



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:33 PM UTC

PDB ID : 7BL7 / pdb_00007bl7
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

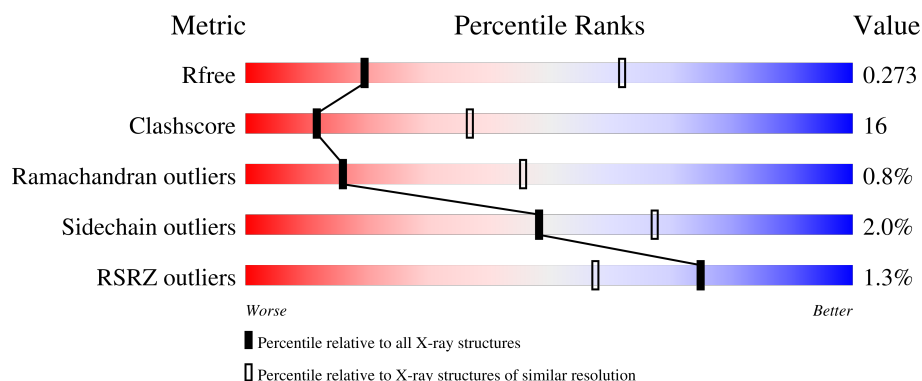
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UDP	C	302	-	-	X	-
2	UDP	H	301	-	-	X	-

2 Entry composition

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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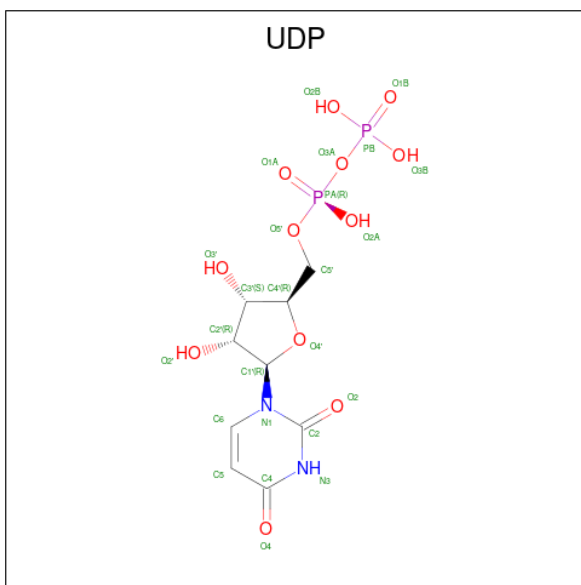
Chain	Residue	Modelled	Actual	Comment	Reference
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K	-5	VAL	-	expression tag	UNP P9WHK5
K	-4	PRO	-	expression tag	UNP P9WHK5
K	-3	ARG	-	expression tag	UNP P9WHK5
K	-2	GLY	-	expression tag	UNP P9WHK5
K	-1	SER	-	expression tag	UNP P9WHK5
K	0	HIS	-	expression 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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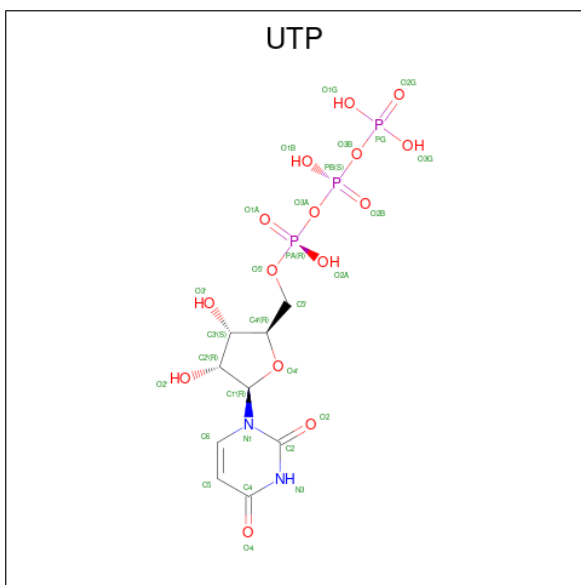
Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	PRO	-	expression tag	UNP P9WHK5
G	-3	ARG	-	expression tag	UNP P9WHK5
G	-2	GLY	-	expression tag	UNP P9WHK5
G	-1	SER	-	expression tag	UNP P9WHK5
G	0	HIS	-	expression tag	UNP P9WHK5
H	-19	MET	-	initiating methionine	UNP P9WHK5
H	-18	GLY	-	expression tag	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 (CCD ID: 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 39	C 9	H 14	N 2	O 12	P 2	0	0
2	E	1	Total 39	C 9	H 14	N 2	O 12	P 2	0	0
2	D	1	Total 39	C 9	H 14	N 2	O 12	P 2	0	0
2	C	1	Total 39	C 9	H 14	N 2	O 12	P 2	0	0
2	I	1	Total 39	C 9	H 14	N 2	O 12	P 2	0	0
2	J	1	Total 39	C 9	H 14	N 2	O 12	P 2	0	0
2	K	1	Total 39	C 9	H 14	N 2	O 12	P 2	0	0
2	H	1	Total 39	C 9	H 14	N 2	O 12	P 2	0	0

- Molecule 3 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: $\text{C}_9\text{H}_{15}\text{N}_2\text{O}_{15}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

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

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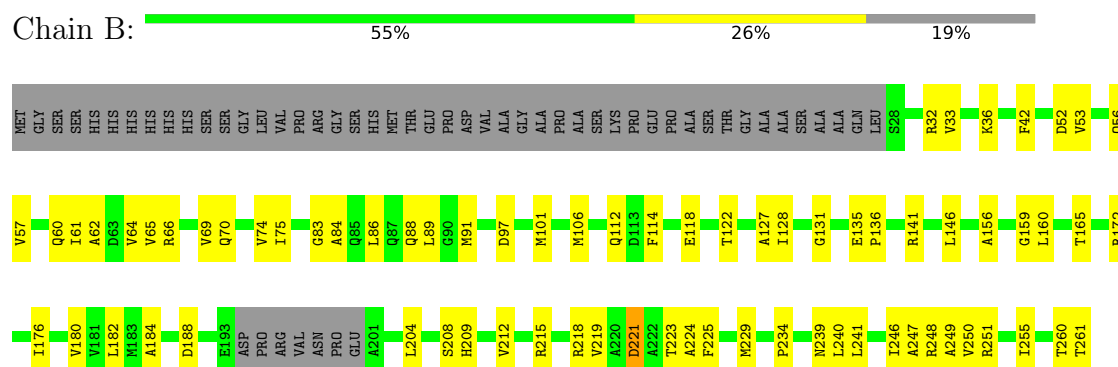
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	6	Total 6	O 6	0	0
4	C	4	Total 4	O 4	0	0
4	I	3	Total 3	O 3	0	0
4	J	3	Total 3	O 3	0	0
4	L	1	Total 1	O 1	0	0
4	G	4	Total 4	O 4	0	0
4	H	5	Total 5	O 5	0	0

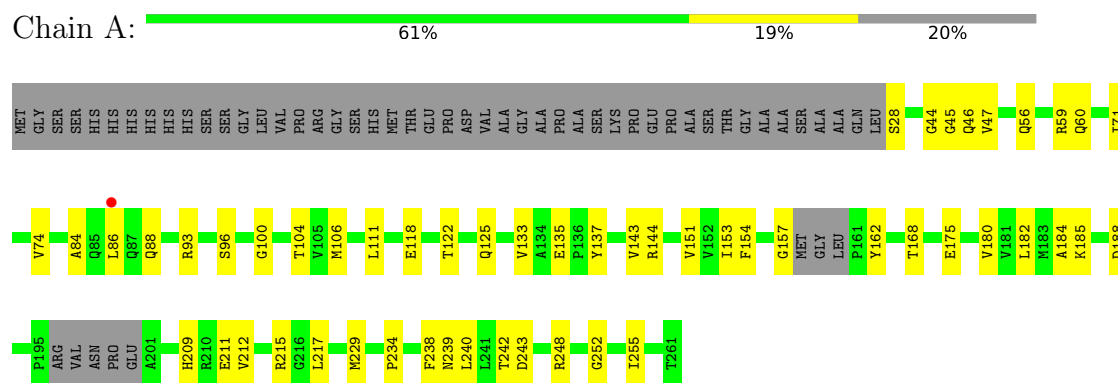
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

