



wwPDB X-ray Structure Validation Summary Report

Feb 21, 2022 – 08:27 pm GMT

PDB ID : 7BL7
Title : Crystal structure of UMPK from *M. tuberculosis* in complex with UDP and UTP (P21212 form)
Authors : Walter, P.; Labesse, G.; Haouz, A.; Mechaly, A.E.; Munier-Lehmann, H.
Deposited on : 2021-01-18
Resolution : 3.33 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.26
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

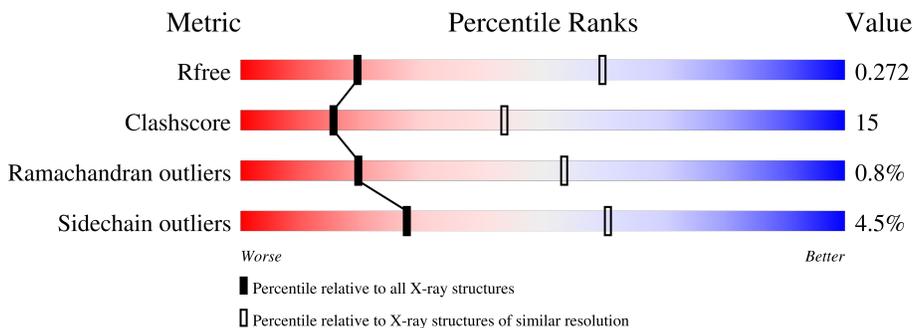
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	281	
1	B	281	
1	C	281	
1	D	281	
1	E	281	
1	F	281	
1	G	281	

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Mol	Chain	Length	Quality of chain
1	H	281	
1	I	281	
1	J	281	
1	K	281	
1	L	281	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UDP	C	302	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19544 atoms, of which 112 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Uridylate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	227	Total 1689	C 1063	N 300	O 315	S 11	0	0	0
1	A	226	Total 1647	C 1038	N 288	O 311	S 10	0	0	0
1	F	216	Total 1552	C 977	N 274	O 290	S 11	0	0	0
1	E	222	Total 1642	C 1035	N 291	O 305	S 11	0	0	0
1	D	228	Total 1690	C 1064	N 301	O 314	S 11	0	0	0
1	C	230	Total 1697	C 1068	N 302	O 316	S 11	0	0	0
1	I	225	Total 1665	C 1049	N 294	O 311	S 11	0	0	0
1	J	227	Total 1674	C 1056	N 297	O 310	S 11	0	0	0
1	K	224	Total 1660	C 1047	N 294	O 308	S 11	0	0	0
1	L	158	Total 1157	C 736	N 201	O 212	S 8	0	0	0
1	G	169	Total 1237	C 785	N 217	O 226	S 9	0	0	0
1	H	222	Total 1649	C 1038	N 295	O 305	S 11	0	0	0

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P9WHK5
B	-18	GLY	-	expression tag	UNP P9WHK5
B	-17	SER	-	expression tag	UNP P9WHK5
B	-16	SER	-	expression tag	UNP P9WHK5
B	-15	HIS	-	expression tag	UNP P9WHK5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P9WHK5
B	-13	HIS	-	expression tag	UNP P9WHK5
B	-12	HIS	-	expression tag	UNP P9WHK5
B	-11	HIS	-	expression tag	UNP P9WHK5
B	-10	HIS	-	expression tag	UNP P9WHK5
B	-9	SER	-	expression tag	UNP P9WHK5
B	-8	SER	-	expression tag	UNP P9WHK5
B	-7	GLY	-	expression tag	UNP P9WHK5
B	-6	LEU	-	expression tag	UNP P9WHK5
B	-5	VAL	-	expression tag	UNP P9WHK5
B	-4	PRO	-	expression tag	UNP P9WHK5
B	-3	ARG	-	expression tag	UNP P9WHK5
B	-2	GLY	-	expression tag	UNP P9WHK5
B	-1	SER	-	expression tag	UNP P9WHK5
B	0	HIS	-	expression tag	UNP P9WHK5
A	-19	MET	-	initiating methionine	UNP P9WHK5
A	-18	GLY	-	expression tag	UNP P9WHK5
A	-17	SER	-	expression tag	UNP P9WHK5
A	-16	SER	-	expression tag	UNP P9WHK5
A	-15	HIS	-	expression tag	UNP P9WHK5
A	-14	HIS	-	expression tag	UNP P9WHK5
A	-13	HIS	-	expression tag	UNP P9WHK5
A	-12	HIS	-	expression tag	UNP P9WHK5
A	-11	HIS	-	expression tag	UNP P9WHK5
A	-10	HIS	-	expression tag	UNP P9WHK5
A	-9	SER	-	expression tag	UNP P9WHK5
A	-8	SER	-	expression tag	UNP P9WHK5
A	-7	GLY	-	expression tag	UNP P9WHK5
A	-6	LEU	-	expression tag	UNP P9WHK5
A	-5	VAL	-	expression tag	UNP P9WHK5
A	-4	PRO	-	expression tag	UNP P9WHK5
A	-3	ARG	-	expression tag	UNP P9WHK5
A	-2	GLY	-	expression tag	UNP P9WHK5
A	-1	SER	-	expression tag	UNP P9WHK5
A	0	HIS	-	expression tag	UNP P9WHK5
F	-19	MET	-	initiating methionine	UNP P9WHK5
F	-18	GLY	-	expression tag	UNP P9WHK5
F	-17	SER	-	expression tag	UNP P9WHK5
F	-16	SER	-	expression tag	UNP P9WHK5
F	-15	HIS	-	expression tag	UNP P9WHK5
F	-14	HIS	-	expression tag	UNP P9WHK5
F	-13	HIS	-	expression tag	UNP P9WHK5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-12	HIS	-	expression tag	UNP P9WHK5
F	-11	HIS	-	expression tag	UNP P9WHK5
F	-10	HIS	-	expression tag	UNP P9WHK5
F	-9	SER	-	expression tag	UNP P9WHK5
F	-8	SER	-	expression tag	UNP P9WHK5
F	-7	GLY	-	expression tag	UNP P9WHK5
F	-6	LEU	-	expression tag	UNP P9WHK5
F	-5	VAL	-	expression tag	UNP P9WHK5
F	-4	PRO	-	expression tag	UNP P9WHK5
F	-3	ARG	-	expression tag	UNP P9WHK5
F	-2	GLY	-	expression tag	UNP P9WHK5
F	-1	SER	-	expression tag	UNP P9WHK5
F	0	HIS	-	expression tag	UNP P9WHK5
E	-19	MET	-	initiating methionine	UNP P9WHK5
E	-18	GLY	-	expression tag	UNP P9WHK5
E	-17	SER	-	expression tag	UNP P9WHK5
E	-16	SER	-	expression tag	UNP P9WHK5
E	-15	HIS	-	expression tag	UNP P9WHK5
E	-14	HIS	-	expression tag	UNP P9WHK5
E	-13	HIS	-	expression tag	UNP P9WHK5
E	-12	HIS	-	expression tag	UNP P9WHK5
E	-11	HIS	-	expression tag	UNP P9WHK5
E	-10	HIS	-	expression tag	UNP P9WHK5
E	-9	SER	-	expression tag	UNP P9WHK5
E	-8	SER	-	expression tag	UNP P9WHK5
E	-7	GLY	-	expression tag	UNP P9WHK5
E	-6	LEU	-	expression tag	UNP P9WHK5
E	-5	VAL	-	expression tag	UNP P9WHK5
E	-4	PRO	-	expression tag	UNP P9WHK5
E	-3	ARG	-	expression tag	UNP P9WHK5
E	-2	GLY	-	expression tag	UNP P9WHK5
E	-1	SER	-	expression tag	UNP P9WHK5
E	0	HIS	-	expression tag	UNP P9WHK5
D	-19	MET	-	initiating methionine	UNP P9WHK5
D	-18	GLY	-	expression tag	UNP P9WHK5
D	-17	SER	-	expression tag	UNP P9WHK5
D	-16	SER	-	expression tag	UNP P9WHK5
D	-15	HIS	-	expression tag	UNP P9WHK5
D	-14	HIS	-	expression tag	UNP P9WHK5
D	-13	HIS	-	expression tag	UNP P9WHK5
D	-12	HIS	-	expression tag	UNP P9WHK5
D	-11	HIS	-	expression tag	UNP P9WHK5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	HIS	-	expression tag	UNP P9WHK5
D	-9	SER	-	expression tag	UNP P9WHK5
D	-8	SER	-	expression tag	UNP P9WHK5
D	-7	GLY	-	expression tag	UNP P9WHK5
D	-6	LEU	-	expression tag	UNP P9WHK5
D	-5	VAL	-	expression tag	UNP P9WHK5
D	-4	PRO	-	expression tag	UNP P9WHK5
D	-3	ARG	-	expression tag	UNP P9WHK5
D	-2	GLY	-	expression tag	UNP P9WHK5
D	-1	SER	-	expression tag	UNP P9WHK5
D	0	HIS	-	expression tag	UNP P9WHK5
C	-19	MET	-	initiating methionine	UNP P9WHK5
C	-18	GLY	-	expression tag	UNP P9WHK5
C	-17	SER	-	expression tag	UNP P9WHK5
C	-16	SER	-	expression tag	UNP P9WHK5
C	-15	HIS	-	expression tag	UNP P9WHK5
C	-14	HIS	-	expression tag	UNP P9WHK5
C	-13	HIS	-	expression tag	UNP P9WHK5
C	-12	HIS	-	expression tag	UNP P9WHK5
C	-11	HIS	-	expression tag	UNP P9WHK5
C	-10	HIS	-	expression tag	UNP P9WHK5
C	-9	SER	-	expression tag	UNP P9WHK5
C	-8	SER	-	expression tag	UNP P9WHK5
C	-7	GLY	-	expression tag	UNP P9WHK5
C	-6	LEU	-	expression tag	UNP P9WHK5
C	-5	VAL	-	expression tag	UNP P9WHK5
C	-4	PRO	-	expression tag	UNP P9WHK5
C	-3	ARG	-	expression tag	UNP P9WHK5
C	-2	GLY	-	expression tag	UNP P9WHK5
C	-1	SER	-	expression tag	UNP P9WHK5
C	0	HIS	-	expression tag	UNP P9WHK5
I	-19	MET	-	initiating methionine	UNP P9WHK5
I	-18	GLY	-	expression tag	UNP P9WHK5
I	-17	SER	-	expression tag	UNP P9WHK5
I	-16	SER	-	expression tag	UNP P9WHK5
I	-15	HIS	-	expression tag	UNP P9WHK5
I	-14	HIS	-	expression tag	UNP P9WHK5
I	-13	HIS	-	expression tag	UNP P9WHK5
I	-12	HIS	-	expression tag	UNP P9WHK5
I	-11	HIS	-	expression tag	UNP P9WHK5
I	-10	HIS	-	expression tag	UNP P9WHK5
I	-9	SER	-	expression tag	UNP P9WHK5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	SER	-	expression tag	UNP P9WHK5
I	-7	GLY	-	expression tag	UNP P9WHK5
I	-6	LEU	-	expression tag	UNP P9WHK5
I	-5	VAL	-	expression tag	UNP P9WHK5
I	-4	PRO	-	expression tag	UNP P9WHK5
I	-3	ARG	-	expression tag	UNP P9WHK5
I	-2	GLY	-	expression tag	UNP P9WHK5
I	-1	SER	-	expression tag	UNP P9WHK5
I	0	HIS	-	expression tag	UNP P9WHK5
J	-19	MET	-	initiating methionine	UNP P9WHK5
J	-18	GLY	-	expression tag	UNP P9WHK5
J	-17	SER	-	expression tag	UNP P9WHK5
J	-16	SER	-	expression tag	UNP P9WHK5
J	-15	HIS	-	expression tag	UNP P9WHK5
J	-14	HIS	-	expression tag	UNP P9WHK5
J	-13	HIS	-	expression tag	UNP P9WHK5
J	-12	HIS	-	expression tag	UNP P9WHK5
J	-11	HIS	-	expression tag	UNP P9WHK5
J	-10	HIS	-	expression tag	UNP P9WHK5
J	-9	SER	-	expression tag	UNP P9WHK5
J	-8	SER	-	expression tag	UNP P9WHK5
J	-7	GLY	-	expression tag	UNP P9WHK5
J	-6	LEU	-	expression tag	UNP P9WHK5
J	-5	VAL	-	expression tag	UNP P9WHK5
J	-4	PRO	-	expression tag	UNP P9WHK5
J	-3	ARG	-	expression tag	UNP P9WHK5
J	-2	GLY	-	expression tag	UNP P9WHK5
J	-1	SER	-	expression tag	UNP P9WHK5
J	0	HIS	-	expression tag	UNP P9WHK5
K	-19	MET	-	initiating methionine	UNP P9WHK5
K	-18	GLY	-	expression tag	UNP P9WHK5
K	-17	SER	-	expression tag	UNP P9WHK5
K	-16	SER	-	expression tag	UNP P9WHK5
K	-15	HIS	-	expression tag	UNP P9WHK5
K	-14	HIS	-	expression tag	UNP P9WHK5
K	-13	HIS	-	expression tag	UNP P9WHK5
K	-12	HIS	-	expression tag	UNP P9WHK5
K	-11	HIS	-	expression tag	UNP P9WHK5
K	-10	HIS	-	expression tag	UNP P9WHK5
K	-9	SER	-	expression tag	UNP P9WHK5
K	-8	SER	-	expression tag	UNP P9WHK5
K	-7	GLY	-	expression tag	UNP P9WHK5

