Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure 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/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:

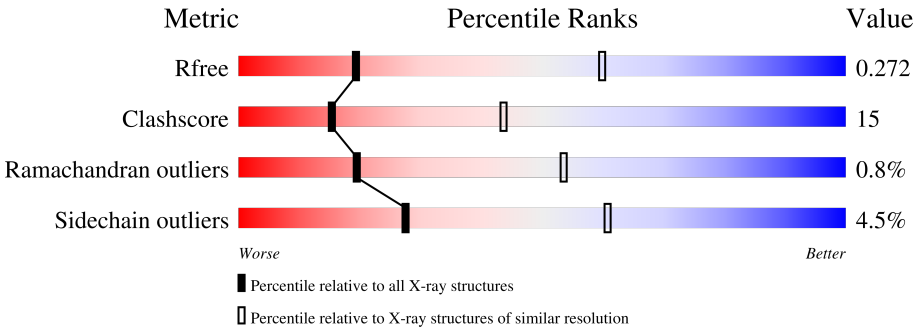
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	281	60% 19% • 20%
1	B	281	53% 27% 19%
1	C	281	59% 21% • 18%
1	D	281	64% 16% • 19%
1	E	281	61% 17% • 21%
1	F	281	58% 17% • 23%
1	G	281	40% 18% • 40%

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Mol	Chain	Length	Quality of chain
1	H	281	45% 30% 21%
1	I	281	54% 25% 20%
1	J	281	58% 21% 19%
1	K	281	59% 20% 20%
1	L	281	34% 20% 44%

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

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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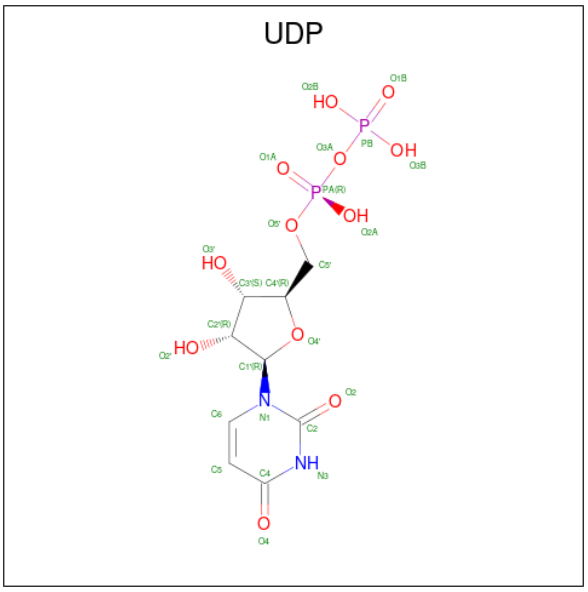
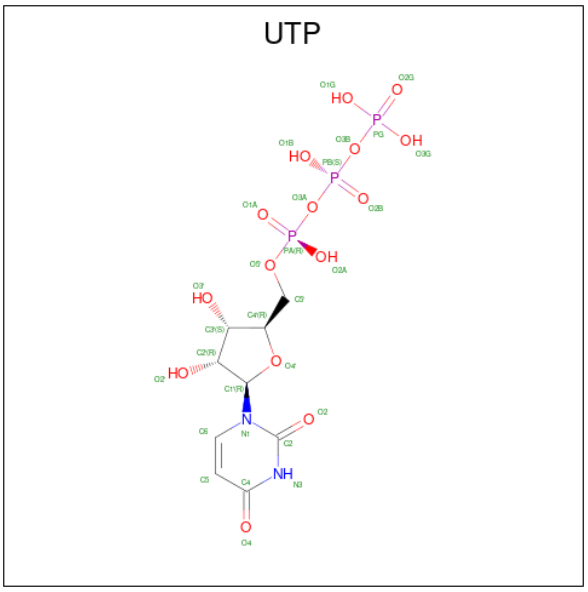
Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	PRO	-	expression tag	UNP P9WHK5
G	-3	ARG	-	expression tag	UNP P9WHK5
G	-2	GLY	-	expression tag	UNP P9WHK5
G	-1	SER	-	expression tag	UNP P9WHK5
G	0	HIS	-	expression tag	UNP P9WHK5
H	-19	MET	-	initiating methionine	UNP P9WHK5
H	-18	GLY	-	expression tag	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: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



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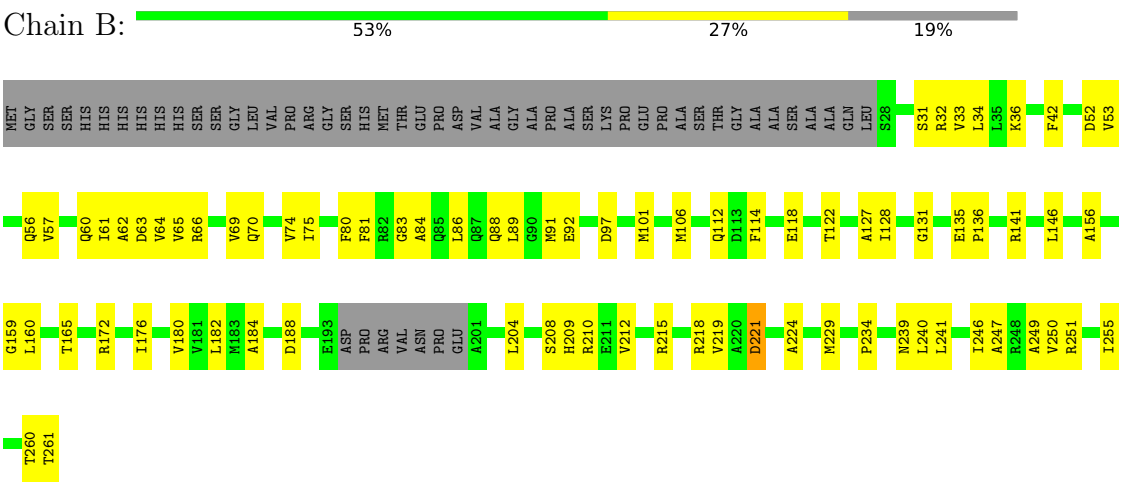
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	6	Total O 6 6	0	0
4	C	4	Total O 4 4	0	0
4	I	3	Total O 3 3	0	0
4	J	3	Total O 3 3	0	0
4	L	1	Total O 1 1	0	0
4	G	4	Total O 4 4	0	0
4	H	5	Total O 5 5	0	0

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. 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. 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.

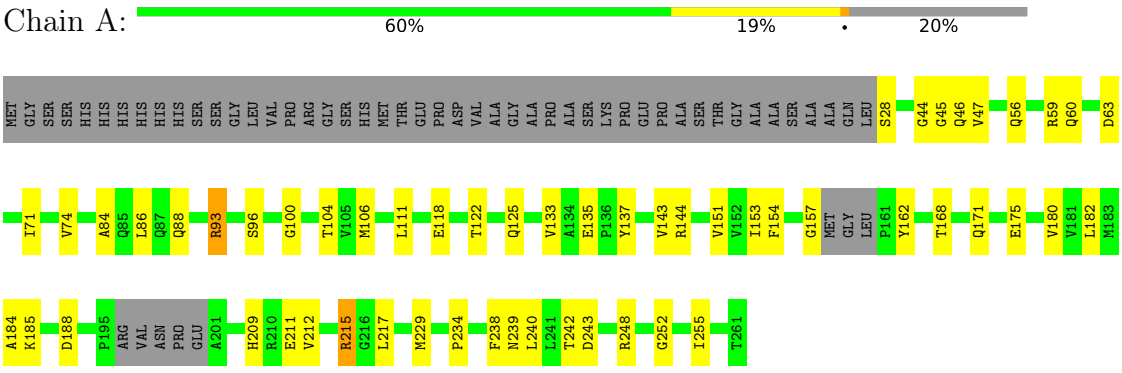
• Molecule 1: Uridylate kinase

Chain B:



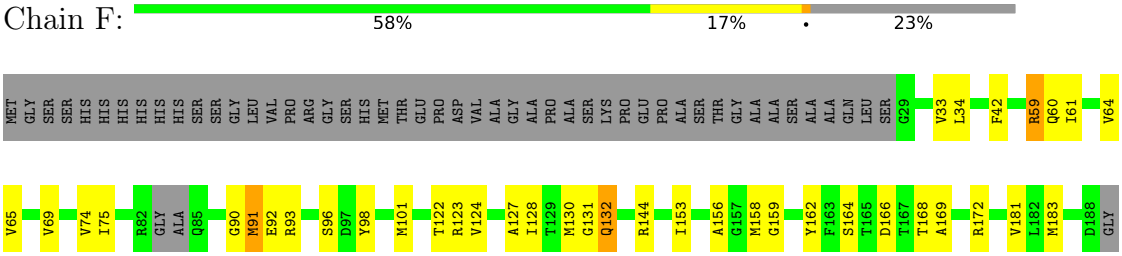
• Molecule 1: Uridylate kinase

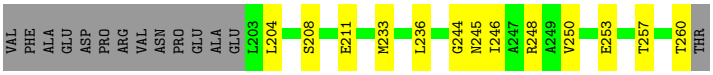
Chain A:



• Molecule 1: Uridylate kinase

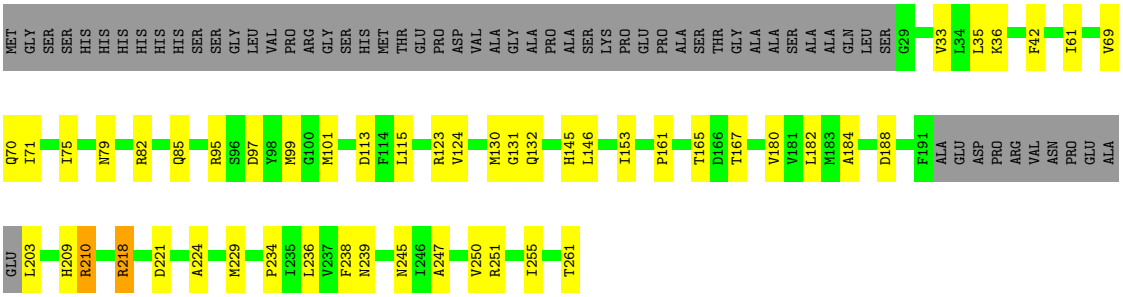
Chain F:





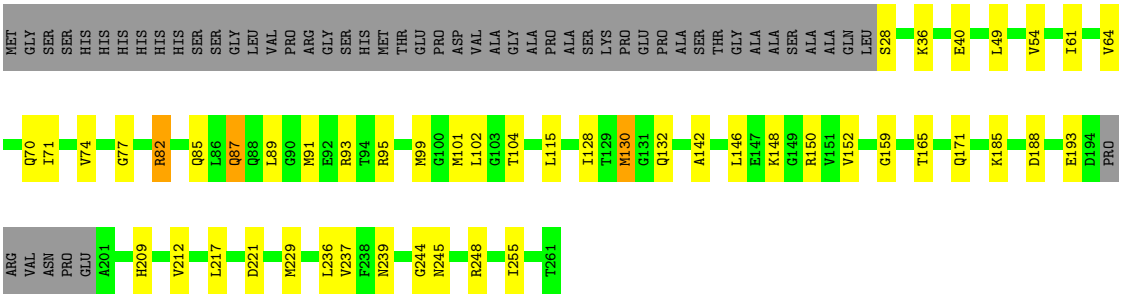
• Molecule 1: Uridylate kinase

Chain E:



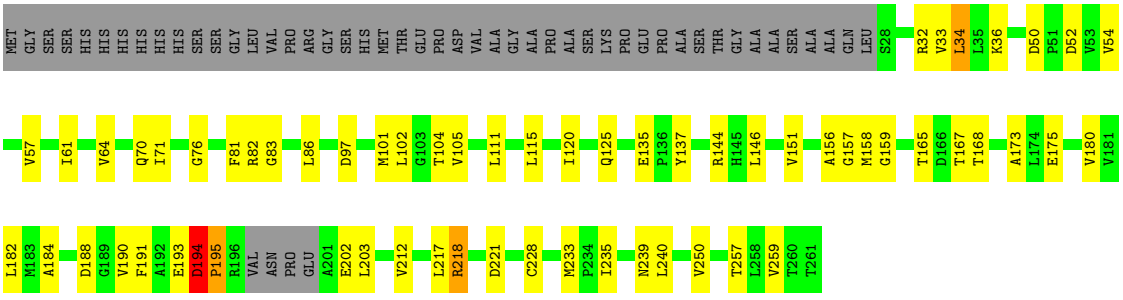
• Molecule 1: Uridylate kinase

Chain D:



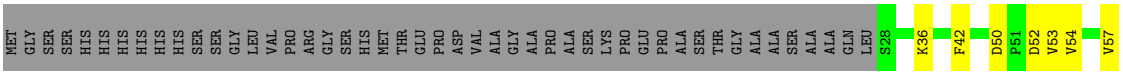
• Molecule 1: Uridylate kinase

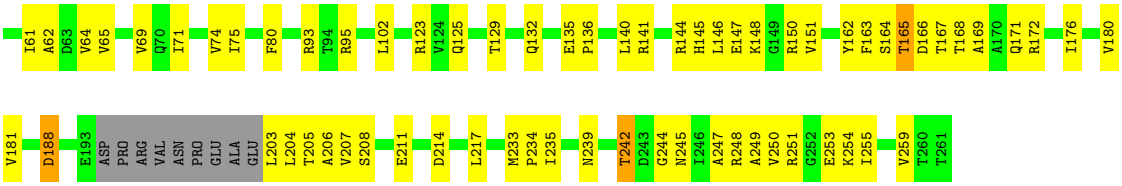
Chain C:



• Molecule 1: Uridylate kinase

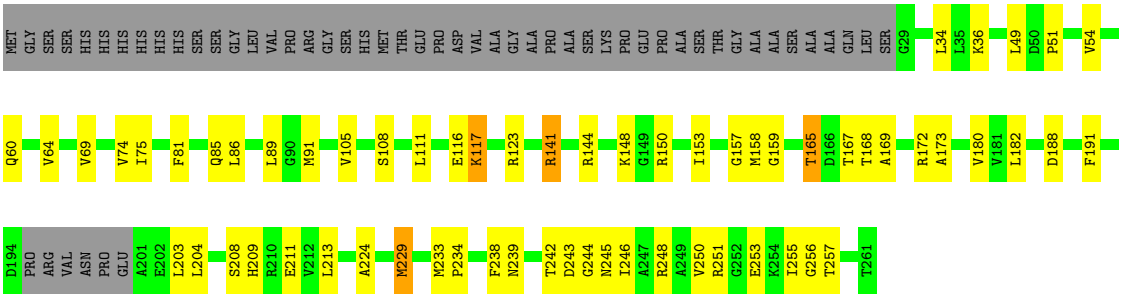
Chain I:





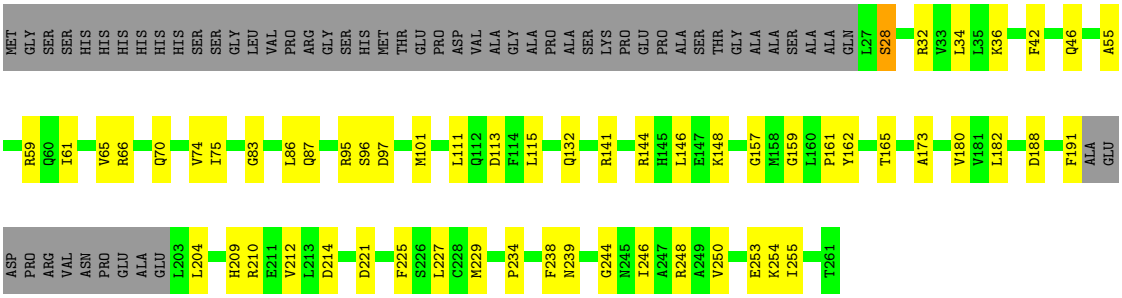
• Molecule 1: Uridylate kinase

Chain J:



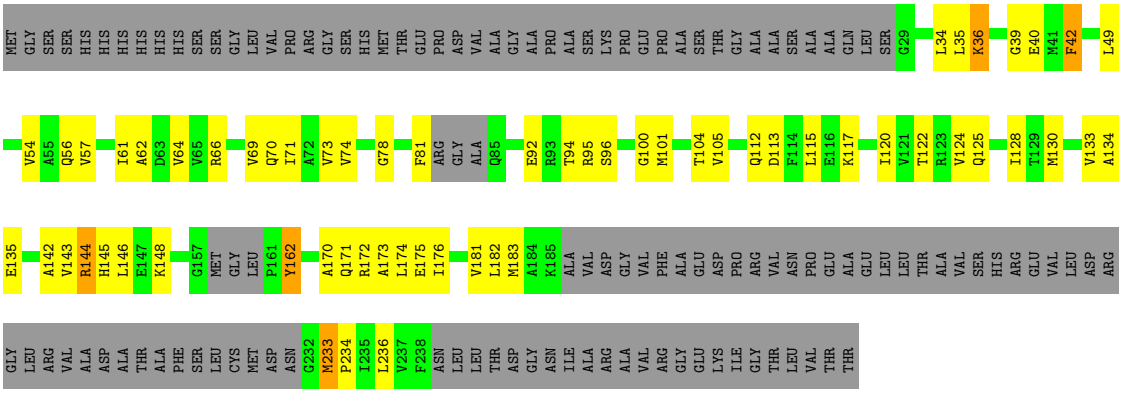
• Molecule 1: Uridylate kinase

Chain K:



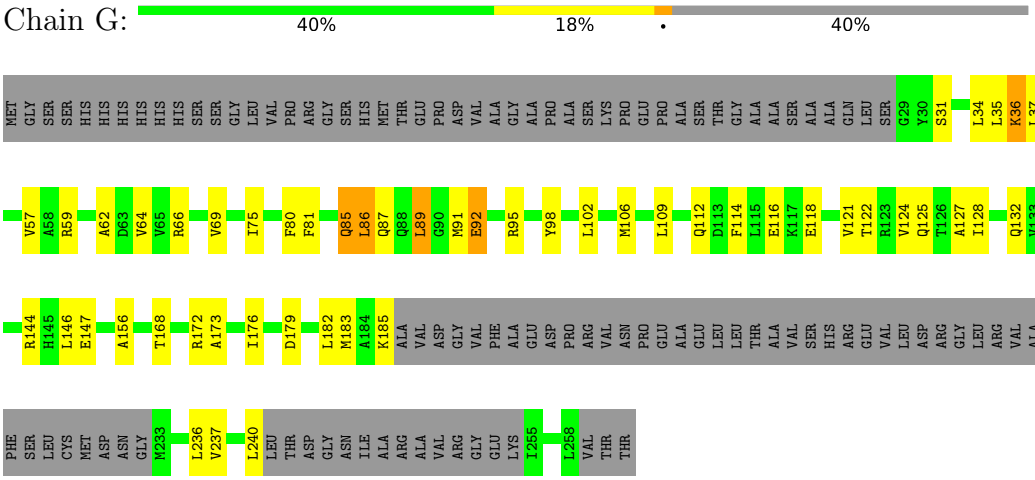
• Molecule 1: Uridylate kinase

Chain L:



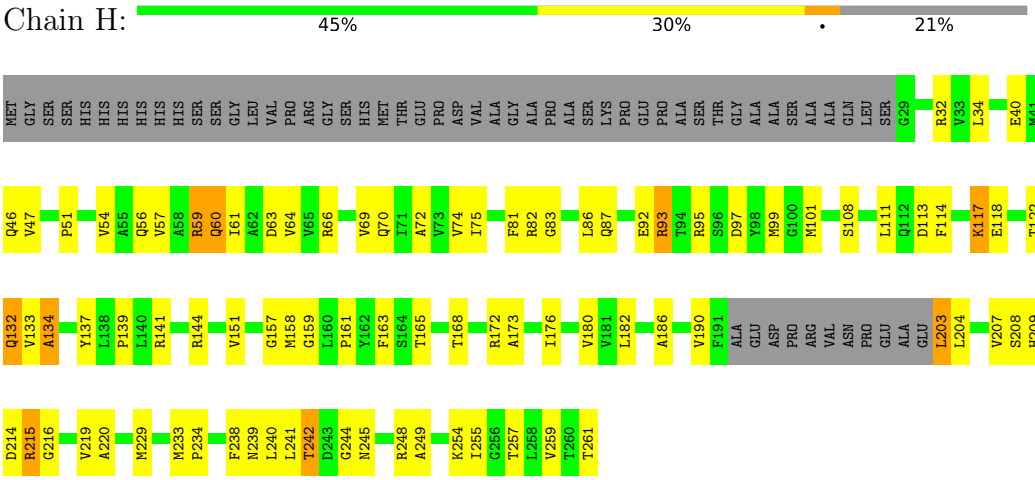
• Molecule 1: Uridylate kinase

Chain G:



- Molecule 1: Uridylate kinase

Chain H:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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.

