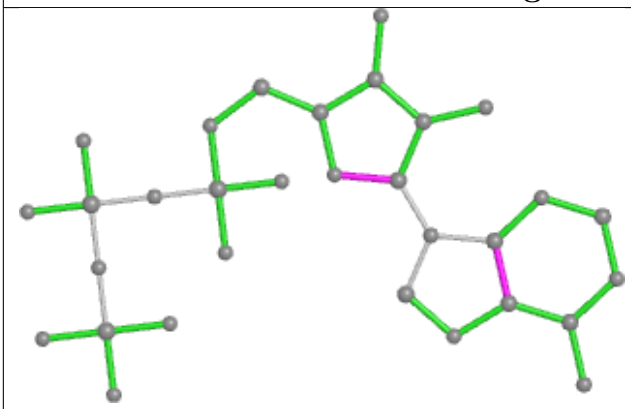


Rings

Ligand ATP N 602



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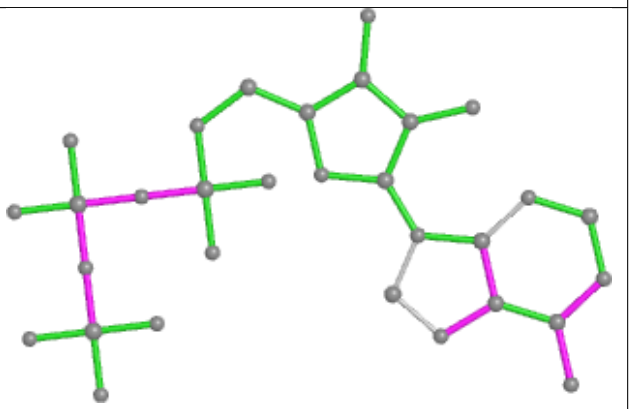

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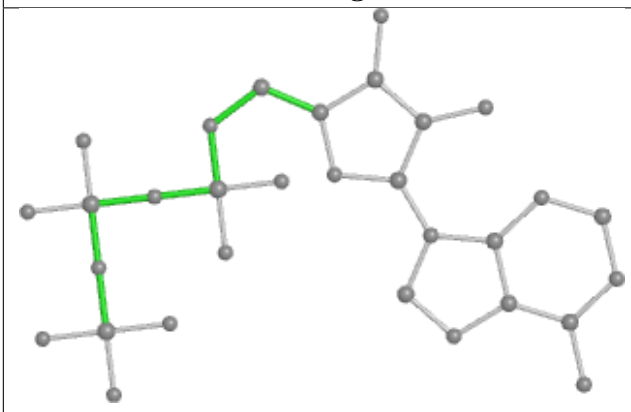

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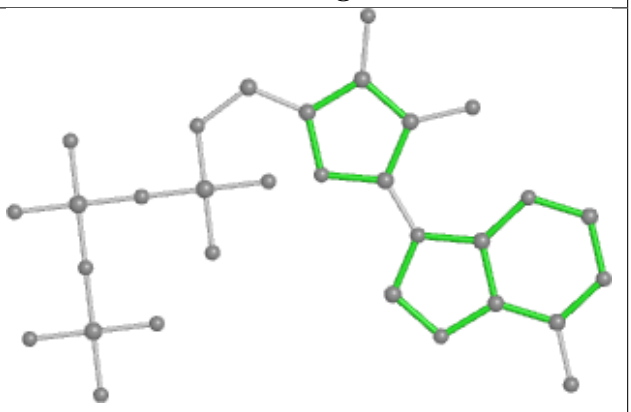
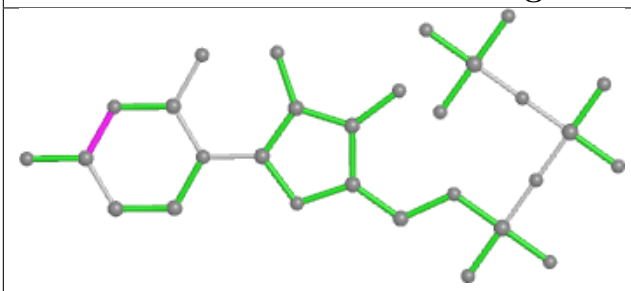


Rings

Ligand UTP Z 603



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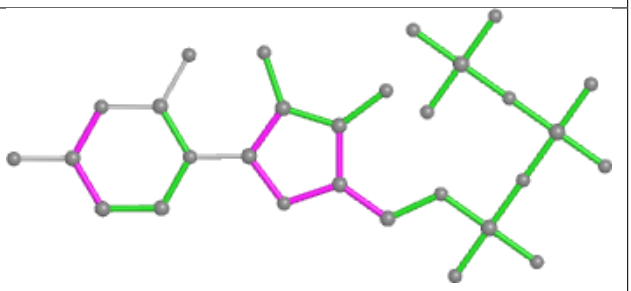

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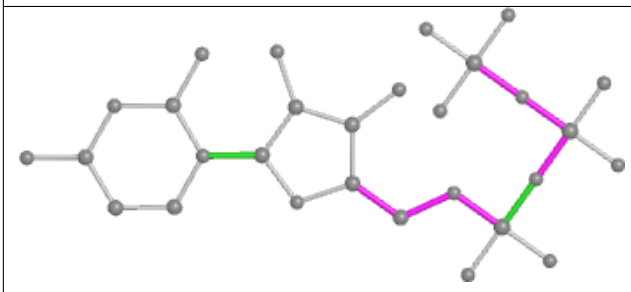

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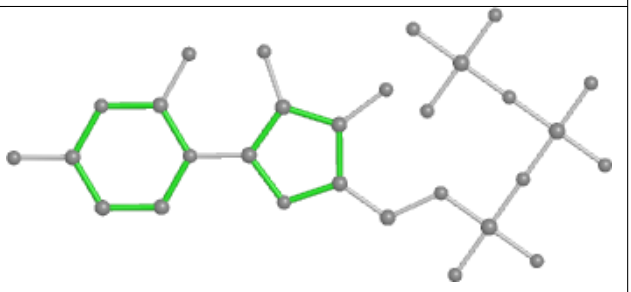
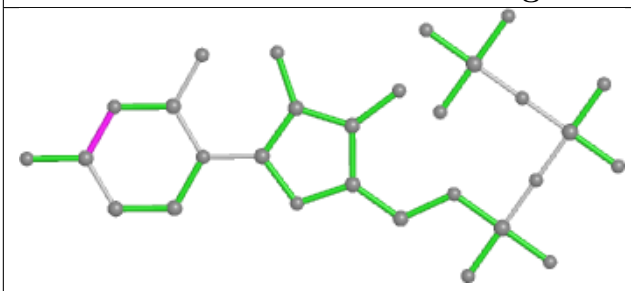


Rings

Ligand UTP A 605



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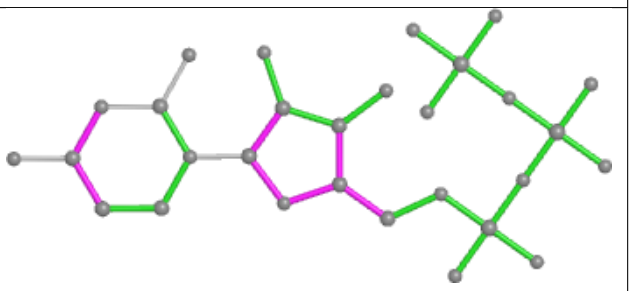

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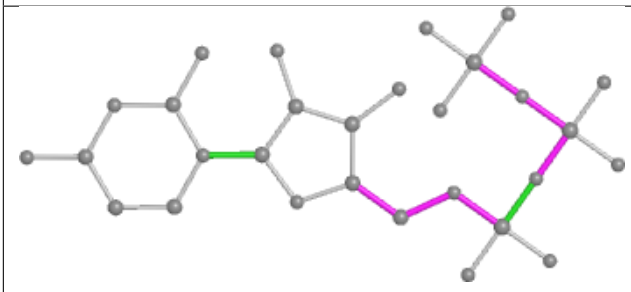

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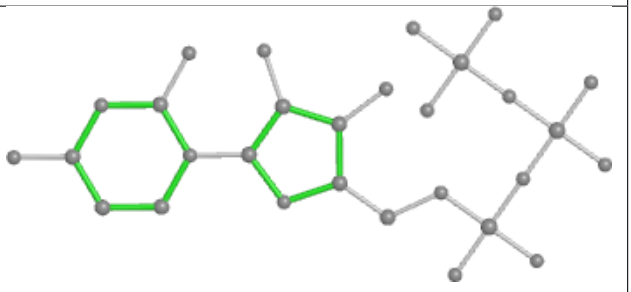

Rings

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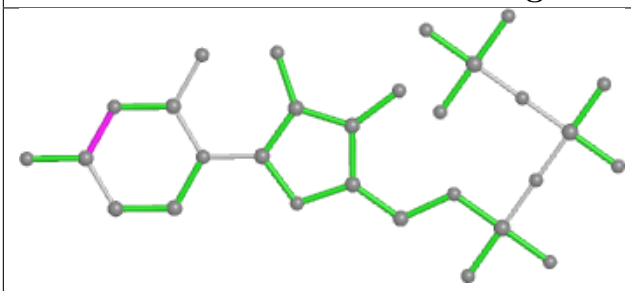

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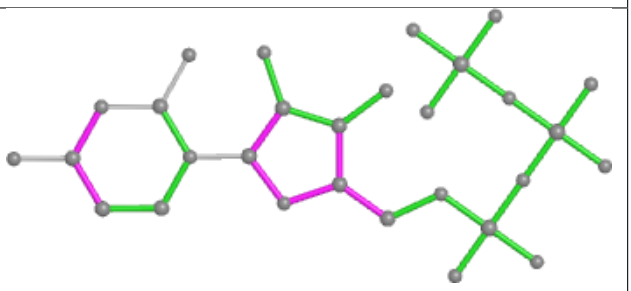

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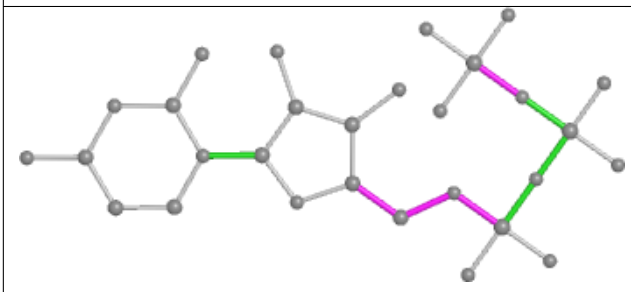

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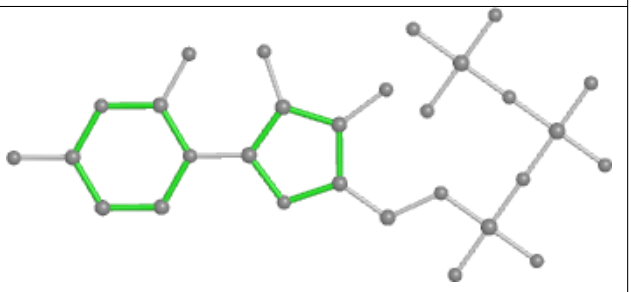

Rings

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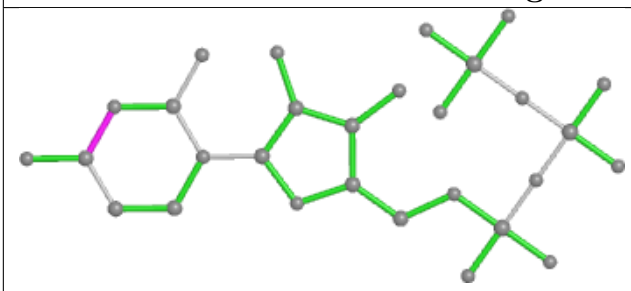

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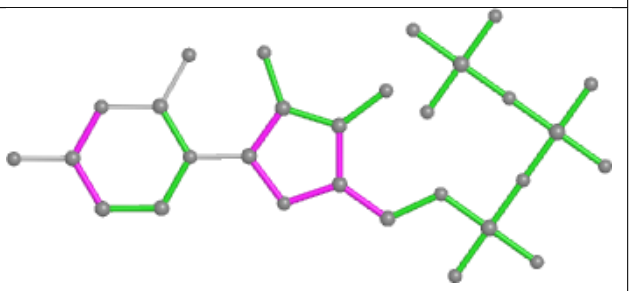

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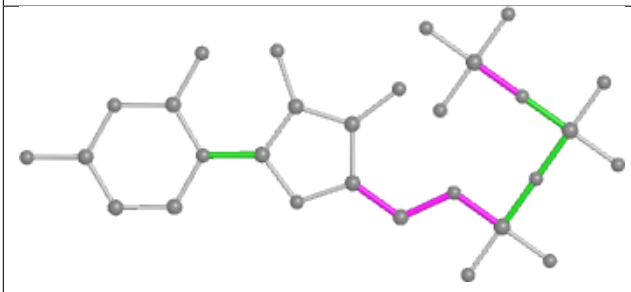

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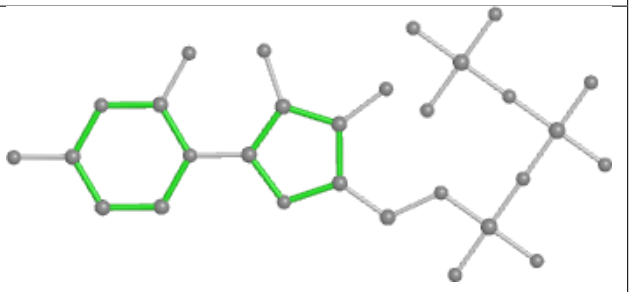
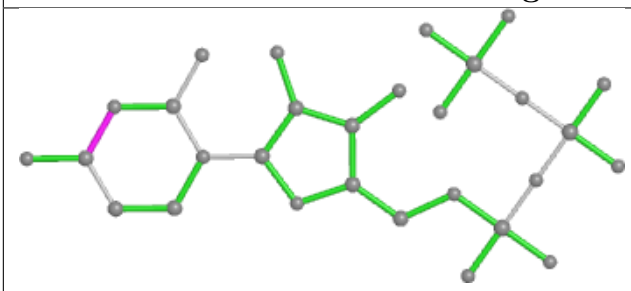


Rings

Ligand UTP Y 603



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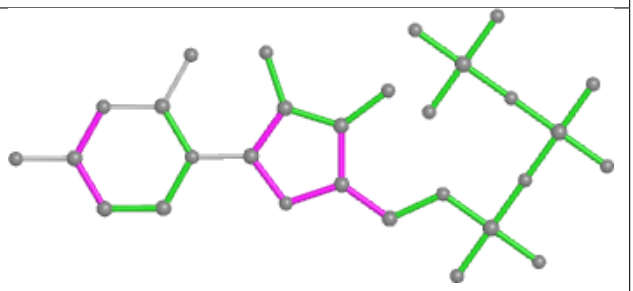