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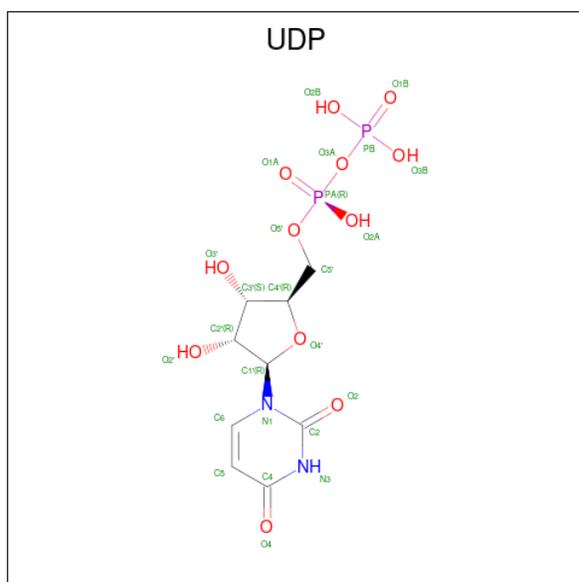
Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	LEU	-	expression tag	UNP P9WHK5
K	-5	VAL	-	expression tag	UNP P9WHK5
K	-4	PRO	-	expression tag	UNP P9WHK5
K	-3	ARG	-	expression tag	UNP P9WHK5
K	-2	GLY	-	expression tag	UNP P9WHK5
K	-1	SER	-	expression tag	UNP P9WHK5
K	0	HIS	-	expression tag	UNP P9WHK5
L	-19	MET	-	initiating methionine	UNP P9WHK5
L	-18	GLY	-	expression tag	UNP P9WHK5
L	-17	SER	-	expression tag	UNP P9WHK5
L	-16	SER	-	expression tag	UNP P9WHK5
L	-15	HIS	-	expression tag	UNP P9WHK5
L	-14	HIS	-	expression tag	UNP P9WHK5
L	-13	HIS	-	expression tag	UNP P9WHK5
L	-12	HIS	-	expression tag	UNP P9WHK5
L	-11	HIS	-	expression tag	UNP P9WHK5
L	-10	HIS	-	expression tag	UNP P9WHK5
L	-9	SER	-	expression tag	UNP P9WHK5
L	-8	SER	-	expression tag	UNP P9WHK5
L	-7	GLY	-	expression tag	UNP P9WHK5
L	-6	LEU	-	expression tag	UNP P9WHK5
L	-5	VAL	-	expression tag	UNP P9WHK5
L	-4	PRO	-	expression tag	UNP P9WHK5
L	-3	ARG	-	expression tag	UNP P9WHK5
L	-2	GLY	-	expression tag	UNP P9WHK5
L	-1	SER	-	expression tag	UNP P9WHK5
L	0	HIS	-	expression tag	UNP P9WHK5
G	-19	MET	-	initiating methionine	UNP P9WHK5
G	-18	GLY	-	expression tag	UNP P9WHK5
G	-17	SER	-	expression tag	UNP P9WHK5
G	-16	SER	-	expression tag	UNP P9WHK5
G	-15	HIS	-	expression tag	UNP P9WHK5
G	-14	HIS	-	expression tag	UNP P9WHK5
G	-13	HIS	-	expression tag	UNP P9WHK5
G	-12	HIS	-	expression tag	UNP P9WHK5
G	-11	HIS	-	expression tag	UNP P9WHK5
G	-10	HIS	-	expression tag	UNP P9WHK5
G	-9	SER	-	expression tag	UNP P9WHK5
G	-8	SER	-	expression tag	UNP P9WHK5
G	-7	GLY	-	expression tag	UNP P9WHK5
G	-6	LEU	-	expression tag	UNP P9WHK5
G	-5	VAL	-	expression tag	UNP P9WHK5

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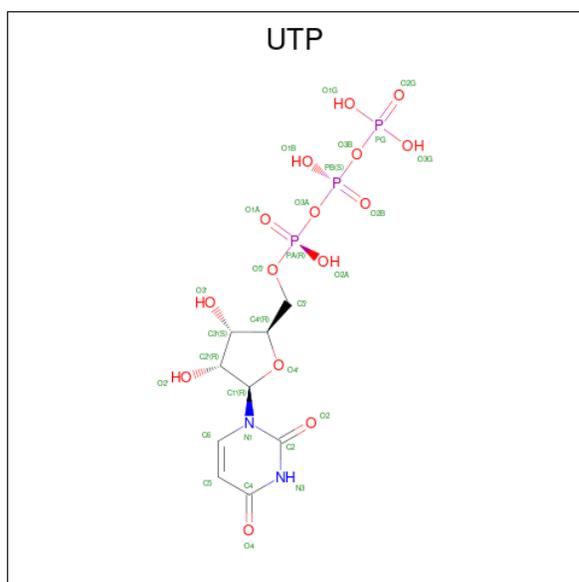
Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	PRO	-	expression tag	UNP P9WHK5
G	-3	ARG	-	expression tag	UNP P9WHK5
G	-2	GLY	-	expression tag	UNP P9WHK5
G	-1	SER	-	expression tag	UNP P9WHK5
G	0	HIS	-	expression tag	UNP P9WHK5
H	-19	MET	-	initiating methionine	UNP P9WHK5
H	-18	GLY	-	expression tag	UNP P9WHK5
H	-17	SER	-	expression tag	UNP P9WHK5
H	-16	SER	-	expression tag	UNP P9WHK5
H	-15	HIS	-	expression tag	UNP P9WHK5
H	-14	HIS	-	expression tag	UNP P9WHK5
H	-13	HIS	-	expression tag	UNP P9WHK5
H	-12	HIS	-	expression tag	UNP P9WHK5
H	-11	HIS	-	expression tag	UNP P9WHK5
H	-10	HIS	-	expression tag	UNP P9WHK5
H	-9	SER	-	expression tag	UNP P9WHK5
H	-8	SER	-	expression tag	UNP P9WHK5
H	-7	GLY	-	expression tag	UNP P9WHK5
H	-6	LEU	-	expression tag	UNP P9WHK5
H	-5	VAL	-	expression tag	UNP P9WHK5
H	-4	PRO	-	expression tag	UNP P9WHK5
H	-3	ARG	-	expression tag	UNP P9WHK5
H	-2	GLY	-	expression tag	UNP P9WHK5
H	-1	SER	-	expression tag	UNP P9WHK5
H	0	HIS	-	expression tag	UNP P9WHK5

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	B	1	Total	C	H	N	O	P	0	0
			39	9	14	2	12	2		
2	E	1	Total	C	H	N	O	P	0	0
			39	9	14	2	12	2		
2	D	1	Total	C	H	N	O	P	0	0
			39	9	14	2	12	2		
2	C	1	Total	C	H	N	O	P	0	0
			39	9	14	2	12	2		
2	I	1	Total	C	H	N	O	P	0	0
			39	9	14	2	12	2		
2	J	1	Total	C	H	N	O	P	0	0
			39	9	14	2	12	2		
2	K	1	Total	C	H	N	O	P	0	0
			39	9	14	2	12	2		
2	H	1	Total	C	H	N	O	P	0	0
			39	9	14	2	12	2		

- Molecule 3 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
3	F	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
3	D	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
3	C	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
3	I	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
3	J	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
3	L	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
3	G	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	7	Total	O	0	0
			7	7		
4	A	1	Total	O	0	0
			1	1		
4	F	1	Total	O	0	0
			1	1		
4	E	6	Total	O	0	0
			6	6		

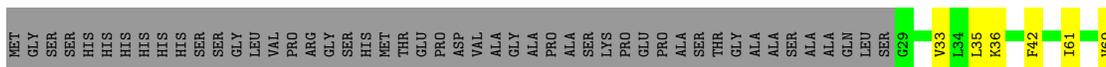
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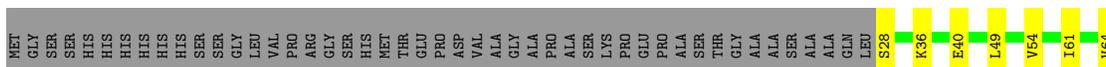
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	6	Total O 6 6	0	0
4	C	4	Total O 4 4	0	0
4	I	3	Total O 3 3	0	0
4	J	3	Total O 3 3	0	0
4	L	1	Total O 1 1	0	0
4	G	4	Total O 4 4	0	0
4	H	5	Total O 5 5	0	0



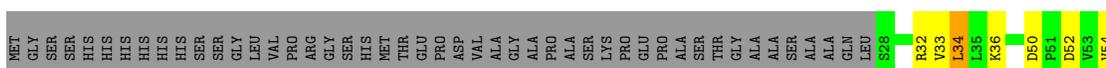
- Molecule 1: Uridylate kinase



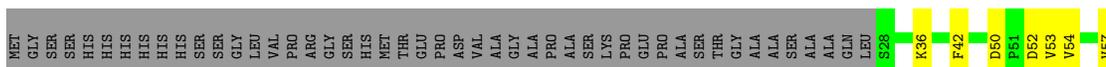
- Molecule 1: Uridylate kinase



- Molecule 1: Uridylate kinase



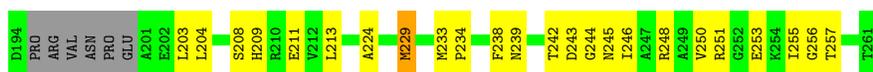
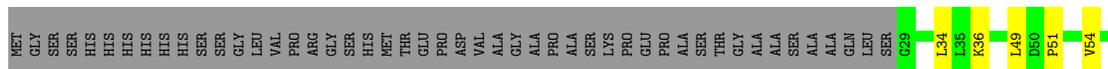
- Molecule 1: Uridylate kinase





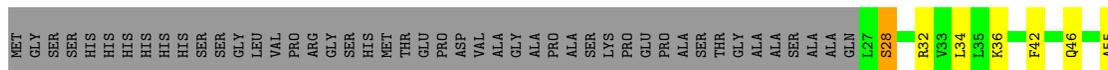
- Molecule 1: Uridylate kinase

Chain J: 58% 21% 19%



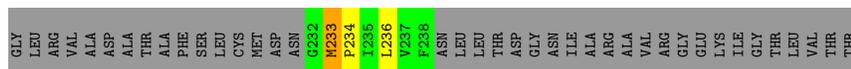
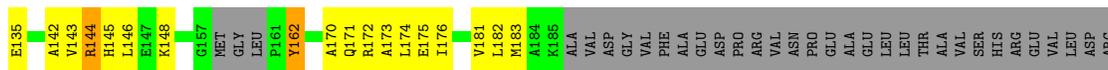
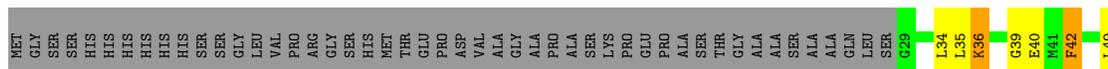
- Molecule 1: Uridylate kinase

Chain K: 59% 20% 20%



- Molecule 1: Uridylate kinase

Chain L: 34% 20% 44%



- Molecule 1: Uridylate kinase

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.23Å 165.75Å 125.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 3.33 48.18 – 2.75	Depositor EDS
% Data completeness (in resolution range)	92.3 (29.95-3.33) 63.3 (48.18-2.75)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.192 , 0.274 0.190 , 0.272	Depositor DCC
R_{free} test set	2604 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19544	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0311e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: UTP, UDP

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	0.45	0/1665	0.65	0/2250
1	B	0.60	0/1707	0.71	0/2302
1	C	0.65	0/1716	0.76	0/2318
1	D	0.65	0/1708	0.71	0/2304
1	E	0.55	0/1660	0.64	0/2241
1	F	0.54	0/1567	0.69	0/2118
1	G	0.46	0/1250	0.67	0/1685
1	H	0.56	0/1666	0.70	0/2247
1	I	0.56	0/1683	0.66	0/2272
1	J	0.59	0/1692	0.72	0/2284
1	K	0.57	0/1678	0.68	0/2264
1	L	0.42	0/1169	0.61	0/1574
All	All	0.56	0/19161	0.69	0/25859

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1647	0	1650	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1689	0	1732	53	0
1	C	1697	0	1726	53	0
1	D	1690	0	1730	38	0
1	E	1642	0	1674	38	0
1	F	1552	0	1532	52	0
1	G	1237	0	1260	51	0
1	H	1649	0	1698	84	0
1	I	1665	0	1699	60	0
1	J	1674	0	1710	55	0
1	K	1660	0	1701	45	0
1	L	1157	0	1173	40	0
2	B	25	14	11	3	0
2	C	25	14	11	9	0
2	D	25	14	11	5	0
2	E	25	14	11	0	0
2	H	25	14	11	6	0
2	I	25	14	11	3	0
2	J	25	14	11	4	0
2	K	25	14	11	6	0
3	A	29	0	11	0	0
3	C	29	0	11	0	0
3	D	29	0	11	1	0
3	F	29	0	11	1	0
3	G	29	0	11	3	0
3	I	29	0	11	4	0
3	J	29	0	11	3	0
3	L	29	0	11	2	0
4	A	1	0	0	0	0
4	B	7	0	0	0	0
4	C	4	0	0	0	0
4	D	6	0	0	0	0
4	E	6	0	0	0	0
4	F	1	0	0	0	0
4	G	4	0	0	1	0
4	H	5	0	0	0	0
4	I	3	0	0	0	0
4	J	3	0	0	0	0
4	L	1	0	0	0	0
All	All	19432	112	19461	579	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 579 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:LYS:HE2	1:I:165:THR:CG2	1.12	1.58
1:C:194:ASP:HB3	1:C:195:PRO:CD	1.56	1.33
1:I:36:LYS:CE	1:I:165:THR:CG2	2.07	1.31
1:C:194:ASP:CB	1:C:195:PRO:HD3	1.71	1.21
1:I:144:ARG:HD2	3:G:301:UTP:H5'1	1.25	1.17

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	220/281 (78%)	209 (95%)	10 (4%)	1 (0%)	29	63
1	B	223/281 (79%)	211 (95%)	11 (5%)	1 (0%)	34	68
1	C	226/281 (80%)	216 (96%)	6 (3%)	4 (2%)	8	37
1	D	224/281 (80%)	216 (96%)	7 (3%)	1 (0%)	34	68
1	E	218/281 (78%)	210 (96%)	7 (3%)	1 (0%)	29	63
1	F	210/281 (75%)	200 (95%)	8 (4%)	2 (1%)	15	49
1	G	163/281 (58%)	145 (89%)	16 (10%)	2 (1%)	13	45
1	H	218/281 (78%)	203 (93%)	11 (5%)	4 (2%)	8	37
1	I	221/281 (79%)	205 (93%)	15 (7%)	1 (0%)	29	63
1	J	223/281 (79%)	215 (96%)	8 (4%)	0	100	100
1	K	220/281 (78%)	209 (95%)	9 (4%)	2 (1%)	17	51
1	L	150/281 (53%)	133 (89%)	17 (11%)	0	100	100
All	All	2516/3372 (75%)	2372 (94%)	125 (5%)	19 (1%)	19	53