All (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
1:J:165:THR:HB	2:J:302:UDP:O2A	1.44	1.14
1:G:86:LEU:HD23	1:G:87:GLN:H	1.05	1.11
1:I:36:LYS:CE	1:I:165:THR:HG22	1.75	1.09
1:I:36:LYS:HE2	1:I:165:THR:HG21	1.35	1.08
1:I:36:LYS:HE2	1:I:165:THR:HG23	1.34	1.03
1:E:36:LYS:HE3	1:E:165:THR:HG22	1.41	1.02
1:I:165:THR:HB	2:I:302:UDP:O2A	1.60	1.00
1:G:86:LEU:HD23	1:G:87:GLN:N	1.79	0.98
1:H:130:MET:CE	1:H:133:VAL:CG2	2.46	0.94
1:I:36:LYS:HE2	1:I:165:THR:HG22	0.94	0.92
1:I:144:ARG:HD2	3:G:301:UTP:C5'	1.99	0.92
1:H:40:GLU:O	1:H:44:GLY:HA2	1.72	0.89
1:I:206:ALA:O	1:I:207:VAL:HG13	1.73	0.88
1:A:209:HIS:HB3	1:A:229:MET:HG3	1.52	0.88
1:H:209:HIS:HB2	1:H:261:THR:HB	1.57	0.87
1:E:36:LYS:HE3	1:E:165:THR:CG2	2.06	0.85
1:F:144:ARG:HH12	1:K:59:ARG:HD2	1.41	0.84
1:I:204:LEU:HD11	1:I:217:LEU:HD11	1.58	0.84
1:H:130:MET:HE2	1:H:133:VAL:CG2	2.07	0.84
1:I:144:ARG:O	1:I:145:HIS:C	2.12	0.83
1:L:54:VAL:HA	1:L:57:VAL:HG12	1.61	0.82
1:F:91:MET:CE	1:F:96:SER:HA	2.10	0.81
1:H:204:LEU:O	1:H:257:THR:HG22	1.81	0.81
1:K:83:GLY:HA3	1:K:97:ASP:OD1	1.81	0.81
1:H:130:MET:HE2	1:H:133:VAL:HG22	1.60	0.81
1:J:36:LYS:HE3	1:J:165:THR:HG22	1.63	0.80
1:B:180:VAL:HG23	1:B:234:PRO:HB2	1.64	0.80
1:H:249:ALA:HB2	1:H:255:ILE:HD11	1.64	0.79
1:J:168:THR:O	1:J:172:ARG:HG2	1.83	0.78
1:J:158:MET:HB2	2:J:302:UDP:O4	1.83	0.77
1:H:130:MET:CE	1:H:133:VAL:HG21	2.14	0.77
1:H:130:MET:CE	1:H:133:VAL:HG22	2.12	0.77
1:H:208:SER:HB2	1:H:211:GLU:HG3	1.66	0.77
1:B:69:VAL:HG21	1:B:250:VAL:HG11	1.67	0.77
1:H:63:ASP:HA	1:H:66:ARG:HG2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:302:UDP:O1A	2:D:302:UDP:O3'	2.04	0.75
1:J:36:LYS:CE	1:J:165:THR:CG2	2.64	0.75
2:H:301:UDP:O1A	2:H:301:UDP:O3'	2.05	0.74
1:G:80:PHE:C	1:G:81:PHE:CD1	2.60	0.74
1:F:59:ARG:HG2	1:F:59:ARG:HH21	1.52	0.74
1:H:130:MET:HE1	1:H:133:VAL:HG21	1.69	0.74
1:E:82:ARG:NH1	1:E:85:GLN:OE1	2.21	0.74
1:J:34:LEU:HD22	1:J:173:ALA:HB2	1.67	0.74
1:F:144:ARG:HH22	1:K:59:ARG:HB3	1.53	0.74
3:I:301:UTP:O2A	1:K:141:ARG:HG3	1.88	0.74
1:G:85:GLN:HA	1:G:89:LEU:HD13	1.68	0.73
1:B:209:HIS:HB3	1:B:229:MET:HG3	1.70	0.73
1:C:144:ARG:O	1:C:144:ARG:HG3	1.88	0.73
1:L:173:ALA:HB1	1:L:233:MET:HE2	1.71	0.73
1:B:249:ALA:HB2	1:B:255:ILE:HD11	1.70	0.72
1:H:87:GLN:HB2	1:H:93:ARG:HG3	1.70	0.72
1:F:90:GLY:O	1:F:91:MET:O	2.08	0.72
1:D:36:LYS:NZ	2:D:302:UDP:O2B	2.22	0.71
1:J:36:LYS:CE	1:J:165:THR:HG22	2.19	0.71
1:H:207:VAL:HG13	1:H:211:GLU:HB2	1.72	0.71
1:K:157:GLY:HA3	2:K:301:UDP:C5	2.26	0.71
1:J:209:HIS:HB3	1:J:229:MET:HG3	1.73	0.71
1:K:157:GLY:HA3	2:K:301:UDP:H5	1.56	0.70
1:I:36:LYS:CE	1:I:165:THR:HG21	1.99	0.70
1:G:35:LEU:HD12	1:G:182:LEU:HG	1.71	0.70
1:B:101:MET:HE3	2:B:301:UDP:N3	2.06	0.70
1:F:59:ARG:HH21	1:F:59:ARG:CG	2.04	0.70
1:J:242:THR:OG1	1:J:245:ASN:ND2	2.24	0.70
1:G:80:PHE:C	1:G:81:PHE:HD1	1.95	0.70
1:G:86:LEU:H	1:G:86:LEU:CD2	2.04	0.70
1:E:182:LEU:HB3	1:E:238:PHE:HE1	1.56	0.70
1:H:215:ARG:HG2	1:H:215:ARG:HH21	1.57	0.70
1:I:123:ARG:NH2	3:I:301:UTP:O1B	2.22	0.70
1:F:92:GLU:O	1:F:96:SER:HB3	1.92	0.69
1:B:101:MET:HE1	1:B:160:LEU:N	2.08	0.69
1:E:209:HIS:HB3	1:E:229:MET:HG3	1.74	0.69
1:H:215:ARG:HG2	1:H:215:ARG:NH2	2.07	0.69
1:J:213:LEU:HD11	1:J:229:MET:HE1	1.75	0.68
1:K:188:ASP:HA	1:K:239:ASN:HB2	1.75	0.68
1:G:80:PHE:O	1:G:81:PHE:HD1	1.76	0.68
1:E:180:VAL:HG23	1:E:234:PRO:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:251:ARG:NH2	1:J:253:GLU:OE2	2.26	0.68
1:H:203:LEU:HD23	1:H:203:LEU:O	1.93	0.68
1:J:36:LYS:HE3	1:J:165:THR:CG2	2.23	0.67
1:H:97:ASP:O	1:H:101:MET:HG3	1.93	0.67
1:L:142:ALA:O	1:L:145:HIS:HB2	1.93	0.67
1:I:144:ARG:O	1:I:147:GLU:N	2.27	0.67
1:C:194:ASP:HB3	1:C:195:PRO:HD3	0.74	0.67
1:B:56:GLN:NE2	1:B:241:LEU:O	2.28	0.67
1:H:75:ILE:HG13	1:H:108:SER:HB3	1.77	0.67
1:K:55:ALA:O	1:K:59:ARG:HG3	1.95	0.66
1:F:130:MET:O	1:F:132:GLN:NE2	2.24	0.66
1:H:190:VAL:HG22	1:H:257:THR:HG21	1.77	0.66
1:C:83:GLY:H	2:C:302:UDP:HO3'	1.41	0.65
1:K:227:LEU:O	1:K:227:LEU:HD12	1.95	0.65
1:H:190:VAL:O	1:H:203:LEU:HA	1.97	0.65
1:C:54:VAL:HA	1:C:57:VAL:HG22	1.77	0.65
1:I:36:LYS:NZ	1:I:165:THR:HG21	2.10	0.65
1:D:77:GLY:HA3	1:D:104:THR:HG22	1.79	0.65
1:G:144:ARG:NH2	1:G:147:GLU:OE1	2.29	0.65
1:H:82:ARG:HH21	1:H:82:ARG:HG3	1.62	0.64
1:A:86:LEU:HD13	1:A:96:SER:OG	1.98	0.64
1:F:91:MET:CE	1:F:96:SER:CA	2.76	0.64
1:I:144:ARG:O	1:I:146:LEU:N	2.30	0.64
1:J:60:GLN:HE21	1:J:246:ILE:HG22	1.62	0.63
1:F:181:VAL:HG23	1:F:233:MET:HE2	1.81	0.63
1:C:194:ASP:CB	1:C:195:PRO:CD	2.47	0.63
1:F:127:ALA:HB2	1:F:172:ARG:HH22	1.63	0.63
1:J:36:LYS:HE2	1:J:165:THR:CG2	2.28	0.63
1:A:184:ALA:HB1	1:A:240:LEU:HB2	1.81	0.63
1:C:83:GLY:N	2:C:302:UDP:O3'	2.19	0.63
1:H:122:THR:HG22	1:H:151:VAL:HG13	1.80	0.63
1:D:146:LEU:CD2	1:D:152:VAL:HG23	2.29	0.63
1:G:146:LEU:HD11	1:G:176:ILE:HD11	1.81	0.63
1:H:51:PRO:HA	1:H:54:VAL:HG12	1.80	0.63
1:H:180:VAL:HG23	1:H:234:PRO:HB2	1.80	0.63
1:K:83:GLY:CA	1:K:97:ASP:OD1	2.46	0.62
1:H:215:ARG:HH21	1:H:215:ARG:CG	2.12	0.62
1:H:182:LEU:HB3	1:H:238:PHE:HE1	1.65	0.62
1:D:188:ASP:HA	1:D:239:ASN:HB2	1.81	0.62
1:G:54:VAL:HA	1:G:57:VAL:HG12	1.81	0.61
1:G:62:ALA:O	1:G:66:ARG:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ARG:NH2	2:D:302:UDP:O1B	2.34	0.61
1:G:86:LEU:CD2	1:G:87:GLN:N	2.61	0.61
1:H:130:MET:O	1:H:132:GLN:N	2.31	0.61
1:H:204:LEU:N	1:H:204:LEU:HD23	2.15	0.61
1:F:144:ARG:NH1	1:K:59:ARG:HD2	2.14	0.61
1:F:60:GLN:HE22	1:F:244:GLY:H	1.48	0.61
1:G:128:ILE:HA	1:H:132:GLN:OE1	2.01	0.61
1:H:101:MET:HE1	1:H:159:GLY:H	1.66	0.61
1:A:56:GLN:NE2	1:A:243:ASP:OD1	2.34	0.60
1:A:211:GLU:OE2	1:A:215:ARG:NH2	2.34	0.60
1:J:191:PHE:CE2	1:J:203:LEU:HG	2.36	0.60
1:D:146:LEU:HD21	1:D:152:VAL:CG2	2.32	0.60
1:B:74:VAL:HG12	1:B:165:THR:CG2	2.31	0.60
1:H:34:LEU:HD23	1:H:173:ALA:HB2	1.84	0.60
1:D:209:HIS:HB3	1:D:229:MET:HG3	1.84	0.60
1:J:188:ASP:HA	1:J:239:ASN:HB2	1.84	0.60
1:H:82:ARG:HG3	1:H:82:ARG:NH2	2.14	0.60
1:F:90:GLY:O	1:F:91:MET:C	2.40	0.60
1:G:34:LEU:HD13	1:G:173:ALA:HA	1.83	0.60
1:F:91:MET:HE3	1:F:96:SER:HA	1.84	0.60
1:I:206:ALA:O	1:I:207:VAL:CG1	2.46	0.60
1:F:166:ASP:OD2	1:F:183:MET:HE1	2.01	0.59
1:E:218:ARG:HH21	1:E:218:ARG:CG	2.15	0.59
1:L:64:VAL:HG22	1:L:69:VAL:HB	1.83	0.59
1:C:83:GLY:HA3	1:C:97:ASP:OD1	2.02	0.59
1:B:204:LEU:HD22	1:B:215:ARG:HH12	1.68	0.59
1:F:59:ARG:HG2	1:F:59:ARG:NH2	2.17	0.59
1:H:60:GLN:OE1	1:H:244:GLY:N	2.33	0.59
1:L:143:VAL:CG2	1:L:144:ARG:N	2.65	0.58
1:I:171:GLN:NE2	1:H:161:PRO:HD2	2.18	0.58
1:J:105:VAL:HA	1:J:108:SER:HB2	1.84	0.58
1:E:247:ALA:O	1:E:251:ARG:HD3	2.03	0.58
1:G:54:VAL:HG23	1:G:114:PHE:CD2	2.39	0.58
1:C:104:THR:HG22	1:C:156:ALA:H	1.69	0.58
1:B:101:MET:HE1	1:B:159:GLY:C	2.23	0.58
1:E:130:MET:O	1:E:132:GLN:N	2.37	0.58
1:D:244:GLY:O	1:D:248:ARG:HG3	2.04	0.58
1:H:133:VAL:O	1:H:134:ALA:HB2	2.03	0.58
1:A:157:GLY:HA3	1:A:168:THR:HG21	1.84	0.58
1:L:115:LEU:HD22	1:L:120:ILE:HD12	1.85	0.58
1:A:84:ALA:O	1:A:88:GLN:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LEU:HD23	1:D:152:VAL:HG23	1.85	0.57
1:C:157:GLY:HA3	2:C:302:UDP:C5	2.38	0.57
1:H:245:ASN:HA	1:H:248:ARG:HD2	1.86	0.57
1:C:180:VAL:HG13	1:C:182:LEU:CD1	2.34	0.57
1:H:204:LEU:HD12	1:H:207:VAL:HG21	1.85	0.57
1:F:91:MET:HE1	1:F:96:SER:HA	1.84	0.57
1:C:61:ILE:O	1:C:64:VAL:HG12	2.05	0.57
1:L:34:LEU:HD11	1:L:74:VAL:HG23	1.86	0.57
1:D:212:VAL:HG13	1:D:217:LEU:HB2	1.85	0.57
1:K:180:VAL:HG23	1:K:234:PRO:HB2	1.87	0.57
1:H:34:LEU:HD12	1:H:72:ALA:O	2.04	0.57
1:J:85:GLN:O	1:J:89:LEU:HD12	2.04	0.57
1:F:128:ILE:HG13	1:F:156:ALA:HB1	1.87	0.57
1:J:255:ILE:HG22	1:J:256:GLY:N	2.20	0.57
1:K:209:HIS:HB3	1:K:229:MET:HG3	1.87	0.57
1:I:165:THR:O	1:I:168:THR:HB	2.05	0.56
1:E:95:ARG:O	1:E:99:MET:HG3	2.04	0.56
1:C:64:VAL:HG23	1:C:250:VAL:HG11	1.87	0.56
1:H:133:VAL:O	1:H:133:VAL:HG23	2.04	0.56
1:D:146:LEU:CD2	1:D:152:VAL:CG2	2.83	0.56
1:G:86:LEU:CD2	1:G:87:GLN:H	1.98	0.56
1:I:165:THR:CB	2:I:302:UDP:O2A	2.45	0.56
1:K:74:VAL:CG1	1:K:165:THR:CG2	2.84	0.56
1:F:144:ARG:NH2	1:K:59:ARG:HB3	2.20	0.56
1:L:173:ALA:O	1:L:176:ILE:HG22	2.06	0.56
1:B:32:ARG:HG3	1:B:70:GLN:HB2	1.88	0.56
1:B:36:LYS:NZ	2:B:301:UDP:O2B	2.38	0.56
1:K:113:ASP:OD1	1:L:95:ARG:NH1	2.39	0.56
1:F:101:MET:HE3	1:F:159:GLY:CA	2.35	0.56
1:C:184:ALA:HB1	1:C:240:LEU:HB2	1.89	0.56
1:I:54:VAL:HA	1:I:57:VAL:HG22	1.87	0.56
1:B:212:VAL:HG11	1:B:219:VAL:CG2	2.35	0.55
1:I:93:ARG:HG2	1:I:162:TYR:CE1	2.41	0.55
1:B:172:ARG:O	1:B:176:ILE:HG12	2.05	0.55
3:J:301:UTP:O1A	1:H:141:ARG:HG3	2.06	0.55
1:C:212:VAL:HA	1:C:217:LEU:HD12	1.87	0.55
1:L:62:ALA:HA	1:L:120:ILE:HD11	1.88	0.55
1:G:86:LEU:HD23	1:G:86:LEU:H	1.71	0.55
1:B:81:PHE:CE2	1:A:106:MET:HE2	2.40	0.55
1:E:69:VAL:HG21	1:E:250:VAL:HB	1.89	0.55
1:G:54:VAL:HA	1:G:57:VAL:CG1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:171:GLN:HE22	1:H:161:PRO:HD2	1.72	0.55
1:D:132:GLN:NE2	1:C:159:GLY:O	2.39	0.55
1:G:168:THR:HG23	1:G:172:ARG:HH11	1.71	0.55
1:L:35:LEU:HB3	1:L:73:VAL:HG12	1.88	0.55
1:H:172:ARG:O	1:H:176:ILE:HG12	2.07	0.55
1:H:209:HIS:HB3	1:H:229:MET:HG3	1.88	0.54
1:B:84:ALA:O	1:B:88:GLN:HG3	2.08	0.54
1:A:125:GLN:HG2	1:A:135:GLU:HG3	1.90	0.54
1:E:36:LYS:CE	1:E:165:THR:CG2	2.85	0.54
1:I:95:ARG:NH2	1:J:116:GLU:OE2	2.41	0.54
1:L:142:ALA:O	1:L:145:HIS:N	2.37	0.54
1:L:39:GLY:HA3	1:L:78:GLY:H	1.73	0.54
1:L:94:THR:HG22	1:L:162:TYR:CZ	2.43	0.54
1:B:33:VAL:HG22	1:B:182:LEU:HG	1.88	0.54
1:J:167:THR:HG22	1:J:167:THR:O	2.06	0.54
1:A:59:ARG:HA	1:A:118:GLU:HG2	1.89	0.54
1:F:90:GLY:C	1:F:91:MET:O	2.46	0.54
1:C:158:MET:HB2	2:C:302:UDP:O4	2.07	0.54
1:C:228:CYS:HB3	1:C:233:MET:HB3	1.88	0.54
1:K:182:LEU:HB3	1:K:238:PHE:HE1	1.72	0.54
1:I:141:ARG:NH2	3:I:301:UTP:O2B	2.41	0.54
1:A:212:VAL:HA	1:A:217:LEU:HD12	1.90	0.54
1:G:91:MET:HB2	1:H:113:ASP:OD2	2.08	0.54
1:C:34:LEU:HD22	1:C:173:ALA:HB2	1.90	0.53
1:I:132:GLN:NE2	1:J:159:GLY:O	2.42	0.53
1:E:209:HIS:HB2	1:E:261:THR:OG1	2.07	0.53
1:H:61:ILE:O	1:H:64:VAL:HG12	2.09	0.53
1:F:208:SER:HA	1:F:260:THR:H	1.73	0.53
1:G:85:GLN:O	1:G:89:LEU:HB2	2.09	0.53
1:G:109:LEU:O	1:H:95:ARG:HD2	2.08	0.53
1:D:245:ASN:ND2	1:D:255:ILE:HD11	2.24	0.53
1:G:62:ALA:CB	1:G:118:GLU:HG2	2.39	0.53
1:G:81:PHE:CD1	1:G:81:PHE:N	2.73	0.53
1:I:50:ASP:HB3	1:I:53:VAL:HG12	1.90	0.53
1:K:244:GLY:O	1:K:248:ARG:HG2	2.09	0.53
1:L:40:GLU:HG3	1:L:78:GLY:O	2.09	0.53
1:F:130:MET:O	1:F:132:GLN:N	2.42	0.53
1:J:167:THR:HA	1:J:224:ALA:HB2	1.90	0.53
1:I:204:LEU:CD1	1:I:217:LEU:HD11	2.35	0.52
1:D:185:LYS:HD3	1:D:237:VAL:HG13	1.90	0.52
1:C:64:VAL:CG2	1:C:250:VAL:HG11	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:THR:HG22	1:A:151:VAL:HB	1.90	0.52
1:A:248:ARG:HD3	1:A:255:ILE:HD11	1.90	0.52
1:H:57:VAL:O	1:H:61:ILE:HG13	2.10	0.52
1:B:74:VAL:CG1	1:B:165:THR:CG2	2.87	0.52
1:A:212:VAL:HG13	1:A:217:LEU:HB2	1.92	0.52
1:L:125:GLN:HG2	1:L:135:GLU:HB3	1.91	0.52
1:C:97:ASP:HA	2:C:302:UDP:O2'	2.09	0.52
1:J:60:GLN:OE1	1:J:243:ASP:HA	2.09	0.52
1:K:42:PHE:HZ	1:K:75:ILE:HD12	1.75	0.52
1:A:93:ARG:HG2	1:A:162:TYR:CE1	2.45	0.51
2:K:301:UDP:H2'	2:K:301:UDP:O2	2.09	0.51
1:K:61:ILE:O	1:K:65:VAL:HG23	2.09	0.51
1:K:74:VAL:CG1	1:K:165:THR:HG23	2.40	0.51
1:F:98:TYR:OH	1:E:132:GLN:OE1	2.28	0.51
1:I:164:SER:OG	1:I:167:THR:HG22	2.11	0.51
1:H:186:ALA:O	1:H:239:ASN:ND2	2.43	0.51
1:B:61:ILE:O	1:B:65:VAL:HG23	2.10	0.51
1:E:210:ARG:O	1:E:210:ARG:HG3	2.10	0.51
1:C:115:LEU:O	1:C:120:ILE:HB	2.10	0.51
1:J:173:ALA:HB1	1:J:233:MET:HE2	1.91	0.51
1:J:182:LEU:HB3	1:J:238:PHE:HE1	1.75	0.51
1:H:83:GLY:N	2:H:301:UDP:O2'	2.41	0.51
1:B:70:GLN:HB3	1:B:146:LEU:HB3	1.92	0.51
1:J:75:ILE:HD11	1:J:108:SER:OG	2.10	0.51
1:C:158:MET:HE3	1:C:167:THR:HG22	1.92	0.51
1:E:218:ARG:CG	1:E:218:ARG:NH2	2.73	0.51
1:I:71:ILE:HG23	1:I:151:VAL:HG13	1.93	0.51
1:L:144:ARG:NH1	1:L:144:ARG:HG2	2.26	0.51
1:H:42:PHE:HE2	1:H:111:LEU:HB2	1.75	0.51
1:B:128:ILE:HG21	1:A:133:VAL:HG23	1.92	0.50
1:D:102:LEU:HD13	1:C:105:VAL:CG2	2.40	0.50
1:I:61:ILE:O	1:I:64:VAL:HG12	2.10	0.50
1:A:188:ASP:HA	1:A:239:ASN:HB2	1.93	0.50
1:C:191:PHE:CE1	1:C:203:LEU:HD12	2.47	0.50
1:K:36:LYS:HE3	1:K:165:THR:CG2	2.42	0.50
1:H:219:VAL:HG23	1:H:220:ALA:H	1.77	0.50
1:C:188:ASP:HA	1:C:239:ASN:HB2	1.94	0.50
1:B:221:ASP:HB2	1:B:224:ALA:HB3	1.94	0.50
1:A:28:SER:HB2	1:A:252:GLY:HA3	1.92	0.50
1:E:33:VAL:HG22	1:E:182:LEU:HG	1.94	0.50
1:F:158:MET:HG2	1:F:168:THR:OG1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:163:PHE:O	2:I:302:UDP:C2	2.64	0.50
1:I:188:ASP:HA	1:I:239:ASN:HB2	1.93	0.50
1:A:185:LYS:O	1:A:239:ASN:HA	2.12	0.49
1:C:71:ILE:HG23	1:C:151:VAL:HG13	1.94	0.49
1:J:255:ILE:CG2	1:J:256:GLY:N	2.75	0.49
1:L:143:VAL:HG23	1:L:144:ARG:N	2.26	0.49