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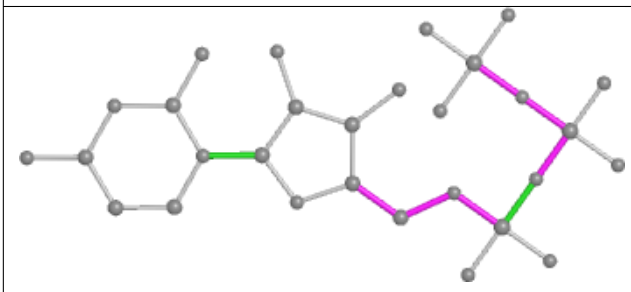

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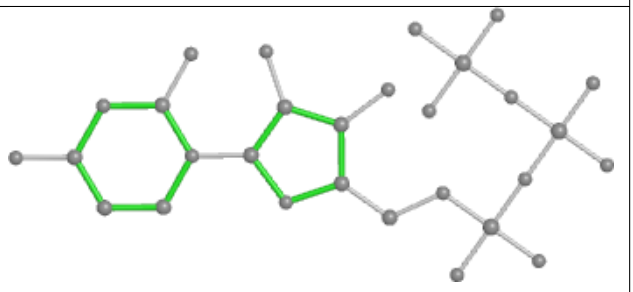
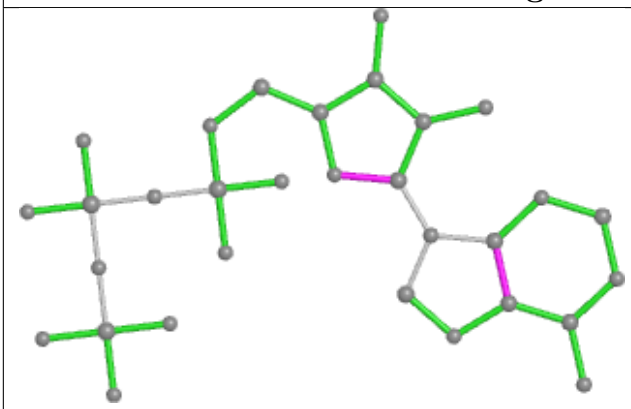


Rings

Ligand ATP F 602



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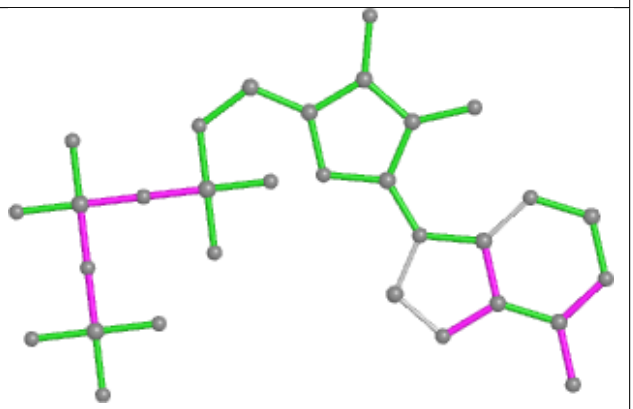

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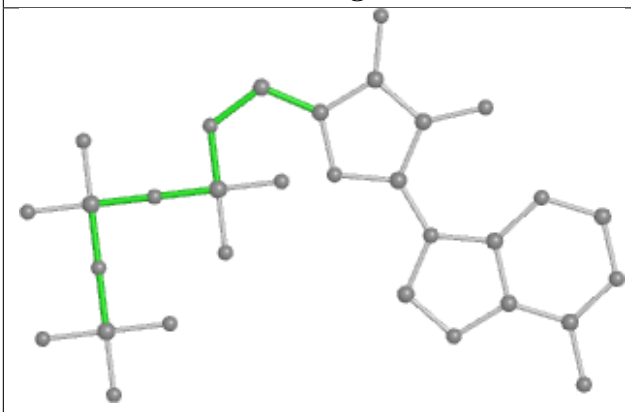

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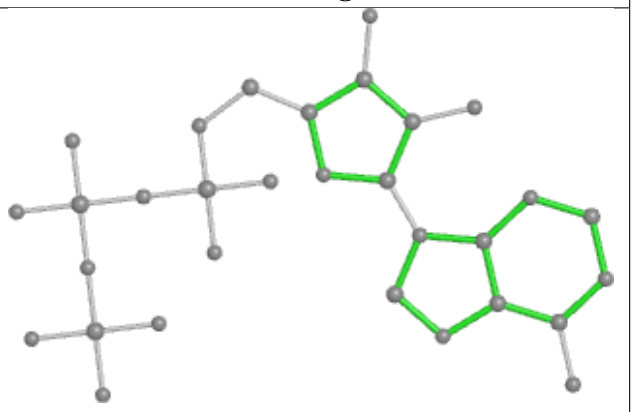
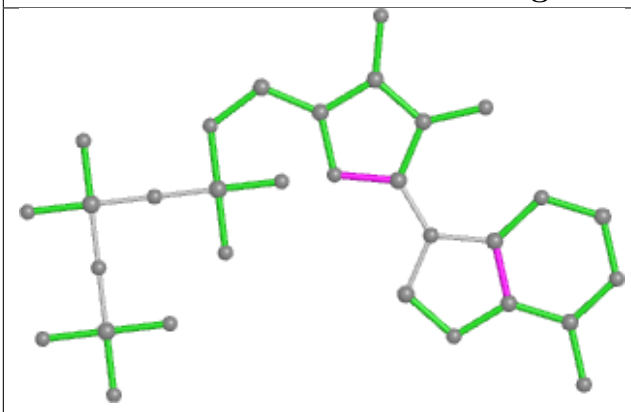


Rings

Ligand ATP I 601



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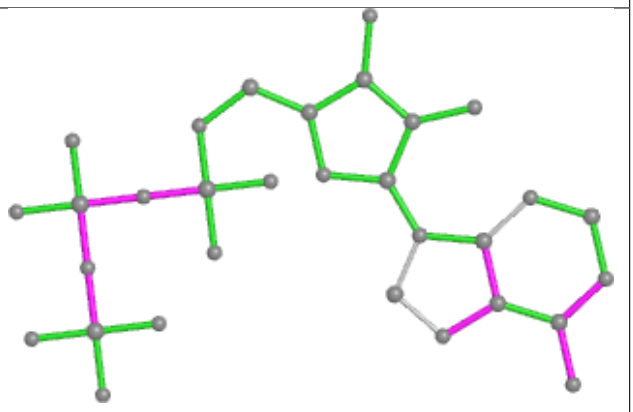
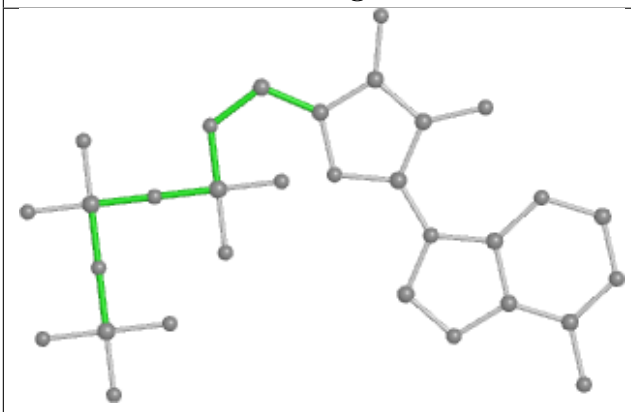


Bond angles



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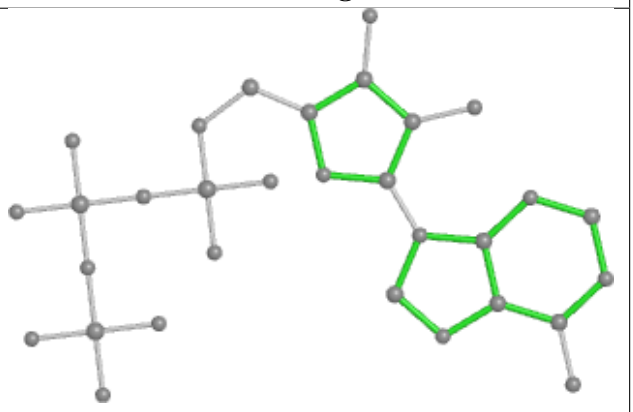
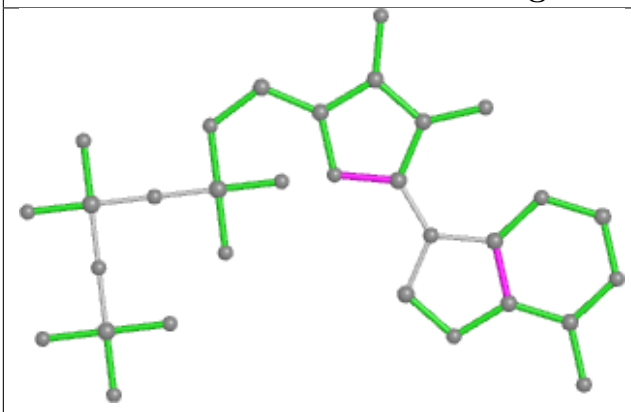


Rings

Ligand ATP g 601



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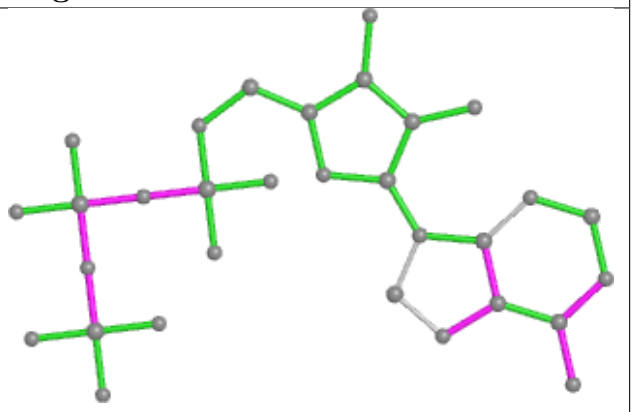

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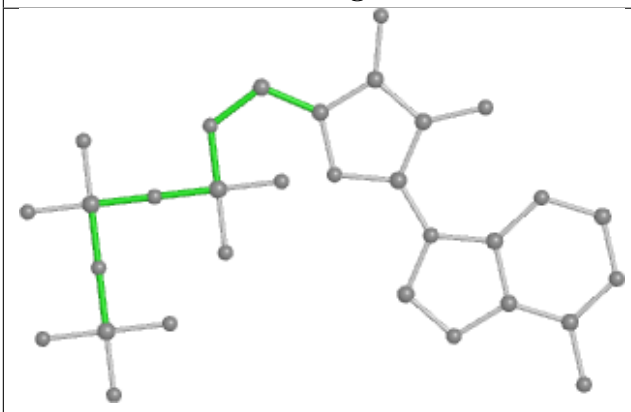
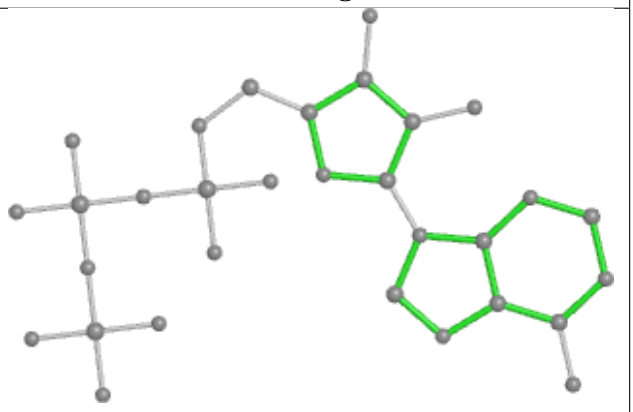
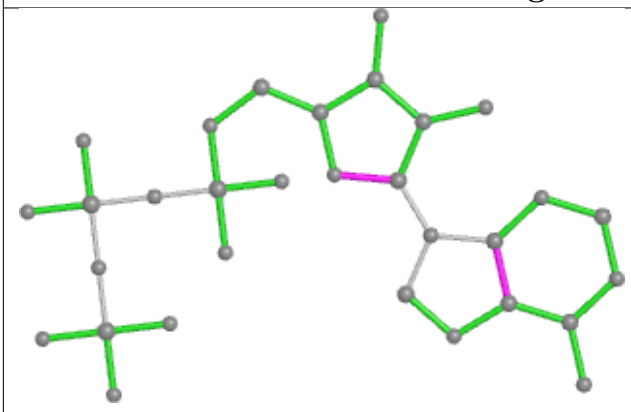


Torsions

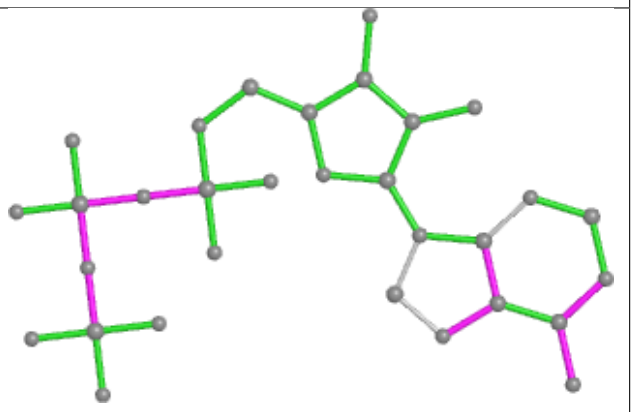


Rings

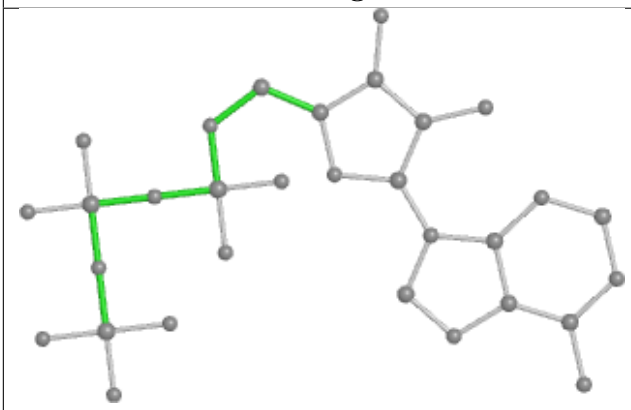
Ligand ATP b 602



Bond lengths



Bond angles



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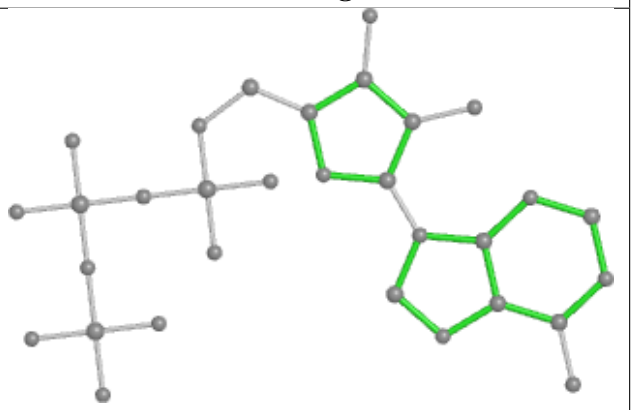
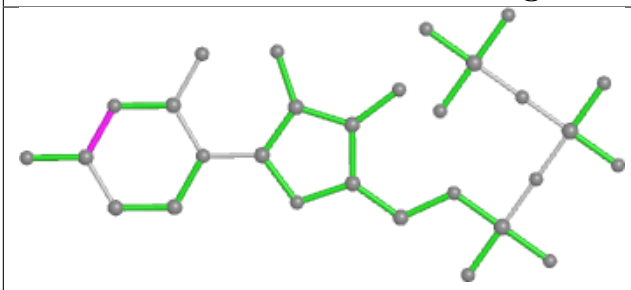