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	91	MET
1	C	194	ASP
1	C	195	PRO
1	K	254	LYS
1	H	44	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	165/215 (77%)	160 (97%)	5 (3%)	41 70
1	B	174/215 (81%)	168 (97%)	6 (3%)	37 67
1	C	173/215 (80%)	169 (98%)	4 (2%)	50 75
1	D	173/215 (80%)	166 (96%)	7 (4%)	31 63
1	E	168/215 (78%)	164 (98%)	4 (2%)	49 75
1	F	150/215 (70%)	144 (96%)	6 (4%)	31 63
1	G	124/215 (58%)	116 (94%)	8 (6%)	17 48
1	H	170/215 (79%)	155 (91%)	15 (9%)	10 36
1	I	171/215 (80%)	164 (96%)	7 (4%)	30 62
1	J	170/215 (79%)	165 (97%)	5 (3%)	42 71
1	K	171/215 (80%)	163 (95%)	8 (5%)	26 60
1	L	116/215 (54%)	105 (90%)	11 (10%)	8 32
All	All	1925/2580 (75%)	1839 (96%)	86 (4%)	27 61

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	96	SER
1	H	46	GLN
1	L	162	TYR
1	G	59	ARG
1	H	92	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	85	GLN
1	G	85	GLN
1	H	56	GLN
1	H	46	GLN
1	D	88	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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	UDP	B	301	-	20,26,26	1.99	6 (30%)	25,40,40	1.37	2 (8%)
2	UDP	C	302	-	20,26,26	2.22	6 (30%)	25,40,40	1.10	2 (8%)
2	UDP	I	302	-	20,26,26	2.12	6 (30%)	25,40,40	1.22	2 (8%)
3	UTP	L	301	-	26,30,30	2.46	6 (23%)	34,47,47	2.06	11 (32%)
3	UTP	J	301	-	26,30,30	2.45	6 (23%)	34,47,47	1.97	11 (32%)
3	UTP	D	301	-	26,30,30	2.31	7 (26%)	34,47,47	1.78	9 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UTP	C	301	-	26,30,30	2.45	4 (15%)	34,47,47	1.71	8 (23%)
3	UTP	I	301	-	26,30,30	2.47	5 (19%)	34,47,47	1.91	7 (20%)
2	UDP	D	302	-	20,26,26	2.28	6 (30%)	25,40,40	1.38	2 (8%)
2	UDP	J	302	-	20,26,26	2.23	6 (30%)	25,40,40	1.05	1 (4%)
3	UTP	F	301	-	26,30,30	2.44	6 (23%)	34,47,47	1.70	8 (23%)
2	UDP	E	301	-	20,26,26	1.83	6 (30%)	25,40,40	1.05	2 (8%)
3	UTP	A	301	-	26,30,30	2.31	4 (15%)	34,47,47	2.00	7 (20%)
2	UDP	K	301	-	20,26,26	1.88	6 (30%)	25,40,40	1.14	2 (8%)
3	UTP	G	301	-	26,30,30	2.47	3 (11%)	34,47,47	1.97	7 (20%)
2	UDP	H	301	-	20,26,26	1.83	7 (35%)	25,40,40	1.15	1 (4%)

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	UDP	B	301	-	-	1/14/32/32	0/2/2/2
2	UDP	C	302	-	-	3/14/32/32	0/2/2/2
2	UDP	I	302	-	-	5/14/32/32	0/2/2/2
3	UTP	L	301	-	-	9/22/38/38	0/2/2/2
3	UTP	J	301	-	-	4/22/38/38	0/2/2/2
3	UTP	D	301	-	-	5/22/38/38	0/2/2/2
3	UTP	C	301	-	-	4/22/38/38	0/2/2/2
3	UTP	I	301	-	-	2/22/38/38	0/2/2/2
2	UDP	D	302	-	-	6/14/32/32	0/2/2/2
2	UDP	J	302	-	-	2/14/32/32	0/2/2/2
3	UTP	F	301	-	-	10/22/38/38	0/2/2/2
2	UDP	E	301	-	-	2/14/32/32	0/2/2/2
3	UTP	A	301	-	-	6/22/38/38	0/2/2/2
2	UDP	K	301	-	-	3/14/32/32	0/2/2/2
3	UTP	G	301	-	-	6/22/38/38	0/2/2/2
2	UDP	H	301	-	-	7/14/32/32	0/2/2/2

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	301	UTP	C2-N1	8.27	1.47	1.35
3	I	301	UTP	C2-N1	7.97	1.47	1.35
3	F	301	UTP	C2-N1	7.95	1.47	1.35
3	L	301	UTP	C2-N1	7.62	1.46	1.35
3	C	301	UTP	C2-N1	7.26	1.46	1.35

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	301	UTP	C4-N3-C2	-7.26	119.77	125.79
3	A	301	UTP	C4-N3-C2	-6.55	120.36	125.79
3	J	301	UTP	C4-N3-C2	-6.16	120.68	125.79
3	G	301	UTP	C4-N3-C2	-6.10	120.73	125.79
3	I	301	UTP	C4-N3-C2	-6.06	120.76	125.79

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

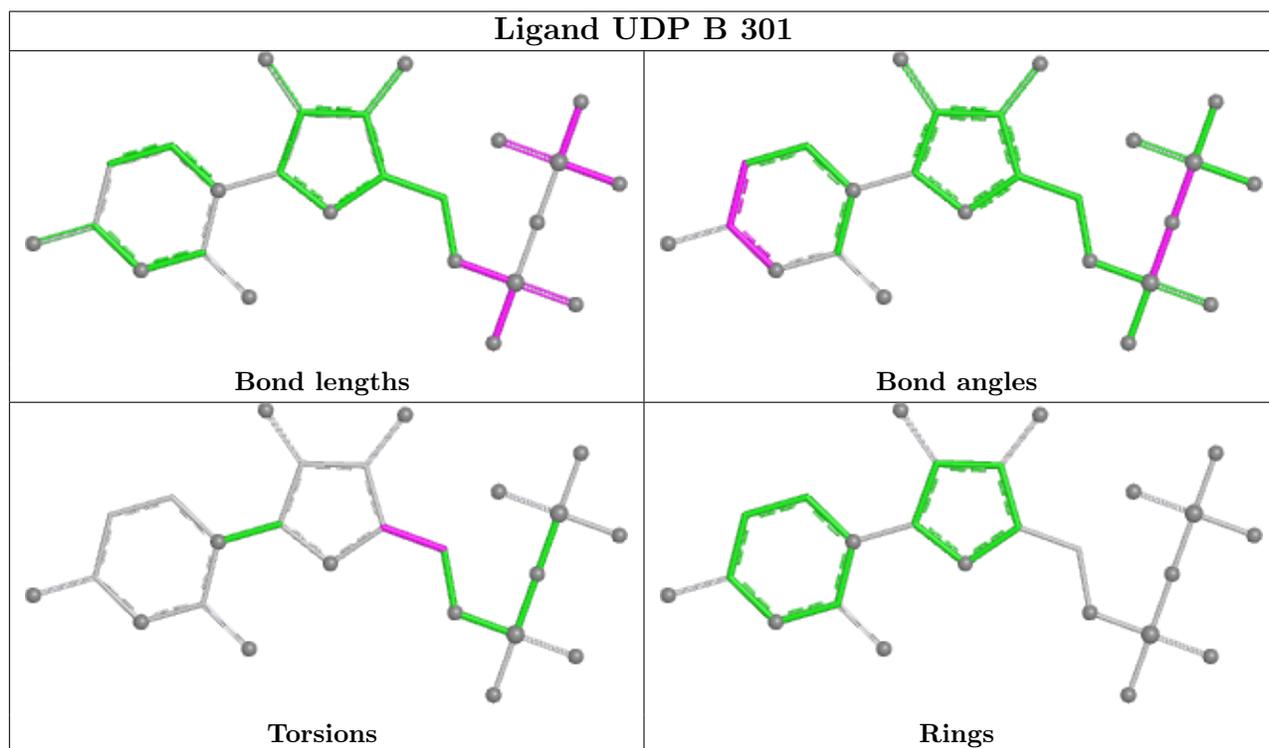
Mol	Chain	Res	Type	Atoms
2	B	301	UDP	O4'-C4'-C5'-O5'
2	D	302	UDP	C5'-O5'-PA-O2A
2	C	302	UDP	C2'-C1'-N1-C6
2	C	302	UDP	O4'-C4'-C5'-O5'
2	I	302	UDP	C5'-O5'-PA-O1A

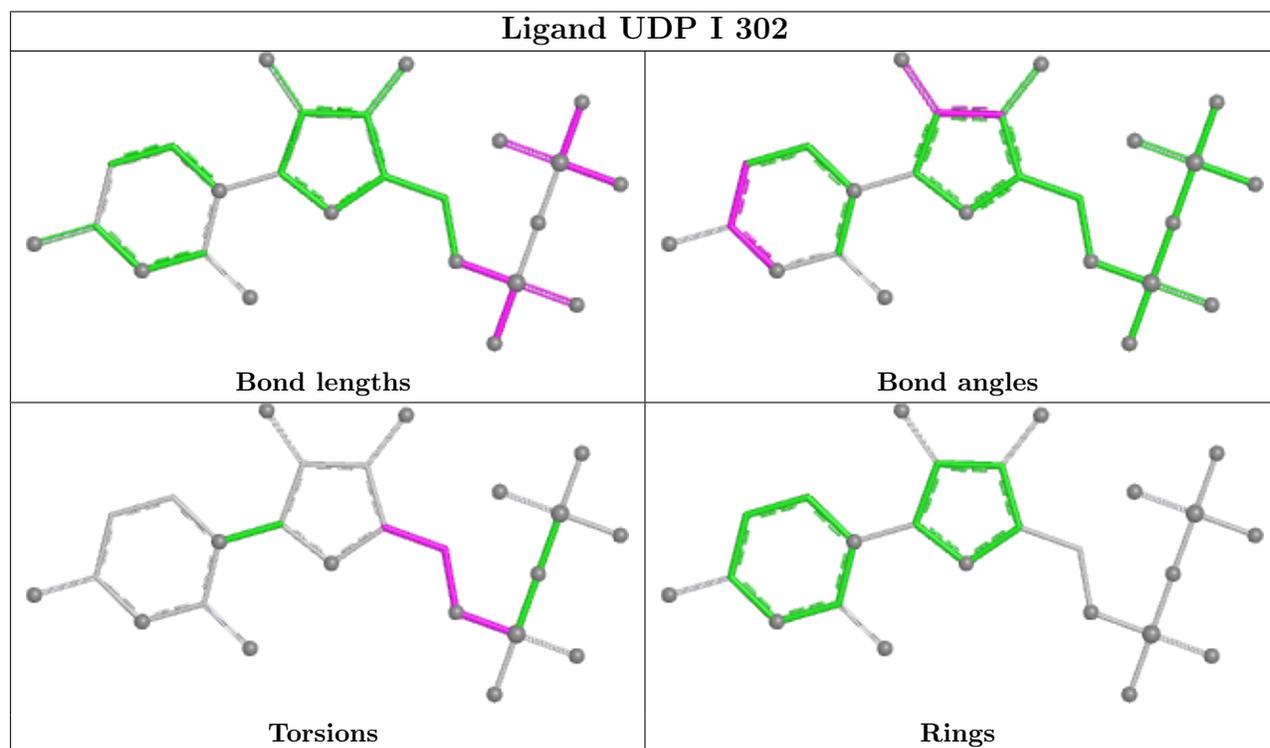
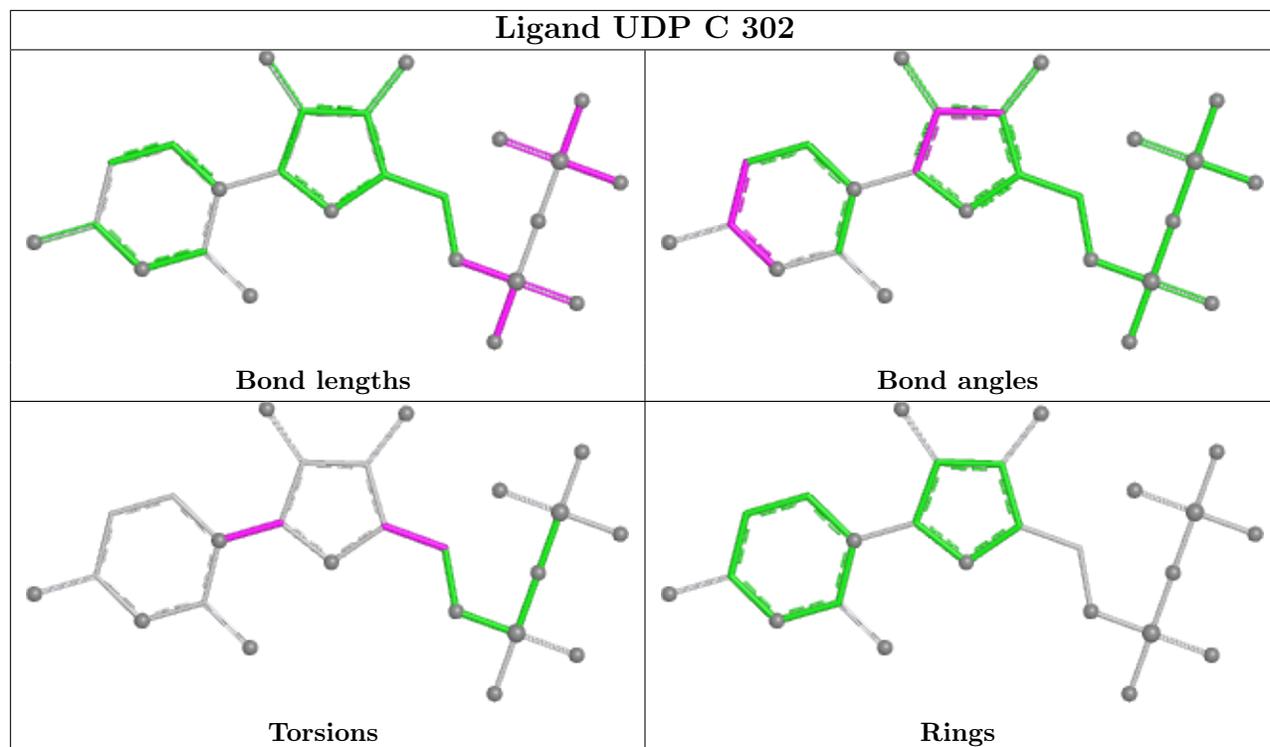
There are no ring outliers.