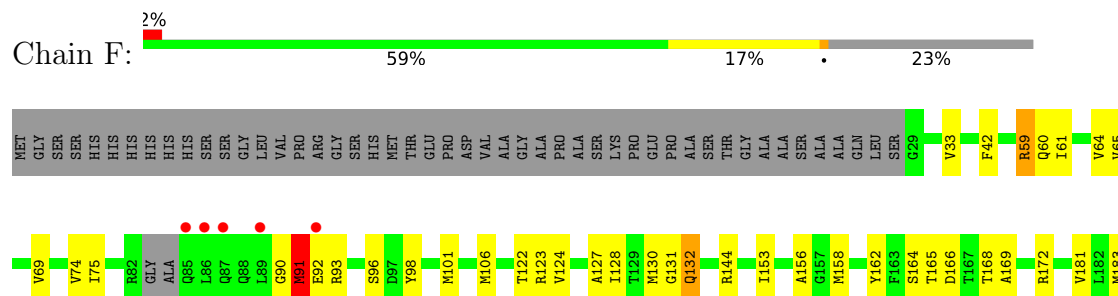
• Molecule 1: Uridylate kinase

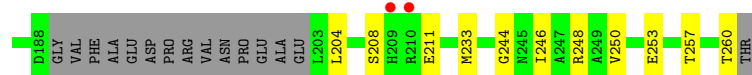


• Molecule 1: Uridylate kinase

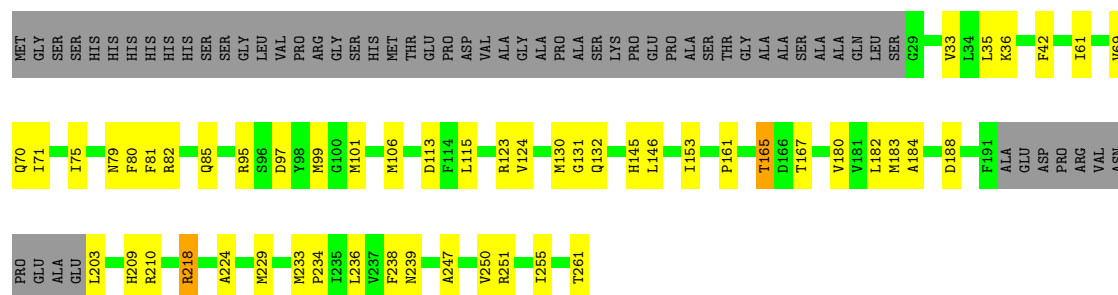


• Molecule 1: Uridylate kinase

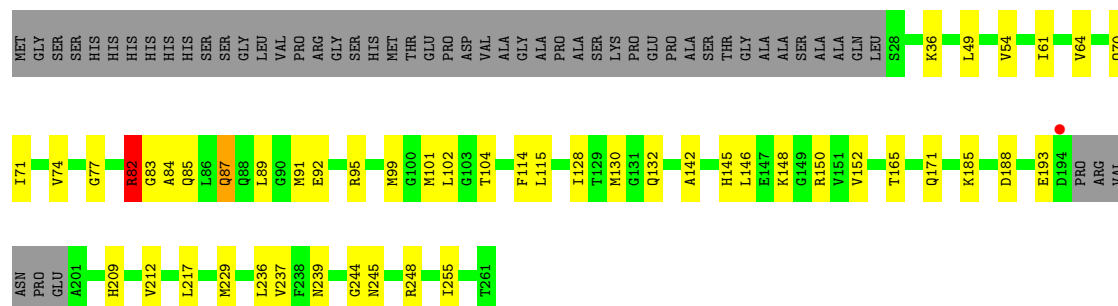




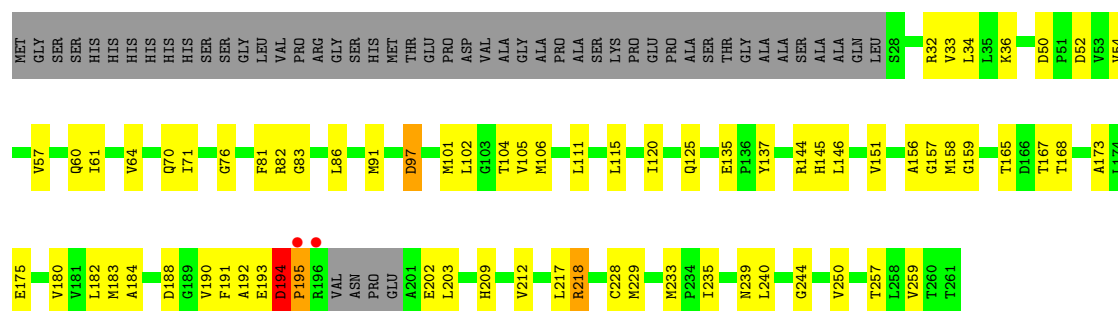
• Molecule 1: Uridylate kinase



• Molecule 1: Uridylate kinase

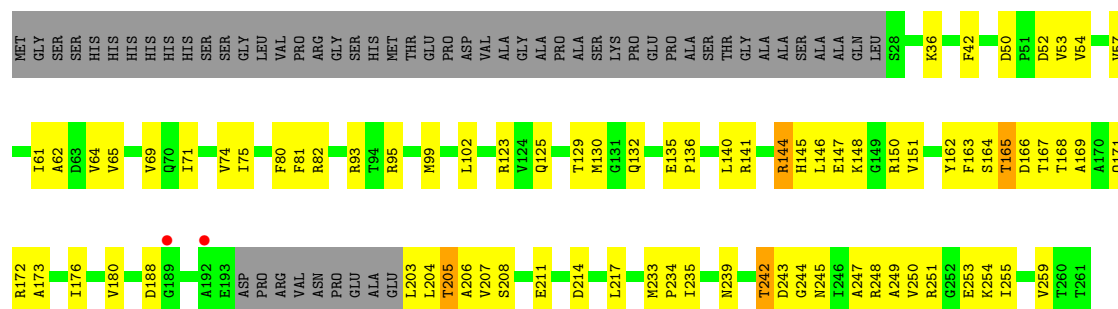


• Molecule 1: Uridylate kinase



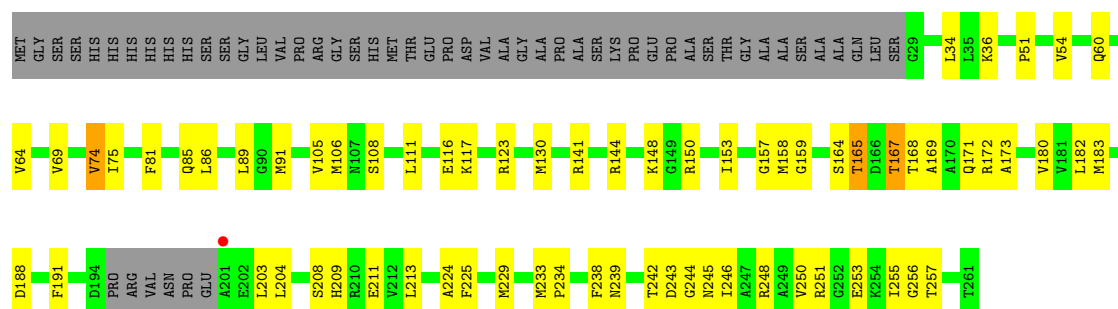
• Molecule 1: Uridylate kinase





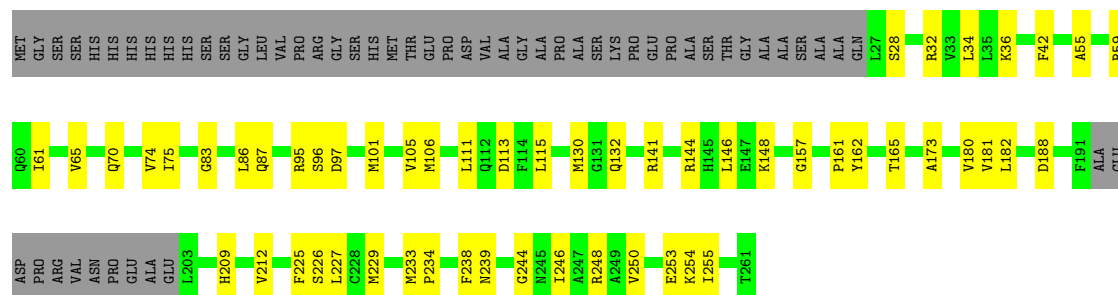
• Molecule 1: Uridylate kinase

Chain J: 57% 23% 19%



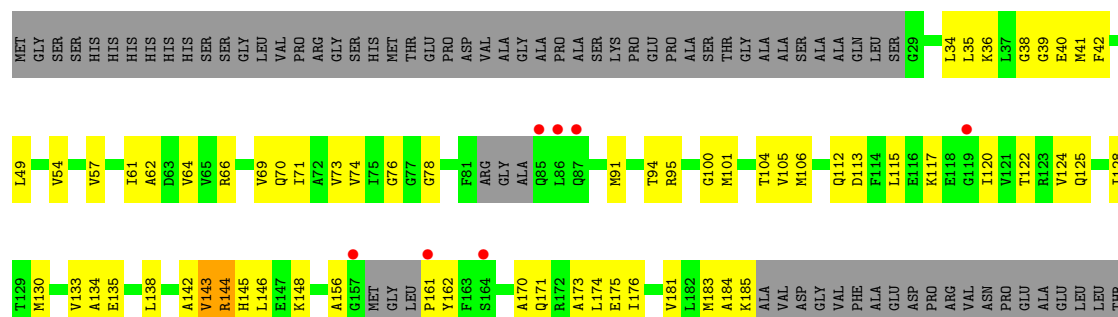
• Molecule 1: Uridylate kinase

Chain K: 60% 20% 20%



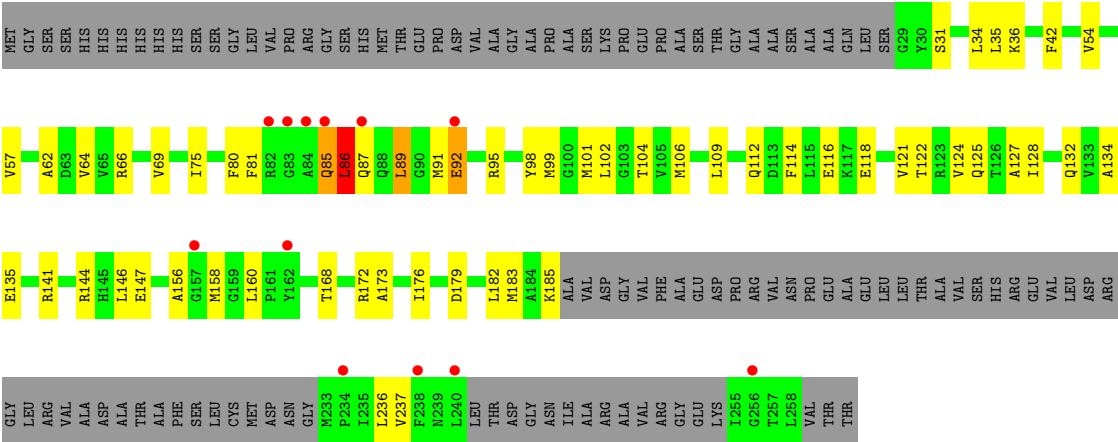
• Molecule 1: Uridylate kinase

Chain L: 33% 23% 44%

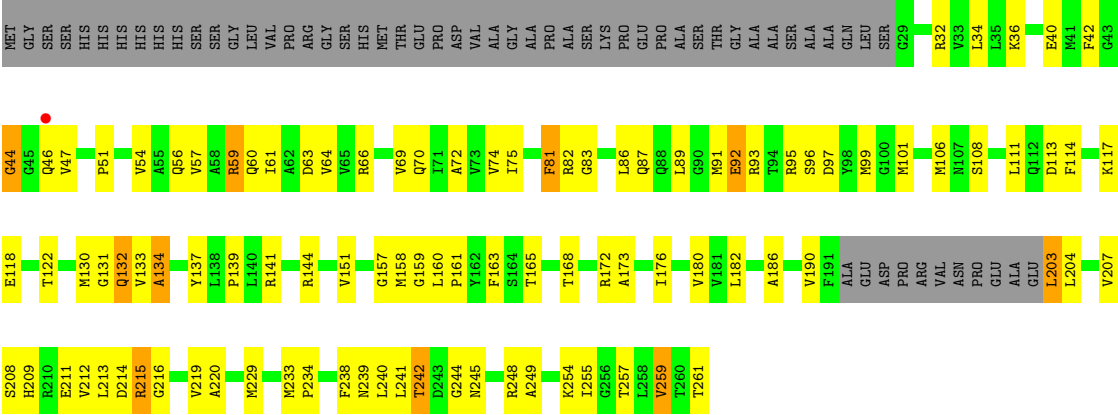




• Molecule 1: Uridylate kinase



• Molecule 1: Uridylate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.23Å 165.75Å 125.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 3.33 29.95 – 3.33	Depositor EDS
% Data completeness (in resolution range)	92.3 (29.95-3.33) 92.2 (29.95-3.33)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.192 , 0.274 0.192 , 0.273	Depositor DCC
R_{free} test set	2604 reflections (3.19%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19544	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.39	0/1665	0.61	0/2250
1	B	0.64	3/1707 (0.2%)	0.74	0/2302
1	C	0.73	2/1716 (0.1%)	0.77	2/2318 (0.1%)
1	D	0.77	5/1708 (0.3%)	0.76	2/2304 (0.1%)
1	E	0.56	0/1660	0.65	0/2241
1	F	0.58	0/1567	0.75	1/2118 (0.0%)
1	G	0.46	0/1250	0.71	1/1685 (0.1%)
1	H	0.68	2/1666 (0.1%)	0.75	1/2247 (0.0%)
1	I	0.62	0/1683	0.70	3/2272 (0.1%)
1	J	0.69	3/1692 (0.2%)	0.76	2/2284 (0.1%)
1	K	0.60	1/1678 (0.1%)	0.67	0/2264
1	L	0.43	0/1169	0.68	2/1574 (0.1%)
All	All	0.61	16/19161 (0.1%)	0.72	14/25859 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	81	PHE	C-N	7.30	1.43	1.33
1	H	89	LEU	C-N	-7.12	1.24	1.33
1	D	145	HIS	CA-C	-6.53	1.44	1.52
1	K	226	SER	C-O	-5.79	1.16	1.24
1	B	223	THR	C-O	-5.71	1.16	1.24
1	D	145	HIS	C-O	-5.60	1.17	1.24
1	C	97	ASP	C-O	-5.59	1.16	1.24
1	D	84	ALA	C-O	-5.40	1.17	1.24
1	B	248	ARG	CA-C	-5.33	1.46	1.52
1	C	145	HIS	C-O	-5.16	1.17	1.24
1	B	248	ARG	C-O	-5.16	1.18	1.24
1	D	92	GLU	CA-C	-5.06	1.46	1.52
1	J	171	GLN	CA-C	-5.05	1.46	1.52
1	D	82	ARG	C-O	-5.04	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	167	THR	C-O	-5.02	1.17	1.24
1	J	164	SER	CA-C	-5.02	1.46	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	145	HIS	N-CA-C	-7.46	103.08	111.14
1	C	192	ALA	N-CA-C	-7.00	99.29	109.59
1	D	83	GLY	N-CA-C	6.62	121.91	113.24
1	I	144	ARG	N-CA-C	-6.03	104.34	111.03
1	C	145	HIS	N-CA-C	-5.95	104.37	111.69
1	F	165	THR	N-CA-C	-5.71	106.86	113.88
1	G	86	LEU	N-CA-C	-5.64	106.07	113.12
1	I	205	THR	N-CA-C	5.52	122.56	110.80
1	I	243	ASP	N-CA-C	5.27	118.11	110.42
1	J	74	VAL	CA-C-N	-5.23	116.36	123.10
1	J	74	VAL	C-N-CA	-5.23	116.36	123.10
1	L	138	LEU	CA-C-N	-5.13	113.26	118.85
1	L	138	LEU	C-N-CA	-5.13	113.26	118.85
1	H	92	GLU	N-CA-C	-5.11	102.81	110.23

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
1	B	1689	0	1732	54	0
1	C	1697	0	1726	58	0
1	D	1690	0	1730	39	0
1	E	1642	0	1674	43	0
1	F	1552	0	1532	51	0
1	G	1237	0	1260	56	0
1	H	1649	0	1698	95	0
1	I	1665	0	1699	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1674	0	1710	61	0
1	K	1660	0	1701	49	0
1	L	1157	0	1173	48	0
2	B	25	14	11	5	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	8	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	619	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 16.

All (619) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ASP:CB	1:C:195:PRO:HD3	1.71	1.21
1:I:144:ARG:HD2	3:G:301:UTP:H5'	1.25	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:I:144:ARG:O	1:I:145:HIS:C	2.12	0.88
1:H:209:HIS:HB2	1:H:261:THR:HB	1.57	0.87
1:H:101:MET:HE3	2:H:301:UDP:C4	2.11	0.85
1:H:130:MET:HE2	1:H:133:VAL:HG22	1.58	0.85
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:B:101:MET:HE3	2:B:301:UDP:N3	1.93	0.82
1:L:54:VAL:HA	1:L:57:VAL:HG12	1.61	0.82
1:F:181:VAL:HG23	1:F:233:MET:HE2	1.62	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:F:91:MET:HE1	1:F:96:SER:HA	1.63	0.80
1:J:36:LYS:HE3	1:J:165:THR:HG22	1.63	0.80
1:H:130:MET:HE2	1:H:133:VAL:CG2	2.10	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:G:80:PHE:C	1:G:81:PHE:CD1	2.60	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:F:101:MET:HE2	1:F:128:ILE:HD11	1.65	0.77
1:H:208:SER:HB2	1:H:211:GLU:HG3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:96:SER:HA	1:H:99:MET:HE2	1.69	0.75
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
1:G:80:PHE:C	1:G:81:PHE:HD1	1.95	0.74
2:H:301:UDP:O1A	2:H:301:UDP:O3'	2.05	0.74
1:H:130:MET:HE1	1:H:133:VAL:HG21	1.67	0.74
1:F:59:ARG:HG2	1:F:59:ARG:HH21	1.52	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:J:213:LEU:HD11	1:J:229:MET:HE1	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: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:D:130:MET:HE1	1:C:102:LEU:HD21	1.71	0.70
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: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: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: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:F:91:MET:HE2	1:F:96:SER:HB2	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:VAL:HG23	1:E:234:PRO:HB2	1.76	0.68
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:173:ALA:HB1	1:H:233:MET:HE3	1.75	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:C:83:GLY:H	2:C:302:UDP:HO3'	1.42	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:B:225:PHE:HE1	1:B:229:MET:HE3	1.60	0.66
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:F:90:GLY:O	1:F:91:MET:C	2.40	0.65
1:G:144:ARG:NH2	1:G:147:GLU:OE1	2.29	0.65
1:L:183:MET:HE3	1:L:185:LYS:HE3	1.79	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: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:L:181:VAL:HG23	1:L:233:MET:HE2	1.80	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:J:158:MET:HE3	1:J:168:THR:HA	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:130:MET:HE2	1:J:130:MET:HE2	1.83	0.60
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:H:86:LEU:HD13	1:H:91:MET:HE2	1.82	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:G:34:LEU:HD13	1:G:173:ALA:HA	1.83	0.60
1:I:206:ALA:O	1:I:207:VAL:CG1	2.46	0.60
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:F:90:GLY:C	1:F:91:MET:O	2.46	0.59
1:B:101:MET:HE1	1:B:160:LEU:N	2.18	0.58
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:I:99:MET:O	1:J:106:MET:HE3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:101:MET:HE2	1:D:128:ILE:HD11	1.85	0.56