1:B:247:ALA:O	1:B:251:ARG:HG3	2.12	0.49
1:E:188:ASP:HB3	1:E:239:ASN:HB2	1.94	0.49
1:D:101:MET:HE2	1:D:128:ILE:HD11	1.94	0.49
1:G:36:LYS:HE3	1:G:183:MET:HG3	1.95	0.49
1:J:148:LYS:HD2	1:J:150:ARG:NH1	2.28	0.49
3:L:301:UTP:C6	3:L:301:UTP:H5'1	2.48	0.49
1:C:111:LEU:O	1:C:115:LEU:HB2	2.12	0.49
1:B:209:HIS:H	1:B:261:THR:HG23	1.78	0.49
1:F:91:MET:HE1	1:F:96:SER:HB2	1.94	0.49
1:F:181:VAL:HG23	1:F:233:MET:CE	2.41	0.49
1:E:188:ASP:OD1	1:E:188:ASP:N	2.35	0.49
1:C:104:THR:CG2	1:C:156:ALA:H	2.25	0.49
1:I:36:LYS:HE3	1:I:166:ASP:OD1	2.12	0.49
1:G:128:ILE:HG23	1:H:132:GLN:HB2	1.94	0.49
1:J:34:LEU:HD11	1:J:74:VAL:HG23	1.95	0.49
1:G:124:VAL:O	1:G:134:ALA:HB1	2.13	0.48
1:J:51:PRO:HA	1:J:54:VAL:HG12	1.94	0.48
1:K:253:GLU:O	1:K:255:ILE:N	2.46	0.48
1:L:101:MET:O	1:L:105:VAL:HG23	2.12	0.48
1:G:95:ARG:NH2	1:H:113:ASP:HA	2.28	0.48
1:H:207:VAL:O	1:H:259:VAL:HA	2.13	0.48
1:K:32:ARG:HD2	1:K:146:LEU:HD13	1.94	0.48
1:K:165:THR:OG1	2:K:301:UDP:O2A	2.25	0.48
1:G:86:LEU:CD2	1:G:86:LEU:N	2.72	0.48
1:H:163:PHE:O	2:H:301:UDP:C2	2.66	0.48
1:K:74:VAL:HG12	1:K:165:THR:CG2	2.43	0.48
1:B:64:VAL:HG12	1:B:247:ALA:HB2	1.96	0.48
1:C:32:ARG:HH21	1:C:146:LEU:HD12	1.77	0.48
1:C:137:TYR:OH	1:C:175:GLU:OE1	2.24	0.48
1:K:111:LEU:HG	1:K:115:LEU:HD12	1.95	0.48
1:K:132:GLN:HB2	1:L:128:ILE:HD11	1.95	0.48
1:F:42:PHE:HZ	1:F:75:ILE:HD12	1.78	0.48
1:C:101:MET:O	1:C:104:THR:HB	2.14	0.48
1:F:93:ARG:NH1	1:F:162:TYR:HD1	2.11	0.48
1:J:208:SER:HB2	1:J:211:GLU:CG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:VAL:HG12	1:G:69:VAL:HB	1.95	0.48
1:G:98:TYR:HE1	1:G:128:ILE:HD11	1.79	0.48
1:B:60:GLN:NE2	1:B:246:ILE:HG22	2.29	0.48
1:E:123:ARG:HD3	1:E:145:HIS:CE1	2.49	0.48
1:K:212:VAL:HG11	1:K:225:PHE:CZ	2.49	0.48
1:H:137:TYR:CZ	1:H:139:PRO:HB3	2.49	0.48
1:B:74:VAL:CG1	1:B:165:THR:HG23	2.44	0.48
1:B:240:LEU:O	1:B:240:LEU:HG	2.13	0.48
1:I:42:PHE:CE2	1:I:75:ILE:HG23	2.49	0.48
1:E:42:PHE:HZ	1:E:75:ILE:HD12	1.78	0.48
1:I:235:ILE:HB	1:I:259:VAL:CG2	2.44	0.48
1:J:244:GLY:O	1:J:248:ARG:HG3	2.14	0.48
1:L:112:GLN:HG3	1:L:122:THR:OG1	2.14	0.48
1:F:42:PHE:CZ	1:F:75:ILE:HD12	2.49	0.47
1:C:218:ARG:HG3	1:C:218:ARG:HH11	1.78	0.47
1:L:171:GLN:O	1:L:175:GLU:HG2	2.14	0.47
1:G:86:LEU:HD23	1:G:86:LEU:N	2.30	0.47
1:G:86:LEU:H	1:G:86:LEU:HD22	1.79	0.47
1:H:99:MET:HE2	1:H:99:MET:HB2	1.41	0.47
1:F:91:MET:HA	1:E:113:ASP:OD2	2.14	0.47
1:A:137:TYR:OH	1:A:175:GLU:OE1	2.25	0.47
1:F:33:VAL:HG11	1:F:250:VAL:CG1	2.45	0.47
1:K:246:ILE:O	1:K:250:VAL:HG23	2.14	0.47
1:L:70:GLN:HB3	1:L:146:LEU:HB3	1.96	0.47
1:F:124:VAL:HG22	1:F:153:ILE:HB	1.97	0.47
1:G:95:ARG:HH21	1:H:113:ASP:HA	1.80	0.47
1:G:121:VAL:HG21	4:G:402:HOH:O	2.14	0.47
1:A:60:GLN:NE2	1:A:243:ASP:HA	2.30	0.47
1:B:83:GLY:N	2:B:301:UDP:O2'	2.45	0.47
1:I:253:GLU:O	1:I:255:ILE:N	2.48	0.47
1:J:34:LEU:HD21	1:J:169:ALA:HB1	1.97	0.47
1:B:188:ASP:HA	1:B:239:ASN:HB2	1.97	0.47
1:B:210:ARG:HA	1:B:229:MET:HE1	1.96	0.47
1:E:124:VAL:HG22	1:E:153:ILE:HB	1.97	0.47
1:C:50:ASP:OD1	1:C:52:ASP:HB2	2.15	0.47
1:L:36:LYS:HD2	1:L:183:MET:SD	2.55	0.47
1:F:60:GLN:NE2	1:F:244:GLY:H	2.12	0.46
1:B:62:ALA:O	1:B:66:ARG:HG3	2.15	0.46
1:F:144:ARG:HA	1:F:144:ARG:HD2	1.75	0.46
1:C:76:GLY:HA2	1:C:165:THR:HG21	1.97	0.46
1:B:86:LEU:HD22	1:B:91:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:ARG:HH21	1:F:59:ARG:CB	2.28	0.46
1:H:165:THR:HB	2:H:301:UDP:O2A	2.15	0.46
1:H:242:THR:O	1:H:245:ASN:HB2	2.16	0.46
1:D:74:VAL:HG12	1:D:165:THR:CG2	2.45	0.46
1:L:66:ARG:HD2	1:L:66:ARG:HA	1.71	0.46
1:J:157:GLY:HA3	2:J:302:UDP:C5	2.51	0.46
1:J:158:MET:N	2:J:302:UDP:O4	2.42	0.46
1:I:144:ARG:CD	3:G:301:UTP:H5'1	2.18	0.46
1:B:221:ASP:HB2	1:B:224:ALA:CB	2.46	0.46
1:A:56:GLN:NE2	1:A:59:ARG:HH22	2.13	0.46
1:A:182:LEU:HB3	1:A:238:PHE:HE1	1.81	0.46
1:J:34:LEU:HD22	1:J:169:ALA:O	2.16	0.46
1:J:168:THR:O	1:J:168:THR:HG22	2.15	0.46
1:L:117:LYS:HD3	1:L:117:LYS:HA	1.62	0.46
1:L:233:MET:HG3	1:L:234:PRO:N	2.29	0.46
1:A:111:LEU:HD23	1:A:153:ILE:HD13	1.98	0.46
1:F:33:VAL:HG11	1:F:250:VAL:HG12	1.98	0.46
1:F:91:MET:HG2	1:E:113:ASP:CG	2.36	0.46
1:F:101:MET:HE3	1:F:159:GLY:HA2	1.97	0.46
1:I:180:VAL:HG23	1:I:234:PRO:HB2	1.98	0.46
1:J:204:LEU:O	1:J:257:THR:HG22	2.16	0.46
1:D:49:LEU:HD11	1:D:54:VAL:HG21	1.97	0.46
1:I:249:ALA:HB2	1:I:255:ILE:HD11	1.97	0.46
1:D:70:GLN:HB3	1:D:146:LEU:HB3	1.97	0.46
1:G:112:GLN:HG3	1:G:122:THR:HG21	1.98	0.46
1:G:116:GLU:OE1	1:H:95:ARG:NH1	2.49	0.45
1:G:185:LYS:HE3	1:G:237:VAL:HG13	1.98	0.45
1:G:182:LEU:HD13	1:G:236:LEU:HD22	1.99	0.45
1:E:35:LEU:HD11	1:E:184:ALA:HB2	1.98	0.45
1:L:130:MET:HG2	1:L:133:VAL:HB	1.98	0.45
1:E:236:LEU:HD11	1:E:255:ILE:O	2.16	0.45
1:D:102:LEU:HD13	1:C:105:VAL:HG23	1.98	0.45
1:L:61:ILE:HG23	1:L:71:ILE:HD13	1.98	0.45
1:H:165:THR:O	1:H:165:THR:HG22	2.16	0.45
1:L:100:GLY:O	1:L:104:THR:HG23	2.17	0.45
1:B:184:ALA:HB1	1:B:240:LEU:HB2	1.98	0.45
1:A:45:GLY:O	1:A:46:GLN:HG3	2.17	0.45
1:A:100:GLY:O	1:A:104:THR:HG23	2.17	0.45
1:C:97:ASP:CG	2:C:302:UDP:O2'	2.55	0.45
1:C:125:GLN:HG2	1:C:135:GLU:HG2	1.98	0.45
1:B:114:PHE:O	1:B:118:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:VAL:HG11	1:B:219:VAL:HG23	1.98	0.45
1:D:245:ASN:HD21	1:D:255:ILE:HD11	1.81	0.45
1:I:148:LYS:HD2	1:I:150:ARG:NH1	2.32	0.45
3:I:301:UTP:O2A	1:K:141:ARG:CG	2.61	0.45
1:H:114:PHE:HA	1:H:117:LYS:HB2	1.99	0.45
1:J:180:VAL:HG23	1:J:234:PRO:HB2	1.99	0.45
1:L:144:ARG:HG2	1:L:144:ARG:HH11	1.82	0.45
1:H:245:ASN:O	1:H:248:ARG:HB2	2.16	0.45
1:D:115:LEU:HD23	1:D:115:LEU:HA	1.74	0.45
1:C:102:LEU:O	1:C:105:VAL:HG22	2.17	0.45
1:I:102:LEU:HD13	1:J:105:VAL:HG23	1.99	0.45
1:B:86:LEU:HD23	1:B:89:LEU:HD12	1.99	0.44
1:J:123:ARG:HD3	3:J:301:UTP:H3'	1.98	0.44
1:K:86:LEU:HD12	1:K:96:SER:HB3	1.98	0.44
1:B:112:GLN:HG3	1:B:122:THR:OG1	2.17	0.44
1:F:208:SER:CB	1:F:211:GLU:HG3	2.47	0.44
1:I:208:SER:HB2	1:I:211:GLU:HG3	1.99	0.44
1:J:117:LYS:HD2	1:J:117:LYS:N	2.32	0.44
1:I:74:VAL:HG21	1:I:169:ALA:HB2	1.98	0.44
1:G:127:ALA:H	1:G:156:ALA:HB3	1.82	0.44
1:H:212:VAL:O	1:H:216:GLY:N	2.50	0.44
1:L:181:VAL:HG23	1:L:233:MET:HE2	1.98	0.44
1:G:31:SER:HB3	1:G:179:ASP:OD2	2.18	0.44
1:H:56:GLN:HE21	1:H:241:LEU:HD23	1.83	0.44
1:D:148:LYS:HD3	1:D:150:ARG:HH21	1.83	0.44
1:I:208:SER:CB	1:I:211:GLU:HG3	2.47	0.44
1:E:61:ILE:HG23	1:E:71:ILE:HD13	2.00	0.44
1:D:95:ARG:O	1:D:99:MET:HG3	2.18	0.44
1:D:101:MET:CE	1:D:128:ILE:HD11	2.47	0.44
1:J:141:ARG:HG3	3:L:301:UTP:H5'2	1.99	0.44
1:J:158:MET:HE2	1:J:168:THR:HA	1.99	0.44
1:B:135:GLU:HG2	1:B:136:PRO:HD2	1.99	0.44
1:C:235:ILE:HB	1:C:259:VAL:CG1	2.48	0.44
1:K:42:PHE:HE2	1:K:111:LEU:HB2	1.83	0.44
1:L:42:PHE:HD2	1:L:49:LEU:HD21	1.82	0.44
1:G:144:ARG:HA	1:G:144:ARG:HD3	1.87	0.44
1:H:101:MET:HE1	1:H:159:GLY:N	2.32	0.44
1:I:80:PHE:HZ	1:J:81:PHE:CE2	2.34	0.44
1:K:70:GLN:HB3	1:K:146:LEU:HB3	2.00	0.44
1:K:95:ARG:HH21	1:L:113:ASP:HA	1.82	0.44
1:B:212:VAL:HG11	1:B:219:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:GLU:O	1:F:96:SER:CB	2.64	0.44
1:D:102:LEU:HD23	1:D:102:LEU:HA	1.78	0.43
1:J:158:MET:CE	1:J:168:THR:HA	2.48	0.43
1:C:190:VAL:HG22	1:C:257:THR:HG21	1.99	0.43
1:K:42:PHE:CZ	1:K:75:ILE:HD12	2.53	0.43
1:E:97:ASP:O	1:E:101:MET:HG3	2.18	0.43
1:E:167:THR:HA	1:E:224:ALA:HB2	1.99	0.43
1:J:64:VAL:HG21	1:J:250:VAL:HG21	2.01	0.43
1:K:165:THR:CB	2:K:301:UDP:O2A	2.66	0.43
1:G:102:LEU:O	1:G:106:MET:HG3	2.18	0.43
3:F:301:UTP:H5'2	3:F:301:UTP:O1B	2.19	0.43
1:I:247:ALA:HB1	1:I:251:ARG:HH11	1.83	0.43
1:J:208:SER:CB	1:J:211:GLU:H	2.31	0.43
1:I:217:LEU:HD23	1:I:217:LEU:HA	1.81	0.43
1:J:111:LEU:HD23	1:J:153:ILE:HD13	2.01	0.43
1:D:87:GLN:HA	1:D:91:MET:O	2.19	0.43
1:B:52:ASP:OD1	1:B:52:ASP:N	2.51	0.43
1:A:143:VAL:HG23	1:A:144:ARG:NH1	2.34	0.43
2:D:302:UDP:C3'	2:D:302:UDP:PA	3.06	0.43
1:C:36:LYS:NZ	2:C:302:UDP:O2B	2.51	0.43
1:I:129:THR:HB	1:I:136:PRO:HB3	2.00	0.43
1:I:140:LEU:HD23	1:I:140:LEU:HA	1.74	0.43
1:J:144:ARG:HH21	1:J:148:LYS:CE	2.32	0.43
1:K:34:LEU:HG	1:K:173:ALA:HB2	2.00	0.43
1:K:161:PRO:O	1:K:162:TYR:HB2	2.19	0.43
1:L:144:ARG:O	1:L:148:LYS:HG3	2.18	0.43
1:H:81:PHE:CD1	1:H:86:LEU:HD11	2.53	0.43
1:C:120:ILE:HD13	1:C:120:ILE:HA	1.89	0.43
1:L:170:ALA:O	1:L:174:LEU:HG	2.18	0.43
1:H:240:LEU:O	1:H:240:LEU:HD23	2.19	0.43
1:B:53:VAL:O	1:B:57:VAL:HG23	2.18	0.43
1:A:46:GLN:HB3	1:A:47:VAL:H	1.69	0.43
1:F:61:ILE:O	1:F:65:VAL:HG23	2.19	0.43
1:D:209:HIS:CB	1:D:229:MET:HG3	2.49	0.43
1:K:182:LEU:HB3	1:K:238:PHE:CE1	2.51	0.43
1:G:80:PHE:O	1:G:81:PHE:CD1	2.64	0.43
1:H:34:LEU:HD11	1:H:74:VAL:HG23	2.01	0.43
1:A:180:VAL:HG23	1:A:234:PRO:HB2	2.01	0.43
1:D:85:GLN:O	1:D:89:LEU:HD13	2.19	0.43
1:D:130:MET:HE3	1:C:102:LEU:HD21	2.01	0.43
1:J:34:LEU:CD2	1:J:169:ALA:HB1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:64:VAL:HG22	1:J:69:VAL:HG11	2.01	0.43
1:B:80:PHE:CZ	1:B:106:MET:HE3	2.54	0.42
1:F:93:ARG:HH11	1:F:162:TYR:HD1	1.66	0.42
1:D:128:ILE:O	1:D:130:MET:HG3	2.19	0.42
1:C:82:ARG:NH1	2:C:302:UDP:O3B	2.51	0.42
1:I:245:ASN:HD22	1:I:245:ASN:HA	1.63	0.42
1:H:40:GLU:O	1:H:44:GLY:CA	2.56	0.42
1:H:133:VAL:O	1:H:134:ALA:CB	2.64	0.42
1:B:221:ASP:HB3	1:B:224:ALA:H	1.83	0.42
1:E:42:PHE:CZ	1:E:75:ILE:HD12	2.53	0.42
1:D:142:ALA:O	1:D:146:LEU:HG	2.19	0.42
1:C:70:GLN:HB3	1:C:146:LEU:HB3	2.01	0.42
1:H:42:PHE:HZ	1:H:75:ILE:HD12	1.83	0.42
1:H:157:GLY:HA3	2:H:301:UDP:H5	1.85	0.42
1:B:249:ALA:CB	1:B:255:ILE:HD11	2.45	0.42
1:I:244:GLY:O	1:I:248:ARG:HG3	2.19	0.42
1:A:60:GLN:HE22	1:A:243:ASP:HA	1.85	0.42
1:I:69:VAL:HG11	1:I:250:VAL:HG21	1.99	0.42
1:B:141:ARG:HG3	3:D:301:UTP:O1A	2.20	0.42
1:B:209:HIS:HB3	1:B:229:MET:HE2	2.01	0.42
1:F:246:ILE:O	1:F:250:VAL:HG22	2.19	0.42
1:L:173:ALA:HB1	1:L:233:MET:CE	2.45	0.42
1:E:36:LYS:CE	1:E:165:THR:HG21	2.49	0.42
1:I:172:ARG:O	1:I:176:ILE:HG12	2.19	0.42
1:A:71:ILE:HG23	1:A:151:VAL:HG13	2.01	0.42
1:J:229:MET:HB2	1:J:229:MET:HE2	1.77	0.42
1:F:74:VAL:HG21	1:F:169:ALA:HA	2.02	0.42
1:I:125:GLN:HG2	1:I:135:GLU:HG2	2.01	0.42
1:F:64:VAL:HG13	1:F:69:VAL:HG11	2.01	0.42
1:C:33:VAL:HG23	1:C:71:ILE:HG13	2.02	0.42
1:K:101:MET:HE1	1:K:159:GLY:HA2	2.02	0.42
1:H:32:ARG:HG3	1:H:70:GLN:HB2	2.02	0.42
1:H:42:PHE:CZ	1:H:75:ILE:HD12	2.55	0.42
1:B:42:PHE:HZ	1:B:75:ILE:HD12	1.85	0.42
1:J:86:LEU:HD22	1:J:91:MET:SD	2.60	0.42
1:E:218:ARG:HH21	1:E:218:ARG:HG2	1.85	0.41
1:G:95:ARG:NH2	1:H:113:ASP:OD1	2.51	0.41
1:I:62:ALA:HA	1:I:65:VAL:HG12	2.02	0.41
1:I:181:VAL:HG23	1:I:233:MET:HE2	2.01	0.41
1:K:87:GLN:O	1:K:87:GLN:HG2	2.19	0.41
1:K:255:ILE:HD12	1:K:255:ILE:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:SER:HA	1:B:260:THR:O	2.20	0.41
1:C:158:MET:CE	1:C:167:THR:HG22	2.51	0.41
1:C:212:VAL:HG13	1:C:217:LEU:HB2	2.02	0.41
3:J:301:UTP:H5'1	1:H:144:ARG:HG2	2.02	0.41
1:L:94:THR:HG22	1:L:162:TYR:CE1	2.55	0.41
1:H:59:ARG:HB2	1:H:118:GLU:OE2	2.20	0.41
1:E:79:ASN:OD1	1:E:79:ASN:N	2.52	0.41
1:L:124:VAL:O	1:L:134:ALA:HB1	2.20	0.41
1:G:132:GLN:NE2	1:H:159:GLY:O	2.53	0.41
1:F:122:THR:O	1:F:123:ARG:NH1	2.47	0.41
1:G:85:GLN:HE21	1:G:85:GLN:HB3	1.65	0.41
1:G:42:PHE:CZ	1:G:75:ILE:HD13	2.56	0.41
1:D:101:MET:HE3	1:D:159:GLY:HA2	2.03	0.41
1:B:83:GLY:HA3	1:B:97:ASP:OD1	2.20	0.41
1:B:127:ALA:H	1:B:156:ALA:HB3	1.85	0.41
1:A:74:VAL:HG22	1:A:154:PHE:HB2	2.03	0.41
1:F:208:SER:O	1:F:211:GLU:N	2.43	0.41
1:E:70:GLN:HB3	1:E:146:LEU:HB3	2.03	0.41
1:D:236:LEU:HD21	1:D:255:ILE:O	2.21	0.41
1:C:218:ARG:HH11	1:C:218:ARG:CG	2.34	0.41
1:K:144:ARG:O	1:K:148:LYS:HG3	2.21	0.41
2:H:301:UDP:O3'	2:H:301:UDP:PA	2.78	0.41
1:A:28:SER:HB2	1:A:252:GLY:CA	2.51	0.41
1:F:248:ARG:O	1:F:253:GLU:HG3	2.21	0.41
1:E:61:ILE:HB	1:E:115:LEU:HD21	2.03	0.41
1:K:101:MET:HG3	2:K:301:UDP:H1'	2.03	0.41
1:H:64:VAL:O	1:H:69:VAL:HG12	2.20	0.41
1:E:161:PRO:HD2	1:D:171:GLN:NE2	2.37	0.40
1:C:81:PHE:CD1	1:C:86:LEU:HD11	2.56	0.40
1:C:158:MET:HG3	1:C:168:THR:OG1	2.21	0.40
1:G:125:GLN:HA	1:G:135:GLU:O	2.21	0.40
2:D:302:UDP:O3'	2:D:302:UDP:PA	2.78	0.40
1:H:158:MET:HG2	1:H:168:THR:HG23	2.02	0.40
1:H:219:VAL:HG23	1:H:220:ALA:N	2.36	0.40
1:F:204:LEU:O	1:F:257:THR:HG23	2.21	0.40
1:D:61:ILE:HG23	1:D:71:ILE:HD13	2.02	0.40
1:I:235:ILE:O	1:I:259:VAL:HG22	2.21	0.40
1:I:239:ASN:HB3	1:I:242:THR:OG1	2.22	0.40
1:G:85:GLN:HA	1:G:89:LEU:CD1	2.45	0.40
1:E:123:ARG:HD3	1:E:145:HIS:NE2	2.35	0.40
1:D:61:ILE:O	1:D:64:VAL:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LYS:HD3	1:D:237:VAL:CG1	2.50	0.40
2:C:302:UDP:O2	2:C:302:UDP:C2'	2.69	0.40
1:L:181:VAL:O	1:L:236:LEU:N	2.52	0.40
1:B:69:VAL:CG2	1:B:250:VAL:HG11	2.43	0.40
1:F:101:MET:HE3	1:F:159:GLY:C	2.42	0.40
1:E:188:ASP:O	1:E:203:LEU:HD21	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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