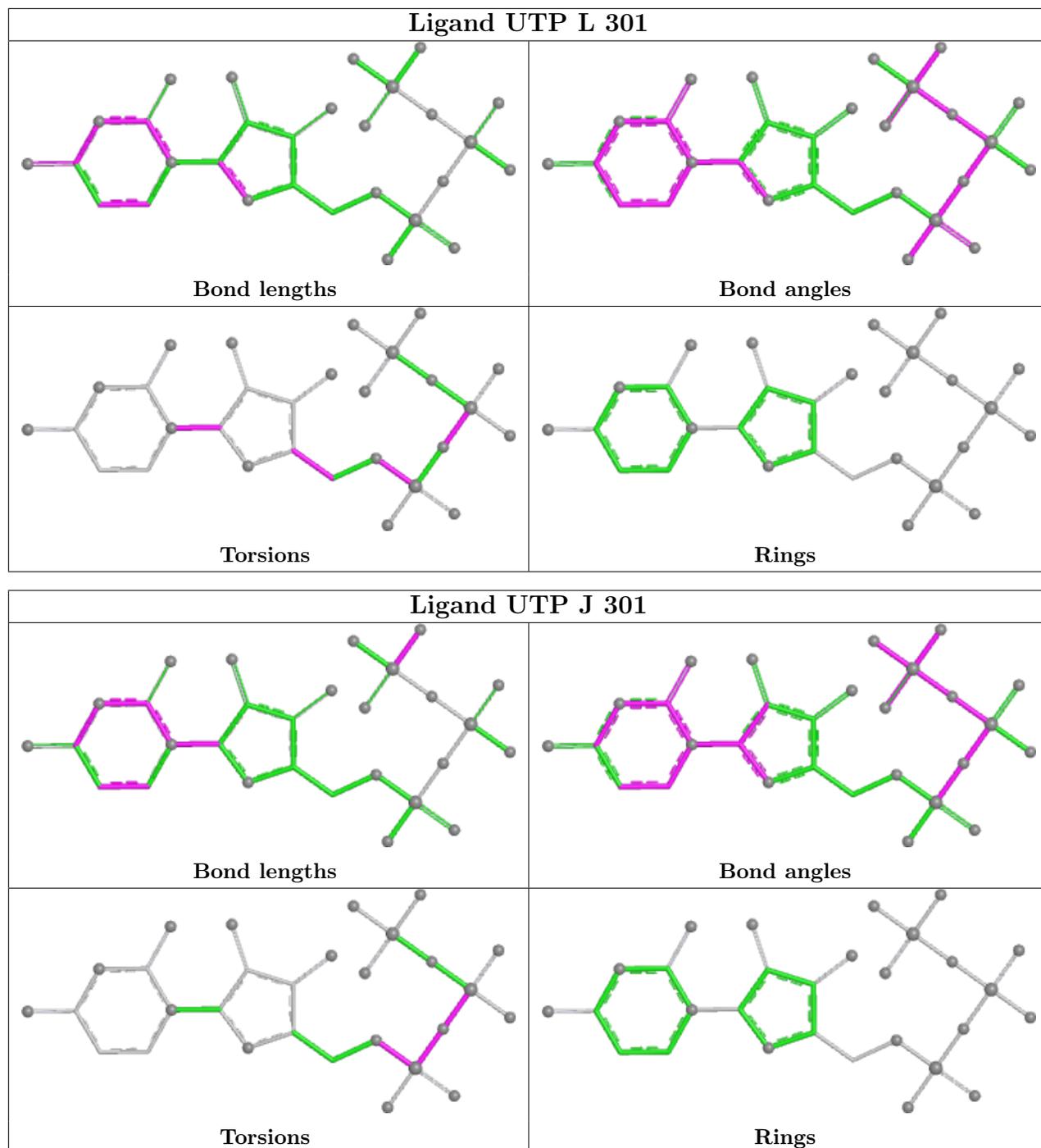
13 monomers are involved in 50 short contacts:

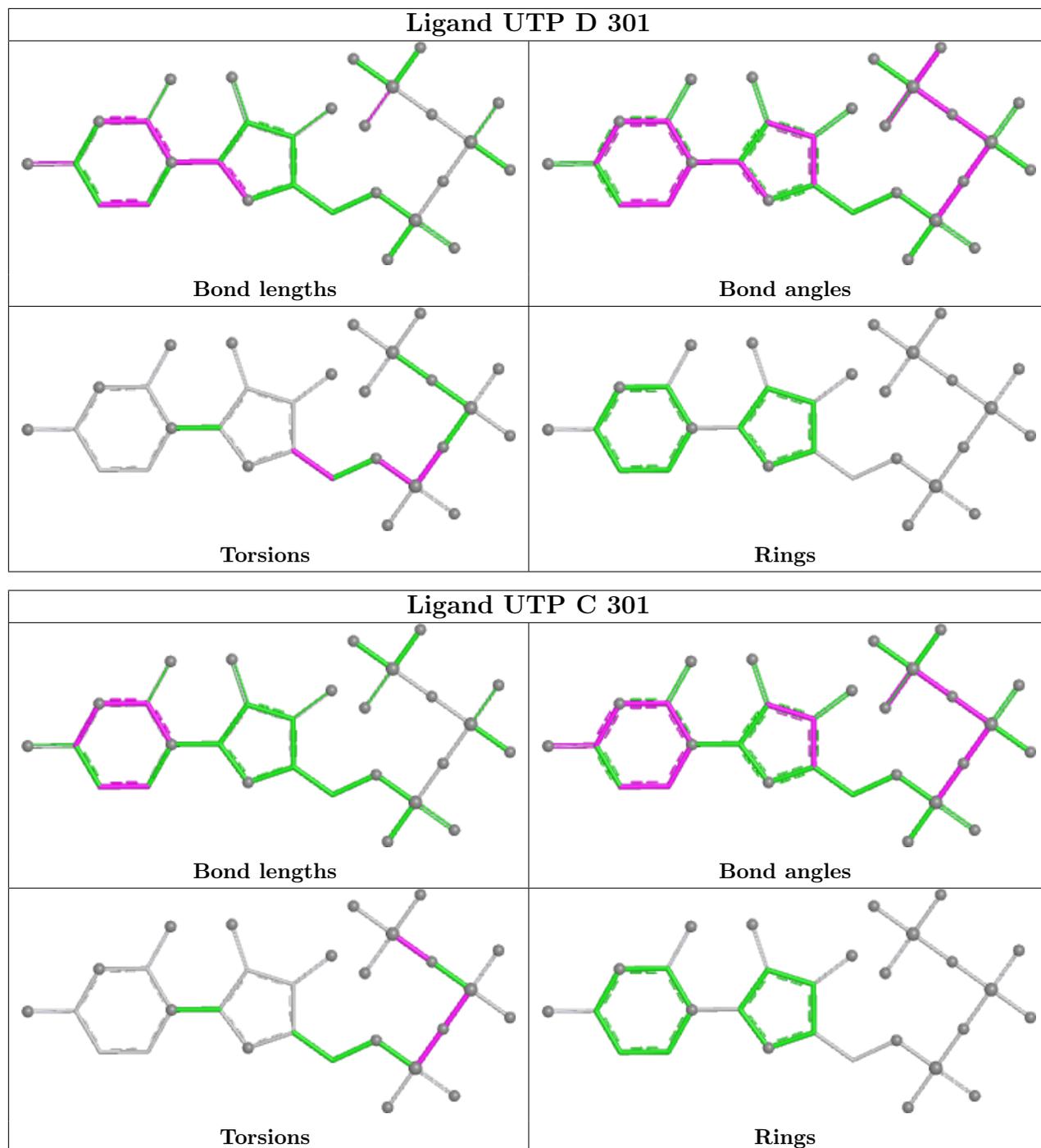
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	UDP	3	0
2	C	302	UDP	9	0
2	I	302	UDP	3	0
3	L	301	UTP	2	0
3	J	301	UTP	3	0
3	D	301	UTP	1	0
3	I	301	UTP	4	0
2	D	302	UDP	5	0
2	J	302	UDP	4	0
3	F	301	UTP	1	0
2	K	301	UDP	6	0
3	G	301	UTP	3	0
2	H	301	UDP	6	0

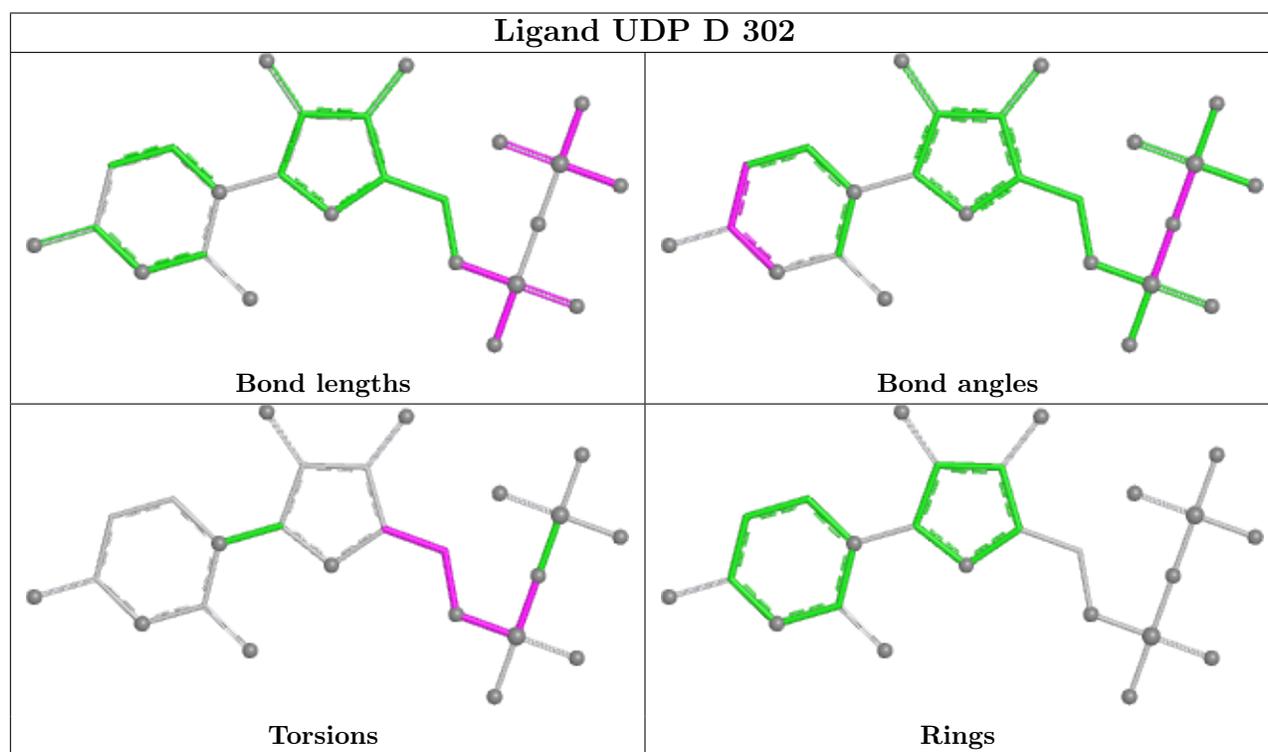
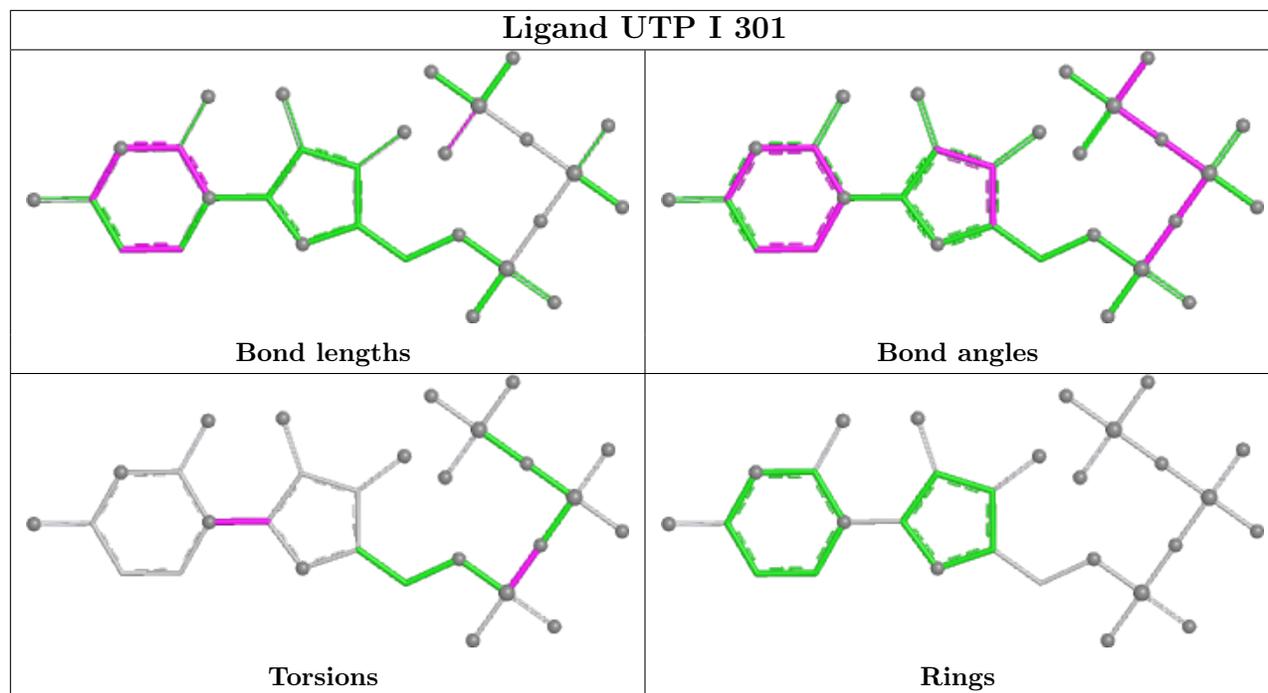
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