Rings

Ligand UTP R 605



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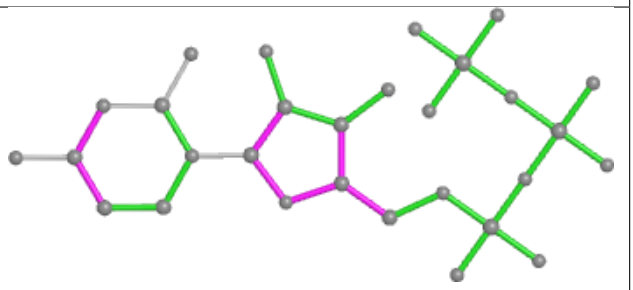

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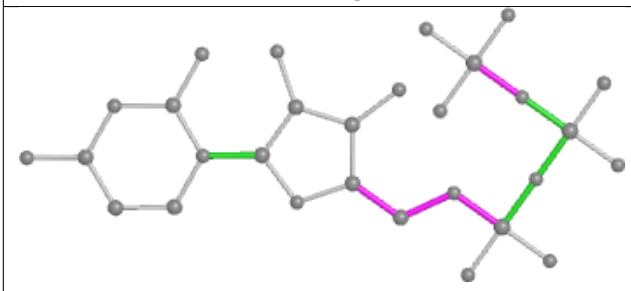

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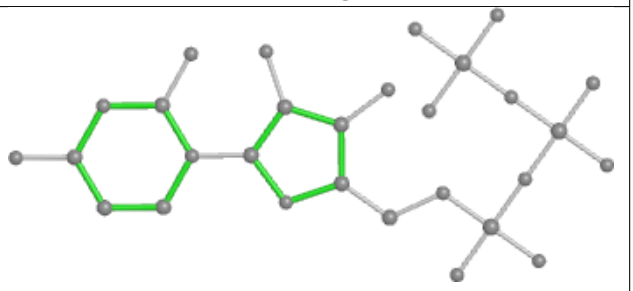
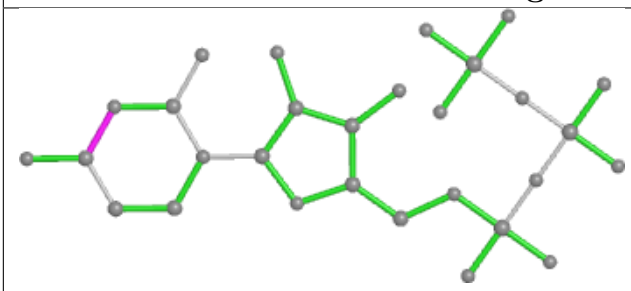


Rings

Ligand UTP J 601



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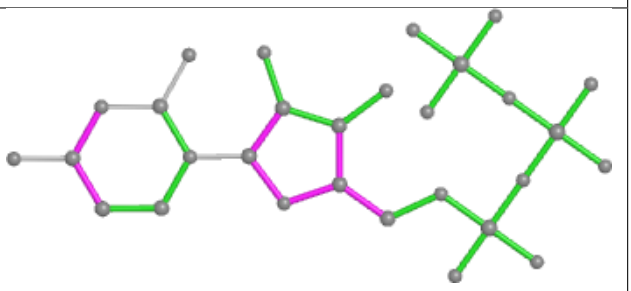

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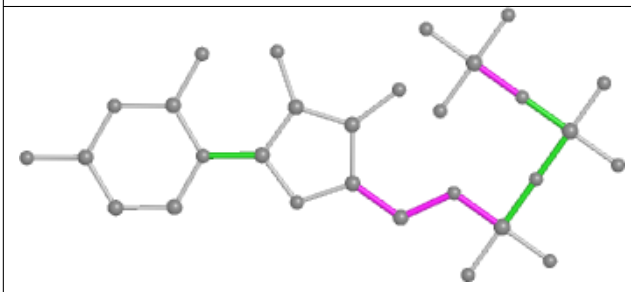

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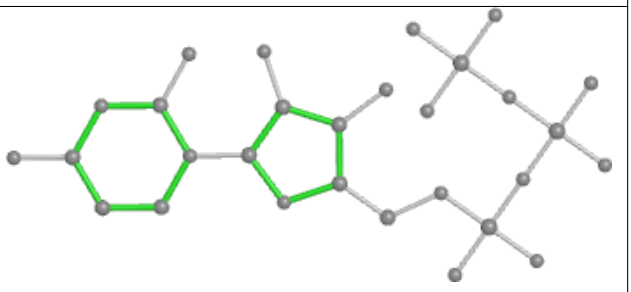

Rings

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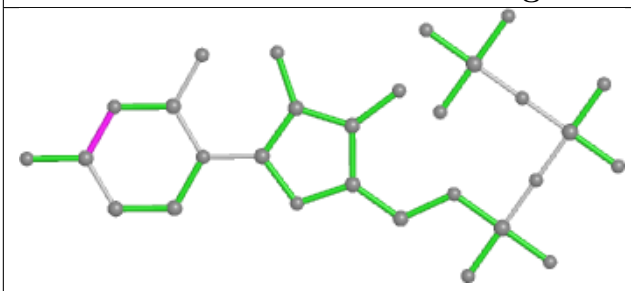

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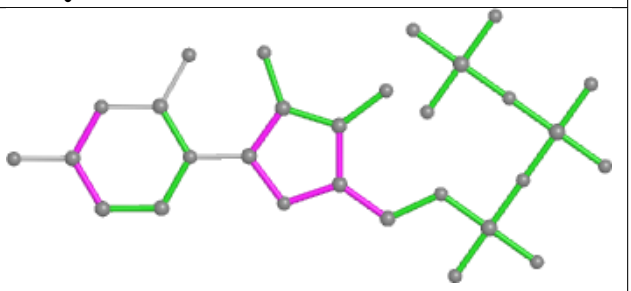

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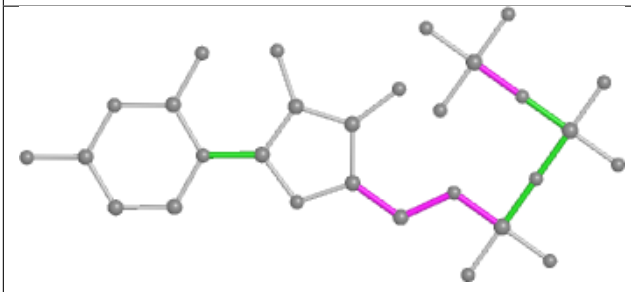

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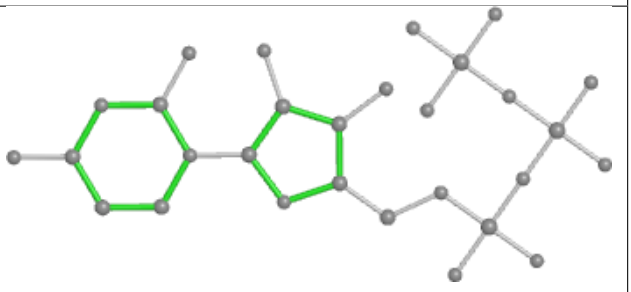
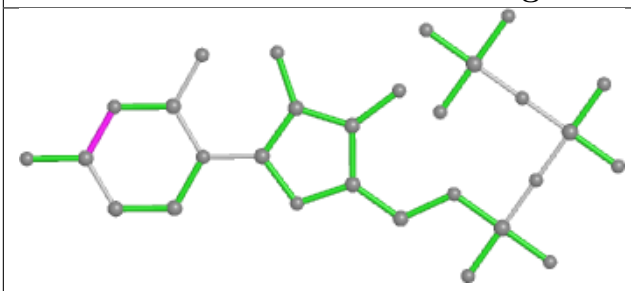


Rings

Ligand UTP N 601



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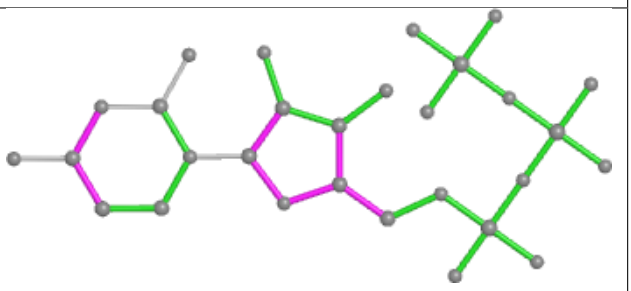

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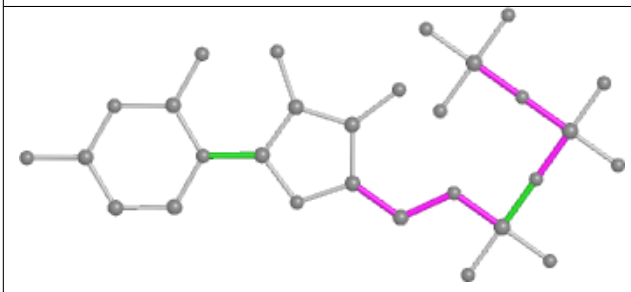

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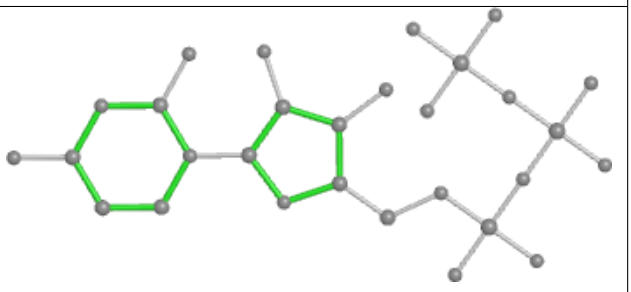
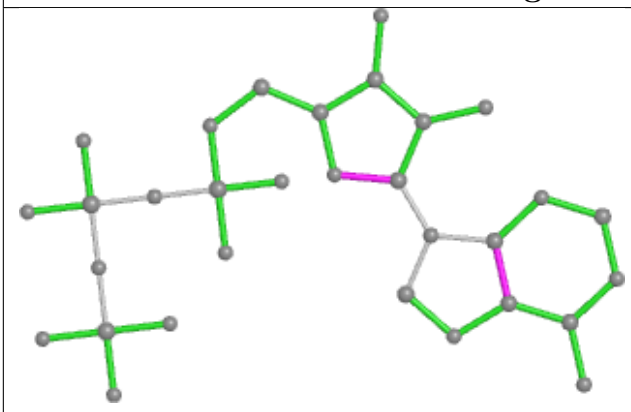


Rings

Ligand ATP A 601



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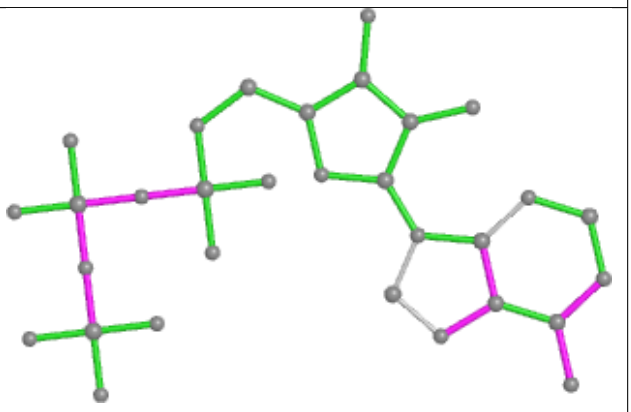

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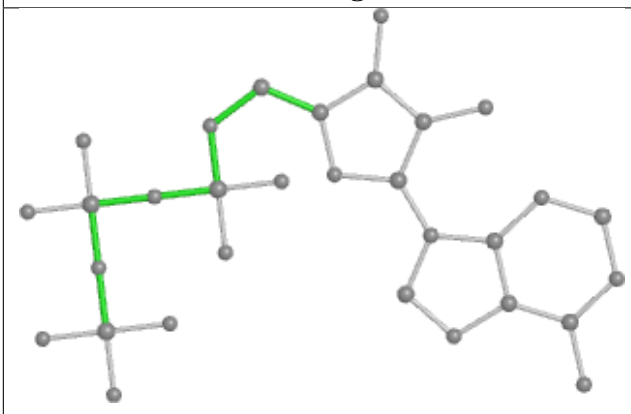

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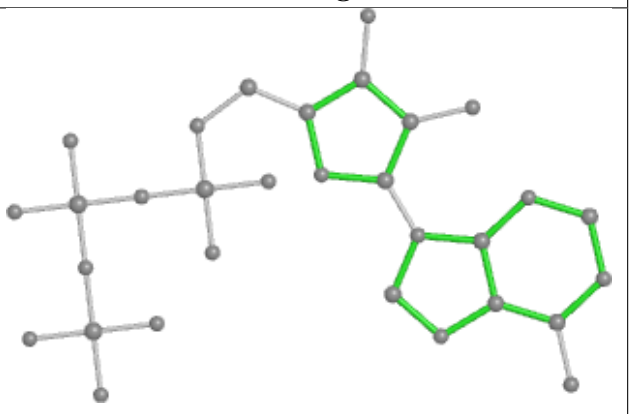
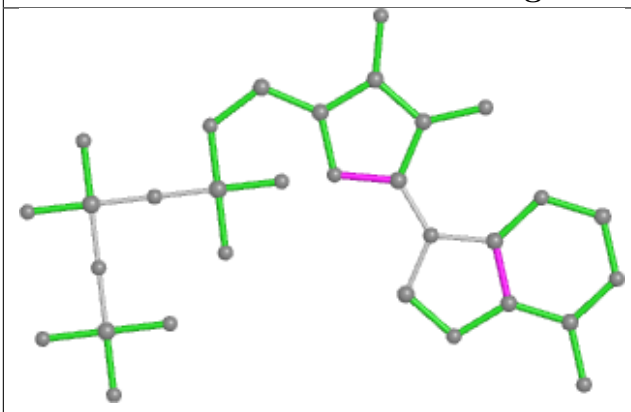


Rings

Ligand ATP Q 601



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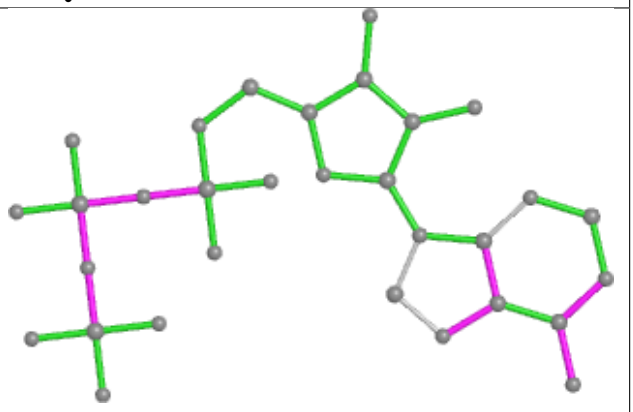