All (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
1	H	131	GLY
1	F	131	GLY
1	E	131	GLY
1	I	254	LYS
1	K	28	SER
1	G	89	LEU
1	H	134	ALA
1	H	254	LYS
1	A	44	GLY
1	D	193	GLU
1	G	92	GLU
1	C	193	GLU
1	C	202	GLU
1	B	131	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	31	SER
1	B	34	LEU
1	B	63	ASP
1	B	92	GLU
1	B	218	ARG
1	B	221	ASP
1	A	63	ASP
1	A	93	ARG
1	A	171	GLN
1	A	215	ARG
1	A	242	THR
1	F	34	LEU
1	F	59	ARG
1	F	132	GLN
1	F	164	SER
1	F	236	LEU
1	F	245	ASN
1	E	210	ARG
1	E	218	ARG
1	E	221	ASP
1	E	245	ASN
1	D	28	SER
1	D	40	GLU
1	D	82	ARG
1	D	87	GLN
1	D	93	ARG
1	D	130	MET
1	D	221	ASP
1	C	34	LEU
1	C	194	ASP
1	C	218	ARG
1	C	221	ASP
1	I	52	ASP
1	I	165	THR

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Mol	Chain	Res	Type
1	I	188	ASP
1	I	203	LEU
1	I	205	THR
1	I	214	ASP
1	I	242	THR
1	J	49	LEU
1	J	117	LYS
1	J	141	ARG
1	J	165	THR
1	J	229	MET
1	K	28	SER
1	K	46	GLN
1	K	66	ARG
1	K	191	PHE
1	K	204	LEU
1	K	210	ARG
1	K	214	ASP
1	K	221	ASP
1	L	36	LYS
1	L	42	PHE
1	L	56	GLN
1	L	81	PHE
1	L	92	GLU
1	L	96	SER
1	L	144	ARG
1	L	162	TYR
1	L	172	ARG
1	L	182	LEU
1	L	233	MET
1	G	36	LYS
1	G	37	LEU
1	G	59	ARG
1	G	85	GLN
1	G	86	LEU
1	G	92	GLU
1	G	141	ARG
1	G	240	LEU
1	H	46	GLN
1	H	47	VAL
1	H	59	ARG
1	H	60	GLN
1	H	92	GLU

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Mol	Chain	Res	Type
1	H	93	ARG
1	H	117	LYS
1	H	123	ARG
1	H	132	GLN
1	H	203	LEU
1	H	213	LEU
1	H	214	ASP
1	H	215	ARG
1	H	233	MET
1	H	242	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	F	125	GLN
1	E	209	HIS
1	D	87	GLN
1	D	88	GLN
1	I	88	GLN
1	J	245	ASN
1	K	85	GLN
1	G	85	GLN
1	H	46	GLN
1	H	56	GLN

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 (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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
3	J	301	UTP	C2-N1	7.01	1.45	1.35
3	A	301	UTP	C2-N1	6.89	1.45	1.35
3	C	301	UTP	C6-C5	-6.87	1.34	1.52
3	D	301	UTP	C6-C5	-6.73	1.34	1.52
3	G	301	UTP	C6-C5	-6.65	1.34	1.52
3	L	301	UTP	C6-C5	-6.56	1.35	1.52
3	J	301	UTP	C6-C5	-6.48	1.35	1.52
3	D	301	UTP	C2-N1	6.48	1.44	1.35
3	A	301	UTP	C6-C5	-6.16	1.36	1.52
3	F	301	UTP	C6-C5	-6.09	1.36	1.52
3	I	301	UTP	C6-C5	-6.06	1.36	1.52
2	J	302	UDP	PB-O1B	-5.81	1.31	1.50
2	B	301	UDP	PB-O1B	-5.16	1.33	1.50
2	I	302	UDP	PB-O1B	-5.10	1.34	1.50
2	D	302	UDP	PA-O5'	-5.00	1.39	1.59
2	C	302	UDP	PB-O1B	-4.60	1.35	1.50
2	I	302	UDP	PA-O5'	-4.43	1.41	1.59
2	D	302	UDP	PB-O1B	-4.42	1.36	1.50
2	C	302	UDP	PB-O3B	-4.17	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	302	UDP	PA-O5'	-4.15	1.42	1.59
2	H	301	UDP	PB-O1B	-4.11	1.37	1.50
2	D	302	UDP	PA-O2A	-4.01	1.36	1.55
2	K	301	UDP	PB-O1B	-3.81	1.38	1.50
2	E	301	UDP	PA-O5'	-3.79	1.44	1.59
2	K	301	UDP	PA-O5'	-3.75	1.44	1.59
2	J	302	UDP	PB-O2B	-3.66	1.40	1.54
2	E	301	UDP	PB-O1B	-3.59	1.38	1.50
2	J	302	UDP	PB-O3B	-3.57	1.41	1.54
2	J	302	UDP	PA-O5'	-3.53	1.45	1.59
2	H	301	UDP	PB-O3B	-3.47	1.41	1.54
2	I	302	UDP	PB-O2B	-3.40	1.41	1.54
2	C	302	UDP	PA-O2A	-3.39	1.39	1.55
2	D	302	UDP	PB-O3B	-3.36	1.41	1.54
2	C	302	UDP	PB-O2B	-3.36	1.41	1.54
2	D	302	UDP	PA-O1A	-3.33	1.39	1.50
2	D	302	UDP	PB-O2B	-3.20	1.42	1.54
2	K	301	UDP	PB-O3B	-3.16	1.42	1.54
2	B	301	UDP	PA-O5'	-3.16	1.46	1.59
2	I	302	UDP	PB-O3B	-3.16	1.42	1.54
2	B	301	UDP	PB-O2B	-3.15	1.42	1.54
2	C	302	UDP	PA-O1A	-3.12	1.39	1.50
2	B	301	UDP	PB-O3B	-3.11	1.42	1.54
3	J	301	UTP	C2-N3	3.07	1.43	1.38
2	H	301	UDP	PA-O5'	-3.07	1.46	1.59
3	J	301	UTP	C4-N3	3.06	1.42	1.37
3	C	301	UTP	C2-N3	3.04	1.43	1.38
2	E	301	UDP	PA-O2A	-3.04	1.41	1.55
2	B	301	UDP	PA-O1A	-3.04	1.40	1.50
2	E	301	UDP	PB-O3B	-3.03	1.43	1.54
2	J	302	UDP	PA-O2A	-2.99	1.41	1.55
3	I	301	UTP	C2-N3	2.94	1.43	1.38
3	C	301	UTP	C4-N3	2.86	1.42	1.37
2	J	302	UDP	PA-O1A	-2.85	1.40	1.50
3	A	301	UTP	O2-C2	-2.75	1.18	1.23
3	L	301	UTP	C2-N3	2.70	1.42	1.38
2	H	301	UDP	PB-O2B	-2.68	1.44	1.54
2	K	301	UDP	PB-O2B	-2.68	1.44	1.54
3	F	301	UTP	C4-N3	2.63	1.42	1.37
2	I	302	UDP	PA-O1A	-2.62	1.41	1.50
2	K	301	UDP	PA-O1A	-2.62	1.41	1.50
3	I	301	UTP	C4-N3	2.54	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	301	UTP	C1'-N1	-2.54	1.42	1.46
2	E	301	UDP	PB-O2B	-2.53	1.45	1.54
3	F	301	UTP	C2-N3	2.50	1.42	1.38
2	E	301	UDP	PA-O1A	-2.50	1.42	1.50
3	D	301	UTP	O4-C4	-2.50	1.18	1.23
2	K	301	UDP	PA-O2A	-2.47	1.43	1.55
3	G	301	UTP	O4-C4	-2.43	1.18	1.23
2	B	301	UDP	PA-O2A	-2.43	1.43	1.55
2	I	302	UDP	PA-O2A	-2.42	1.43	1.55
3	L	301	UTP	C4-N3	2.39	1.41	1.37
2	H	301	UDP	PA-O1A	-2.37	1.42	1.50
3	A	301	UTP	C4-N3	2.29	1.41	1.37
2	H	301	UDP	PA-O2A	-2.27	1.44	1.55
3	L	301	UTP	O4-C4	-2.27	1.18	1.23
3	D	301	UTP	C2-N3	2.26	1.42	1.38
3	D	301	UTP	O4'-C1'	2.20	1.47	1.42
3	J	301	UTP	PG-O1G	-2.18	1.46	1.54
3	F	301	UTP	PG-O1G	-2.18	1.46	1.54
3	I	301	UTP	PG-O3G	-2.18	1.46	1.54
3	D	301	UTP	PG-O3G	-2.05	1.46	1.54
2	H	301	UDP	C4-N3	2.04	1.36	1.33
3	F	301	UTP	PA-O5'	2.04	1.67	1.59
3	L	301	UTP	O4'-C1'	2.01	1.46	1.42
3	D	301	UTP	C1'-N1	-2.01	1.43	1.46

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
3	F	301	UTP	C4-N3-C2	-4.95	121.69	125.79
3	A	301	UTP	N3-C2-N1	4.86	121.79	116.65
3	D	301	UTP	C4-N3-C2	-4.78	121.83	125.79
3	C	301	UTP	C4-N3-C2	-4.75	121.85	125.79
2	B	301	UDP	PA-O3A-PB	-4.72	116.65	132.83
3	G	301	UTP	O4'-C1'-N1	-4.31	103.43	109.30
3	G	301	UTP	O1G-PG-O3B	4.04	118.17	104.64
3	D	301	UTP	PB-O3B-PG	-4.03	118.99	132.83
2	C	302	UDP	C5-C4-N3	-3.94	114.64	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	302	UDP	C5-C4-N3	-3.92	114.68	123.31
2	I	302	UDP	C5-C4-N3	-3.91	114.71	123.31
2	D	302	UDP	C5-C4-N3	-3.89	114.76	123.31
3	I	301	UTP	N3-C2-N1	3.87	120.75	116.65
2	H	301	UDP	C5-C4-N3	-3.87	114.79	123.31
2	K	301	UDP	C5-C4-N3	-3.84	114.85	123.31
2	E	301	UDP	C5-C4-N3	-3.82	114.91	123.31
2	D	302	UDP	PA-O3A-PB	3.82	145.92	132.83
2	B	301	UDP	C5-C4-N3	-3.78	114.99	123.31
3	C	301	UTP	PB-O3A-PA	-3.67	120.22	132.83
3	L	301	UTP	N3-C2-N1	3.64	120.50	116.65
3	F	301	UTP	PB-O3B-PG	-3.38	121.22	132.83
3	I	301	UTP	PB-O3A-PA	-3.37	121.28	132.83
3	D	301	UTP	PB-O3A-PA	-3.34	121.37	132.83
3	J	301	UTP	PB-O3A-PA	-3.07	122.30	132.83
3	J	301	UTP	O2-C2-N1	-3.02	119.31	123.11
3	C	301	UTP	C5-C6-N1	3.02	121.57	111.61
3	C	301	UTP	PB-O3B-PG	-2.95	122.70	132.83
3	I	301	UTP	O1G-PG-O3B	2.94	114.51	104.64
3	G	301	UTP	C5-C4-N3	2.94	119.95	116.65
3	J	301	UTP	N3-C2-N1	2.93	119.75	116.65
3	J	301	UTP	PB-O3B-PG	-2.92	122.80	132.83
3	A	301	UTP	O3G-PG-O3B	2.90	114.35	104.64
3	F	301	UTP	C5-C6-N1	2.84	120.97	111.61
3	J	301	UTP	O3G-PG-O3B	2.79	114.00	104.64
3	L	301	UTP	C5-C4-N3	2.77	119.76	116.65
3	F	301	UTP	N3-C2-N1	2.73	119.54	116.65
3	D	301	UTP	C5-C6-N1	2.73	120.60	111.61
3	A	301	UTP	C5-C6-N1	2.68	120.45	111.61
3	L	301	UTP	O3G-PG-O3B	2.67	113.59	104.64
3	I	301	UTP	PB-O3B-PG	-2.63	123.80	132.83
3	J	301	UTP	O4'-C1'-C2'	-2.63	100.92	106.64
3	C	301	UTP	O3G-PG-O3B	2.58	113.28	104.64
3	L	301	UTP	C5-C6-N1	2.57	120.07	111.61
3	L	301	UTP	O2-C2-N1	-2.56	119.90	123.11
3	I	301	UTP	C5-C6-N1	2.55	120.02	111.61
3	J	301	UTP	C5-C6-N1	2.54	120.00	111.61
3	G	301	UTP	C5-C6-N1	2.46	119.73	111.61
3	F	301	UTP	O3G-PG-O3B	2.45	112.86	104.64
3	L	301	UTP	PB-O3B-PG	-2.43	124.48	132.83
3	A	301	UTP	O2A-PA-O1A	-2.42	100.30	112.24
3	D	301	UTP	C2'-C3'-C4'	2.41	107.33	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	301	UTP	C2'-C3'-C4'	2.40	107.30	102.64
3	L	301	UTP	O4'-C1'-N1	2.40	112.56	109.30
3	G	301	UTP	N3-C2-N1	2.40	119.19	116.65
3	L	301	UTP	PB-O3A-PA	-2.39	124.62	132.83
3	L	301	UTP	O1G-PG-O3B	2.32	112.41	104.64
3	A	301	UTP	O2-C2-N1	-2.31	120.20	123.11
2	E	301	UDP	O2'-C2'-C3'	-2.31	104.36	111.82
3	C	301	UTP	N3-C2-N1	2.31	119.09	116.65
3	C	301	UTP	O4-C4-N3	2.28	123.90	120.28
3	G	301	UTP	O3G-PG-O3B	2.28	112.28	104.64
3	D	301	UTP	O3G-PG-O3B	2.26	112.22	104.64
3	D	301	UTP	N3-C2-N1	2.24	119.02	116.65
2	K	301	UDP	O2'-C2'-C3'	-2.23	104.62	111.82
3	D	301	UTP	O4'-C1'-N1	2.22	112.33	109.30
3	F	301	UTP	C5-C4-N3	2.22	119.14	116.65
3	F	301	UTP	O1B-PB-O2B	-2.22	101.28	112.24
3	D	301	UTP	O1G-PG-O3B	2.18	111.95	104.64
3	J	301	UTP	O1G-PG-O3B	2.18	111.94	104.64
2	C	302	UDP	C3'-C2'-C1'	2.16	104.23	100.98
3	F	301	UTP	O1G-PG-O3B	2.16	111.88	104.64
3	A	301	UTP	C3'-C2'-C1'	2.12	105.45	101.43
2	I	302	UDP	O2'-C2'-C3'	-2.09	105.06	111.82
3	J	301	UTP	O1G-PG-O2G	-2.05	102.66	110.68
3	C	301	UTP	C2'-C3'-C4'	2.03	106.58	102.64
3	L	301	UTP	O2A-PA-O1A	-2.02	102.27	112.24
3	J	301	UTP	O4'-C1'-N1	2.01	112.03	109.30

There are no chirality outliers.