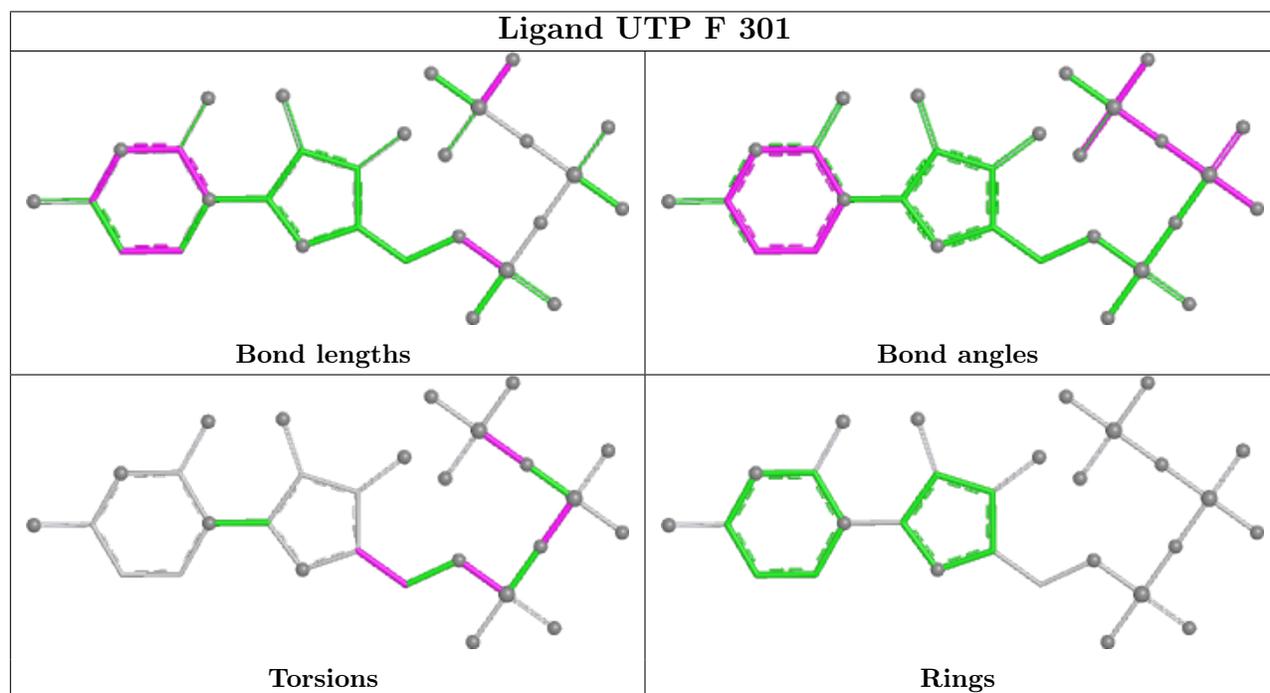
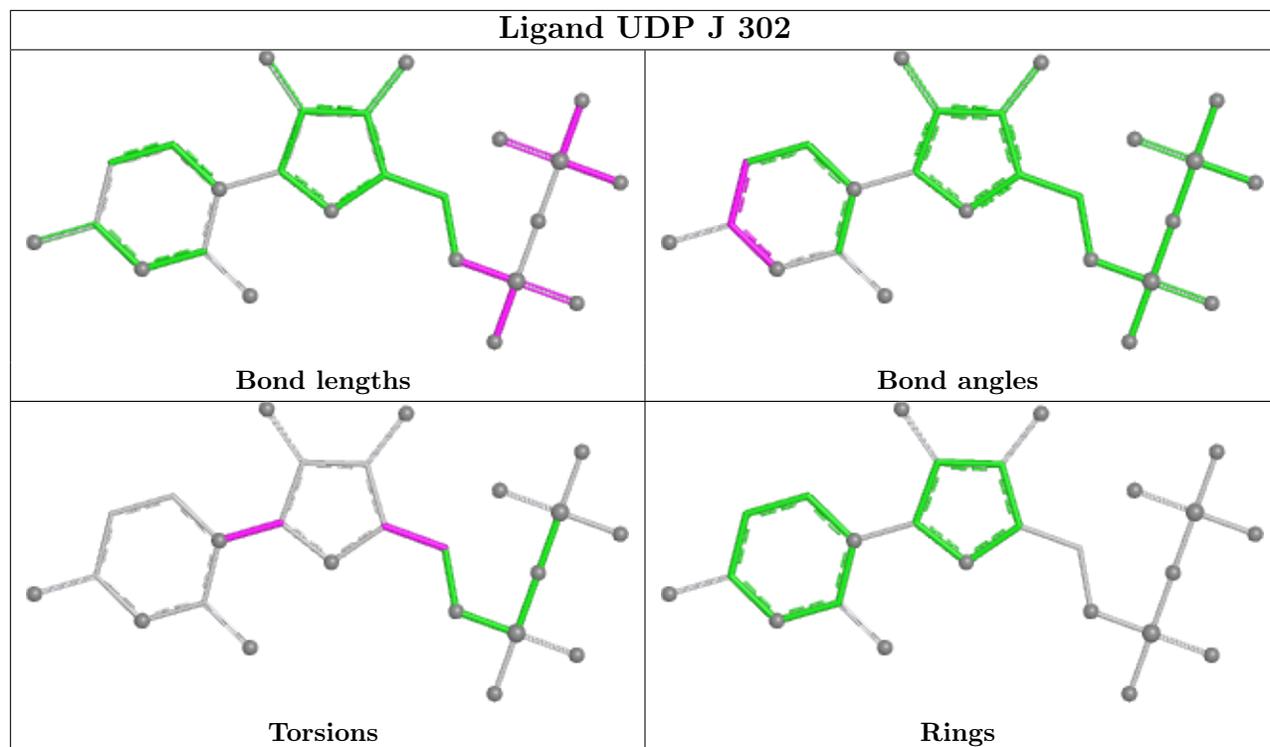


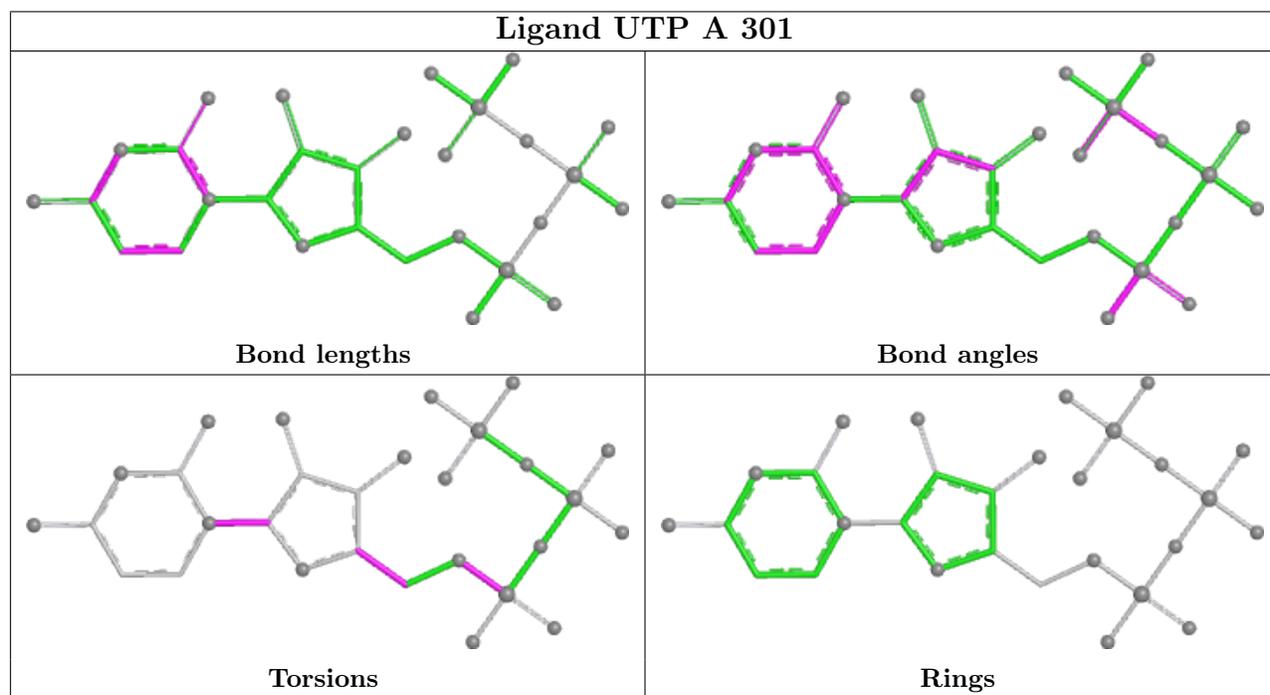
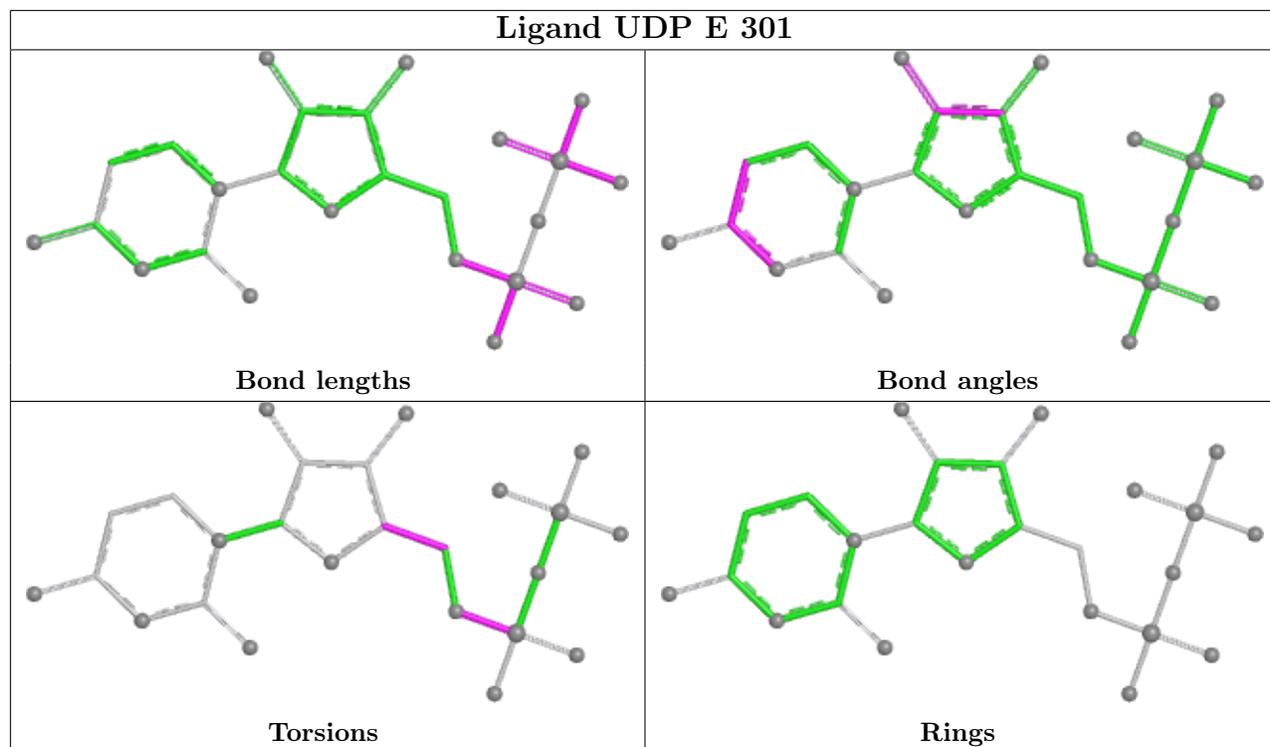