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:B:101:MET:HE3	2:B:301:UDP:C4	2.39	0.56
1:D:146:LEU:CD2	1:D:152:VAL:CG2	2.83	0.56
1:L:101:MET:HE3	1:L:156:ALA:HB1	1.87	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: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:G:101:MET:HE1	1:G:160:LEU:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:I:81:PHE:CD2	1:J:106:MET:HE2	2.41	0.55
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:J:158:MET:HE1	1:J:167:THR:HG22	1.89	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: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:F:166:ASP:OD2	1:F:183:MET:HE1	2.08	0.53
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:I:81:PHE:CE2	1:J:106:MET:HE2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:106:MET:HE2	1:A:106:MET:SD	2.50	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: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:K:180:VAL:C	1:K:233:MET:HE1	2.36	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:F:91:MET:HG2	1:E:113:ASP:CG	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:106:MET:HE2	1:L:106:MET:SD	2.51	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:J:173:ALA:HB1	1:J:233:MET:HE2	1.92	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
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:C:97:ASP:CG	2:C:302:UDP:O2'	2.55	0.49
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: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:L:41:MET:HE1	1:L:184:ALA:O	2.13	0.49
1:B:209:HIS:H	1:B:261:THR:HG23	1.78	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:B:101:MET:HE3	2:B:301:UDP:C2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:209:HIS:C	1:B:229:MET:HE2	2.39	0.47
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:101:MET:HE3	2:H:301:UDP:C5	2.49	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:C:158:MET:HE3	1:C:168:THR:HA	1.95	0.47
1:L:173:ALA:HB1	1:L:233:MET:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:38:GLY:HA3	1:L:41:MET:HE2	1.97	0.47
1:B:188:ASP:HA	1:B:239:ASN:HB2	1.97	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
1:F:59:ARG:HH21	1:F:59:ARG:CB	2.28	0.46
1:D:114:PHE:CE2	1:C:91:MET:HE3	2.50	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:F:106:MET:HE2	1:E:81:PHE:CE2	2.51	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:G:106:MET:HE3	1:H:99:MET:O	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:101:MET:HE1	1:L:161:PRO:HD2	1.98	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:101:MET:O	1:G:104:THR:OG1	2.31	0.45
1:G:182:LEU:HD13	1:G:236:LEU:HD22	1.99	0.45
1:H:130:MET:HE1	1:H:133:VAL:CG2	2.27	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:F:91:MET:HE2	1:F:96:SER:CB	2.45	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: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
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:K:181:VAL:N	1:K:233:MET:HE1	2.32	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:G:99:MET:O	1:H:106:MET:HE3	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:233:MET:HE2	1:E:233:MET:HB2	1.76	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:C:36:LYS:NZ	2:C:302:UDP:O2B	2.51	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:J:141:ARG:HG3	3:L:301:UTP:H5'2	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: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
1:F:92:GLU:O	1:F:96:SER:CB	2.64	0.44
1:K:105:VAL:HG21	1:K:130:MET:HE1	2.00	0.44
1:D:102:LEU:HD23	1:D:102:LEU:HA	1.78	0.43
1:H:204:LEU:C	1:H:257:THR:HG22	2.42	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
1:F:233:MET:HB3	1:F:233:MET:HE3	1.60	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:E:80:PHE:CZ	1:E:106:MET:HE3	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:302:UDP:C3'	2:D:302:UDP:PA	3.06	0.43
1:C:209:HIS:HB3	1:C:229:MET:HE3	2.00	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:I:173:ALA:HB1	1:I:233:MET:HE2	2.00	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:J:34:LEU:CD2	1:J:169:ALA:HB1	2.49	0.43
1:J:64:VAL:HG22	1:J:69:VAL:HG11	2.01	0.43
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:K:233:MET:HB3	1:K:233:MET:HE3	1.73	0.42
1:A:60:GLN:HE22	1:A:243:ASP:HA	1.85	0.42
1:D:99:MET:O	1:C:106:MET:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:246:ILE:O	1:F:250:VAL:HG22	2.19	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:H:36:LYS:HD3	1:H:36:LYS:C	2.45	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:L:76:GLY:C	1:L:104:THR:HG22	2.45	0.42
1:F:64:VAL:HG13	1:F:69:VAL:HG11	2.01	0.42
1:D:101:MET:CE	1:D:128:ILE:HD11	2.47	0.42
1:C:33:VAL:HG23	1:C:71:ILE:HG13	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:J:225:PHE:CE2	1:J:229:MET:HE2	2.55	0.42
1:H:91:MET:CE	1:H:99:MET:HE1	2.50	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:E:99:MET:HE2	1:E:99:MET:HB3	1.83	0.41
1:I:62:ALA:HA	1:I:65:VAL:HG12	2.02	0.41
1:G:86:LEU:O	1:G:87:GLN:C	2.62	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
1:L:39:GLY:C	1:L:41:MET:H	2.28	0.41
1:B:208:SER:HA	1:B:260:THR:O	2.20	0.41
1:C:60:GLN:CD	1:C:244:GLY:H	2.29	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:H:101:MET:HE1	1:H:160:LEU:N	2.36	0.41
1:F:122:THR:O	1:F:123:ARG:NH1	2.47	0.41
1:G:42:PHE:CZ	1:G:75:ILE:HD13	2.56	0.41
1:H:130:MET:C	1:H:132:GLN:H	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:91:MET:HE3	1:L:91:MET:HB2	1.80	0.41
1:H:203:LEU:C	1:H:204:LEU:HD23	2.46	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:B:101:MET:HE1	1:B:159:GLY:C	2.45	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:J:158:MET:CE	1:J:168:THR:HA	2.48	0.40
1:J:183:MET:HE3	1:J:183:MET:HB3	1.76	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:C:183:MET:HE3	1:C:183:MET:HB3	1.81	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:G:158:MET:HB2	1:G:158:MET:HE3	1.80	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
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:I:144:ARG:C	1:I:146:LEU:N	2.78	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:E:183:MET:HE2	1:E:183:MET:HB2	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	24	55
1	B	223/281 (79%)	211 (95%)	11 (5%)	1 (0%)	30	59
1	C	226/281 (80%)	216 (96%)	6 (3%)	4 (2%)	6	30
1	D	224/281 (80%)	216 (96%)	7 (3%)	1 (0%)	30	59
1	E	218/281 (78%)	210 (96%)	7 (3%)	1 (0%)	24	55
1	F	210/281 (75%)	200 (95%)	8 (4%)	2 (1%)	12	41
1	G	163/281 (58%)	145 (89%)	16 (10%)	2 (1%)	10	37
1	H	218/281 (78%)	203 (93%)	11 (5%)	4 (2%)	6	30
1	I	221/281 (79%)	205 (93%)	15 (7%)	1 (0%)	24	55
1	J	223/281 (79%)	215 (96%)	8 (4%)	0	100	100
1	K	220/281 (78%)	209 (95%)	9 (4%)	2 (1%)	14	43
1	L	150/281 (53%)	133 (89%)	17 (11%)	0	100	100
All	All	2516/3372 (75%)	2372 (94%)	125 (5%)	19 (1%)	16	46