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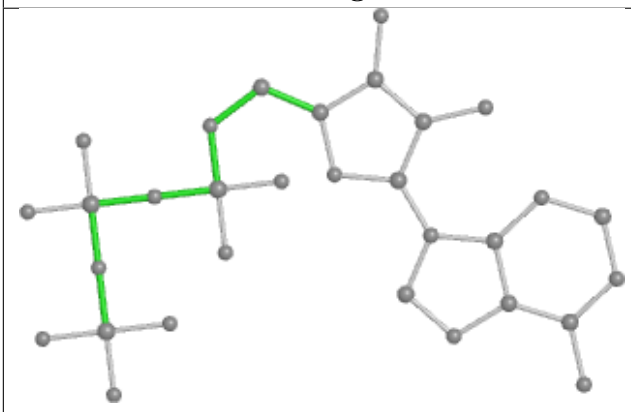

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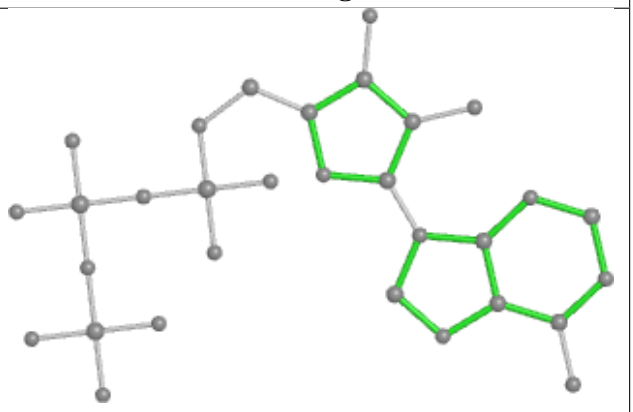
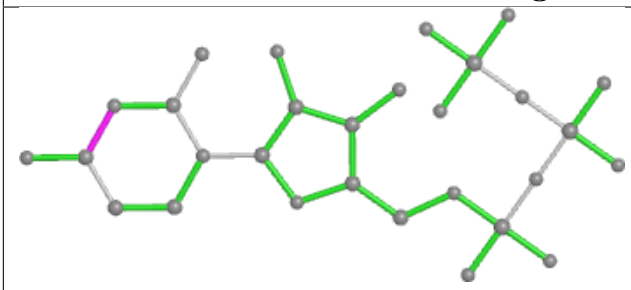


Rings

Ligand UTP l 601



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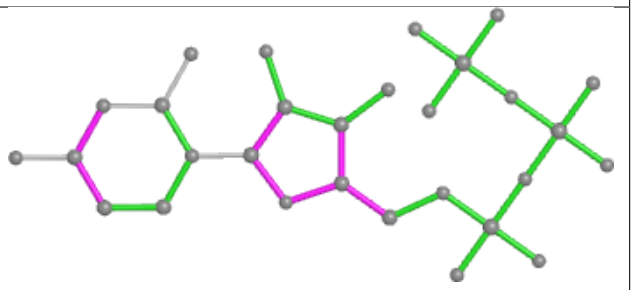

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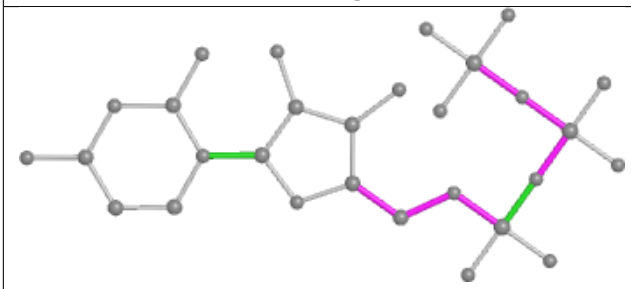

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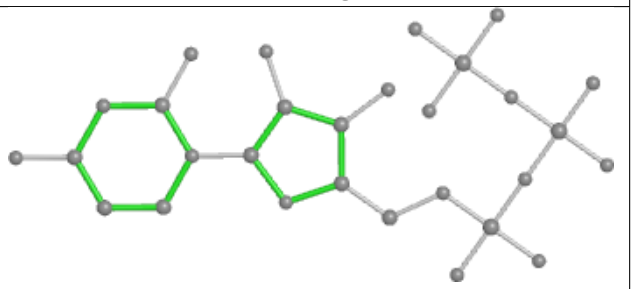
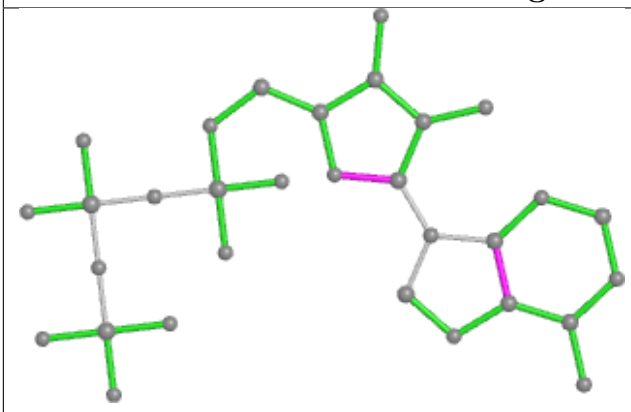


Rings

Ligand ATP J 602



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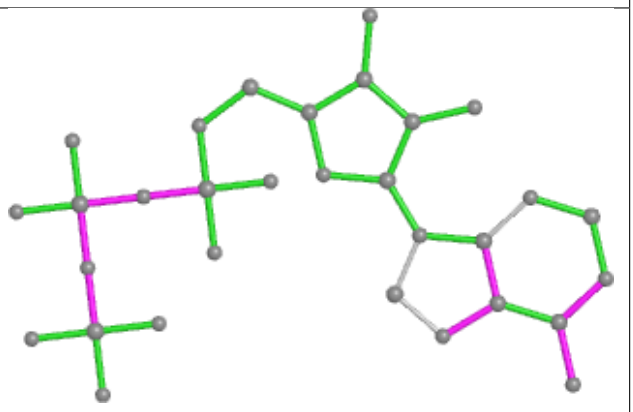

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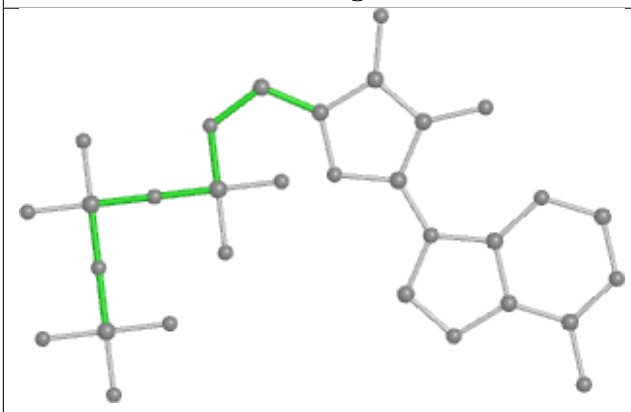

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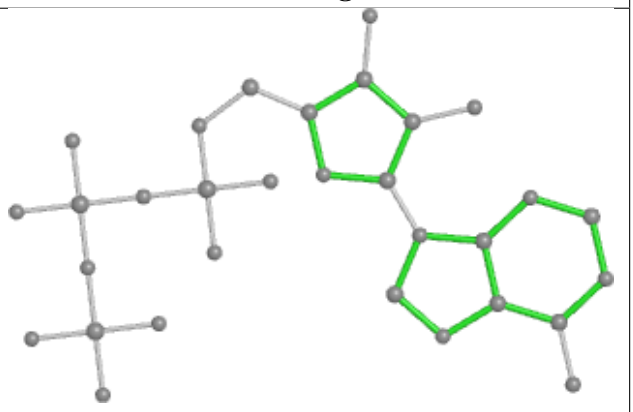
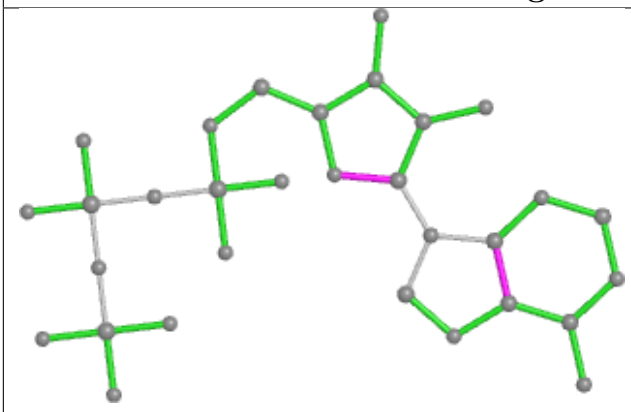


Rings

Ligand ATP S 602



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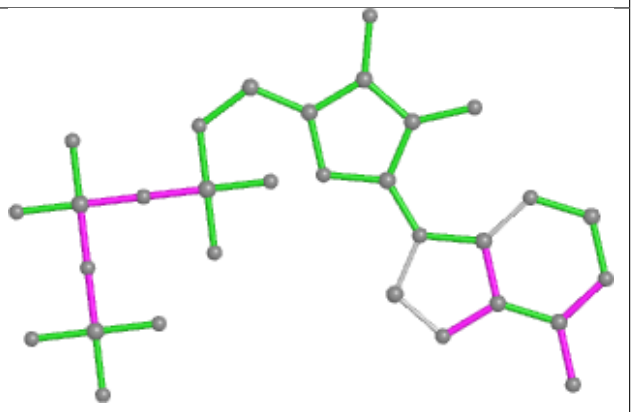

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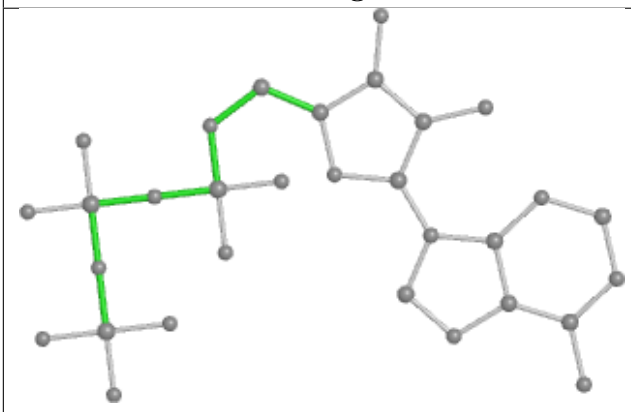

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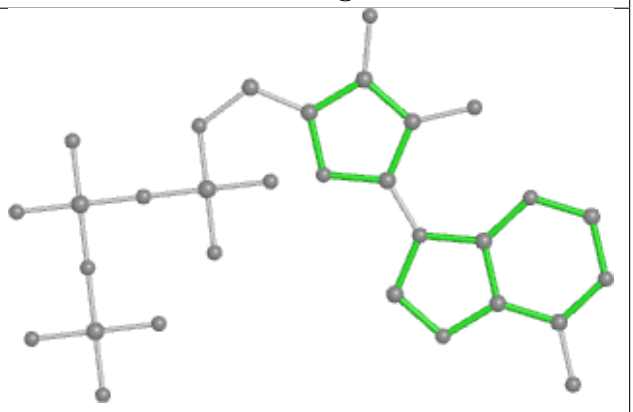
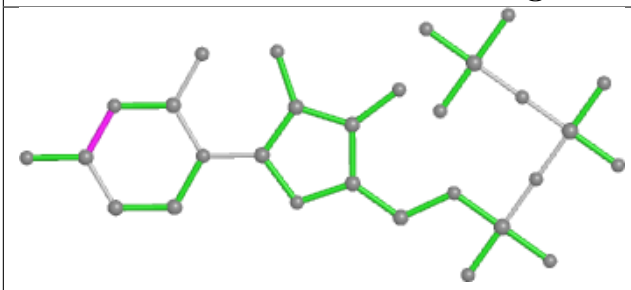


Rings

Ligand UTP k 603



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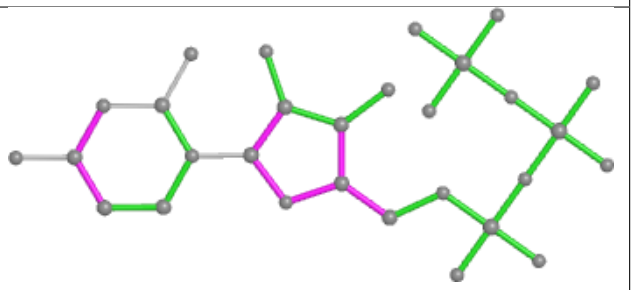

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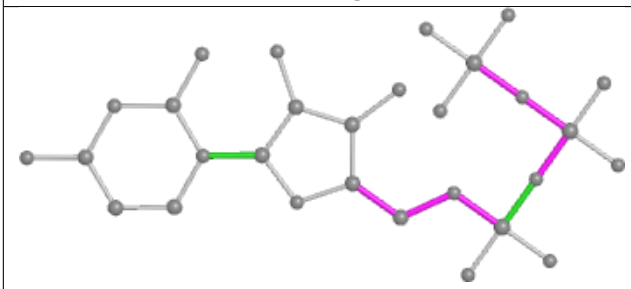

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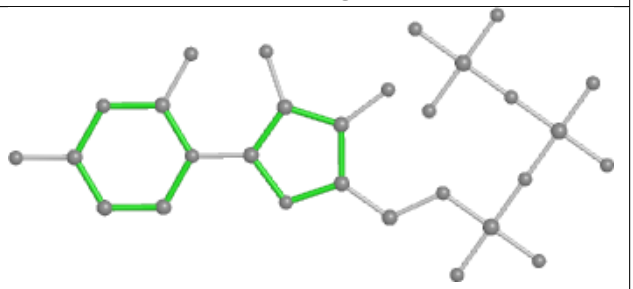
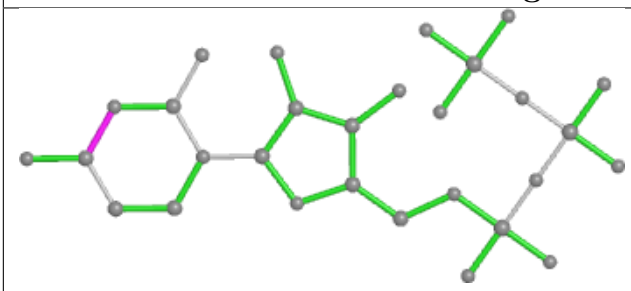


Rings

Ligand UTP T 601



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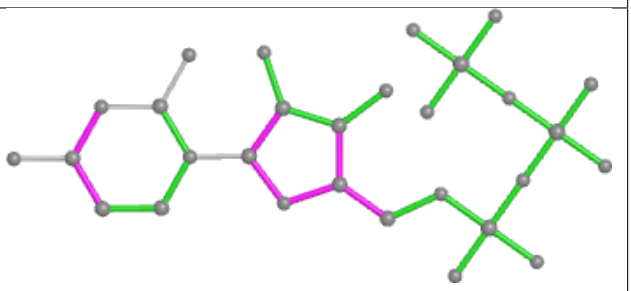