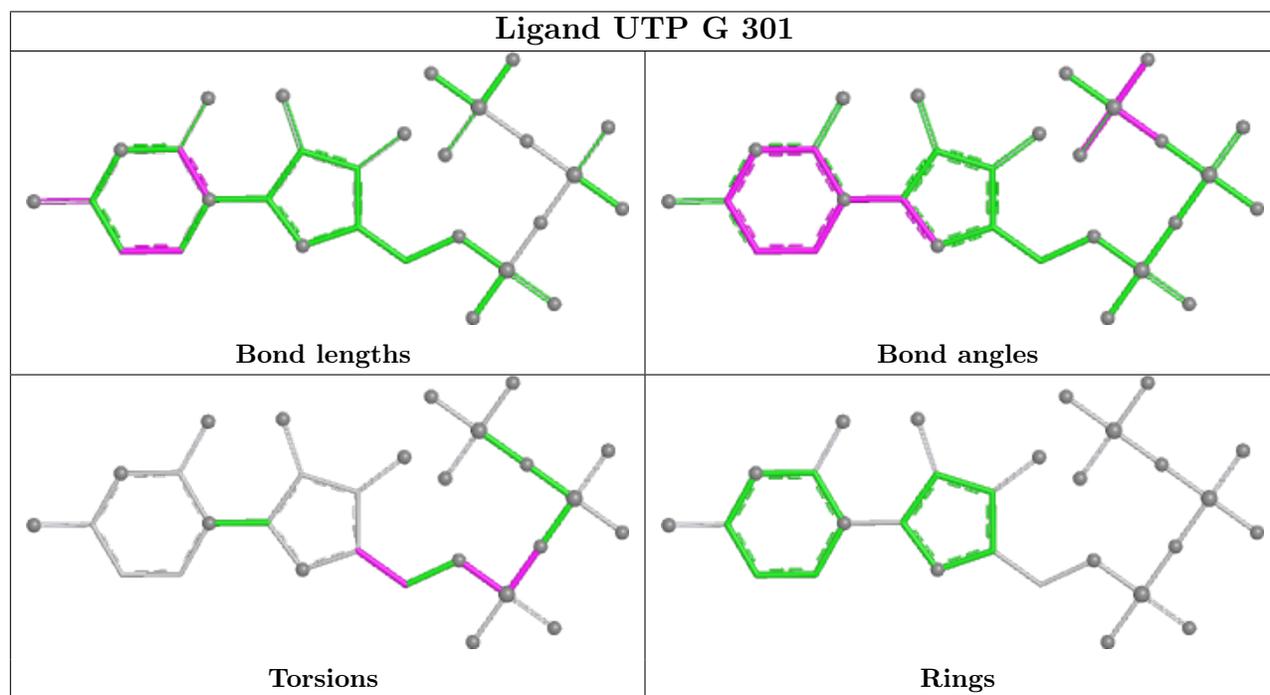
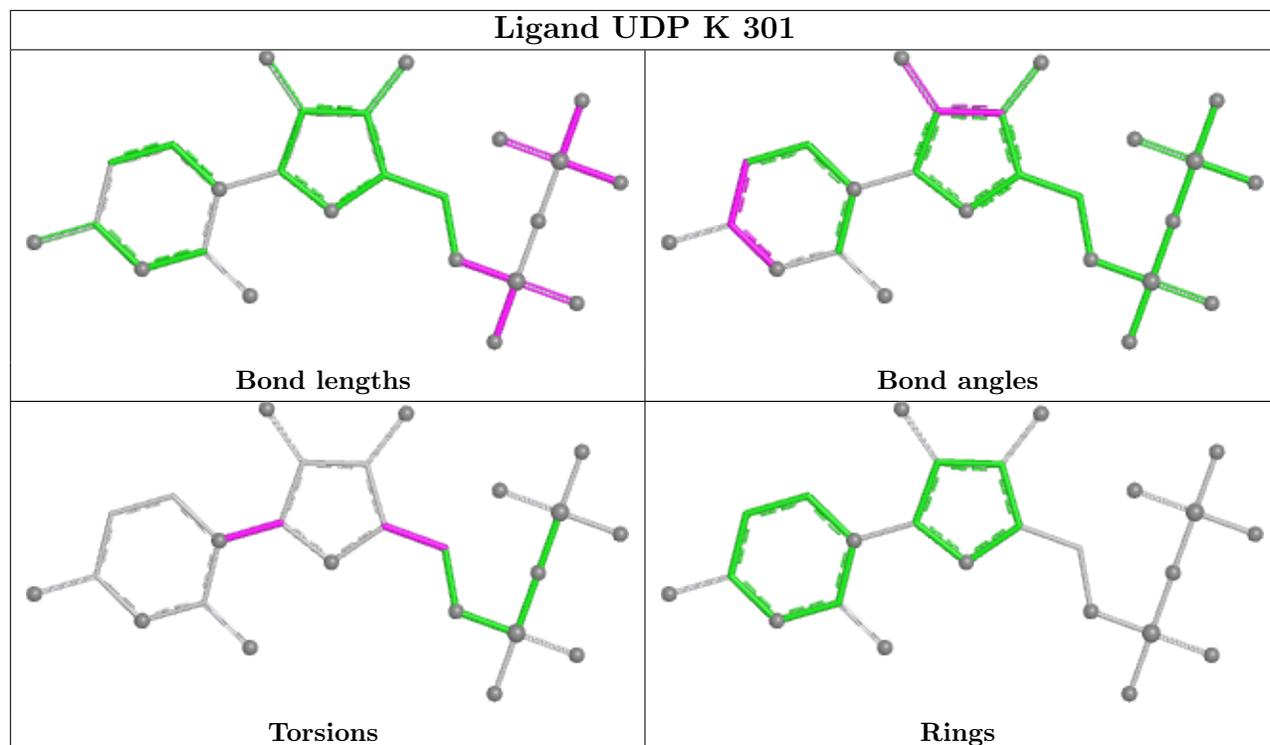


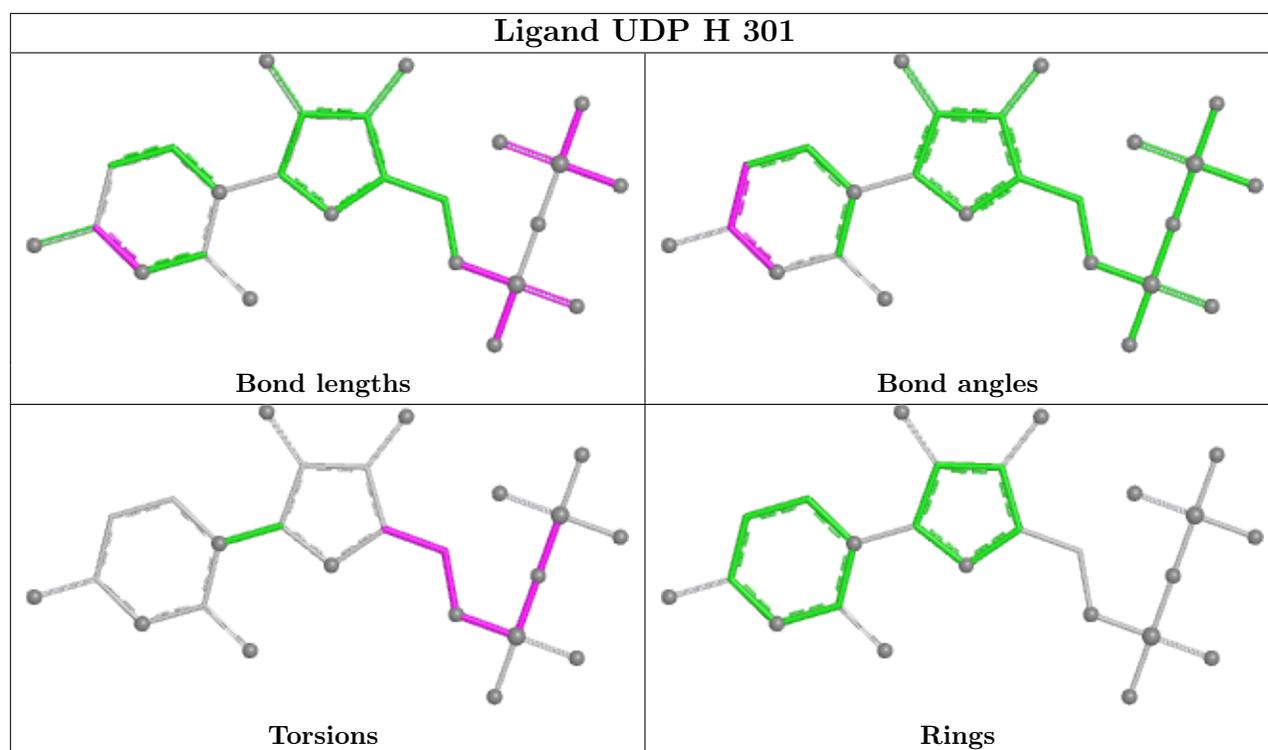












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

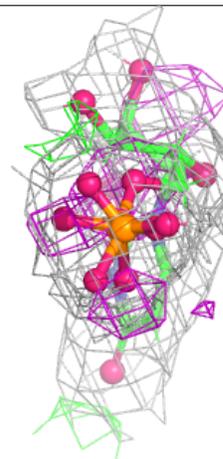
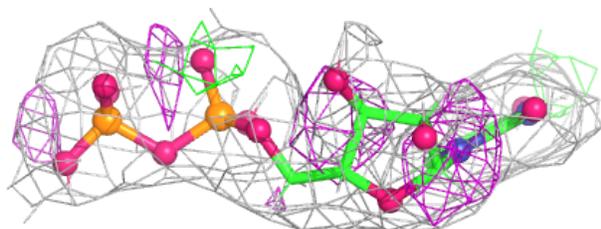
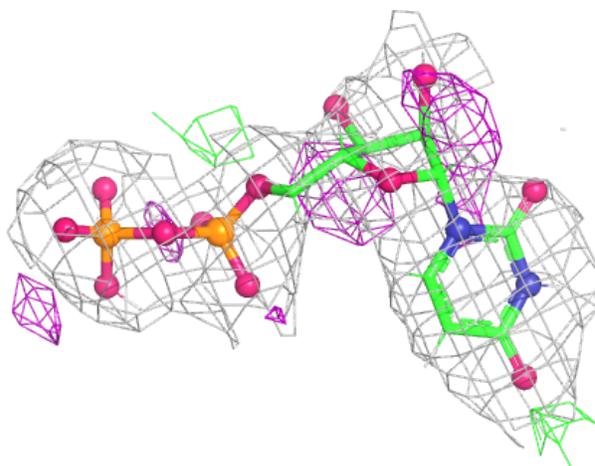
6.4 Ligands

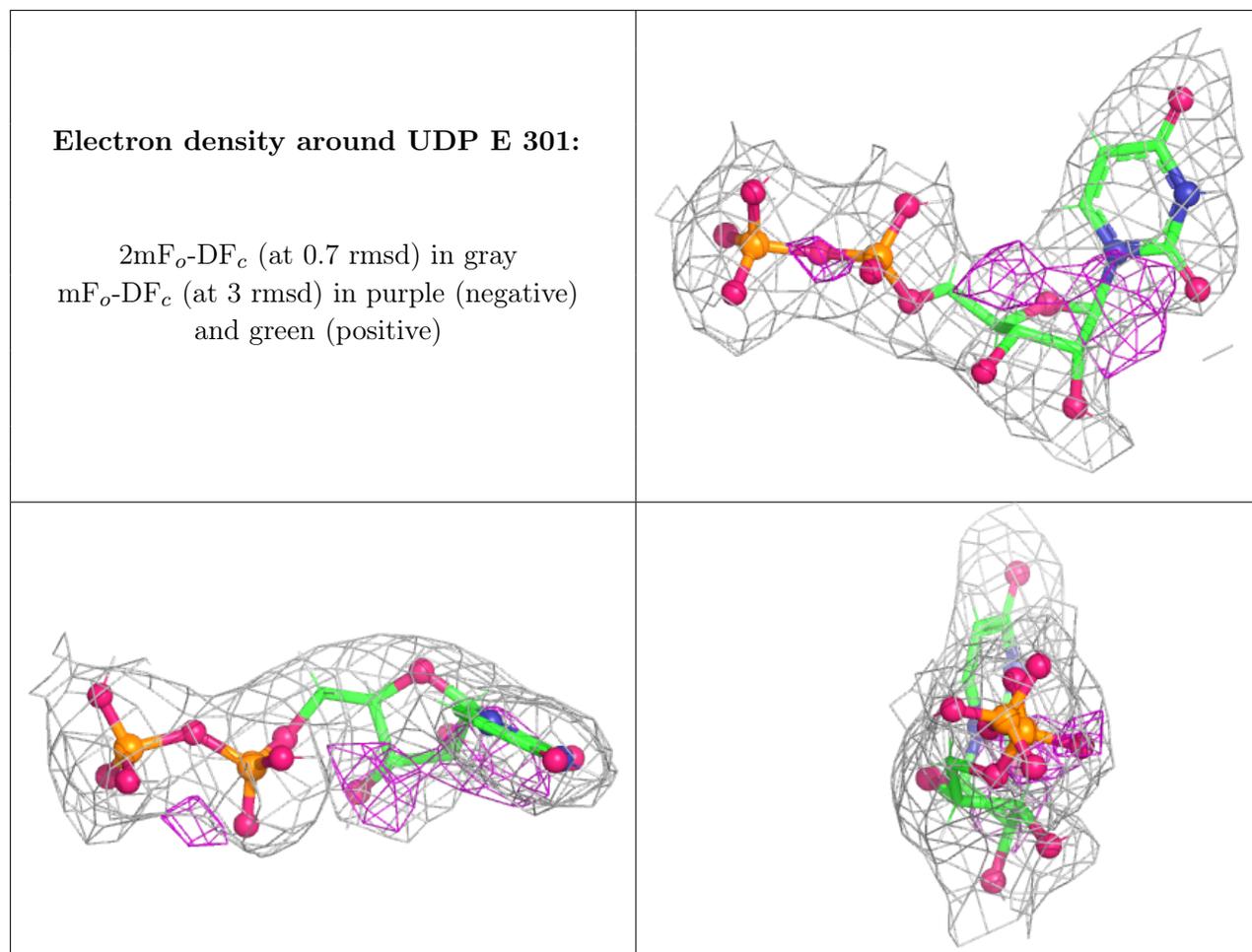
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UDP B 301:

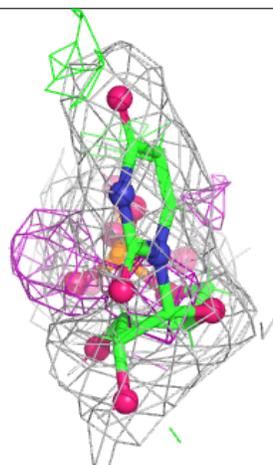
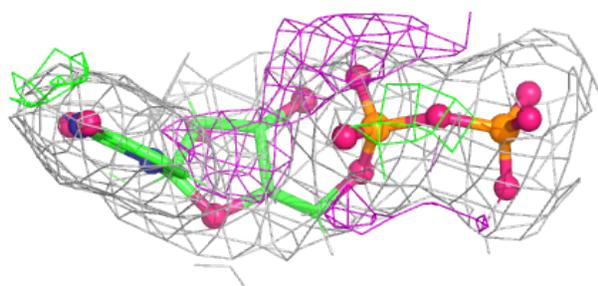
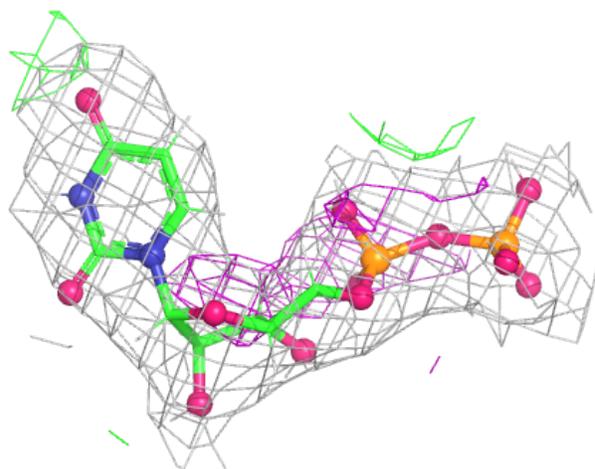
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