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	91	MET
1	C	194	ASP
1	C	195	PRO

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Mol	Chain	Res	Type
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 ⓘ

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%)	164 (99%)	1 (1%)	78	81
1	B	174/215 (81%)	172 (99%)	2 (1%)	65	75
1	C	173/215 (80%)	171 (99%)	2 (1%)	63	74
1	D	173/215 (80%)	171 (99%)	2 (1%)	63	74
1	E	168/215 (78%)	166 (99%)	2 (1%)	63	74
1	F	150/215 (70%)	146 (97%)	4 (3%)	39	63
1	G	124/215 (58%)	120 (97%)	4 (3%)	34	60
1	H	170/215 (79%)	159 (94%)	11 (6%)	15	44
1	I	171/215 (80%)	164 (96%)	7 (4%)	27	55
1	J	170/215 (79%)	169 (99%)	1 (1%)	78	81
1	K	171/215 (80%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	116/215 (54%)	114 (98%)	2 (2%)	53 70
All	All	1925/2580 (75%)	1887 (98%)	38 (2%)	48 67

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	218	ARG
1	B	221	ASP
1	A	242	THR
1	F	59	ARG
1	F	91	MET
1	F	132	GLN
1	F	164	SER
1	E	165	THR
1	E	218	ARG
1	D	82	ARG
1	D	87	GLN
1	C	194	ASP
1	C	218	ARG
1	I	52	ASP
1	I	82	ARG
1	I	165	THR
1	I	203	LEU
1	I	205	THR
1	I	214	ASP
1	I	242	THR
1	J	165	THR
1	L	143	VAL
1	L	144	ARG
1	G	85	GLN
1	G	86	LEU
1	G	92	GLU
1	G	141	ARG
1	H	46	GLN
1	H	47	VAL
1	H	59	ARG
1	H	92	GLU
1	H	132	GLN
1	H	203	LEU
1	H	213	LEU
1	H	214	ASP
1	H	215	ARG

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Mol	Chain	Res	Type
1	H	242	THR
1	H	259	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	GLN
1	B	209	HIS
1	A	56	GLN
1	A	60	GLN
1	A	125	GLN
1	A	145	HIS
1	A	231	ASN
1	E	112	GLN
1	E	125	GLN
1	D	87	GLN
1	D	88	GLN
1	C	231	ASN
1	I	56	GLN
1	I	70	GLN
1	I	88	GLN
1	I	239	ASN
1	I	245	ASN
1	J	70	GLN
1	J	112	GLN
1	J	245	ASN
1	K	60	GLN
1	K	85	GLN
1	K	132	GLN
1	G	85	GLN
1	G	112	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	C	302	-	25,26,26	2.09	6 (24%)	38,40,40	0.59	0
3	UTP	L	301	-	29,30,30	2.72	10 (34%)	43,47,47	1.79	10 (23%)
3	UTP	A	301	-	29,30,30	2.73	10 (34%)	43,47,47	1.76	9 (20%)
3	UTP	D	301	-	29,30,30	2.29	11 (37%)	43,47,47	1.49	9 (20%)
3	UTP	G	301	-	29,30,30	2.72	8 (27%)	43,47,47	1.71	8 (18%)
2	UDP	K	301	-	25,26,26	1.70	6 (24%)	38,40,40	0.64	1 (2%)
3	UTP	I	301	-	29,30,30	2.59	9 (31%)	43,47,47	1.62	5 (11%)
2	UDP	J	302	-	25,26,26	2.08	6 (24%)	38,40,40	0.60	0
3	UTP	F	301	-	29,30,30	2.88	11 (37%)	43,47,47	1.59	8 (18%)
3	UTP	C	301	-	29,30,30	2.55	9 (31%)	43,47,47	1.67	9 (20%)
2	UDP	I	302	-	25,26,26	1.96	6 (24%)	38,40,40	0.76	1 (2%)
2	UDP	H	301	-	25,26,26	1.64	6 (24%)	38,40,40	0.66	0
2	UDP	D	302	-	25,26,26	2.14	7 (28%)	38,40,40	0.82	0
3	UTP	J	301	-	29,30,30	2.68	10 (34%)	43,47,47	1.76	12 (27%)
2	UDP	B	301	-	25,26,26	1.88	7 (28%)	38,40,40	0.61	0
2	UDP	E	301	-	25,26,26	1.72	7 (28%)	38,40,40	0.62	1 (2%)

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	C	302	-	-	3/16/32/32	0/2/2/2
3	UTP	L	301	-	-	8/22/38/38	0/2/2/2
3	UTP	A	301	-	-	7/22/38/38	0/2/2/2
3	UTP	D	301	-	-	4/22/38/38	0/2/2/2
3	UTP	G	301	-	-	6/22/38/38	0/2/2/2
2	UDP	K	301	-	-	4/16/32/32	0/2/2/2
3	UTP	I	301	-	-	4/22/38/38	0/2/2/2
2	UDP	J	302	-	-	3/16/32/32	0/2/2/2
3	UTP	F	301	-	-	10/22/38/38	0/2/2/2
3	UTP	C	301	-	-	4/22/38/38	0/2/2/2
2	UDP	I	302	-	-	5/16/32/32	0/2/2/2
2	UDP	H	301	-	-	6/16/32/32	0/2/2/2
2	UDP	D	302	-	-	7/16/32/32	0/2/2/2
3	UTP	J	301	-	-	4/22/38/38	0/2/2/2
2	UDP	B	301	-	-	2/16/32/32	0/2/2/2
2	UDP	E	301	-	-	2/16/32/32	0/2/2/2