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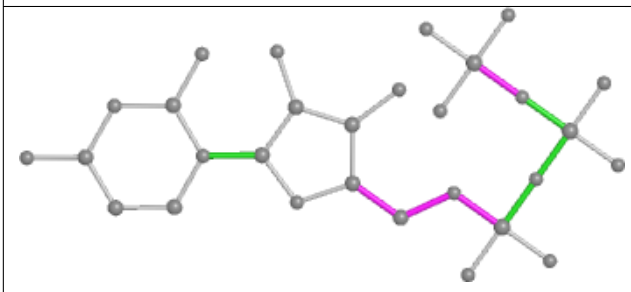

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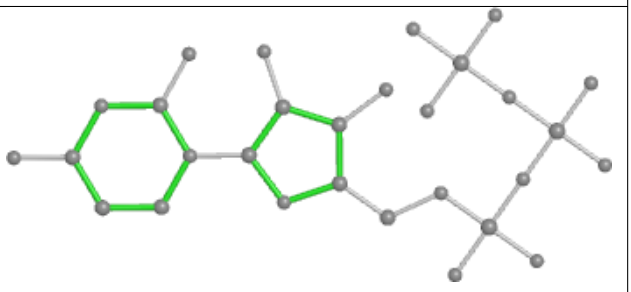
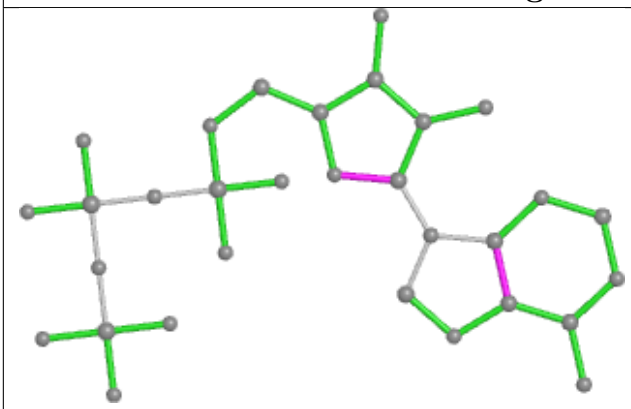


Rings

Ligand ATP E 601



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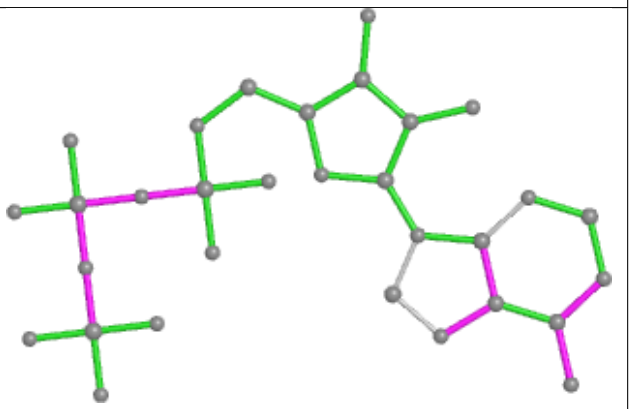

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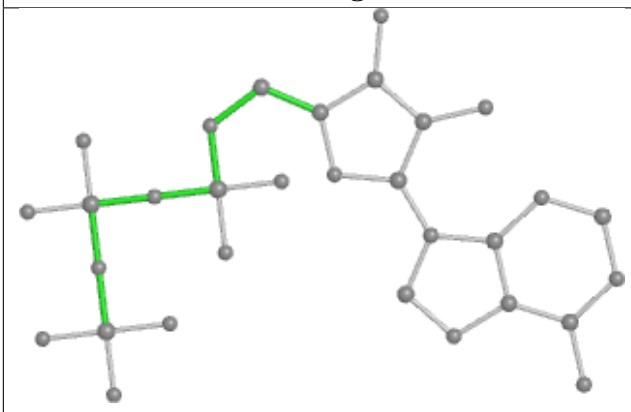

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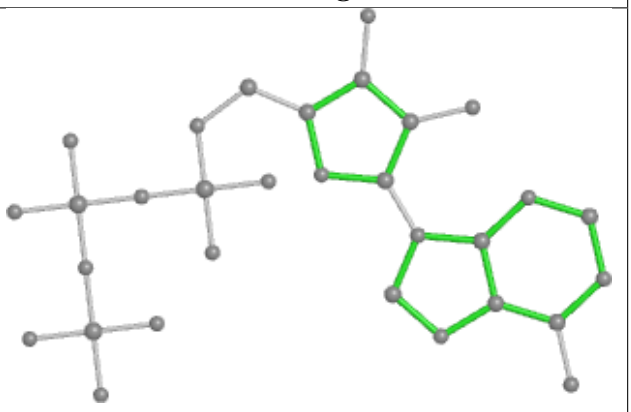
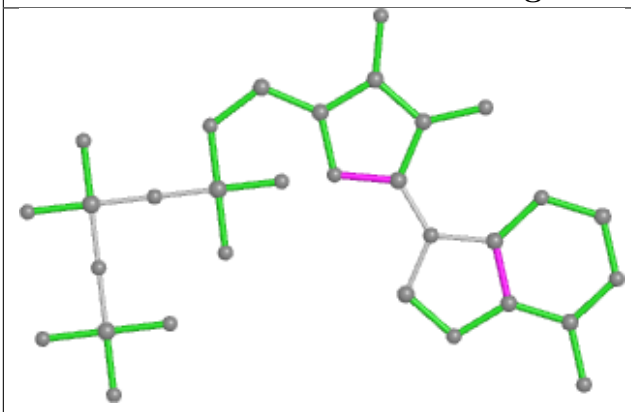


Rings

Ligand ATP R 601



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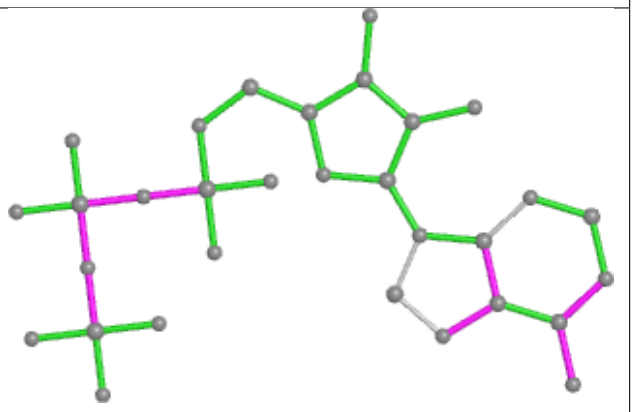
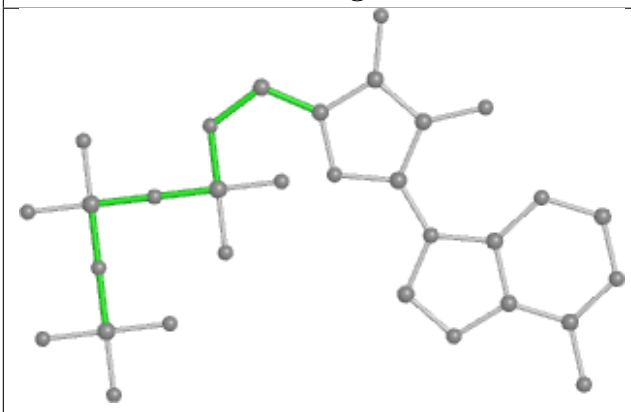


Bond angles



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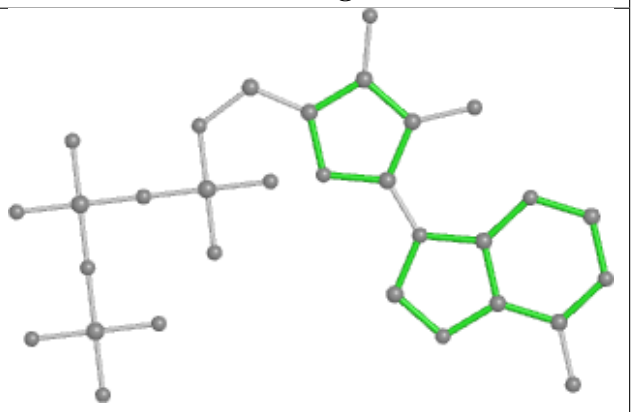
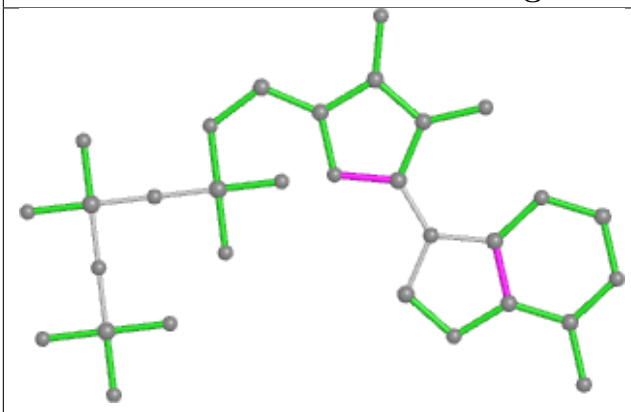
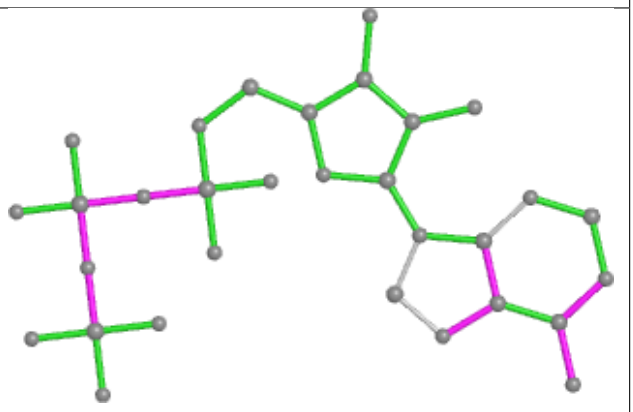