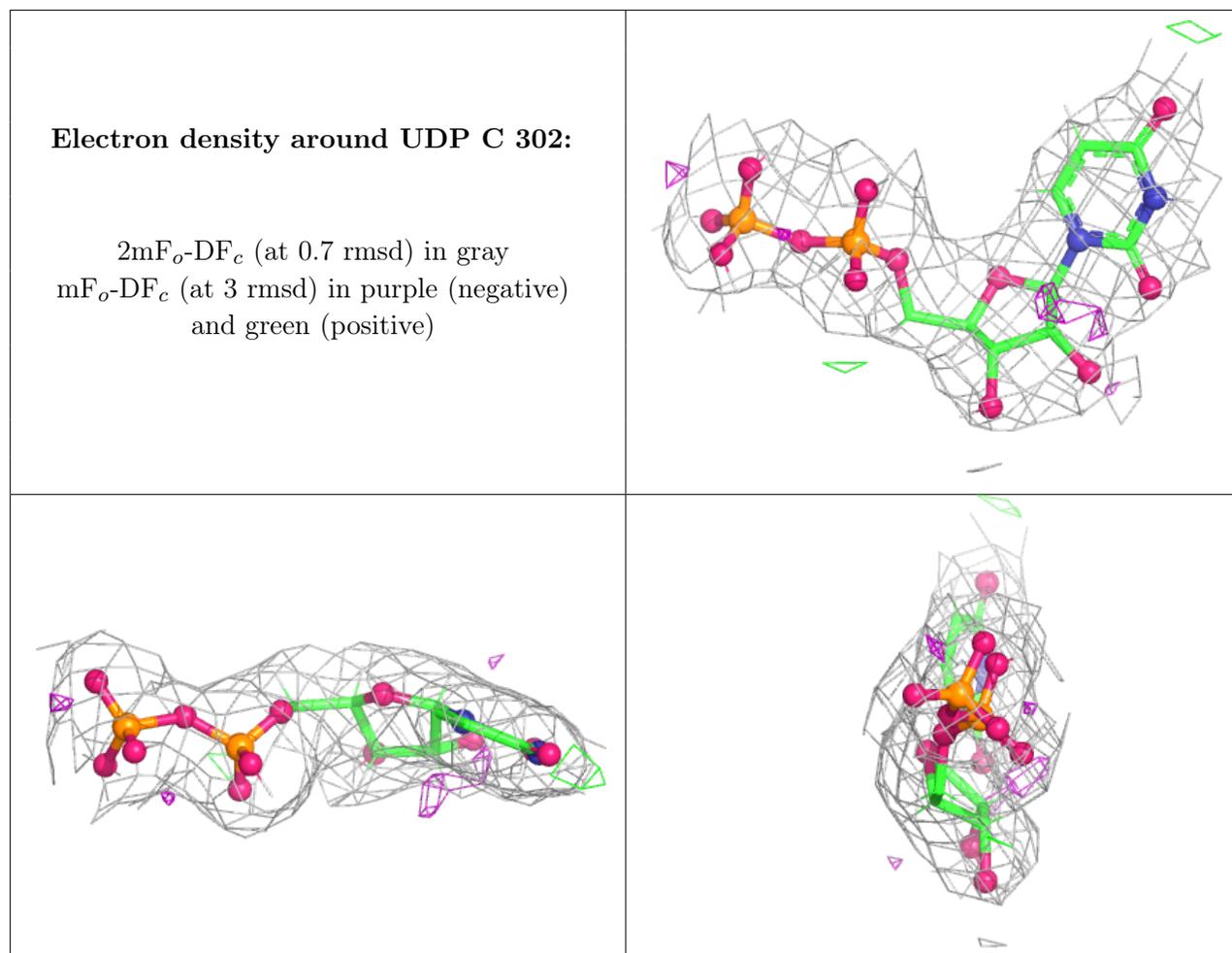




Electron density around UDP D 302:

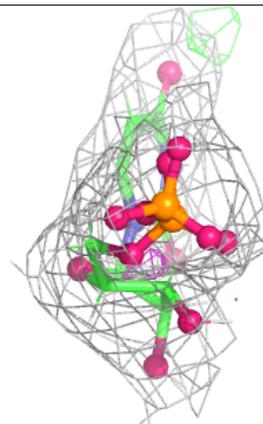
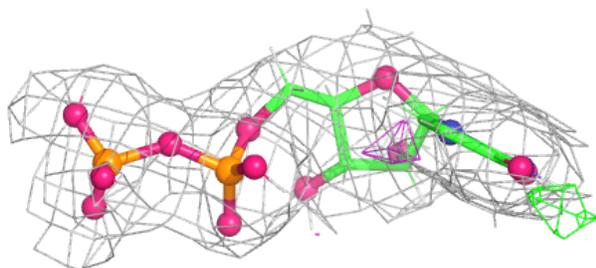
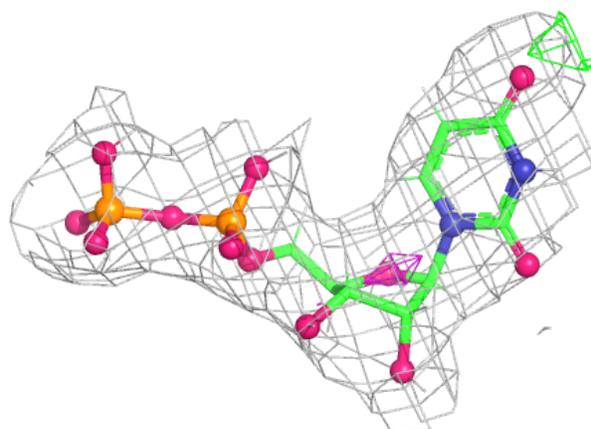
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





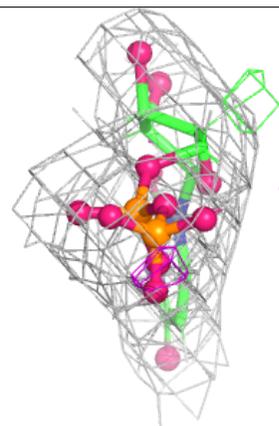
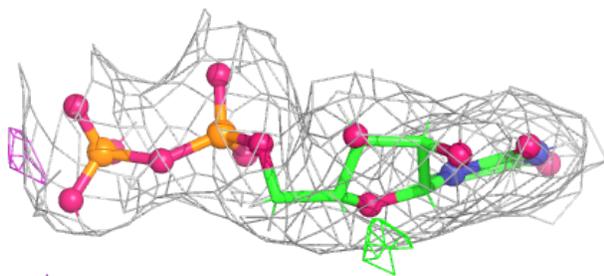
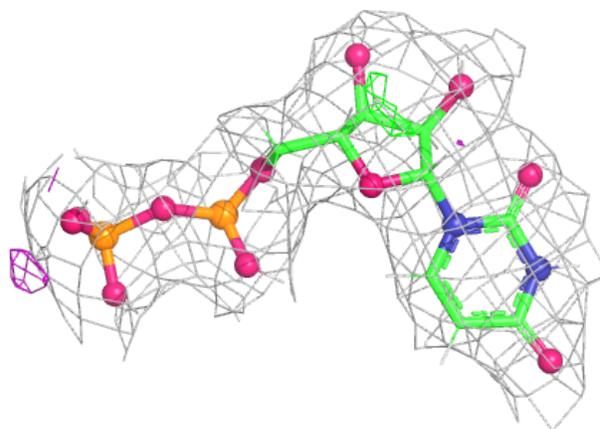
Electron density around UDP I 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



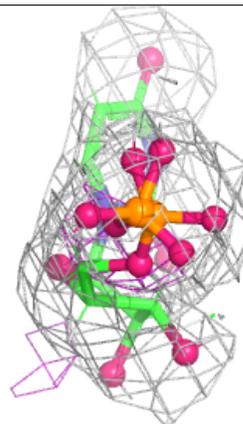
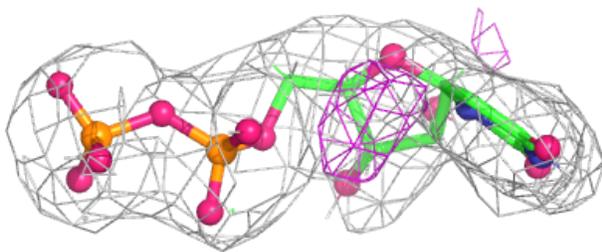
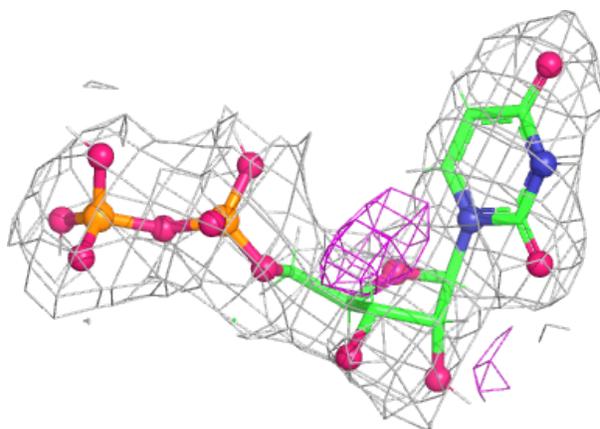
Electron density around UDP J 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



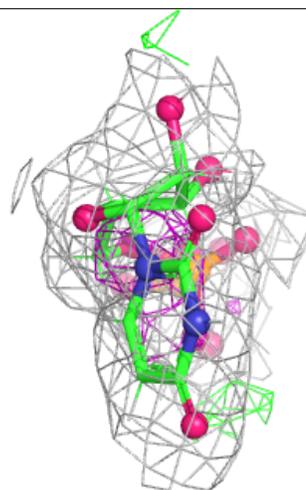
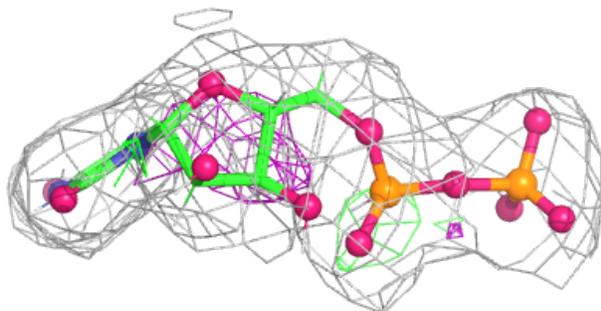
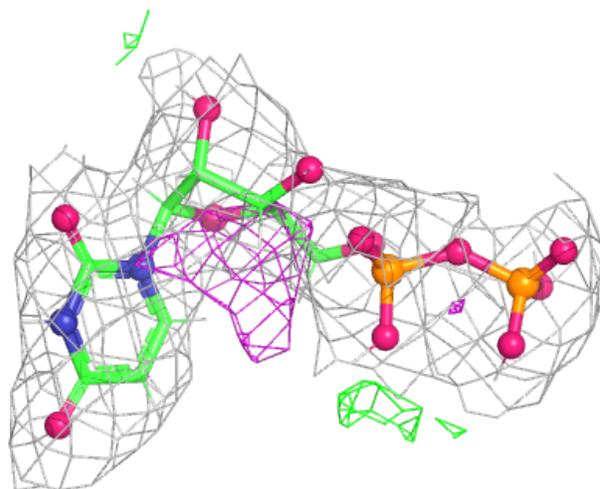
Electron density around UDP K 301:

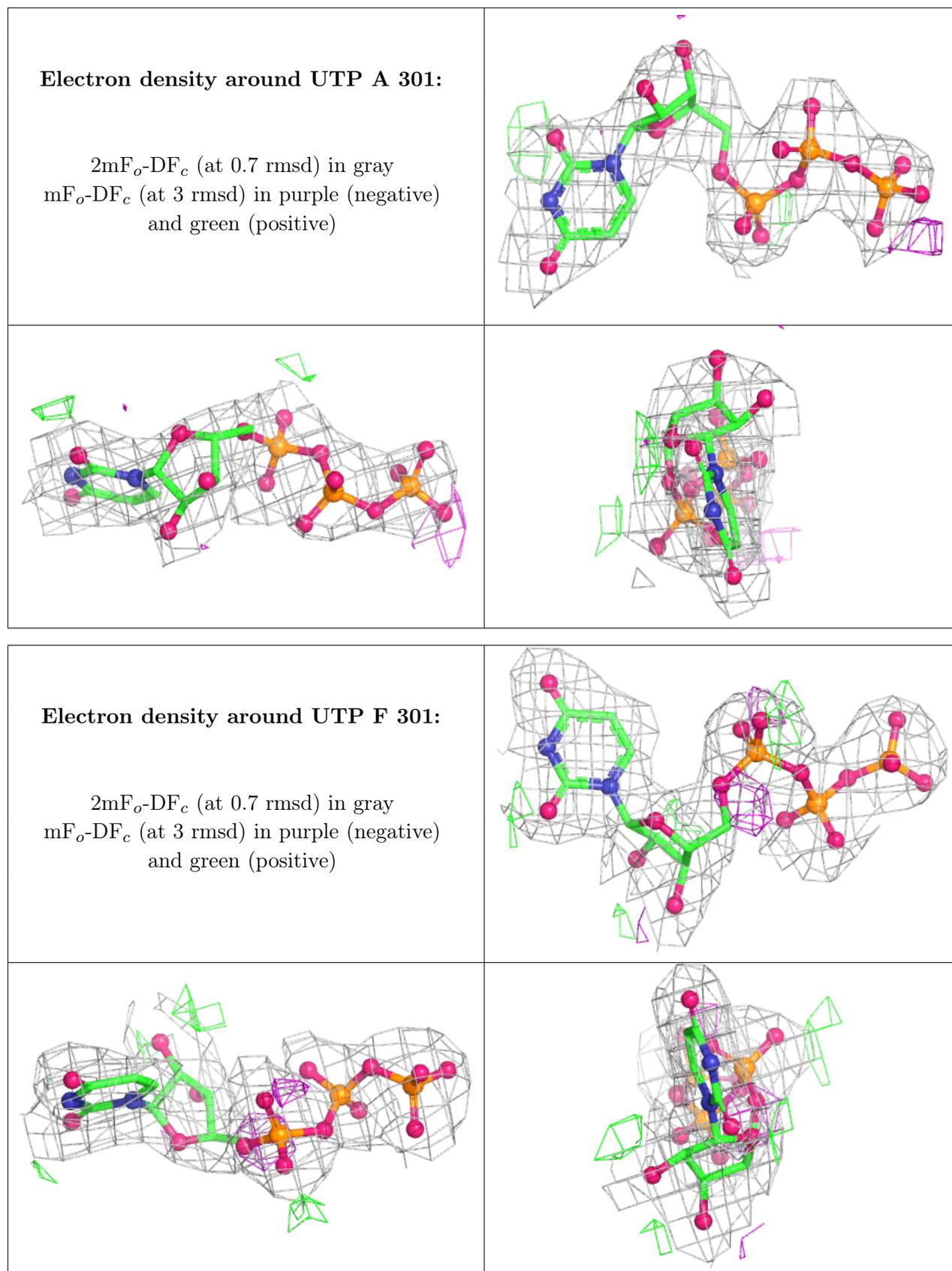
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