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	301	UTP	PA-O3A	7.04	1.67	1.59
3	F	301	UTP	PB-O3A	6.64	1.66	1.59
3	G	301	UTP	PB-O3A	6.53	1.66	1.59
3	A	301	UTP	PA-O3A	6.19	1.66	1.59
3	A	301	UTP	PB-O3A	6.17	1.66	1.59
2	J	302	UDP	PB-O1B	-6.00	1.31	1.50
3	C	301	UTP	PA-O3A	5.99	1.66	1.59
3	L	301	UTP	PB-O3B	5.82	1.65	1.59
3	C	301	UTP	PB-O3B	5.75	1.65	1.59
3	G	301	UTP	C2-N1	5.73	1.47	1.38
3	I	301	UTP	PA-O3A	5.68	1.65	1.59
3	J	301	UTP	PB-O3B	5.63	1.65	1.59
3	G	301	UTP	PA-O3A	5.58	1.65	1.59
3	J	301	UTP	PA-O3A	5.53	1.65	1.59
3	L	301	UTP	PB-O3A	5.52	1.65	1.59
3	L	301	UTP	PA-O3A	5.49	1.65	1.59
3	I	301	UTP	C2-N1	5.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	301	UTP	C2-N1	5.44	1.47	1.38
3	J	301	UTP	PB-O3A	5.40	1.65	1.59
2	B	301	UDP	PB-O1B	-5.33	1.33	1.50
2	I	302	UDP	PB-O1B	-5.26	1.34	1.50
2	D	302	UDP	PA-O5'	-5.20	1.39	1.59
3	G	301	UTP	PB-O3B	5.16	1.65	1.59
3	L	301	UTP	C2-N1	5.14	1.46	1.38
3	F	301	UTP	C6-N1	5.11	1.50	1.38
3	A	301	UTP	PB-O3B	5.05	1.65	1.59
3	C	301	UTP	C2-N1	4.81	1.46	1.38
2	C	302	UDP	PB-O1B	-4.74	1.35	1.50
3	D	301	UTP	PA-O3A	4.67	1.64	1.59
2	I	302	UDP	PA-O5'	-4.60	1.41	1.59
3	F	301	UTP	PB-O3B	4.60	1.64	1.59
3	J	301	UTP	C2-N1	4.58	1.45	1.38
2	D	302	UDP	PB-O1B	-4.56	1.36	1.50
3	A	301	UTP	C5-C4	4.55	1.53	1.43
3	L	301	UTP	C6-N1	4.54	1.48	1.38
3	A	301	UTP	C6-N1	4.54	1.48	1.38
3	I	301	UTP	C5-C4	4.53	1.53	1.43
3	C	301	UTP	PB-O3A	4.51	1.64	1.59
3	A	301	UTP	C2-N1	4.48	1.45	1.38
3	I	301	UTP	C6-N1	4.48	1.48	1.38
3	F	301	UTP	C5-C4	4.43	1.53	1.43
2	C	302	UDP	PA-O5'	-4.32	1.42	1.59
2	C	302	UDP	PB-O3B	-4.31	1.38	1.54
3	I	301	UTP	PB-O3A	4.26	1.64	1.59
2	H	301	UDP	PB-O1B	-4.24	1.37	1.50
3	G	301	UTP	C6-N1	4.24	1.48	1.38
3	D	301	UTP	PB-O3B	4.17	1.64	1.59
3	J	301	UTP	C5-C4	4.16	1.52	1.43
3	L	301	UTP	C5-C4	4.13	1.52	1.43
3	D	301	UTP	C2-N1	4.10	1.44	1.38
3	J	301	UTP	C6-N1	4.10	1.47	1.38
3	I	301	UTP	PB-O3B	4.08	1.63	1.59
2	D	302	UDP	PA-O2A	-4.07	1.36	1.55
3	D	301	UTP	PB-O3A	4.00	1.63	1.59
3	G	301	UTP	C5-C4	3.99	1.52	1.43
3	D	301	UTP	C6-N1	3.95	1.47	1.38
2	E	301	UDP	PA-O5'	-3.94	1.44	1.59
2	K	301	UDP	PB-O1B	-3.92	1.38	1.50
2	K	301	UDP	PA-O5'	-3.90	1.44	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	302	UDP	PB-O2B	-3.78	1.40	1.54
2	E	301	UDP	PB-O1B	-3.70	1.38	1.50
2	J	302	UDP	PB-O3B	-3.69	1.41	1.54
2	J	302	UDP	PA-O5'	-3.68	1.45	1.59
2	H	301	UDP	PB-O3B	-3.58	1.41	1.54
2	I	302	UDP	PB-O2B	-3.52	1.41	1.54
2	D	302	UDP	PB-O3B	-3.48	1.41	1.54
2	C	302	UDP	PB-O2B	-3.47	1.41	1.54
2	C	302	UDP	PA-O2A	-3.44	1.39	1.55
2	D	302	UDP	PA-O1A	-3.38	1.39	1.50
2	D	302	UDP	PB-O2B	-3.30	1.42	1.54
2	B	301	UDP	PA-O5'	-3.29	1.46	1.59
3	D	301	UTP	C5-C4	3.29	1.50	1.43
2	K	301	UDP	PB-O3B	-3.27	1.42	1.54
2	I	302	UDP	PB-O3B	-3.26	1.42	1.54
2	B	301	UDP	PB-O2B	-3.26	1.42	1.54
3	C	301	UTP	C6-N1	3.26	1.45	1.38
3	D	301	UTP	O4-C4	-3.24	1.18	1.24
2	B	301	UDP	PB-O3B	-3.22	1.42	1.54
2	H	301	UDP	PA-O5'	-3.20	1.46	1.59
3	C	301	UTP	C5-C4	3.18	1.50	1.43
3	G	301	UTP	O4-C4	-3.17	1.18	1.24
2	C	302	UDP	PA-O1A	-3.16	1.39	1.50
3	J	301	UTP	C2-N3	3.14	1.43	1.38
2	E	301	UDP	PB-O3B	-3.13	1.43	1.54
3	C	301	UTP	C2-N3	3.11	1.43	1.38
2	E	301	UDP	PA-O2A	-3.08	1.41	1.55
2	B	301	UDP	PA-O1A	-3.08	1.40	1.50
2	J	302	UDP	PA-O2A	-3.04	1.41	1.55
3	I	301	UTP	C2-N3	3.01	1.43	1.38
3	L	301	UTP	O4-C4	-3.00	1.18	1.24
2	J	302	UDP	PA-O1A	-2.89	1.40	1.50
3	A	301	UTP	O2-C2	-2.85	1.18	1.23
2	H	301	UDP	PB-O2B	-2.77	1.44	1.54
2	K	301	UDP	PB-O2B	-2.76	1.44	1.54
3	L	301	UTP	C2-N3	2.76	1.42	1.38
2	I	302	UDP	PA-O1A	-2.65	1.41	1.50
2	K	301	UDP	PA-O1A	-2.65	1.41	1.50
2	E	301	UDP	PB-O2B	-2.62	1.45	1.54
3	F	301	UTP	C2-N3	2.56	1.42	1.38
2	E	301	UDP	PA-O1A	-2.53	1.42	1.50
3	F	301	UTP	O4-C4	-2.51	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301	UDP	PA-O2A	-2.51	1.43	1.55
2	B	301	UDP	PA-O2A	-2.46	1.43	1.55
2	I	302	UDP	PA-O2A	-2.46	1.43	1.55
3	J	301	UTP	C4-N3	2.45	1.42	1.38
3	A	301	UTP	O4-C4	-2.44	1.19	1.24
2	H	301	UDP	PA-O1A	-2.40	1.42	1.50
3	C	301	UTP	O4-C4	-2.33	1.20	1.24
3	I	301	UTP	O4-C4	-2.32	1.20	1.24
2	H	301	UDP	PA-O2A	-2.31	1.44	1.55
3	D	301	UTP	C2-N3	2.31	1.42	1.38
3	D	301	UTP	O4'-C1'	2.25	1.47	1.42
3	J	301	UTP	PG-O1G	-2.25	1.46	1.54
3	F	301	UTP	PG-O1G	-2.25	1.46	1.54
3	I	301	UTP	PG-O3G	-2.25	1.46	1.54
3	C	301	UTP	C4-N3	2.24	1.42	1.38
3	J	301	UTP	O4-C4	-2.21	1.20	1.24
3	D	301	UTP	PG-O3G	-2.12	1.46	1.54
2	D	302	UDP	C4-N3	-2.09	1.35	1.38
3	F	301	UTP	PA-O5'	2.08	1.67	1.59
3	L	301	UTP	O4'-C1'	2.06	1.46	1.42
2	B	301	UDP	C4-N3	-2.06	1.35	1.38
3	A	301	UTP	PG-O1G	-2.04	1.47	1.54
3	G	301	UTP	PG-O1G	-2.04	1.47	1.54
3	L	301	UTP	O2-C2	-2.03	1.19	1.23
3	F	301	UTP	C4-N3	2.02	1.42	1.38
3	A	301	UTP	C2-N3	2.02	1.41	1.38
2	E	301	UDP	C4-N3	-2.00	1.35	1.38
3	D	301	UTP	PG-O1G	-2.00	1.47	1.54

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	301	UTP	C4-N3-C2	-5.51	119.77	126.61
3	A	301	UTP	N3-C2-N1	5.30	121.79	114.89
3	A	301	UTP	C4-N3-C2	-5.03	120.36	126.61
3	J	301	UTP	C4-N3-C2	-4.78	120.68	126.61
3	G	301	UTP	C4-N3-C2	-4.74	120.73	126.61
3	I	301	UTP	C4-N3-C2	-4.71	120.76	126.61
3	I	301	UTP	N3-C2-N1	4.50	120.75	114.89
3	L	301	UTP	N3-C2-N1	4.31	120.50	114.89
3	G	301	UTP	O1G-PG-O3B	4.04	118.17	104.64
3	F	301	UTP	C4-N3-C2	-3.97	121.69	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	UTP	C4-N3-C2	-3.86	121.83	126.61
3	C	301	UTP	C4-N3-C2	-3.83	121.85	126.61
3	J	301	UTP	N3-C2-N1	3.73	119.75	114.89
3	G	301	UTP	C5-C4-N3	3.68	119.95	114.80
3	C	301	UTP	C1'-N1-C2	3.66	124.17	117.59
3	F	301	UTP	N3-C2-N1	3.57	119.54	114.89
3	L	301	UTP	C5-C4-N3	3.54	119.76	114.80
3	C	301	UTP	O4-C4-C5	-3.53	119.07	125.16
3	F	301	UTP	O2A-PA-O3A	3.45	116.60	107.27
3	G	301	UTP	N3-C2-N1	3.30	119.19	114.89
3	C	301	UTP	N3-C2-N1	3.23	119.09	114.89
3	C	301	UTP	O4-C4-N3	3.19	123.90	119.27
3	D	301	UTP	N3-C2-N1	3.17	119.02	114.89
3	J	301	UTP	O4-C4-C5	-3.10	119.81	125.16
3	F	301	UTP	C5-C4-N3	3.10	119.14	114.80
3	I	301	UTP	O1G-PG-O3B	2.94	114.51	104.64
3	L	301	UTP	O4-C4-C5	-2.94	120.09	125.16
3	A	301	UTP	O3G-PG-O3B	2.90	114.35	104.64
3	J	301	UTP	O3G-PG-O3B	2.79	114.00	104.64
3	A	301	UTP	C5-C4-N3	2.75	118.64	114.80
3	D	301	UTP	C5-C4-N3	2.68	118.55	114.80
3	J	301	UTP	O2-C2-N1	-2.68	119.31	122.80
3	L	301	UTP	O3G-PG-O3B	2.67	113.59	104.64
3	C	301	UTP	O1B-PB-O3B	2.67	114.49	107.27
3	J	301	UTP	O4'-C1'-C2'	-2.66	100.92	106.62
3	A	301	UTP	O2A-PA-O1A	-2.61	100.30	112.44
3	G	301	UTP	O4-C4-C5	-2.59	120.70	125.16
3	C	301	UTP	O3G-PG-O3B	2.58	113.28	104.64
3	D	301	UTP	O4-C4-C5	-2.50	120.85	125.16
3	J	301	UTP	C5-C4-N3	2.45	118.24	114.80
3	F	301	UTP	O3G-PG-O3B	2.45	112.86	104.64
3	D	301	UTP	C2'-C3'-C4'	2.44	107.33	102.61
3	I	301	UTP	C2'-C3'-C4'	2.43	107.30	102.61
3	I	301	UTP	C5-C4-N3	2.43	118.20	114.80
3	F	301	UTP	O1B-PB-O2B	-2.40	101.28	112.44
3	J	301	UTP	O1B-PB-O3A	2.37	113.68	107.27
2	E	301	UDP	O2'-C2'-C3'	-2.33	104.36	111.82
3	L	301	UTP	O1G-PG-O3B	2.32	112.41	104.64
3	F	301	UTP	O1B-PB-O3A	2.29	113.47	107.27
3	G	301	UTP	O3G-PG-O3B	2.28	112.28	104.64
3	A	301	UTP	C6-N1-C2	-2.28	118.22	121.00
3	D	301	UTP	O3G-PG-O3B	2.26	112.22	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	301	UDP	O2'-C2'-C3'	-2.25	104.62	111.82
3	L	301	UTP	O2-C2-N1	-2.23	119.90	122.80
3	L	301	UTP	O2A-PA-O1A	-2.19	102.27	112.44
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
3	G	301	UTP	O4'-C1'-N1	-2.18	103.43	108.36
3	F	301	UTP	O1G-PG-O3B	2.16	111.88	104.64
3	G	301	UTP	C1'-N1-C2	2.16	121.46	117.59
3	D	301	UTP	O2A-PA-O1A	-2.13	102.52	112.44
3	A	301	UTP	O1B-PB-O2B	-2.13	102.56	112.44
3	J	301	UTP	O1B-PB-O2B	-2.11	102.63	112.44
2	I	302	UDP	O2'-C2'-C3'	-2.11	105.06	111.82
3	A	301	UTP	C3'-C2'-C1'	2.11	105.45	101.46
3	L	301	UTP	O1B-PB-O2B	-2.10	102.68	112.44
3	J	301	UTP	O1G-PG-O2G	-2.10	102.66	110.83
3	A	301	UTP	O1B-PB-O3A	2.07	112.87	107.27
3	D	301	UTP	O1B-PB-O3B	2.06	112.84	107.27
3	C	301	UTP	C2'-C3'-C4'	2.05	106.58	102.61
3	C	301	UTP	O1B-PB-O2B	-2.02	103.03	112.44
3	L	301	UTP	O2A-PA-O3A	2.02	112.74	107.27
3	J	301	UTP	O2A-PA-O1A	-2.02	103.07	112.44