Rings

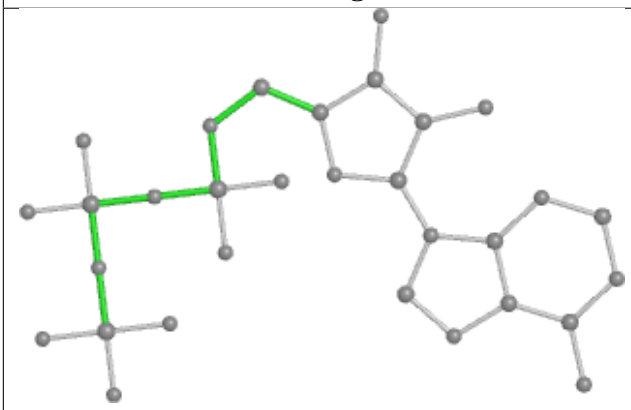
Ligand ATP Y 601



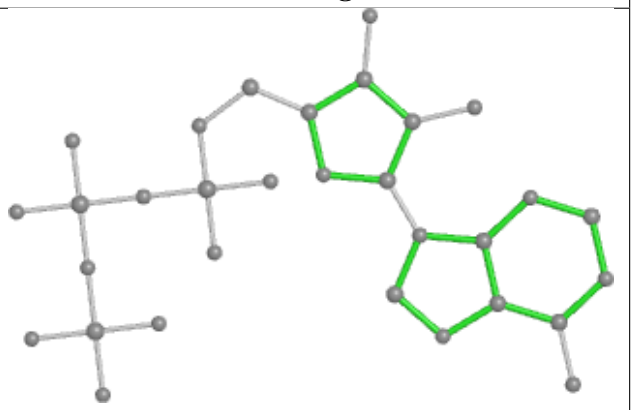
Bond lengths



Bond angles

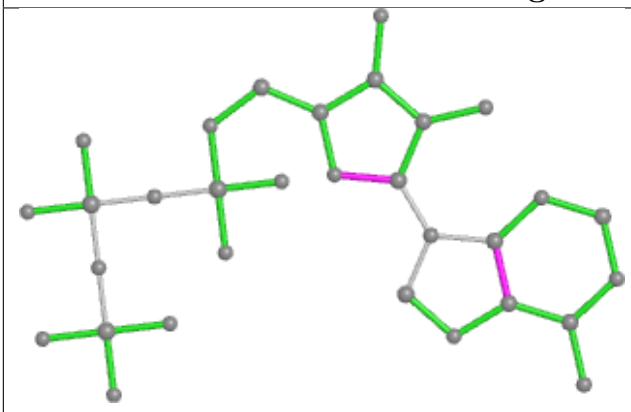


Torsions

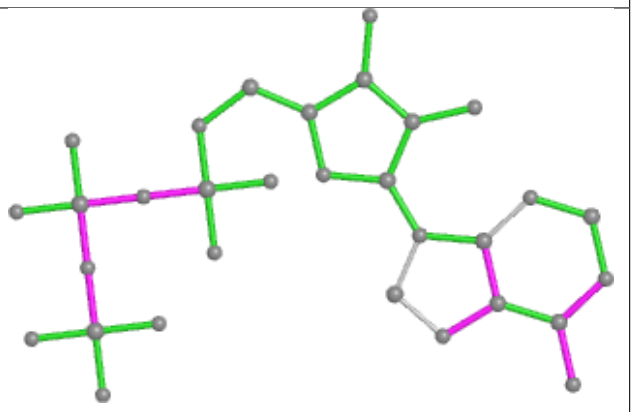


Rings

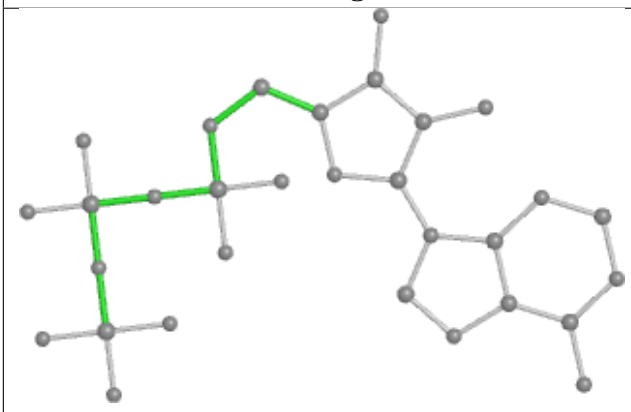
Ligand ATP k 601



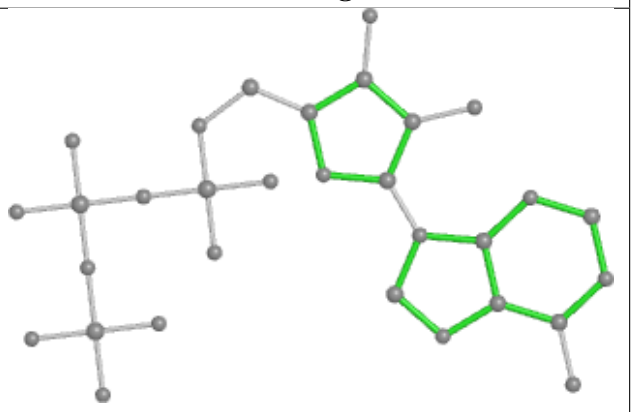
Bond lengths



Bond angles

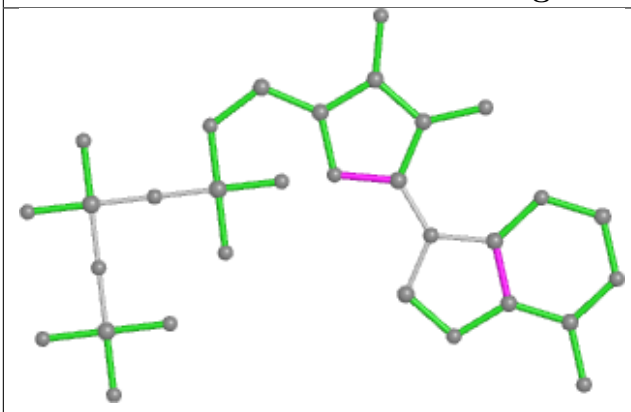


Torsions

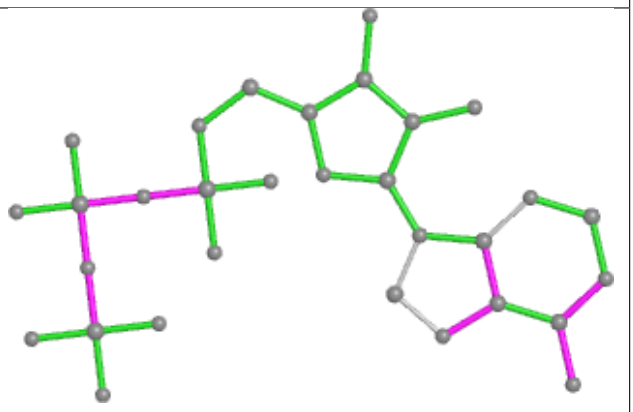


Rings

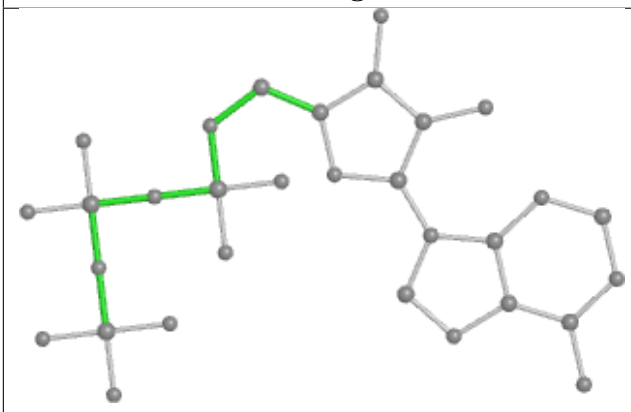
Ligand ATP l 602



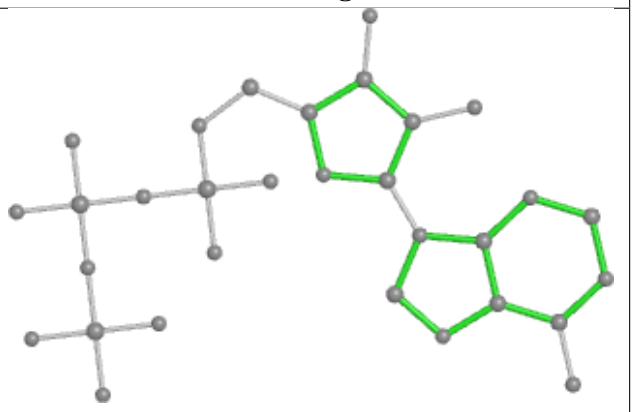
Bond lengths



Bond angles

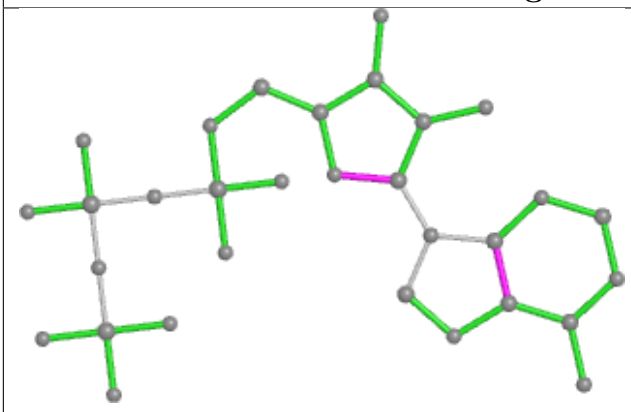


Torsions

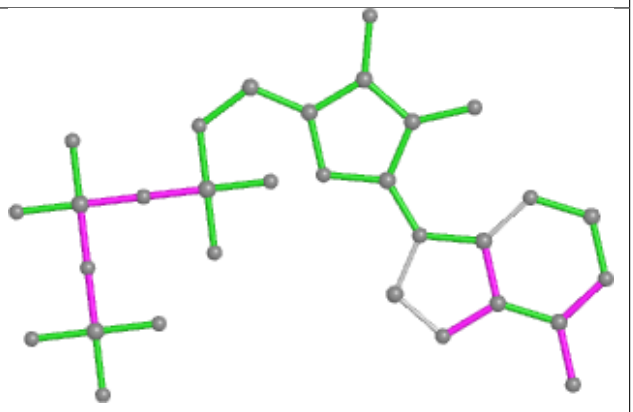


Rings

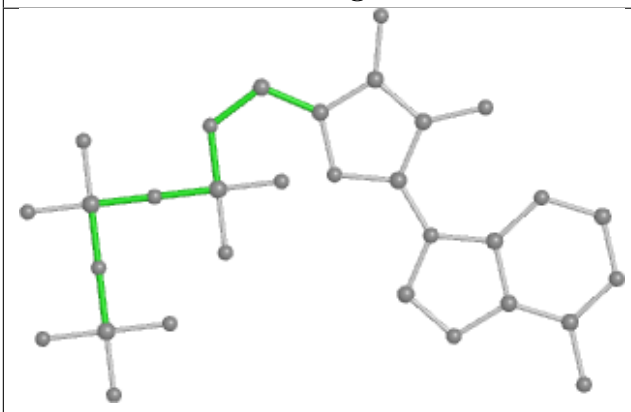
Ligand ATP B 602



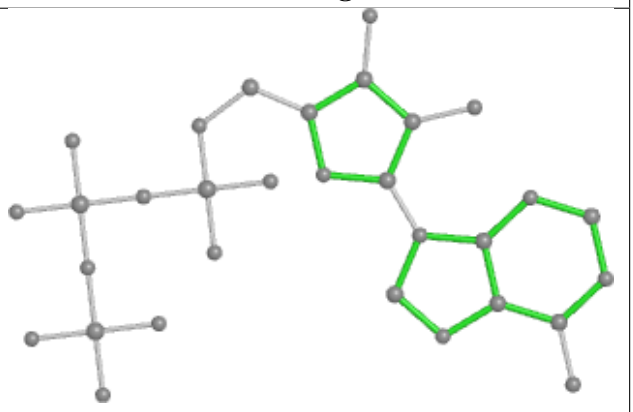
Bond lengths



Bond angles

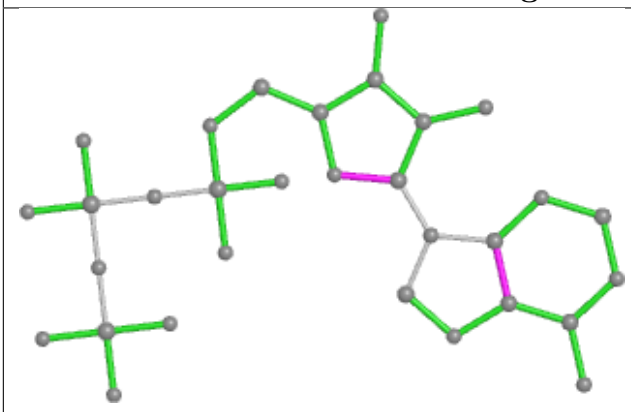


Torsions

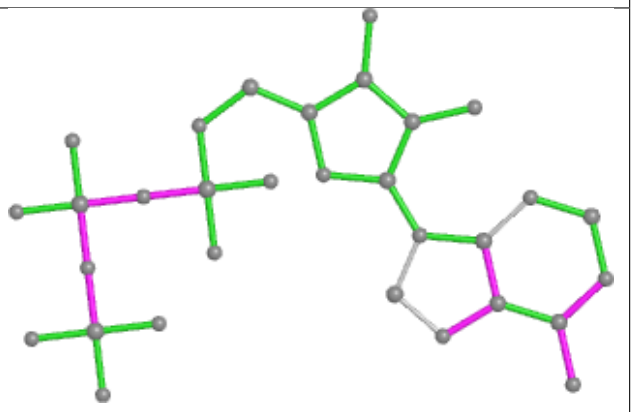


Rings

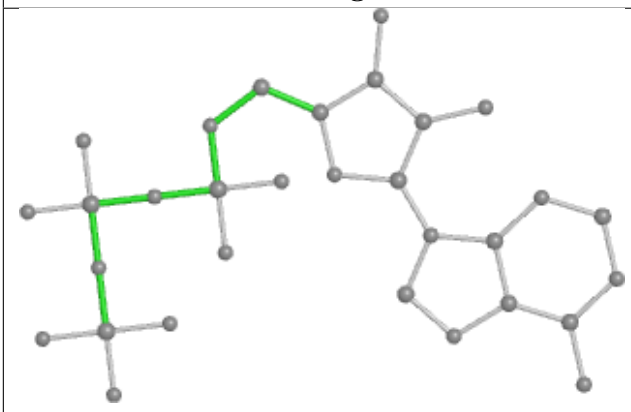
Ligand ATP M 601



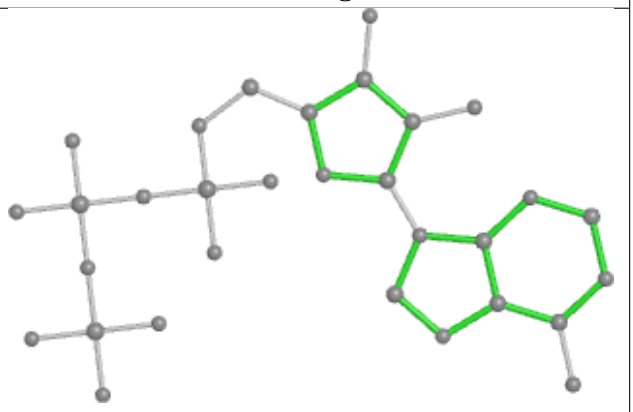
Bond lengths



Bond angles

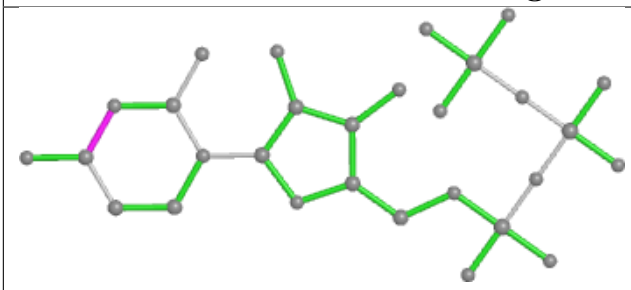


Torsions

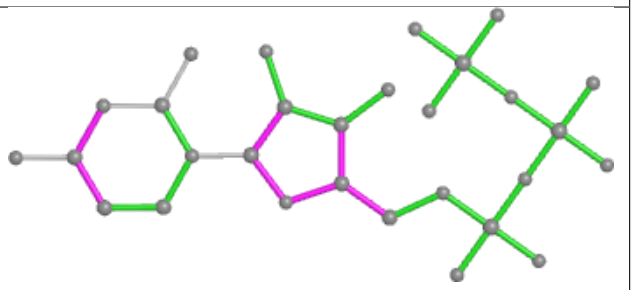


Rings

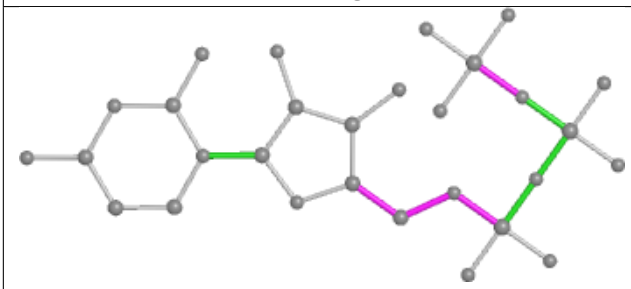
Ligand UTP b 601



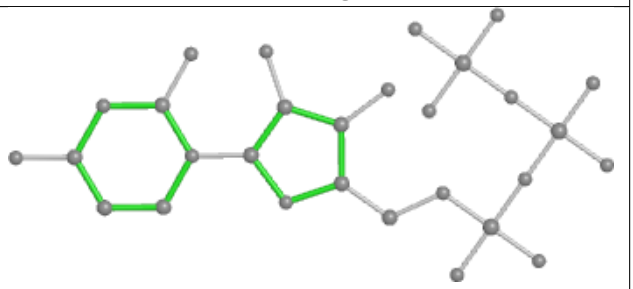
Bond lengths



Bond angles

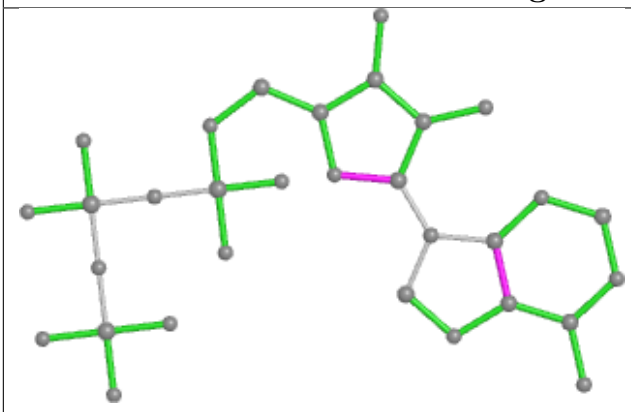


Torsions

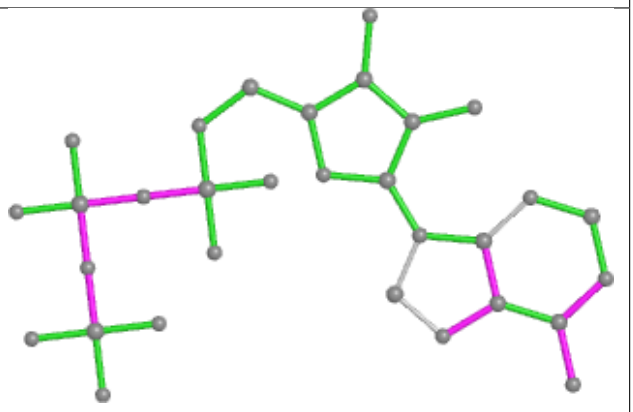


Rings

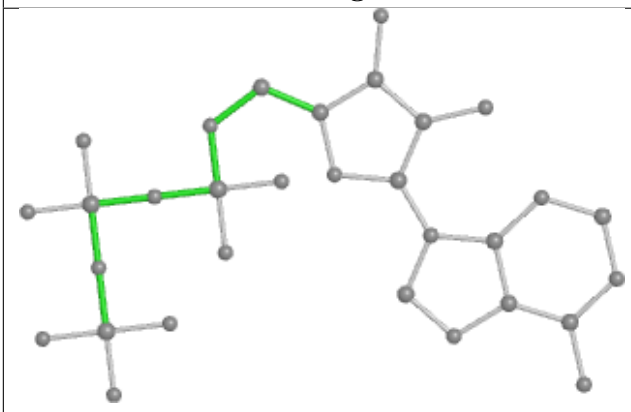
Ligand ATP a 602



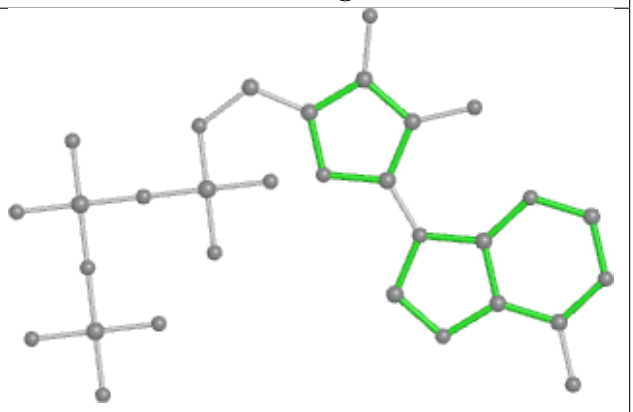
Bond lengths



Bond angles

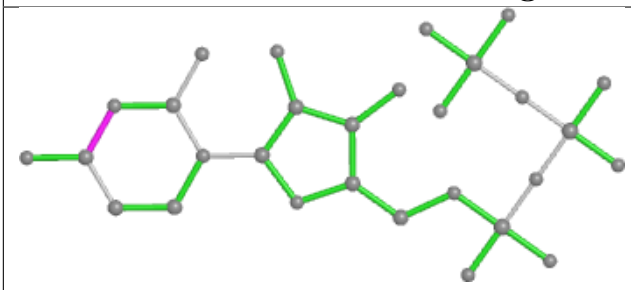