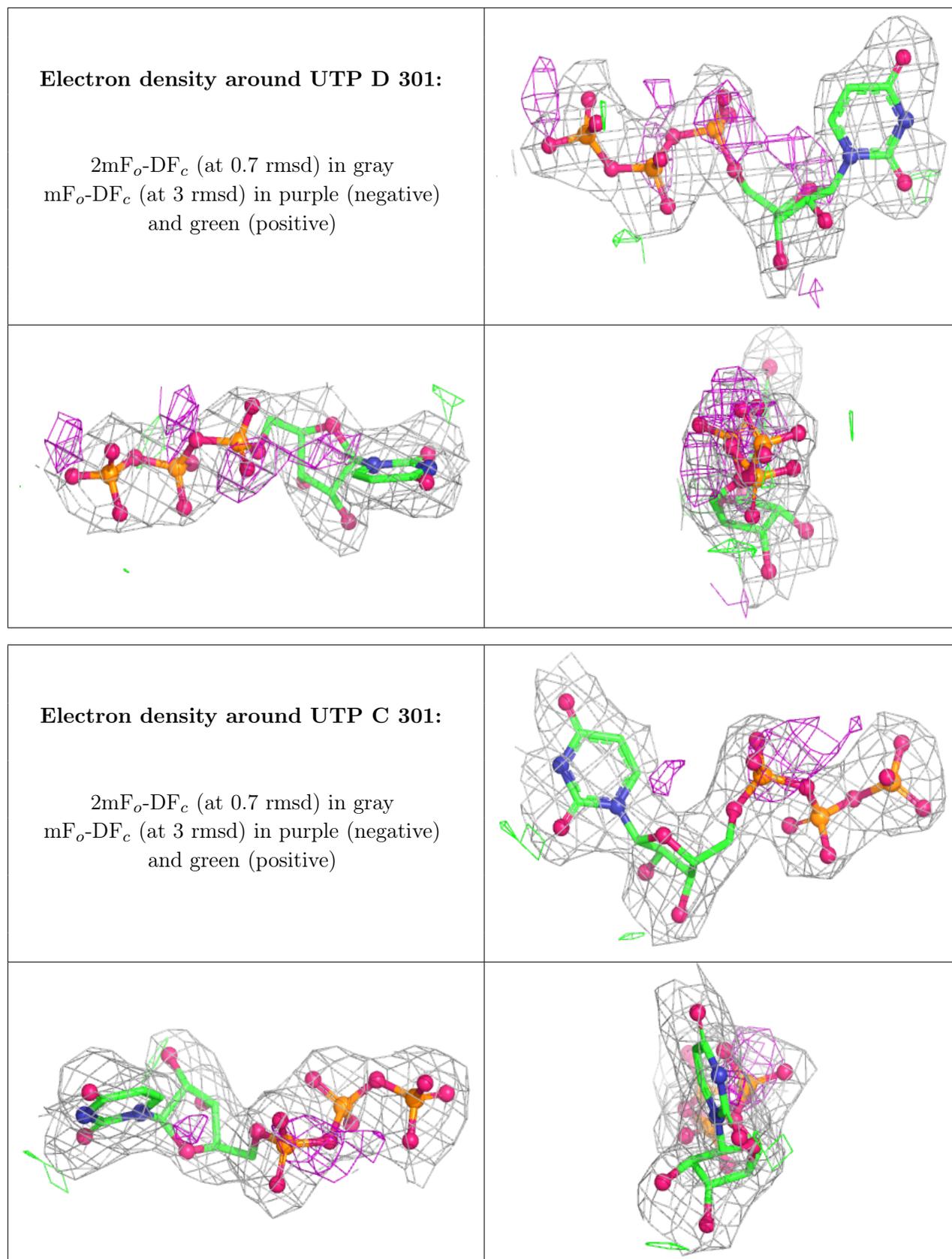


Electron density around UDP H 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

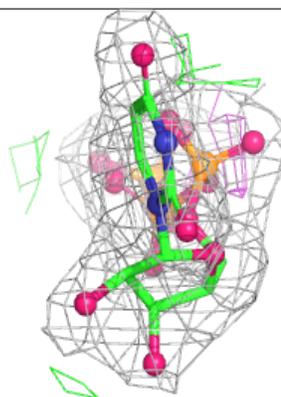
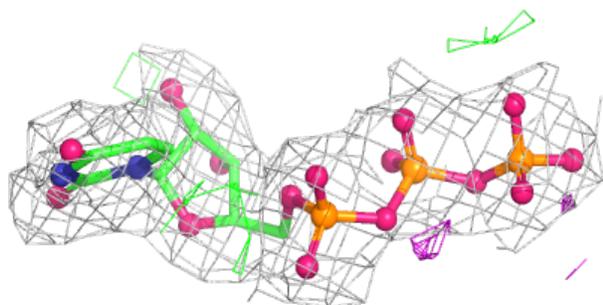
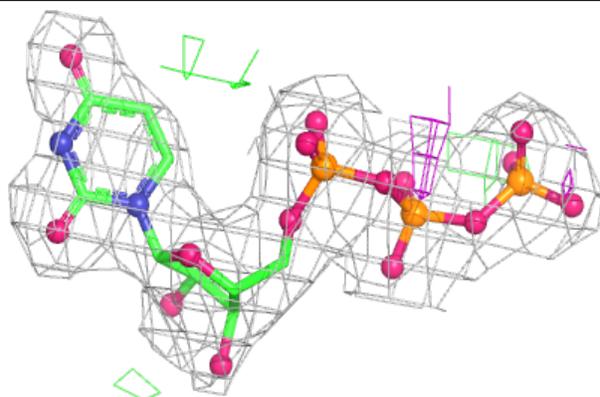




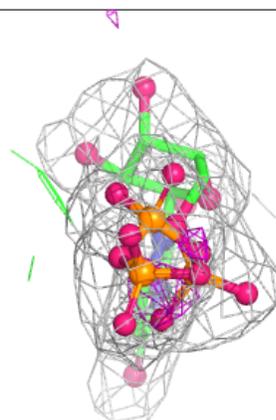
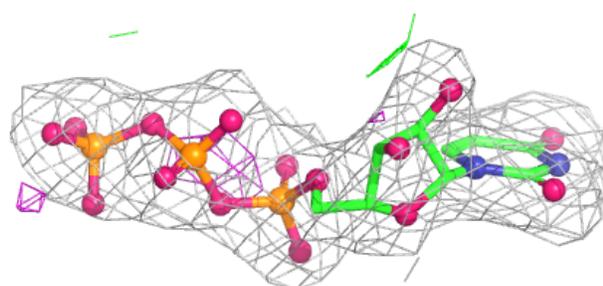
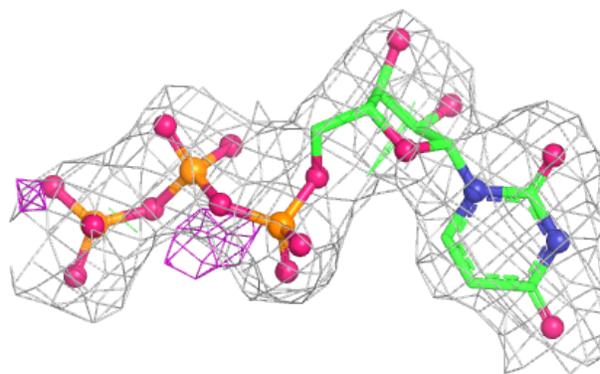


Electron density around UTP I 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

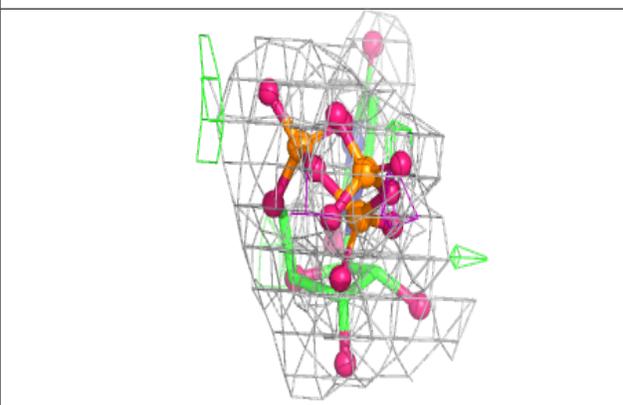
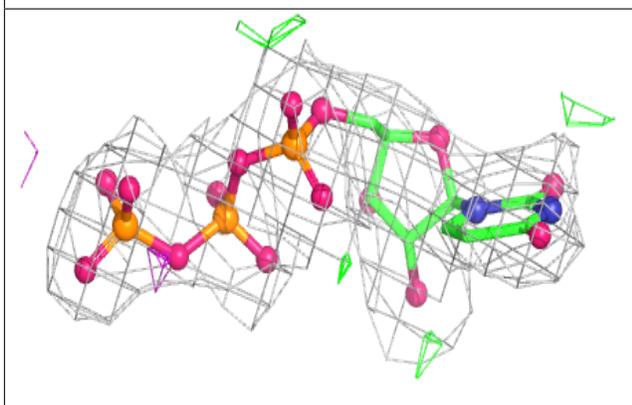
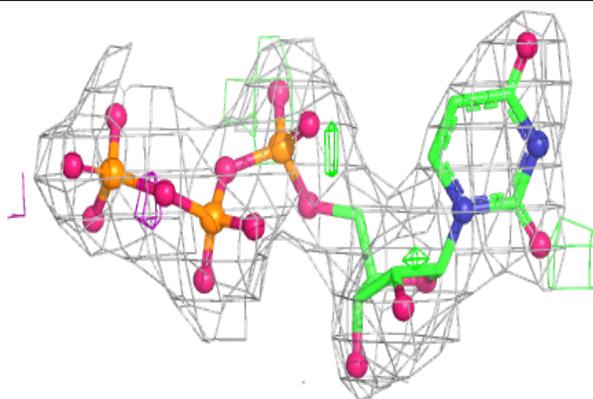
**Electron density around UTP J 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

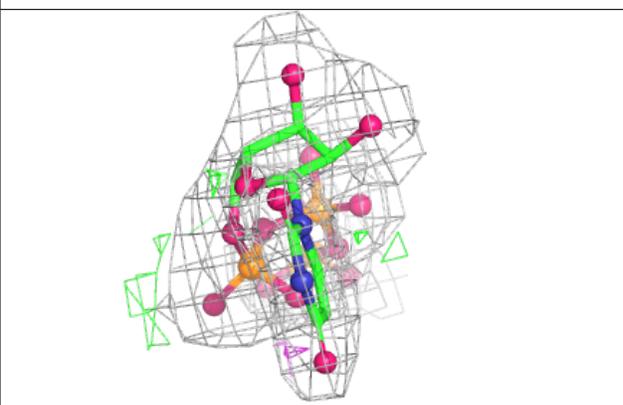
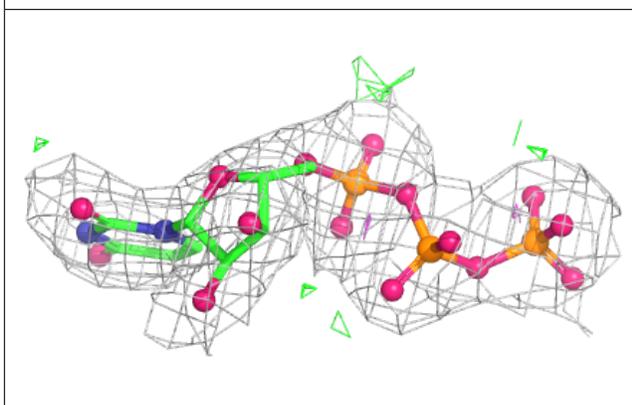
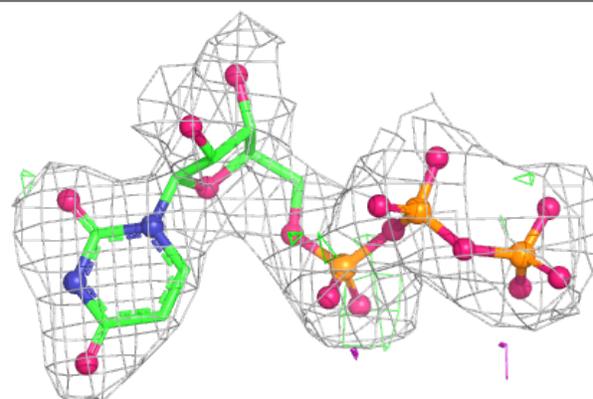


Electron density around UTP L 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around UTP G 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.