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	302	UDP	C5'-O5'-PA-O2A
2	D	302	UDP	C5'-O5'-PA-O3A
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	I	302	UDP	C5'-O5'-PA-O3A
2	H	301	UDP	C5'-O5'-PA-O1A
2	H	301	UDP	PA-O3A-PB-O2B
3	A	301	UTP	C5'-O5'-PA-O1A
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	PB-O3B-PG-O1G
3	F	301	UTP	PB-O3B-PG-O3G

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

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

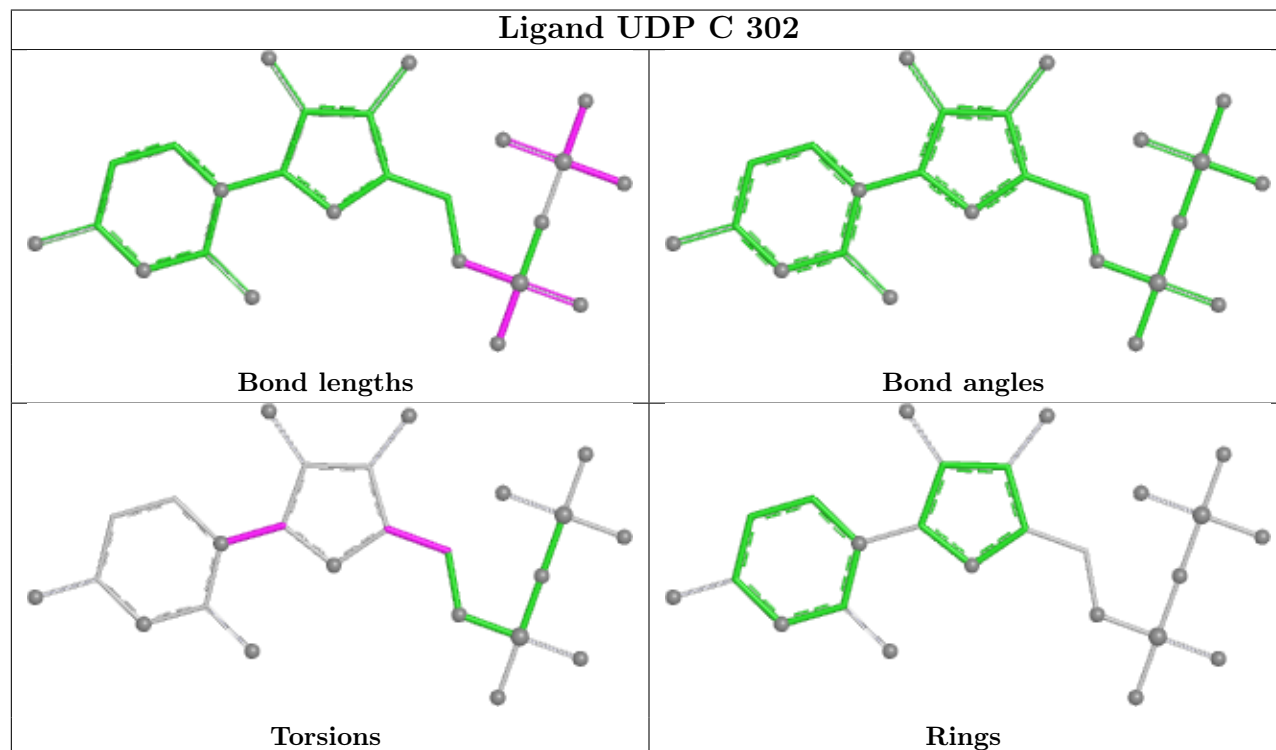
There are no ring outliers.

13 monomers are involved in 54 short contacts:

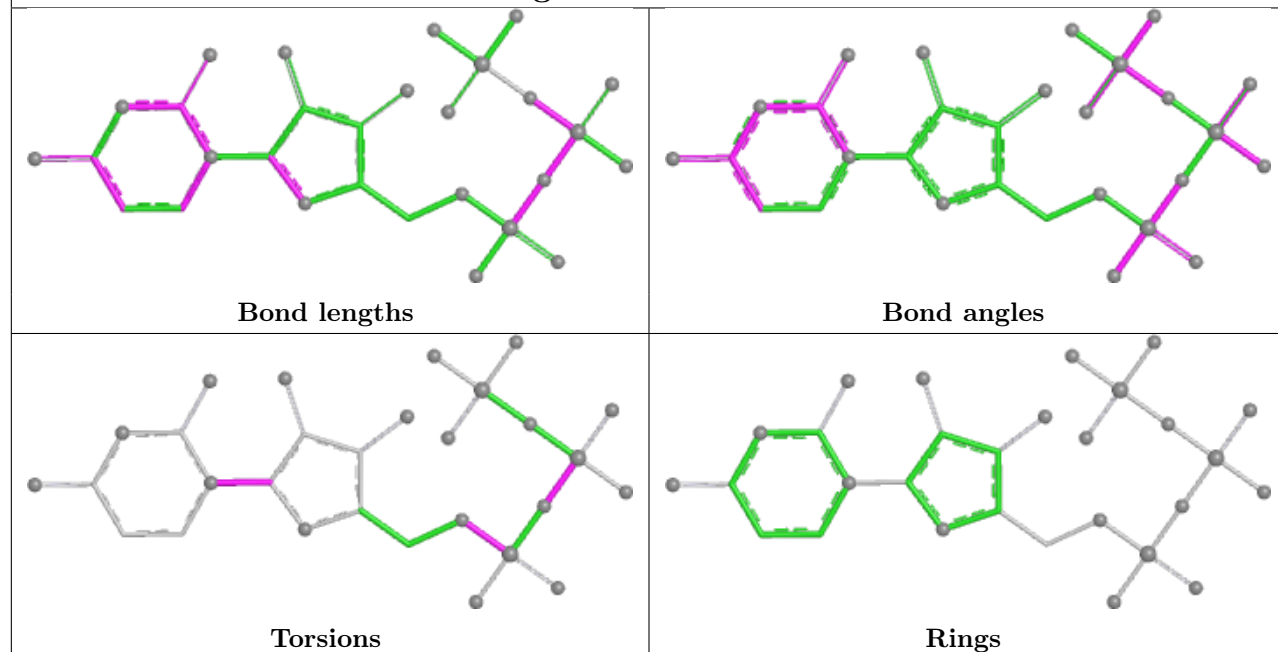
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	302	UDP	9	0
3	L	301	UTP	2	0
3	D	301	UTP	1	0
3	G	301	UTP	3	0
2	K	301	UDP	6	0
3	I	301	UTP	4	0
2	J	302	UDP	4	0
3	F	301	UTP	1	0
2	I	302	UDP	3	0
2	H	301	UDP	8	0
2	D	302	UDP	5	0
3	J	301	UTP	3	0
2	B	301	UDP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

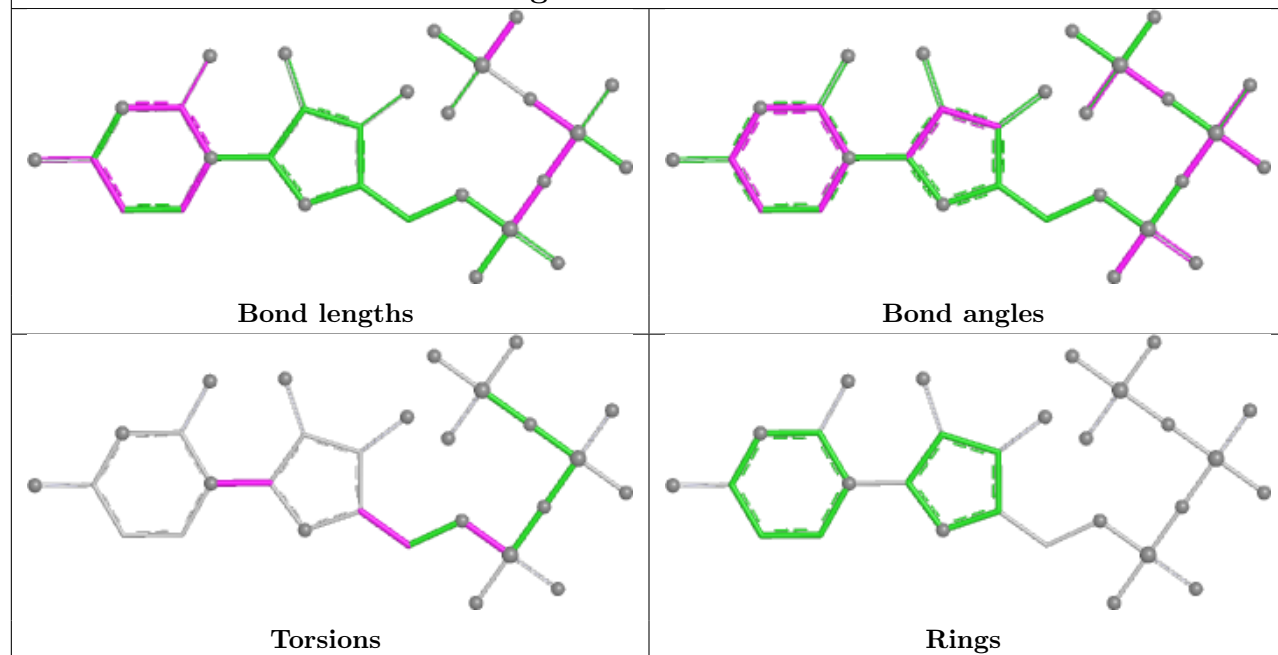
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