All (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
2	I	302	UDP	C5'-O5'-PA-O2A
2	J	302	UDP	C2'-C1'-N1-C6
2	K	301	UDP	C2'-C1'-N1-C6
2	H	301	UDP	C5'-O5'-PA-O1A
2	H	301	UDP	PA-O3A-PB-O2B
3	A	301	UTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	301	UTP	C5'-O5'-PA-O2A
3	A	301	UTP	C5'-O5'-PA-O3A
3	A	301	UTP	O4'-C4'-C5'-O5'
3	F	301	UTP	C5'-O5'-PA-O1A
3	F	301	UTP	C5'-O5'-PA-O2A
3	F	301	UTP	C5'-O5'-PA-O3A
3	F	301	UTP	PB-O3B-PG-O1G
3	F	301	UTP	PB-O3B-PG-O3G
3	F	301	UTP	O4'-C4'-C5'-O5'
3	C	301	UTP	PB-O3B-PG-O1G
3	I	301	UTP	PB-O3A-PA-O5'
3	J	301	UTP	PB-O3A-PA-O5'
3	L	301	UTP	C5'-O5'-PA-O2A
3	L	301	UTP	C5'-O5'-PA-O3A
3	L	301	UTP	O4'-C1'-N1-C6
3	G	301	UTP	C5'-O5'-PA-O1A
3	G	301	UTP	C5'-O5'-PA-O3A
3	G	301	UTP	O4'-C4'-C5'-O5'
3	G	301	UTP	C3'-C4'-C5'-O5'
2	C	302	UDP	C3'-C4'-C5'-O5'
2	K	301	UDP	O4'-C4'-C5'-O5'
3	A	301	UTP	C3'-C4'-C5'-O5'
3	F	301	UTP	C3'-C4'-C5'-O5'
2	K	301	UDP	C3'-C4'-C5'-O5'
3	L	301	UTP	C2'-C1'-N1-C6
2	E	301	UDP	O4'-C4'-C5'-O5'
3	D	301	UTP	O4'-C4'-C5'-O5'
3	D	301	UTP	C3'-C4'-C5'-O5'
2	D	302	UDP	C4'-C5'-O5'-PA
2	D	302	UDP	PB-O3A-PA-O5'
3	D	301	UTP	PB-O3A-PA-O5'
3	C	301	UTP	PB-O3A-PA-O5'
3	L	301	UTP	C2'-C1'-N1-C2
2	I	302	UDP	O4'-C4'-C5'-O5'
2	I	302	UDP	C5'-O5'-PA-O3A
3	D	301	UTP	C5'-O5'-PA-O3A
2	D	302	UDP	O4'-C4'-C5'-O5'
2	H	301	UDP	C4'-C5'-O5'-PA
2	E	301	UDP	C5'-O5'-PA-O1A
2	D	302	UDP	C5'-O5'-PA-O1A
3	D	301	UTP	C5'-O5'-PA-O2A
3	L	301	UTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	G	301	UTP	C5'-O5'-PA-O2A
2	H	301	UDP	PA-O3A-PB-O1B
3	L	301	UTP	O4'-C1'-N1-C2
2	H	301	UDP	PB-O3A-PA-O2A
3	F	301	UTP	PA-O3A-PB-O1B
3	J	301	UTP	PA-O3A-PB-O2B
3	L	301	UTP	PA-O3A-PB-O1B
3	A	301	UTP	C2'-C1'-N1-C6
2	J	302	UDP	C3'-C4'-C5'-O5'
3	I	301	UTP	C2'-C1'-N1-C6
2	D	302	UDP	C5'-O5'-PA-O3A
2	H	301	UDP	C5'-O5'-PA-O3A
2	I	302	UDP	C4'-C5'-O5'-PA
3	F	301	UTP	PA-O3A-PB-O2B
3	C	301	UTP	PA-O3A-PB-O2B
3	J	301	UTP	PA-O3A-PB-O1B
3	G	301	UTP	PB-O3A-PA-O2A
3	J	301	UTP	C5'-O5'-PA-O1A
2	H	301	UDP	O4'-C4'-C5'-O5'
3	L	301	UTP	O4'-C4'-C5'-O5'
3	F	301	UTP	PB-O3B-PG-O2G
3	C	301	UTP	PB-O3B-PG-O2G

There are no ring outliers.

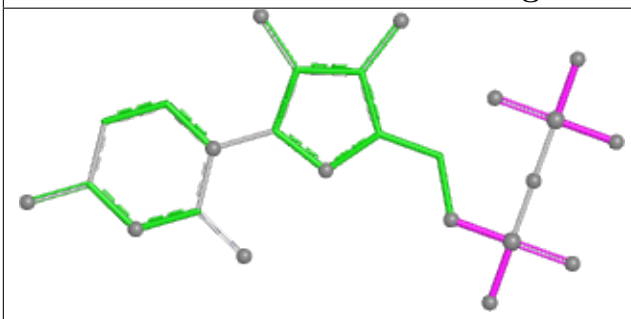
13 monomers are involved in 50 short contacts:

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

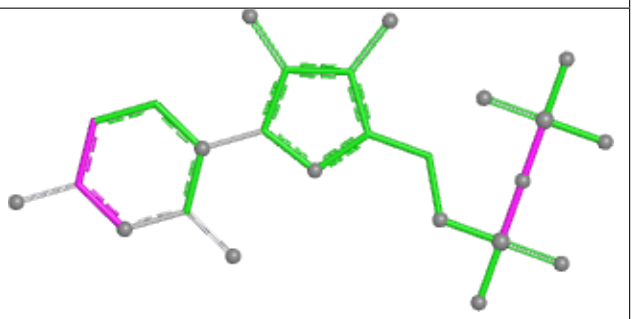
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 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.

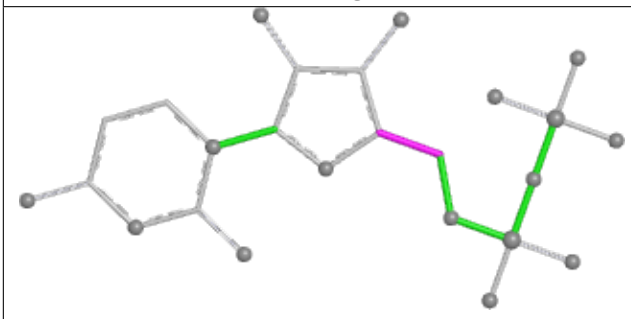
Ligand UDP B 301



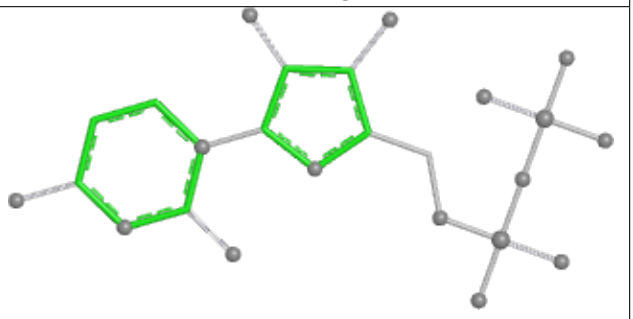
Bond lengths



Bond angles



Torsions



Rings

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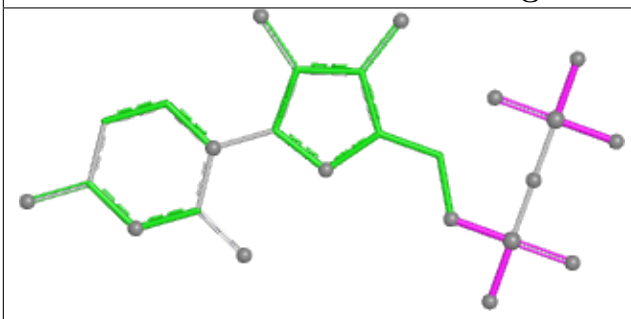
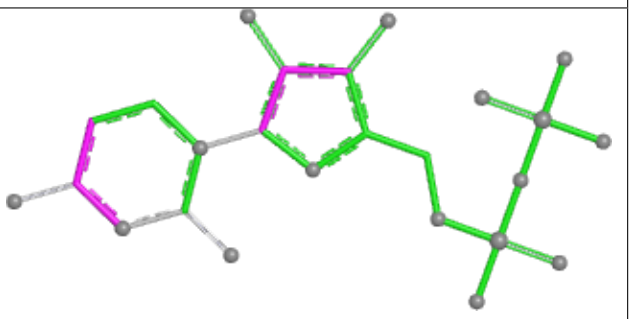
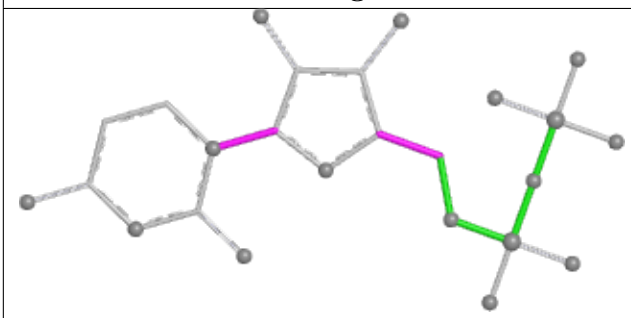
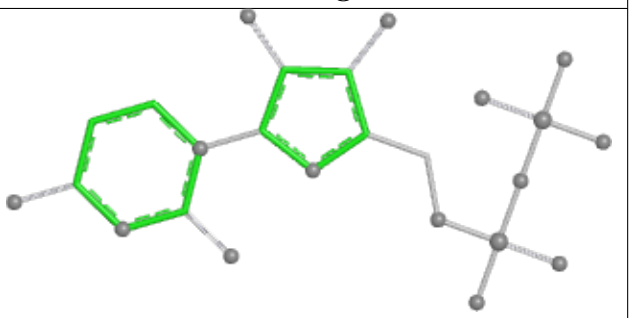
 Bond lengths	 Bond angles
 Torsions	 Rings

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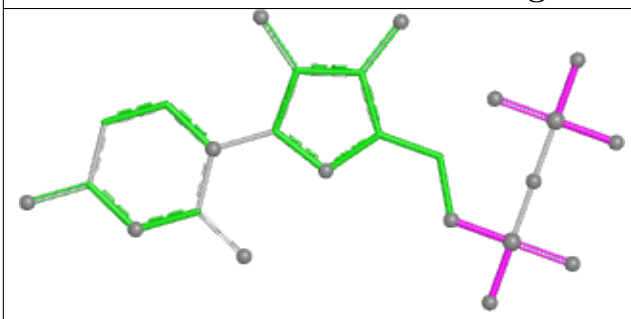
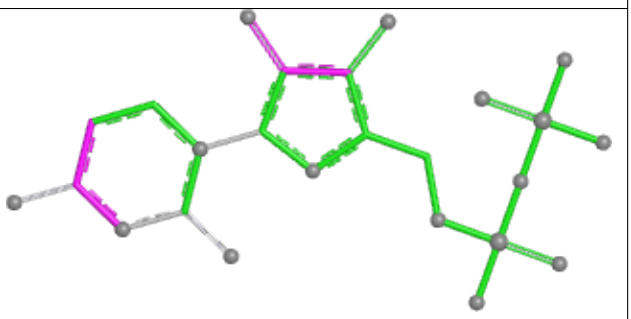
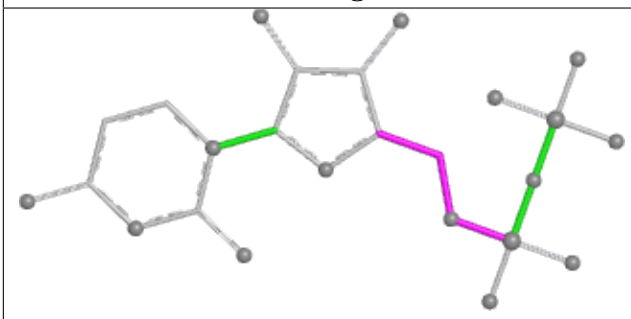
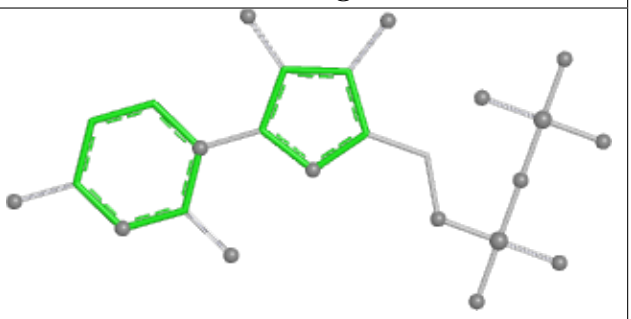
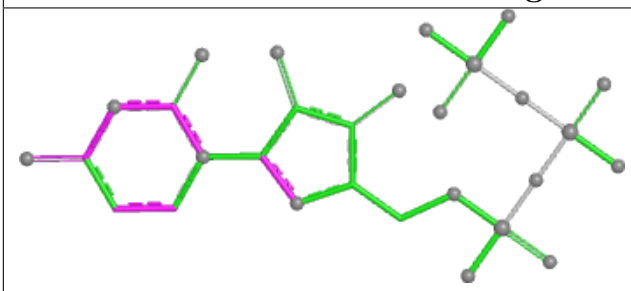
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UTP L 301



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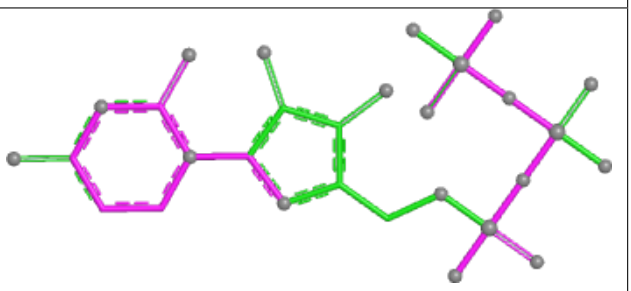

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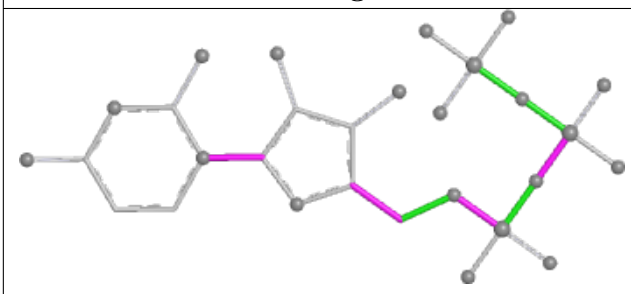

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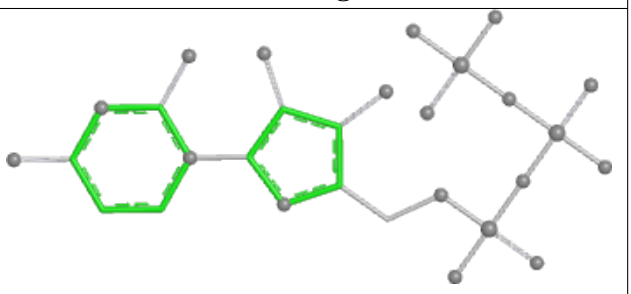
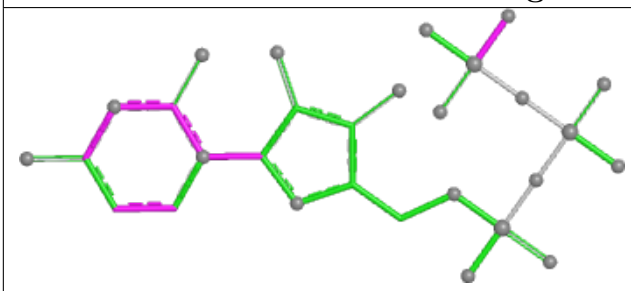


Rings

Ligand UTP J 301



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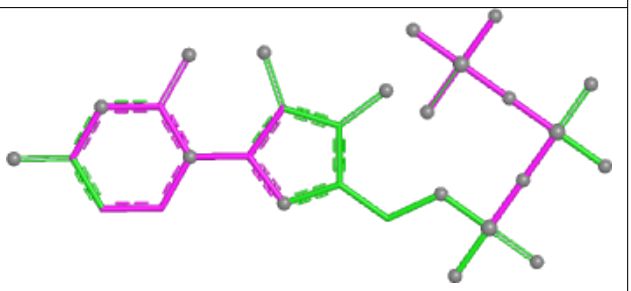

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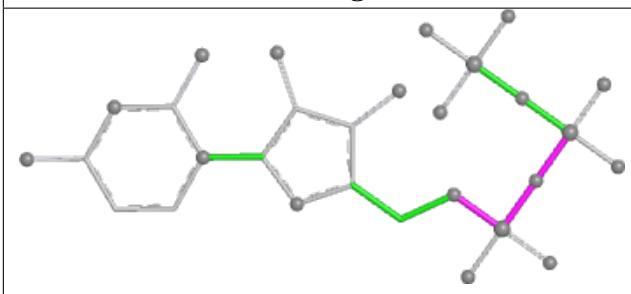

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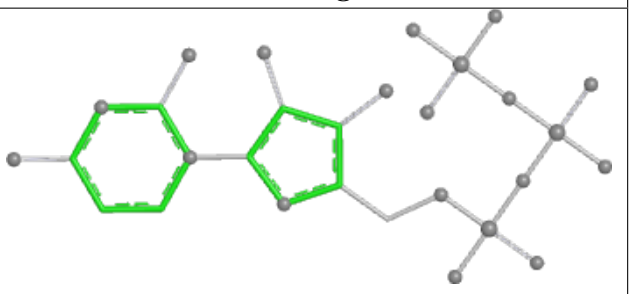