Torsions

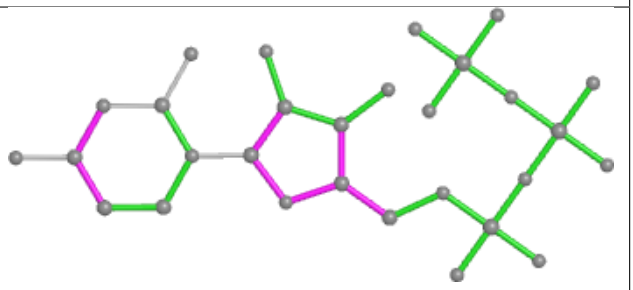


Rings

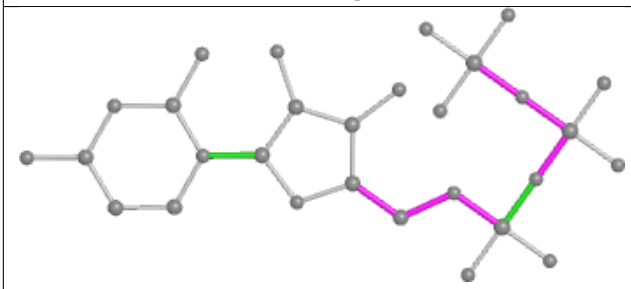
Ligand UTP M 603



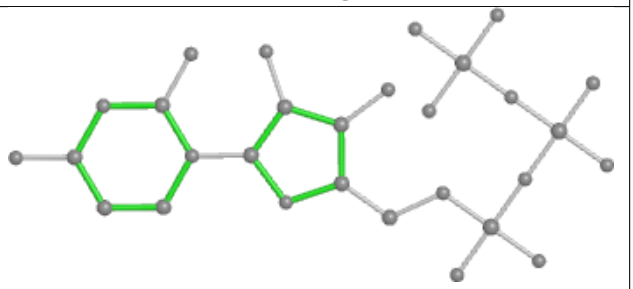
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

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

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

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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

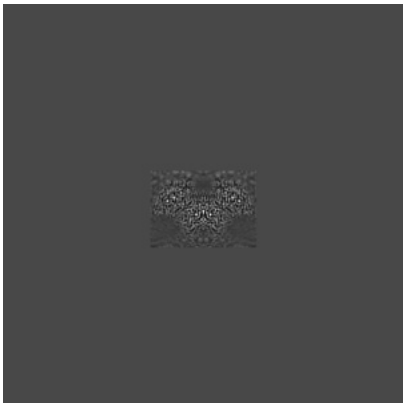
6 Map visualisation

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.

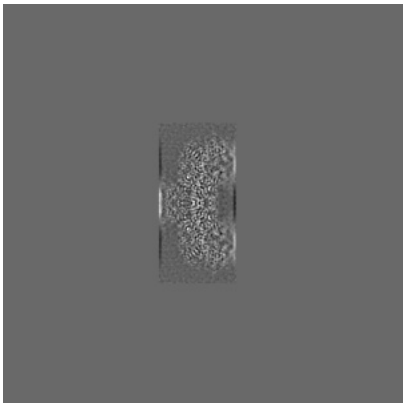
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

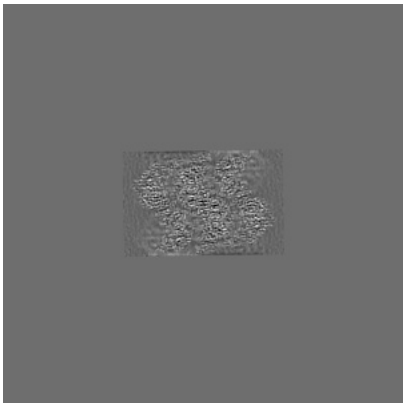
6.1.1 Primary map



X



Y

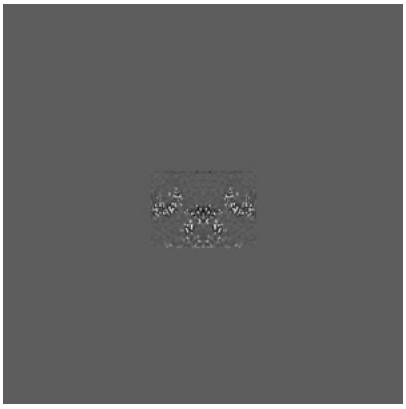


Z

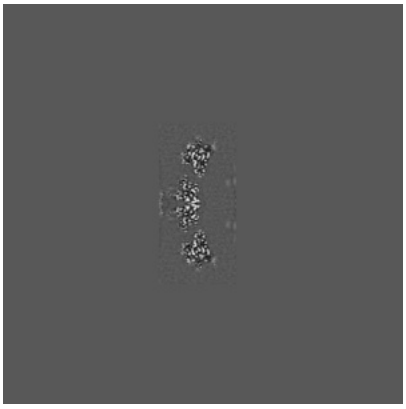
The images above show the map projected in three orthogonal directions.

6.2 Central slices

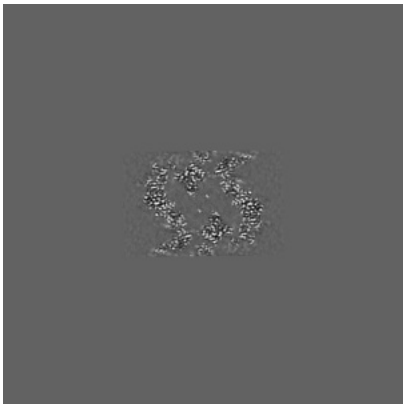
6.2.1 Primary map



X Index: 256



Y Index: 256

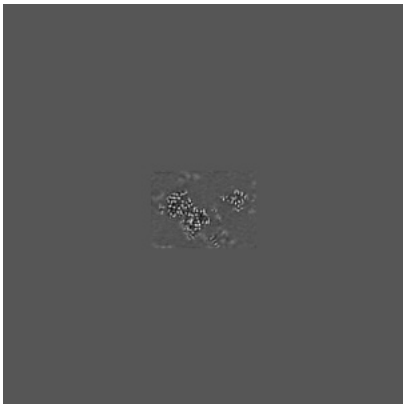


Z Index: 256

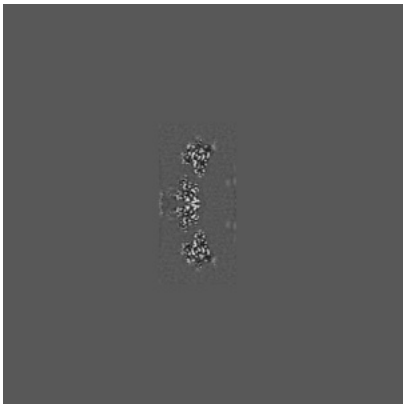
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

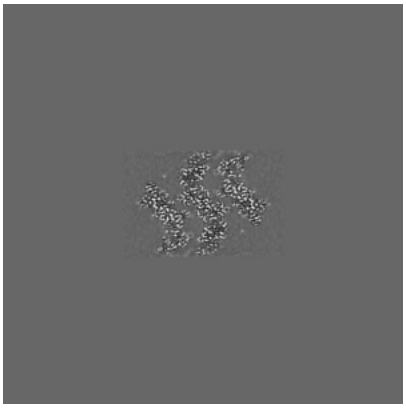
6.3.1 Primary map



X Index: 275



Y Index: 256

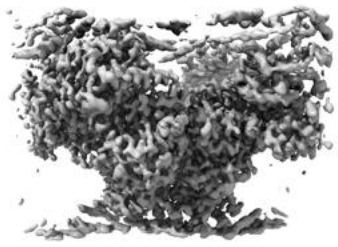


Z Index: 248

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

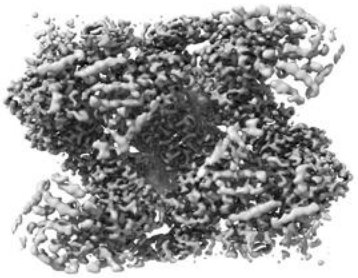
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

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

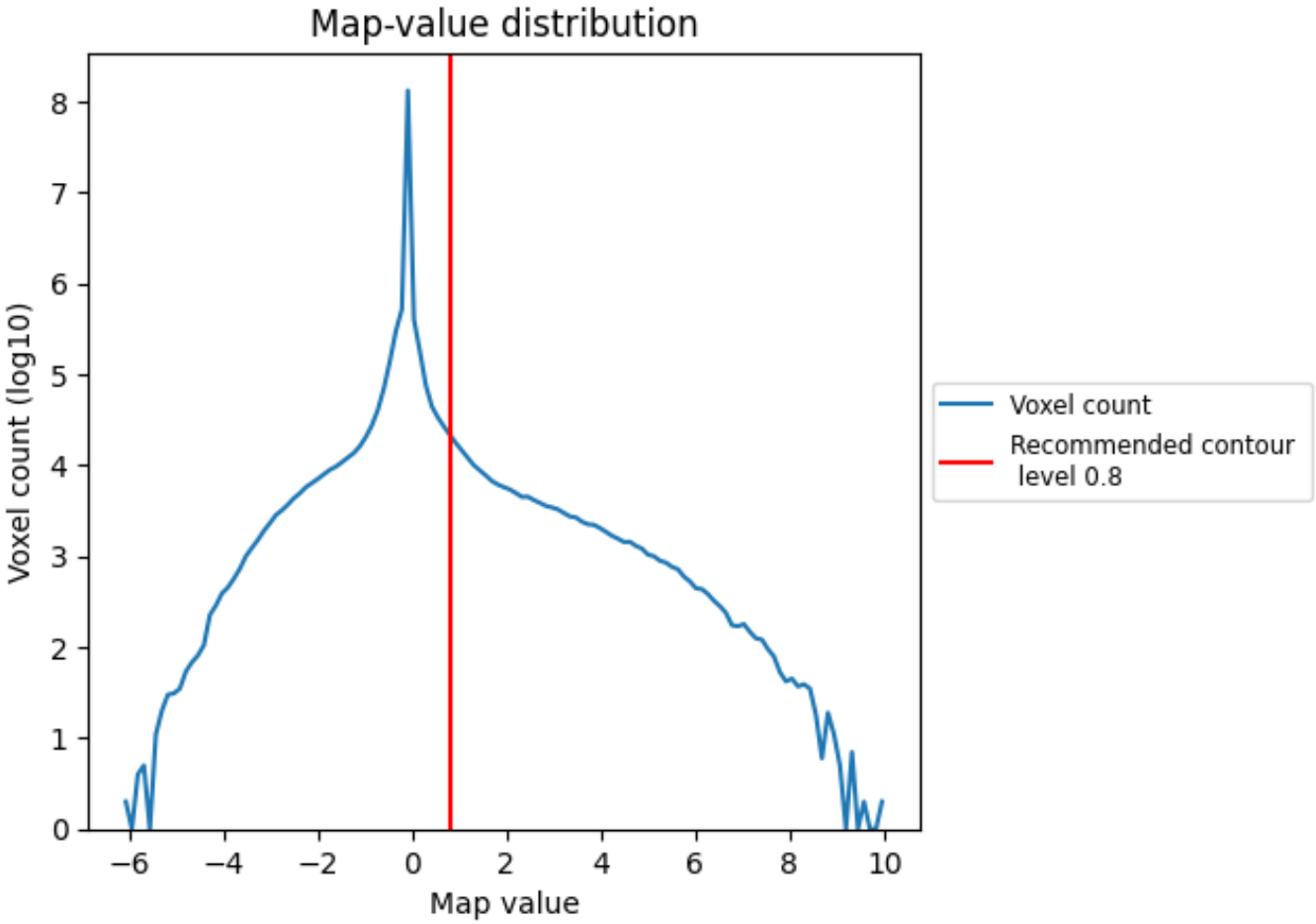
6.5 Mask visualisation (i)