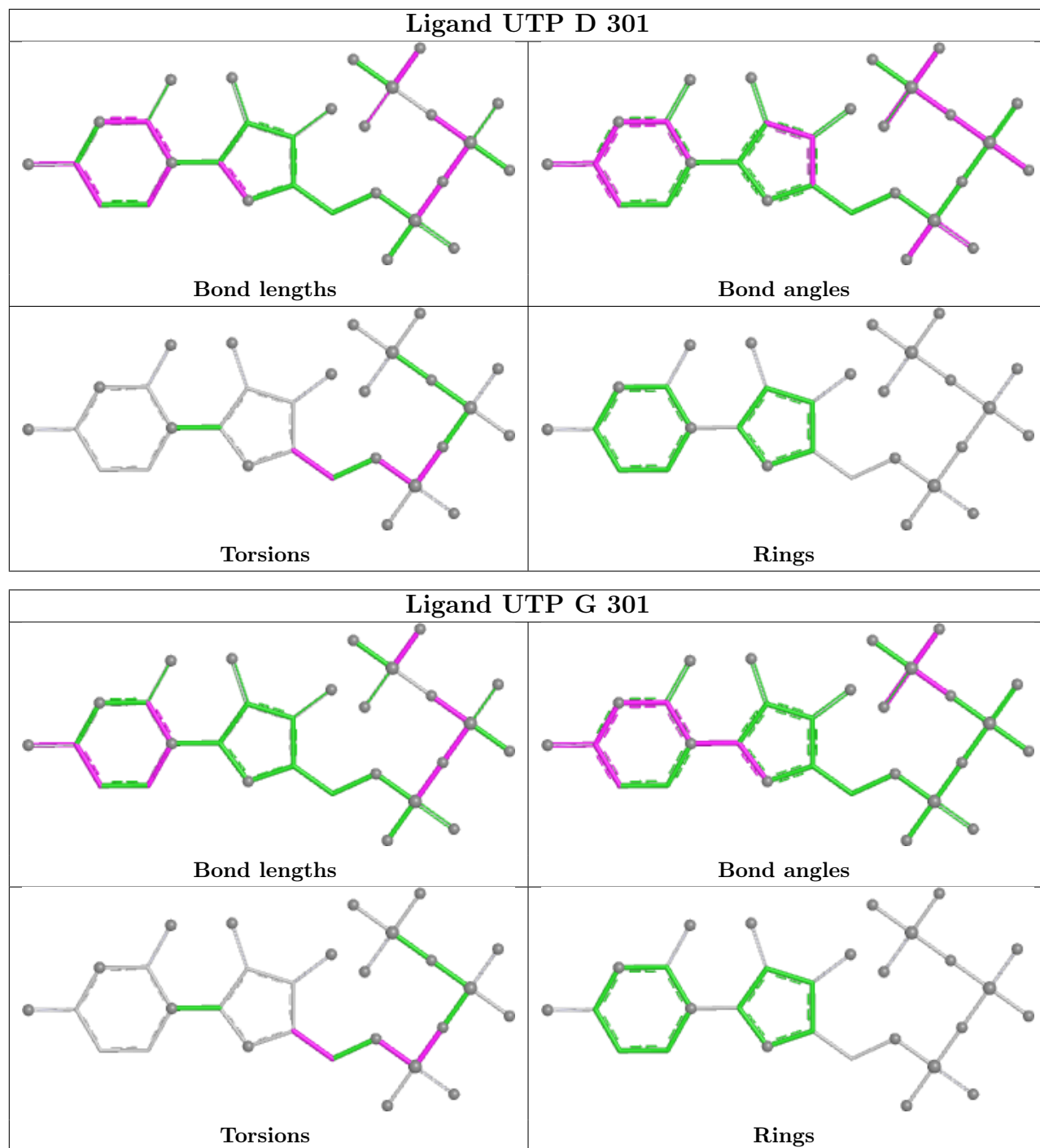


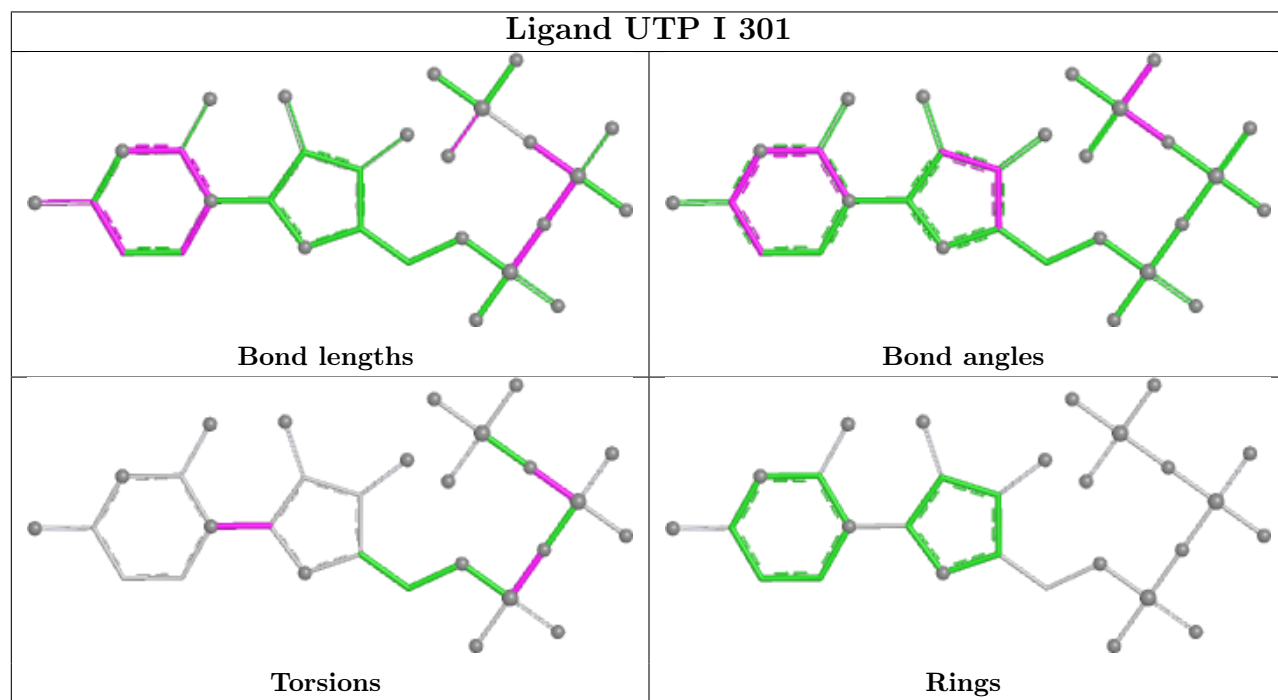
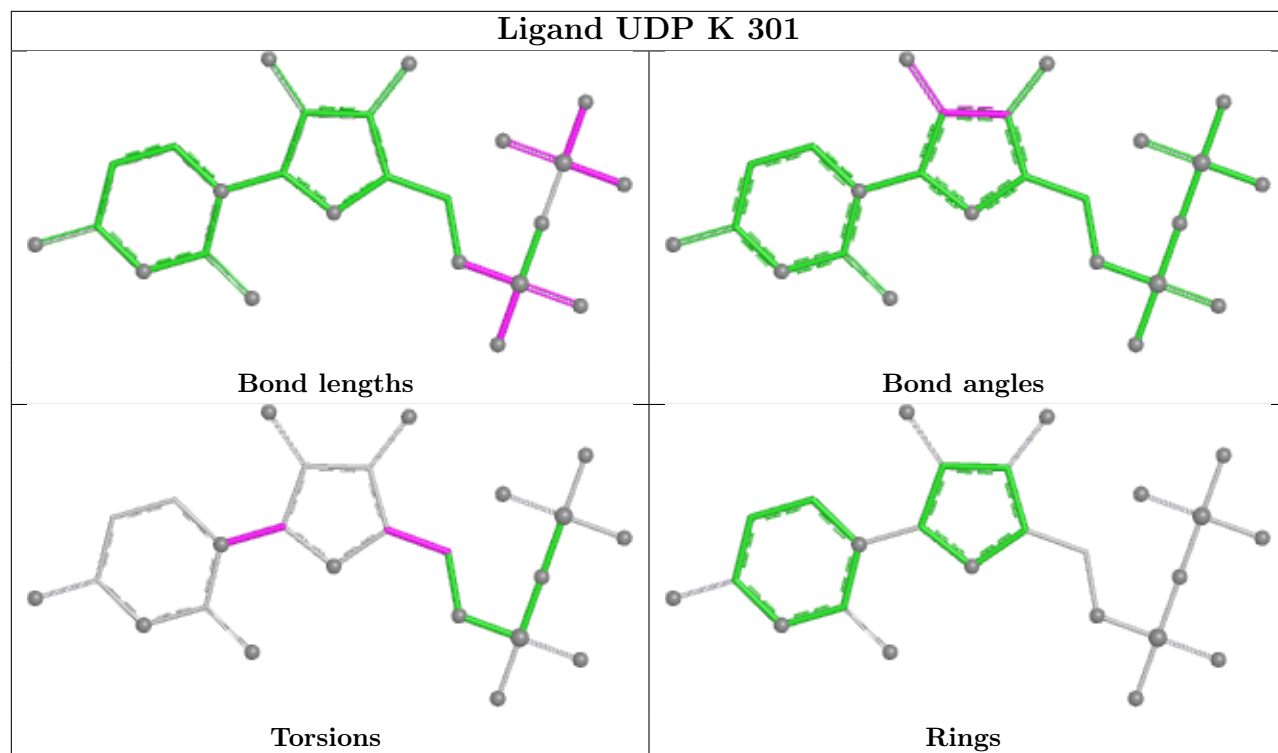
Ligand UTP L 301