Rings

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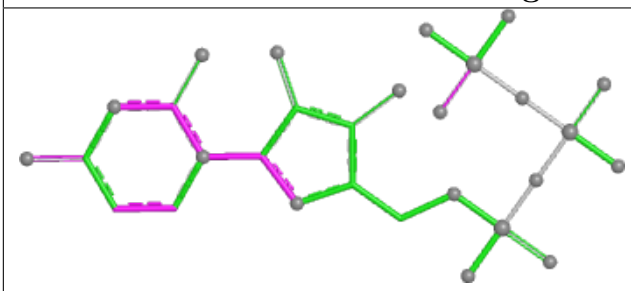
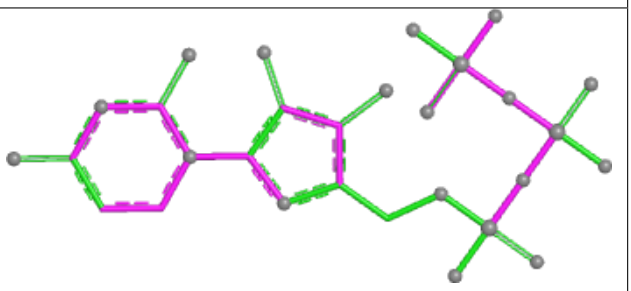
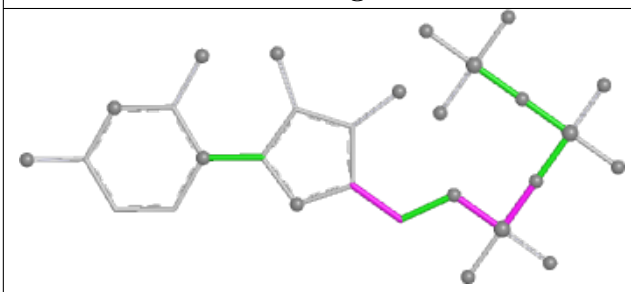
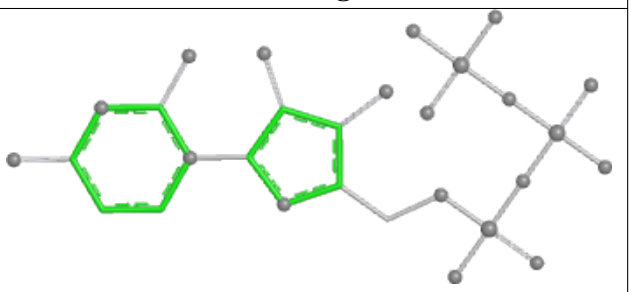
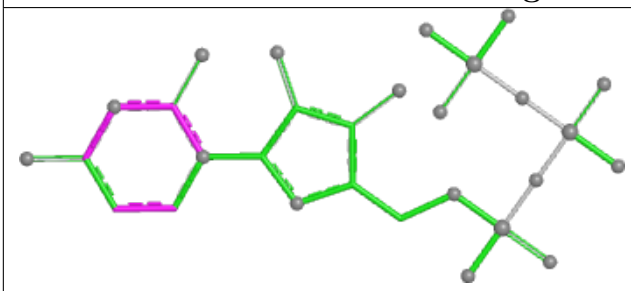
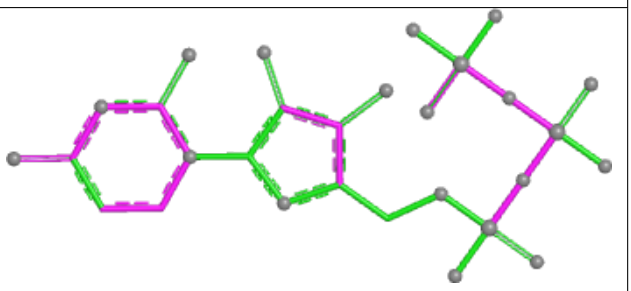
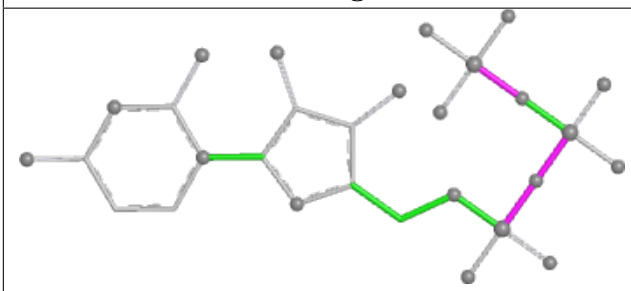
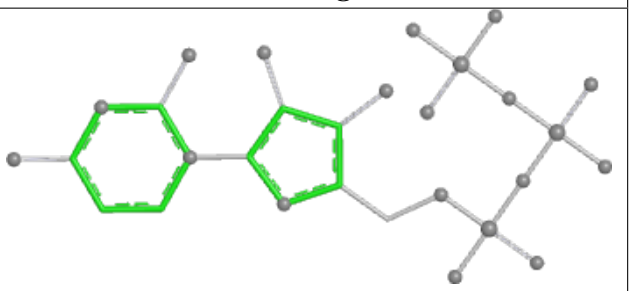
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UTP C 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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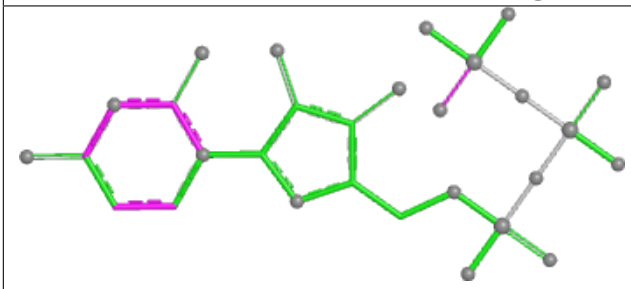
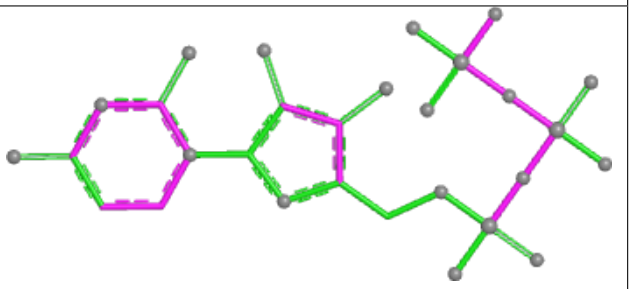
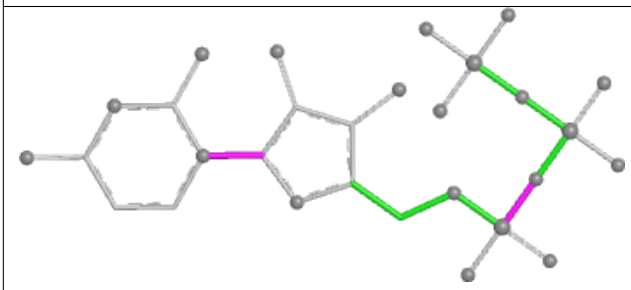
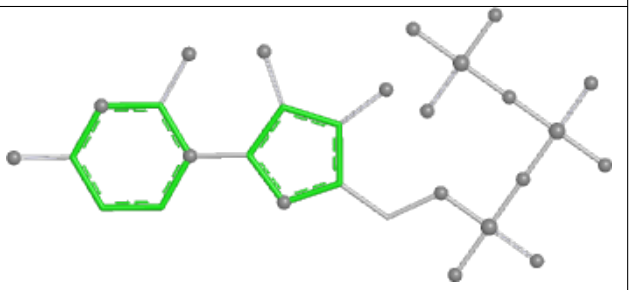
 Bond lengths	 Bond angles
 Torsions	 Rings

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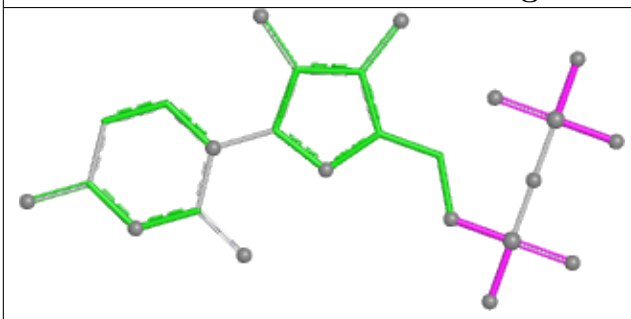
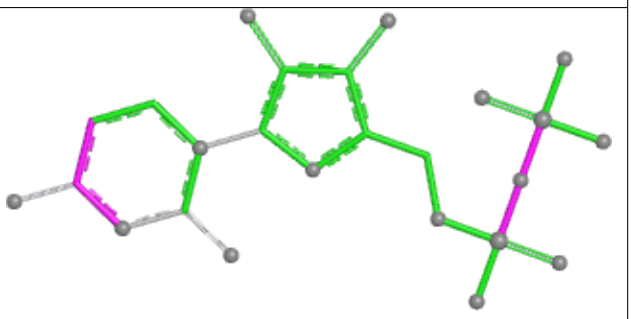
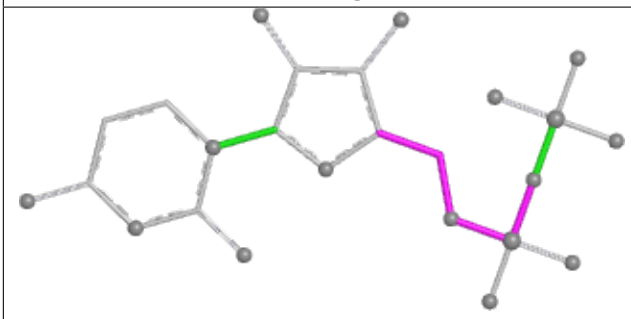
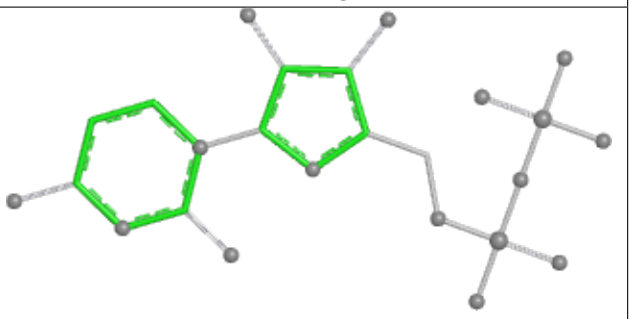
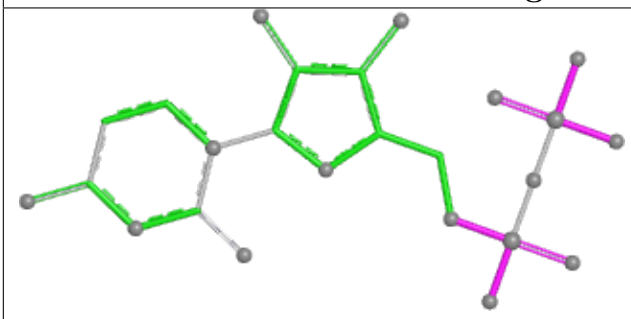
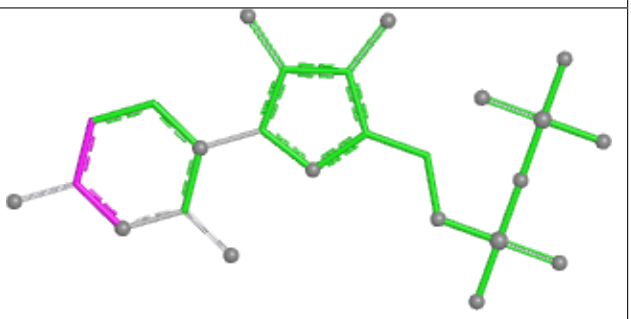
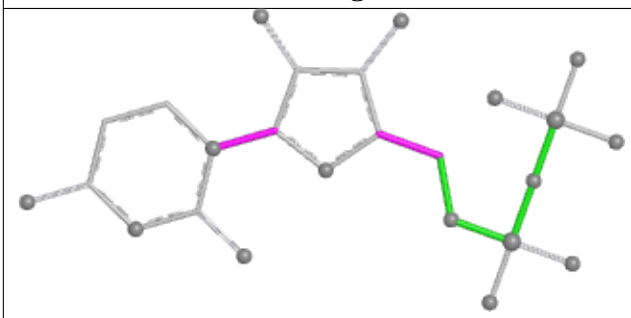
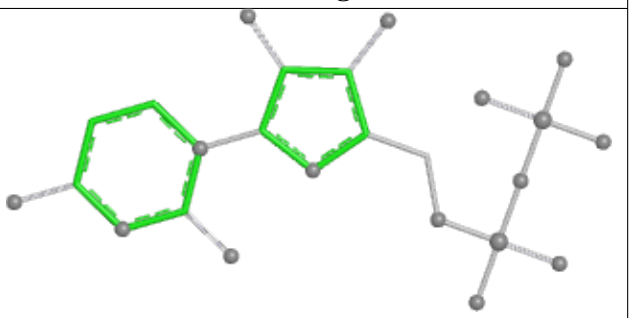
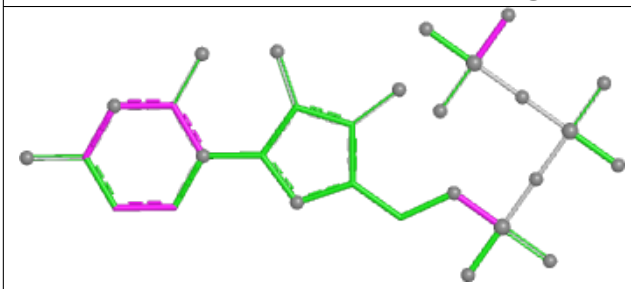
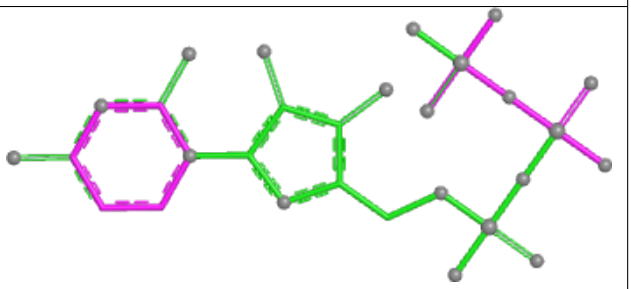
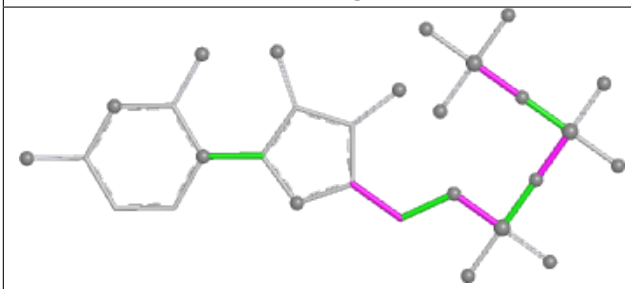
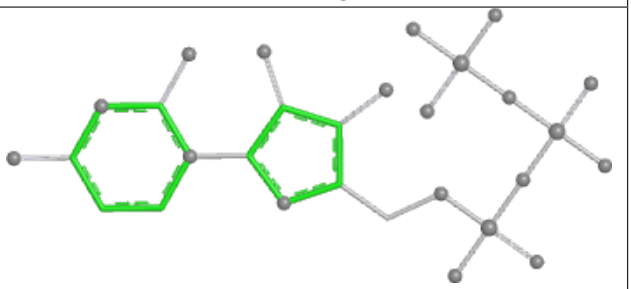
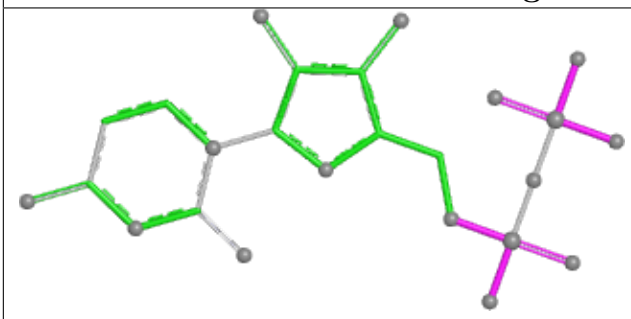
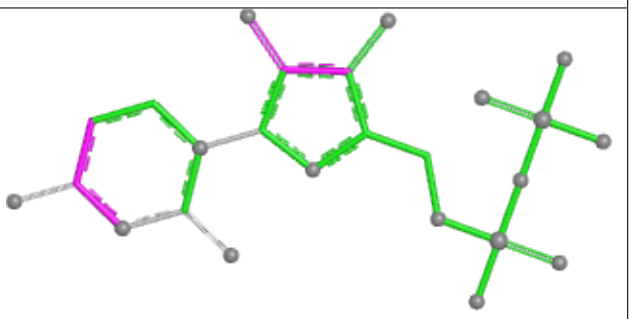
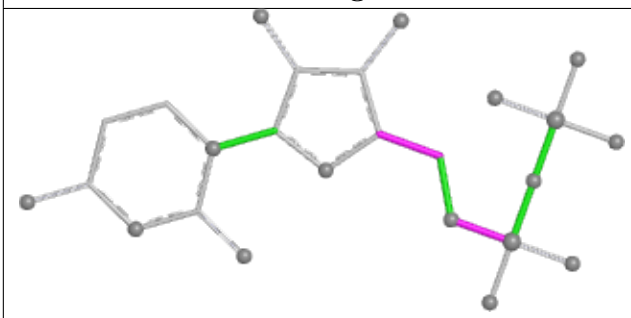
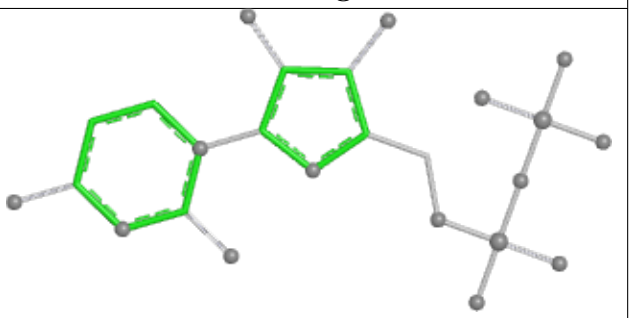
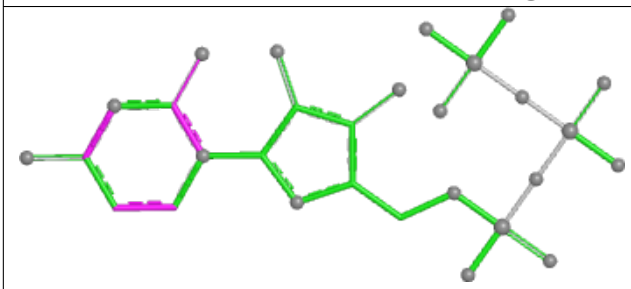
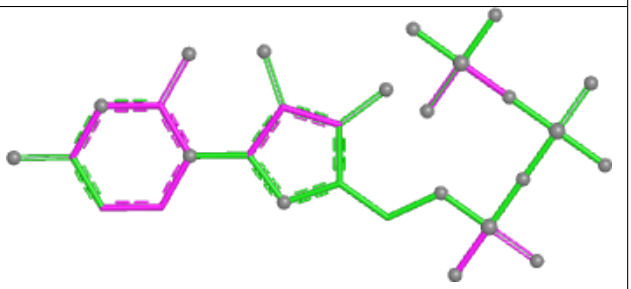
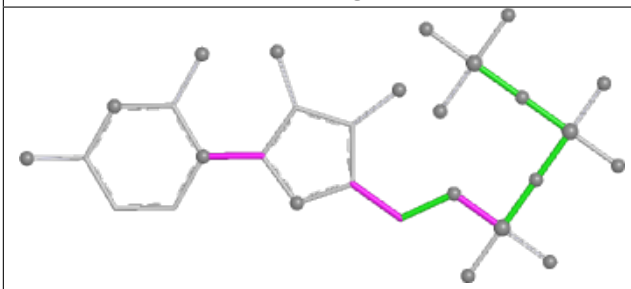
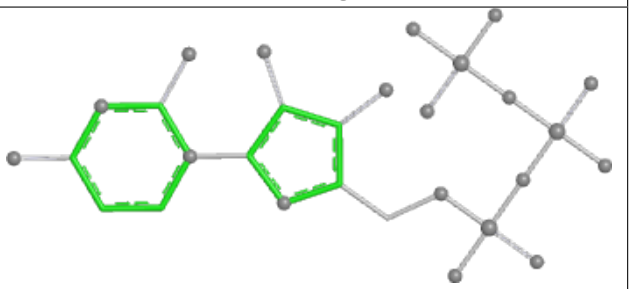
 Bond lengths	 Bond angles
 Torsions	 Rings