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

7 Map analysis

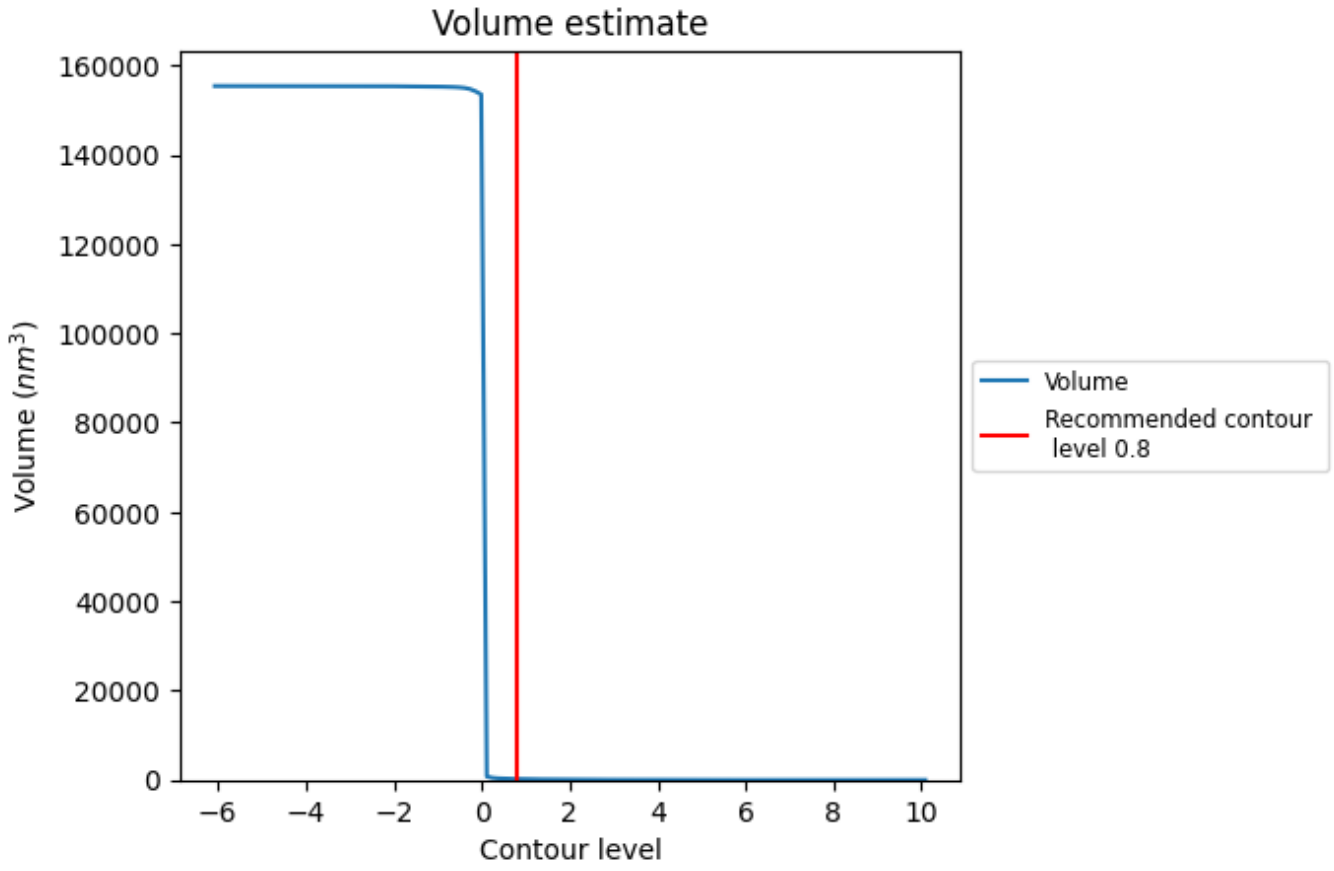
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

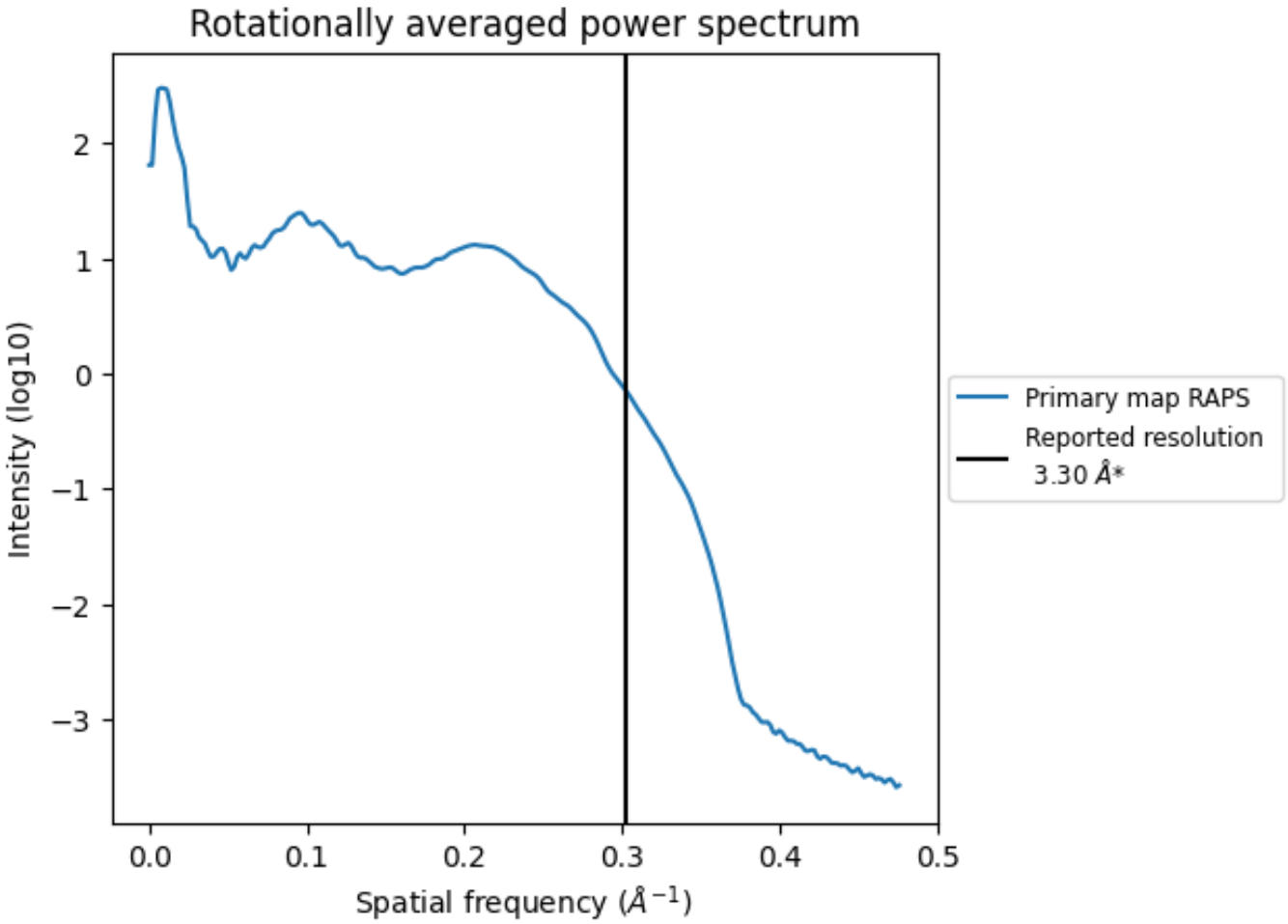
7.2 Volume estimate



The volume at the recommended contour level is 216 nm^3; this corresponds to an approximate mass of 195 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

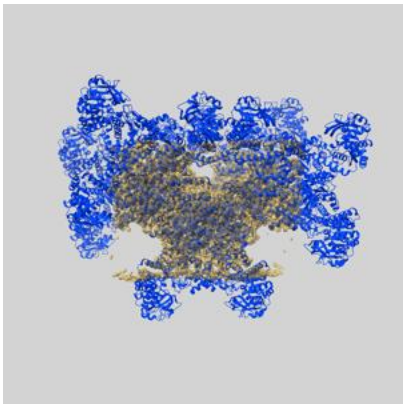
8 Fourier-Shell correlation (i)

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

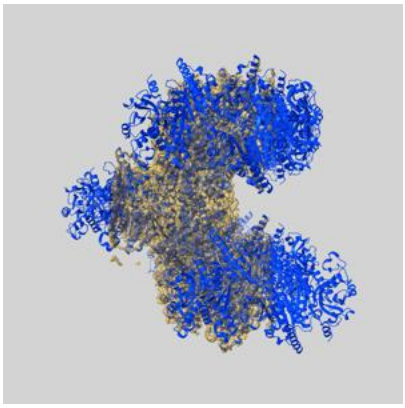
9 Map-model fit

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.

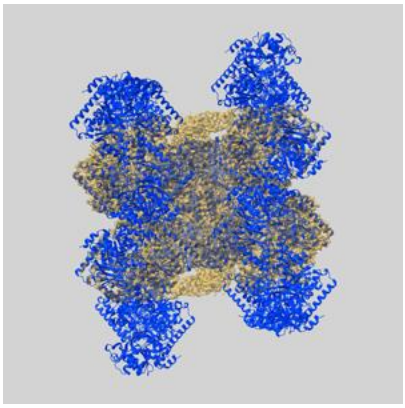
9.1 Map-model overlay



X



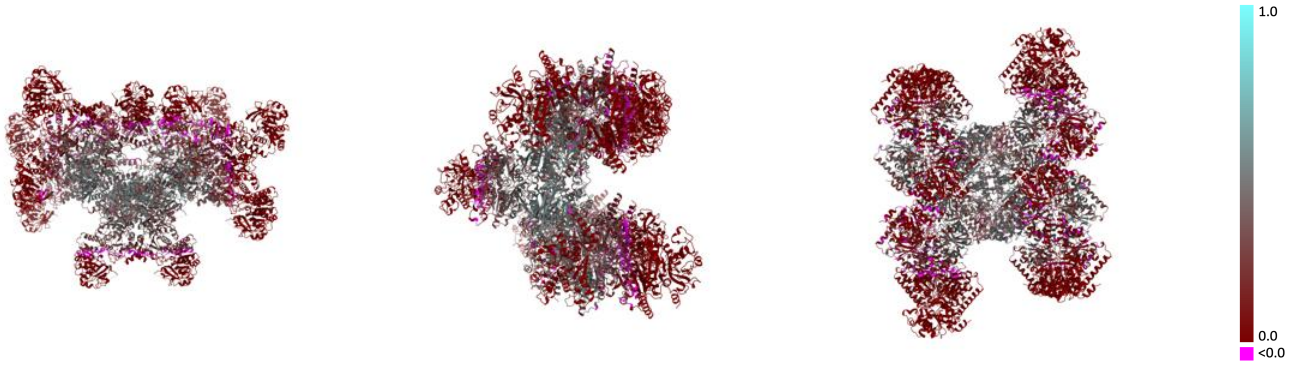
Y



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.

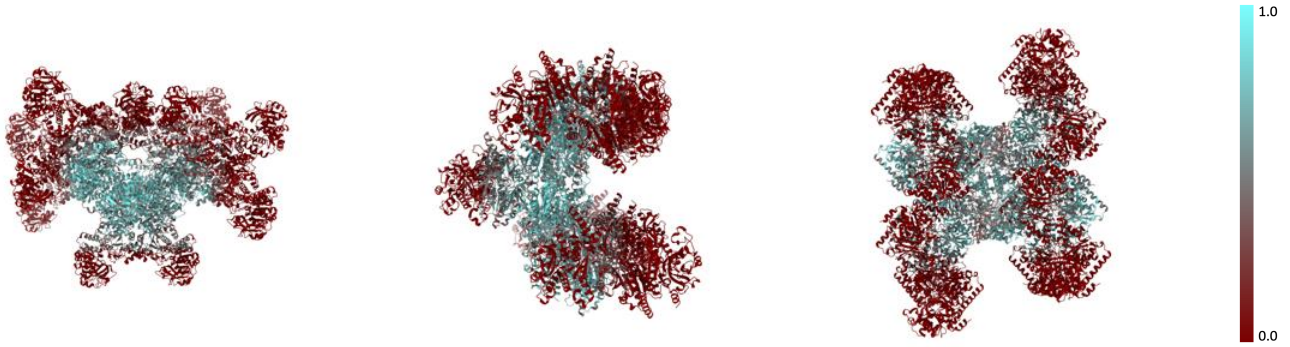
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

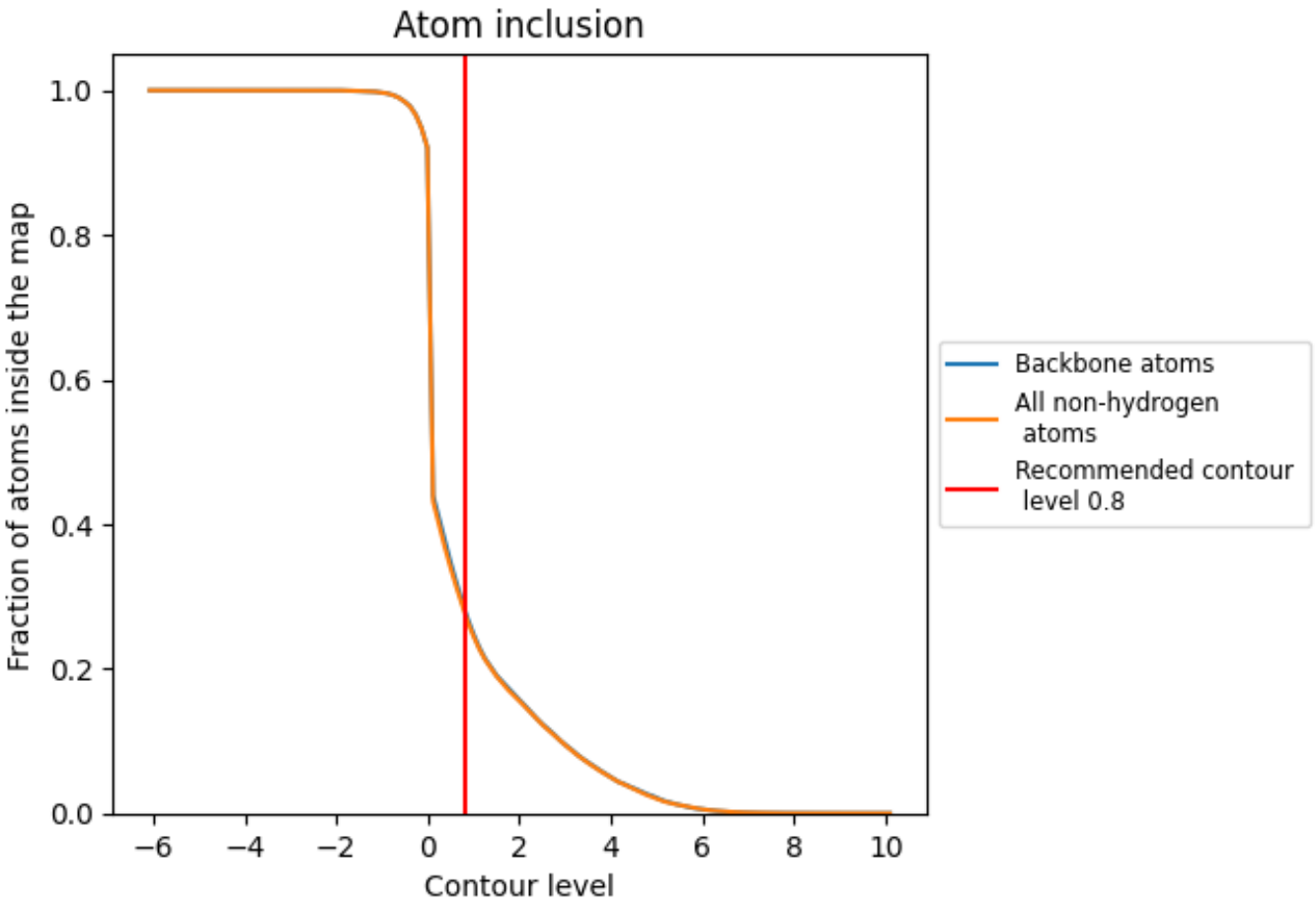
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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