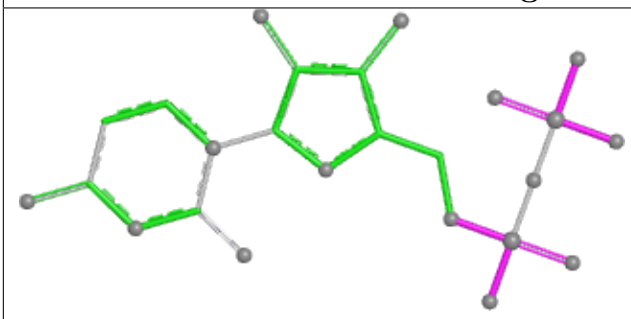
Ligand UDP J 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UTP F 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

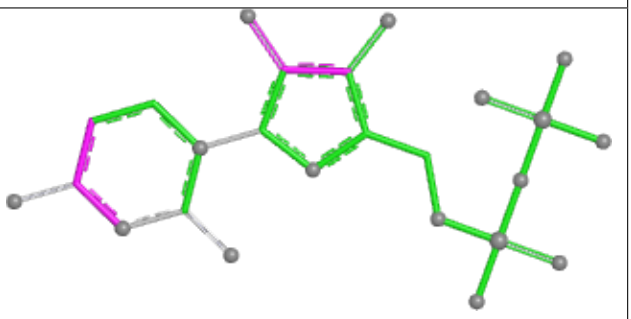
Ligand UDP E 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UTP A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

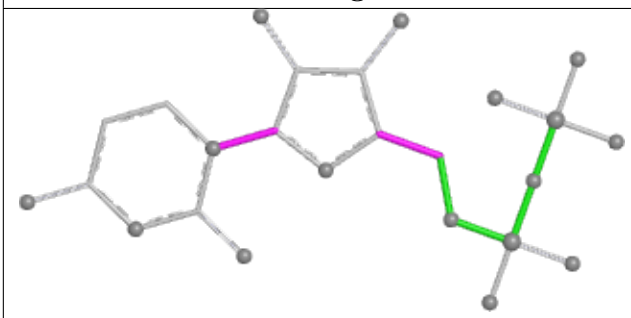
Ligand UDP K 301



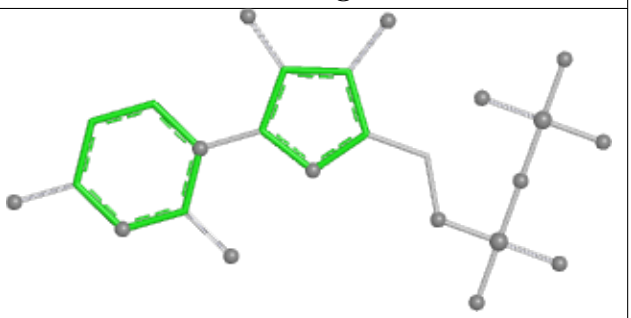
Bond lengths



Bond angles

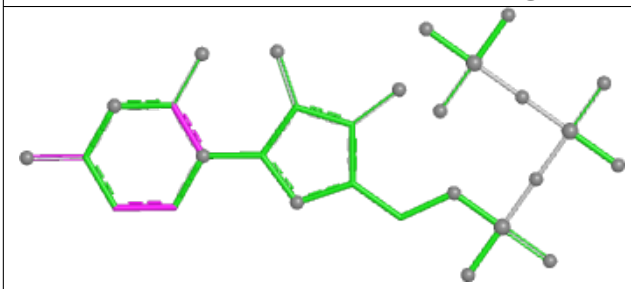


Torsions

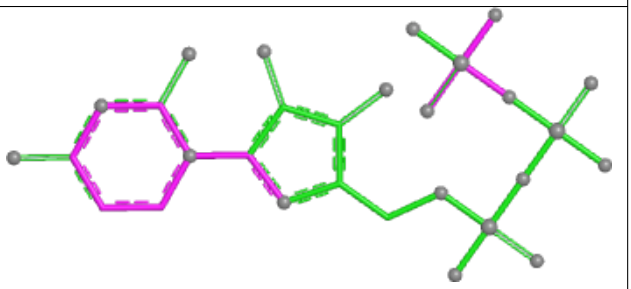


Rings

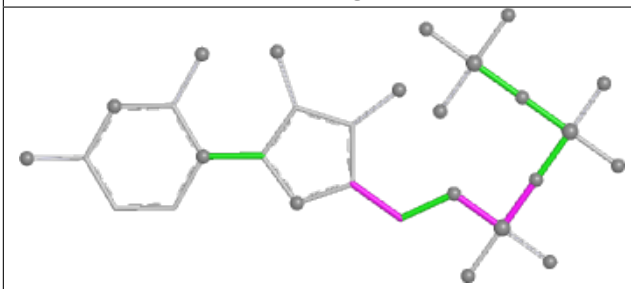
Ligand UTP G 301



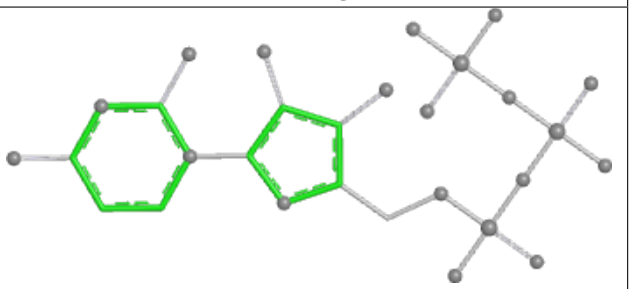
Bond lengths



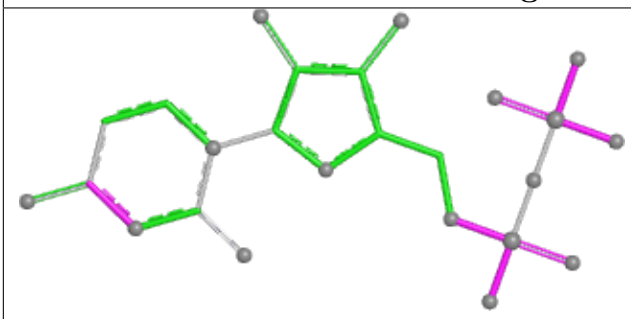
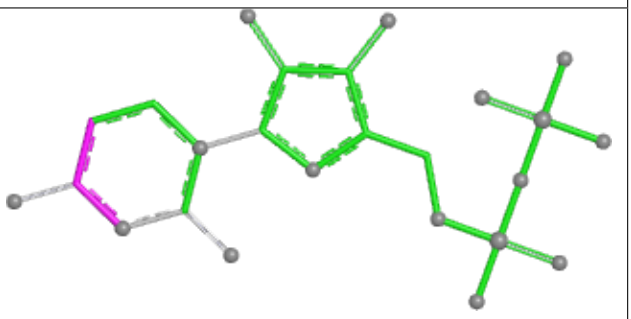
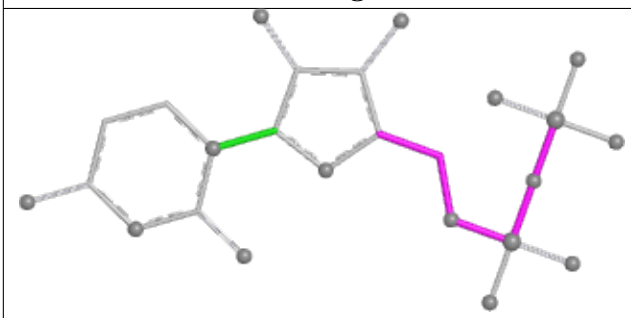
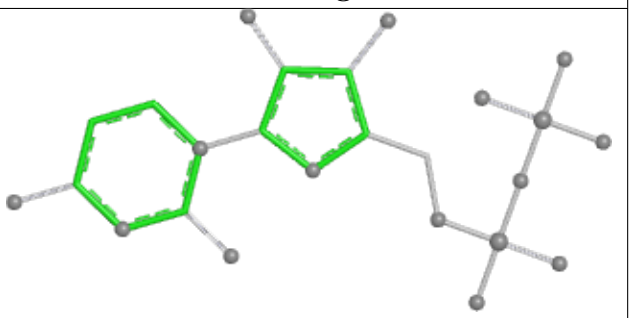
Bond angles



Torsions



Rings

Ligand UDP H 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.

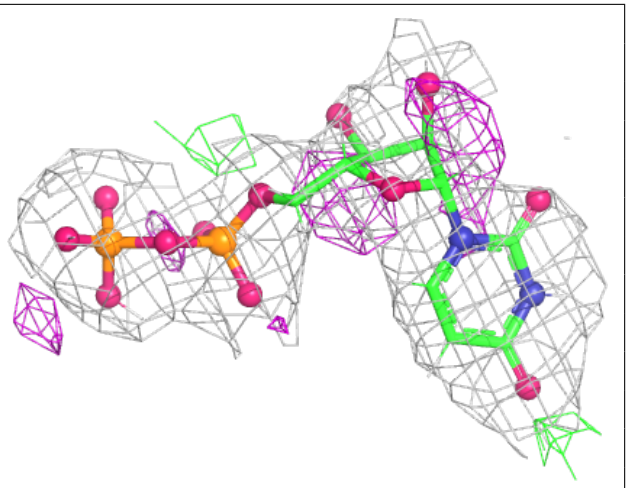
6.4 Ligands

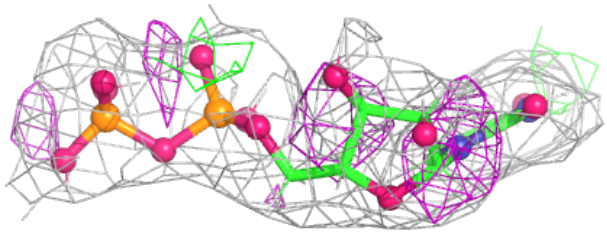
Unable to reproduce the depositors R factor - this section is therefore empty.

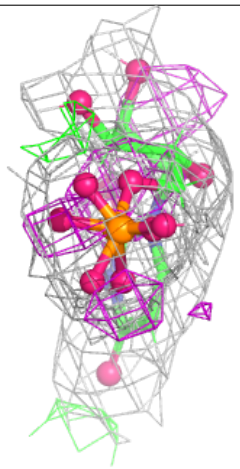
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

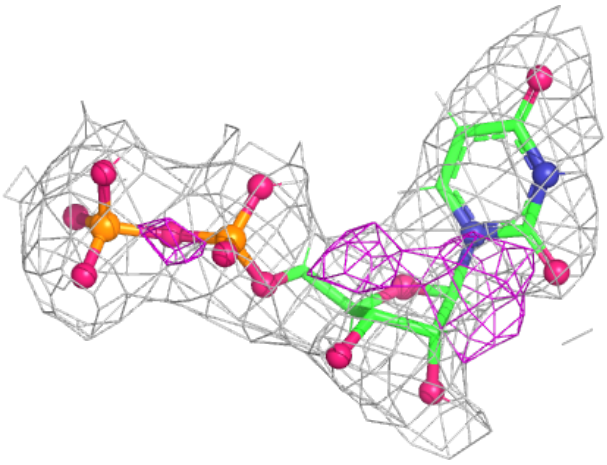


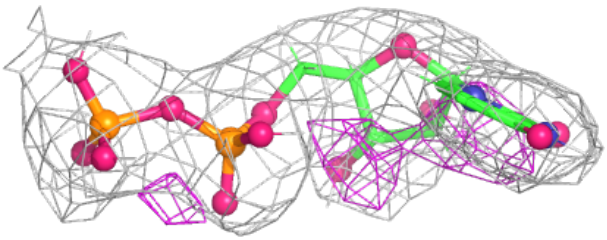


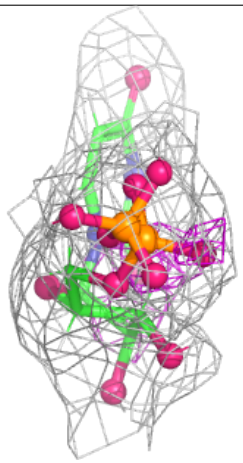


Electron density around UDP E 301:

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

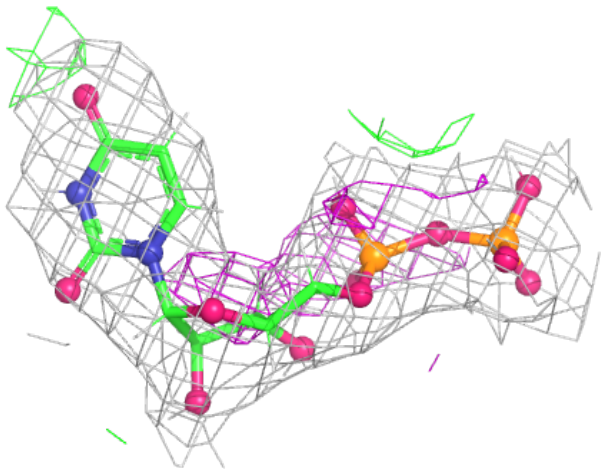


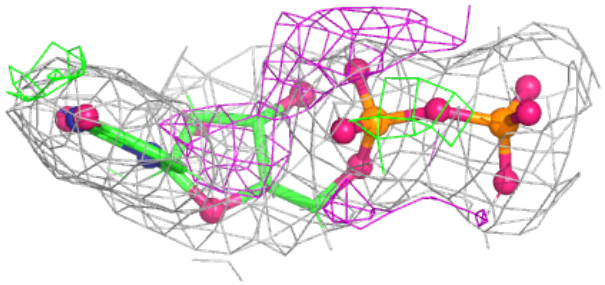


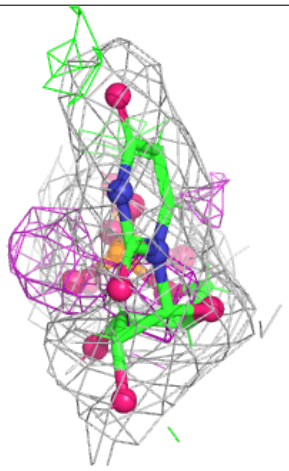


Electron density around UDP D 302:

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

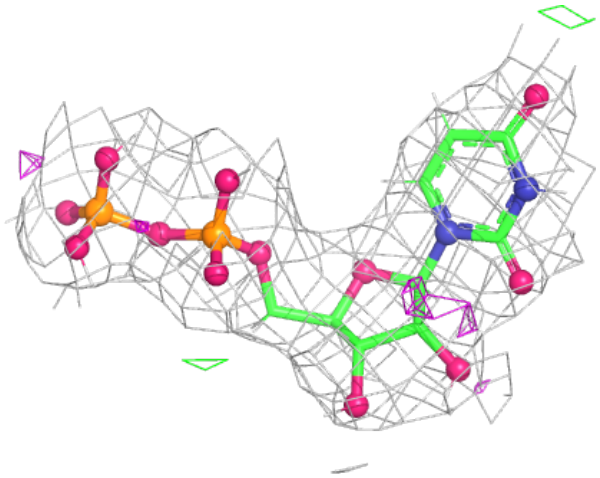


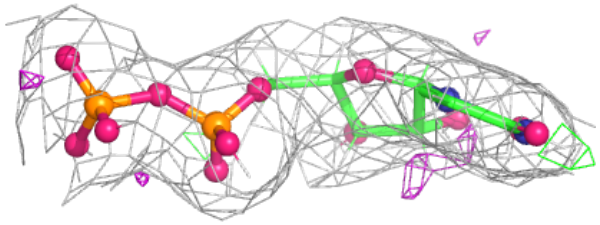


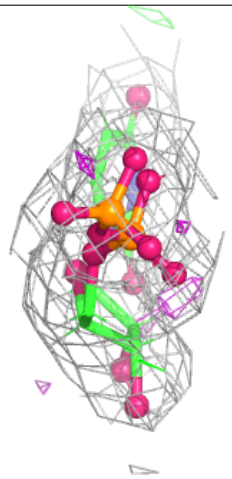


Electron density around UDP C 302:

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

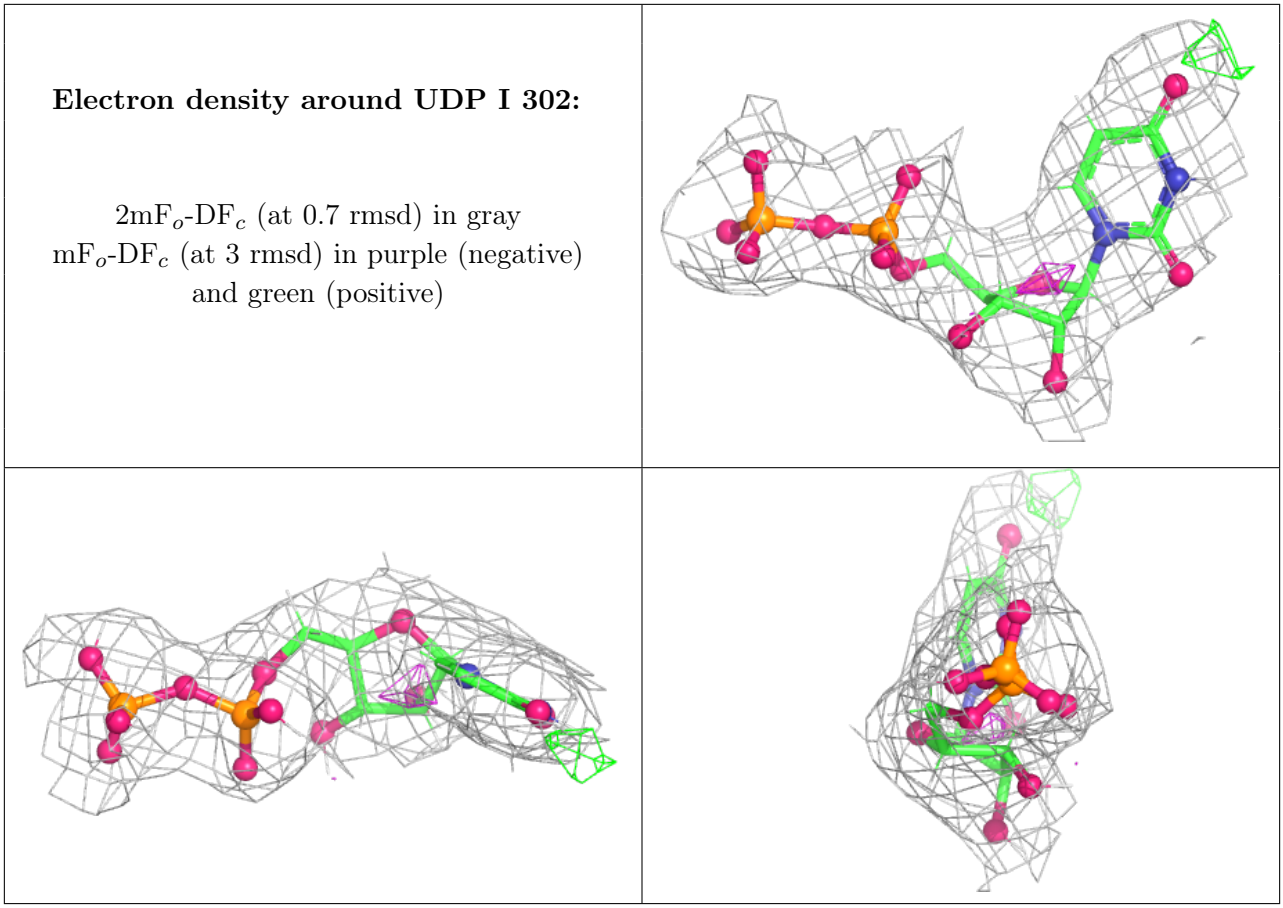






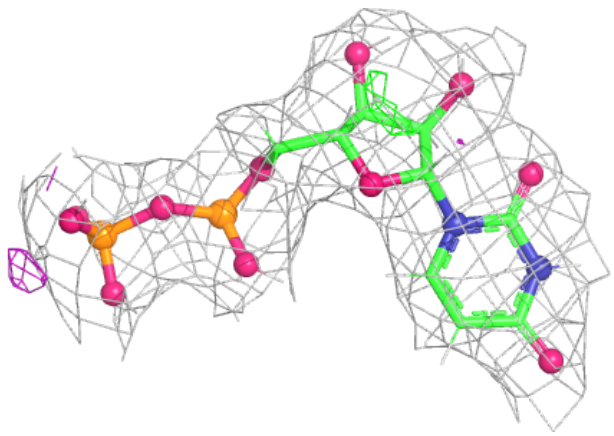
Electron density around UDP I 302:

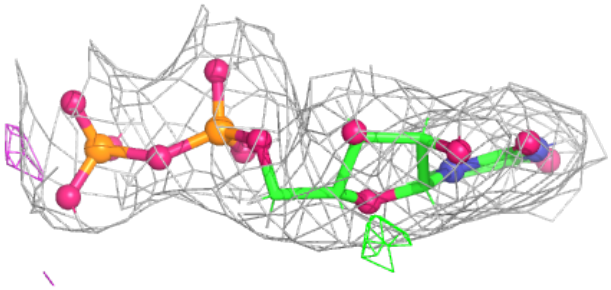
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

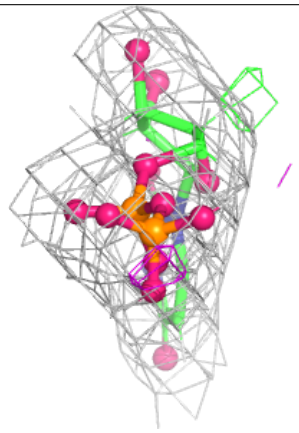


Electron density around UDP J 302:

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

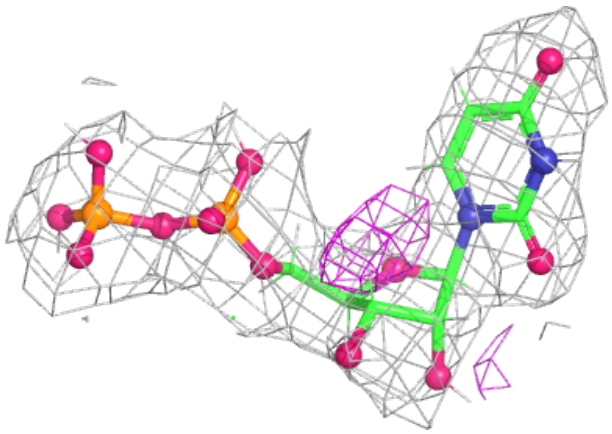


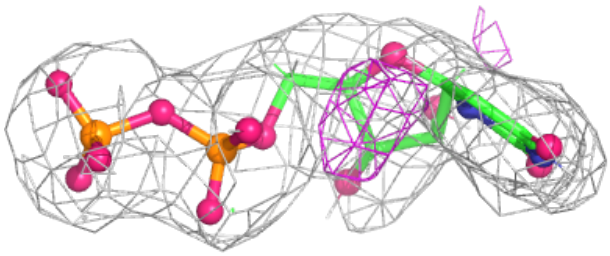


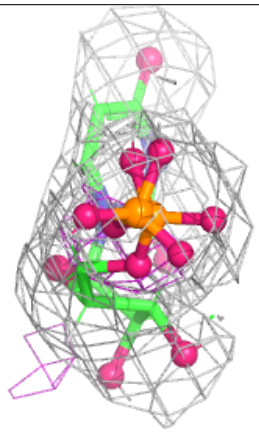


Electron density around UDP K 301:

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

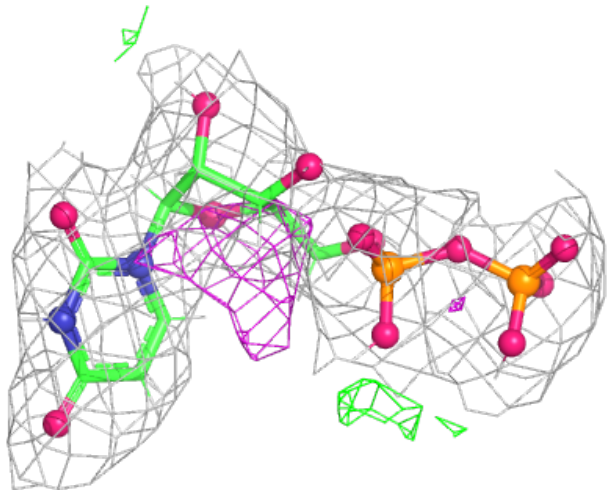


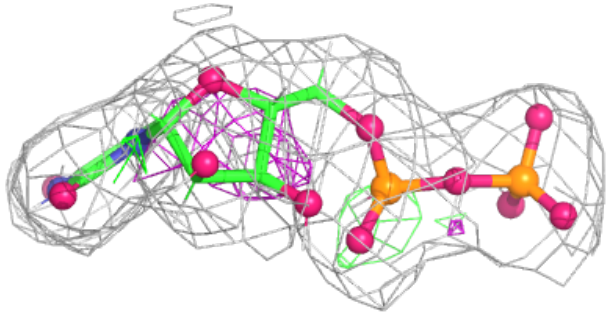


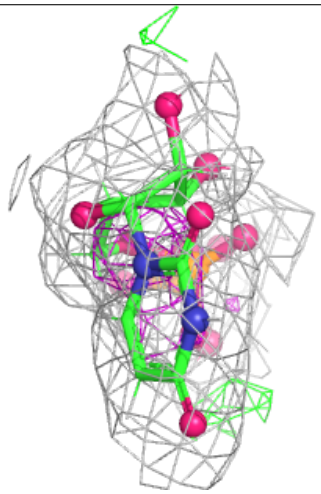


Electron density around UDP H 301:

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

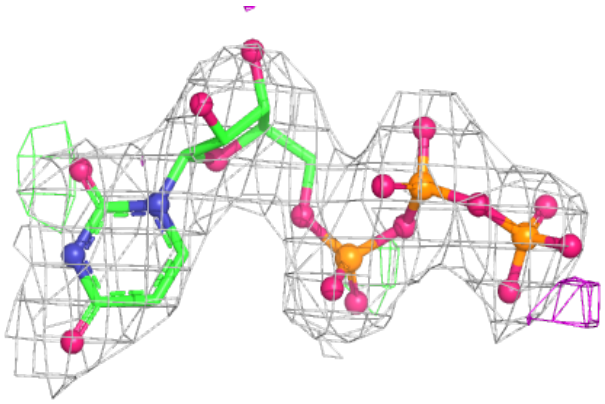


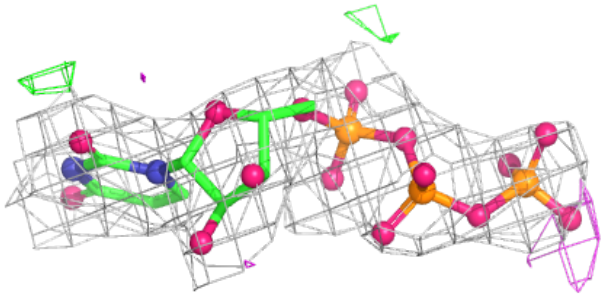


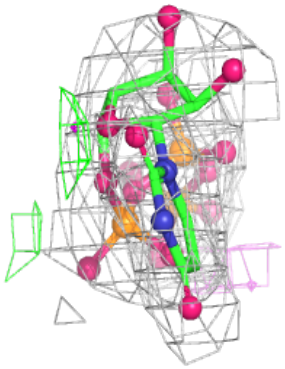


Electron density around UTP A 301:

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

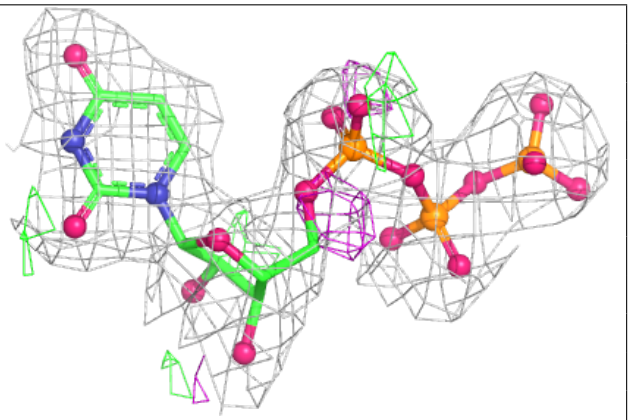


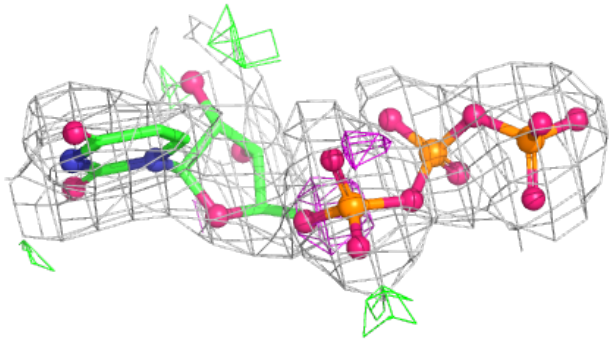


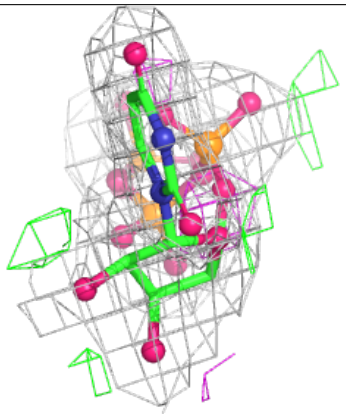


Electron density around UTP F 301:

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

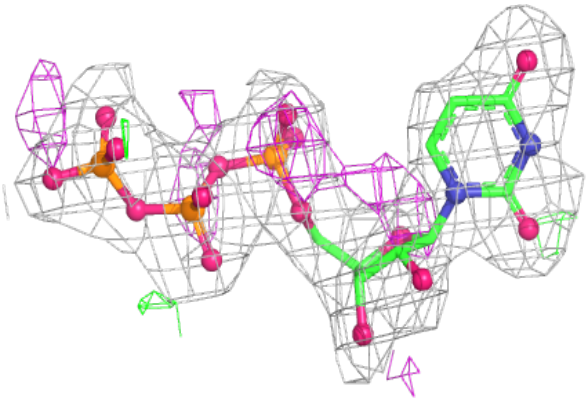


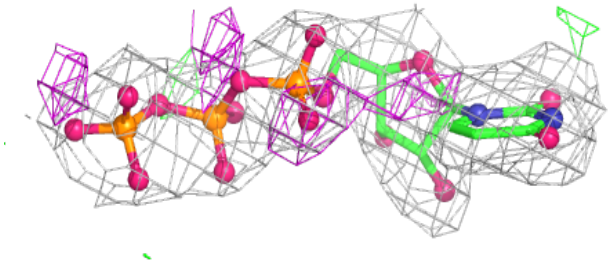


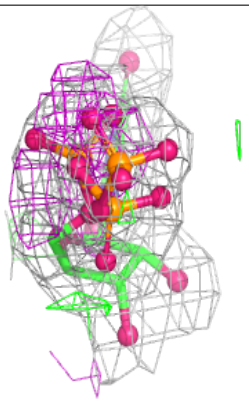


Electron density around UTP D 301:

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

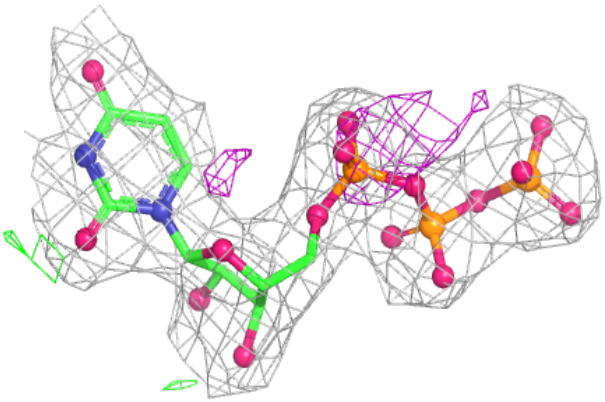


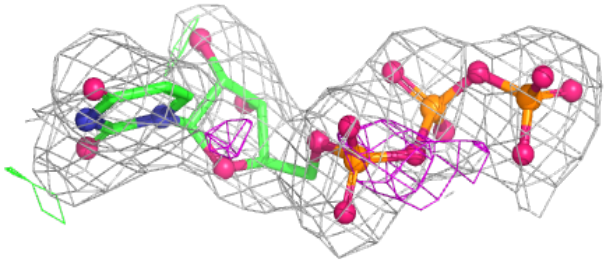


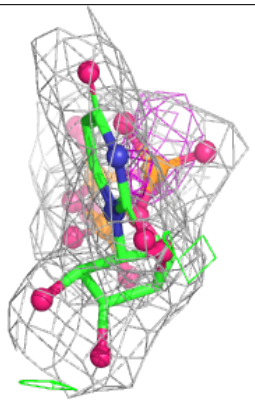


Electron density around UTP C 301:

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

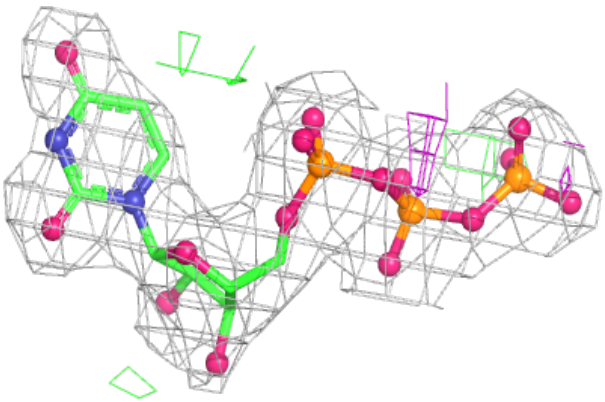


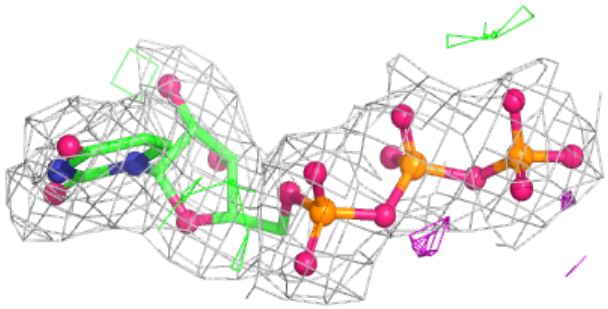


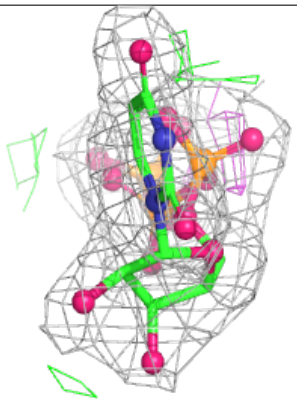


Electron density around UTP I 301:

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

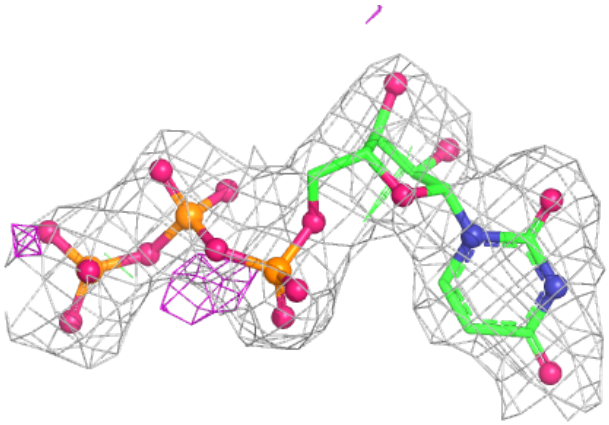


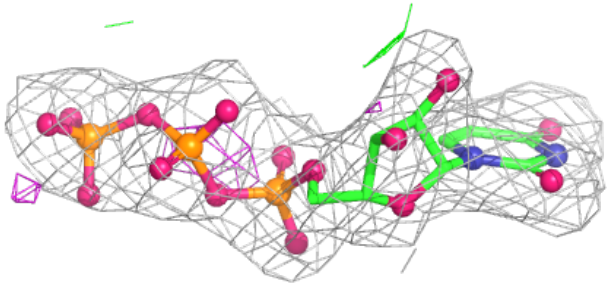


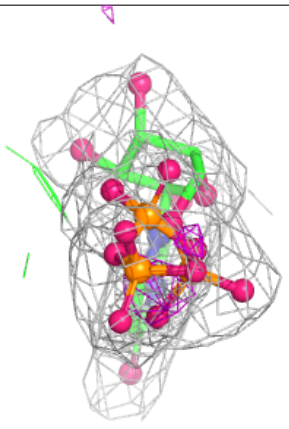


Electron density around UTP J 301:

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

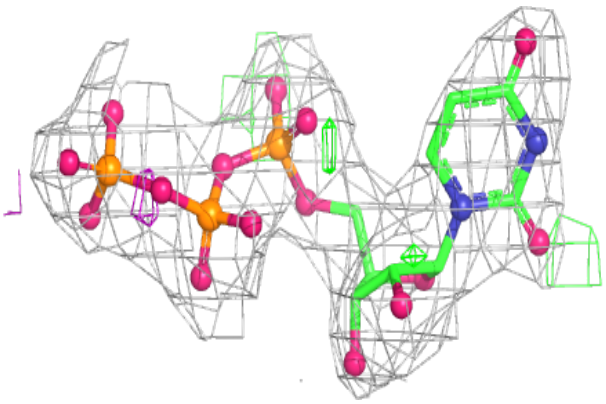


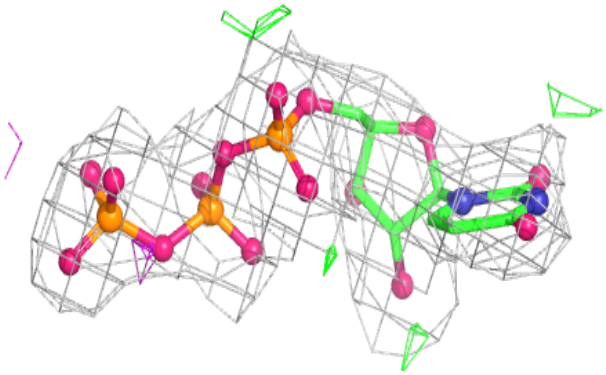


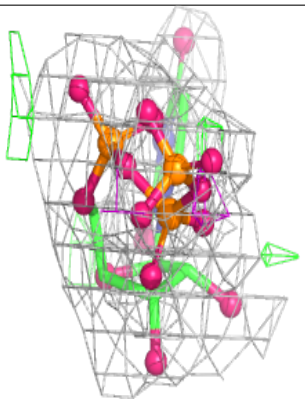


Electron density around UTP L 301:

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

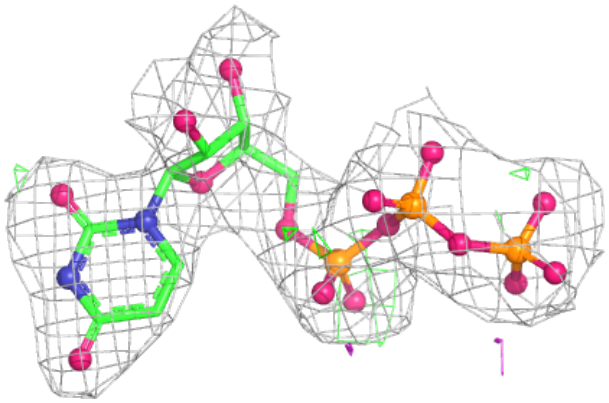


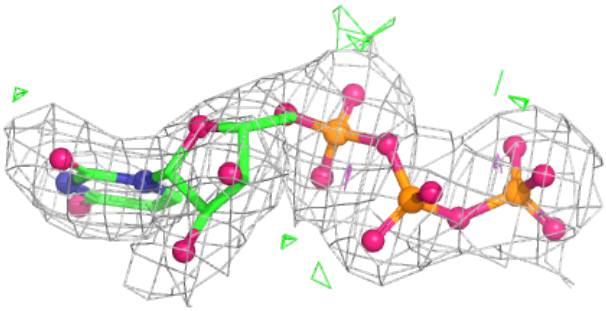


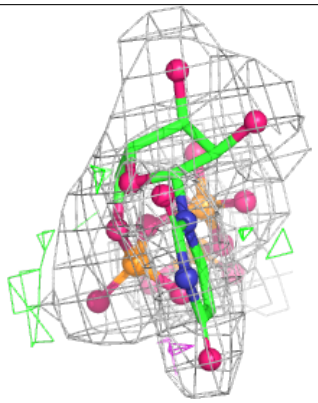


Electron density around UTP G 301:

$2mF_o$-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 (i)

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