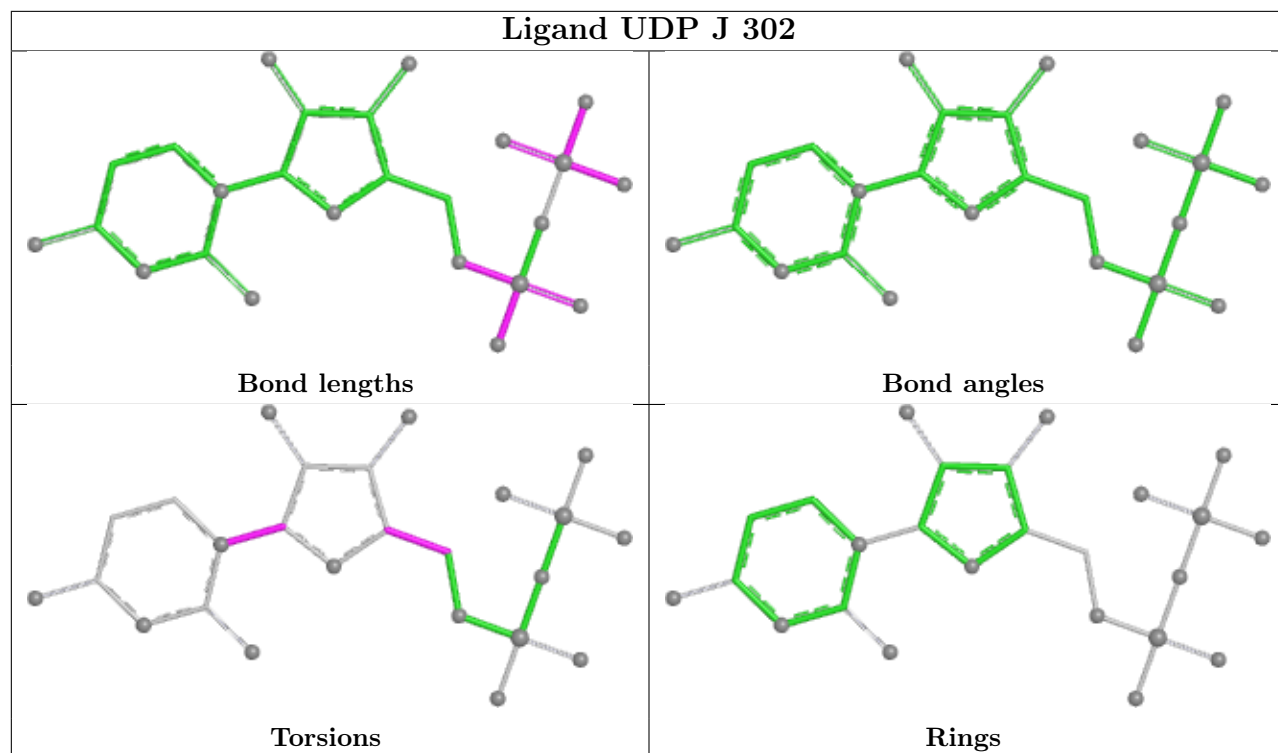
Ligand UTP A 301



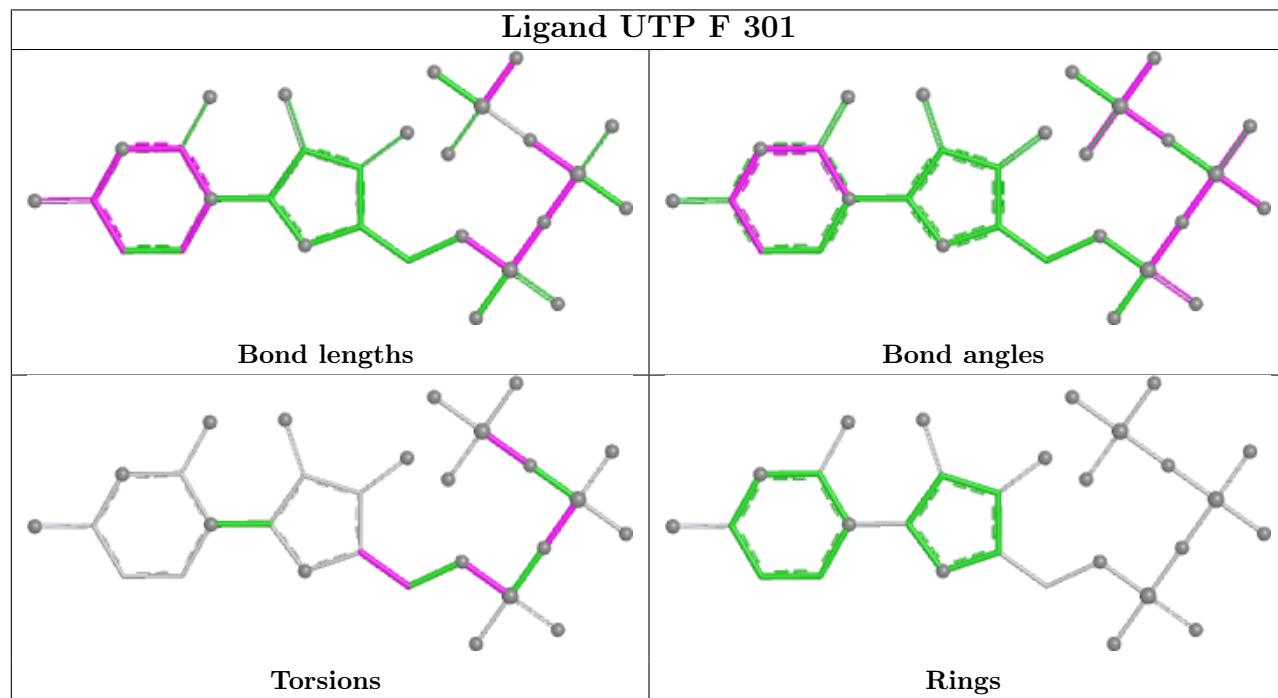




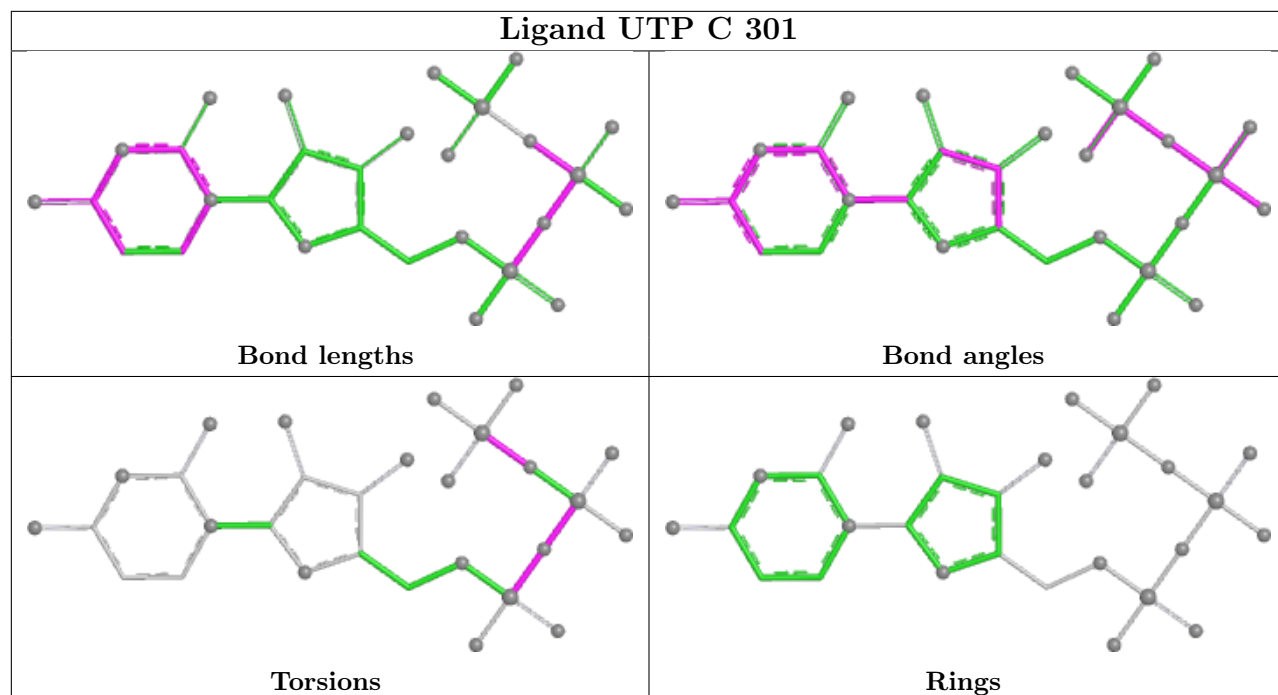
Ligand UDP J 302



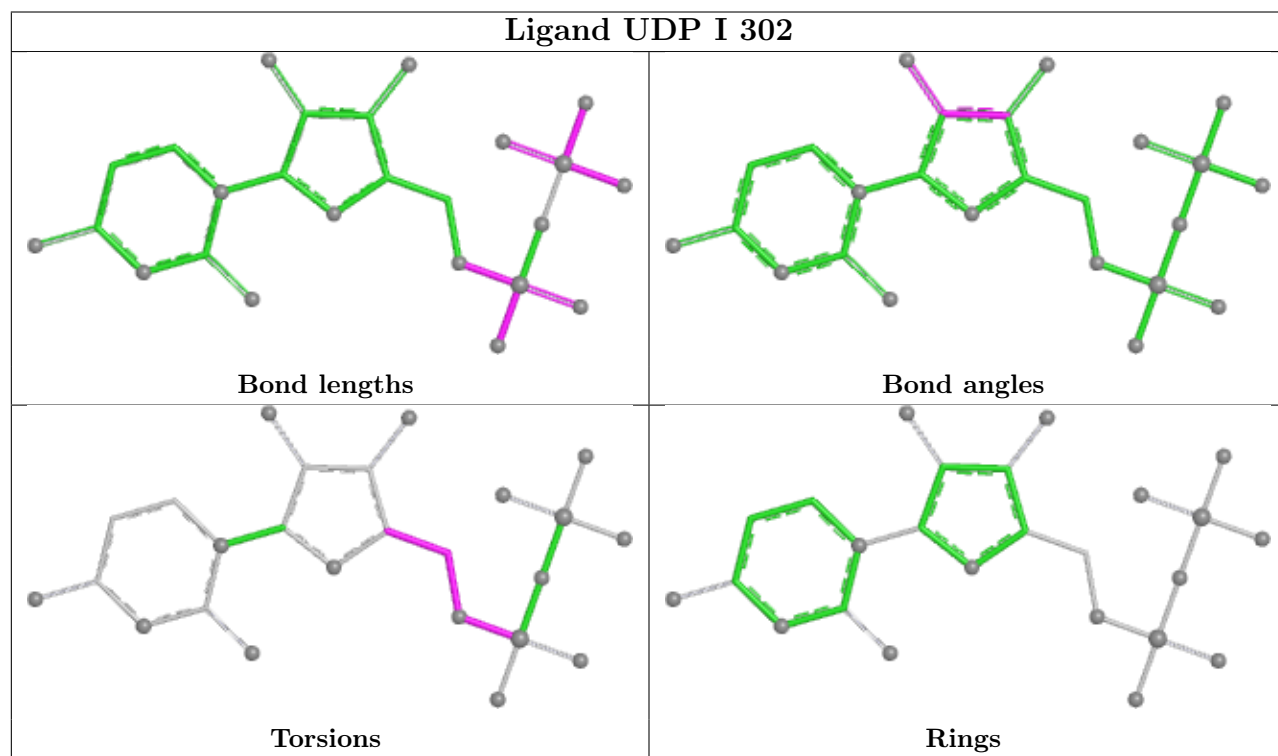
Ligand UTP F 301

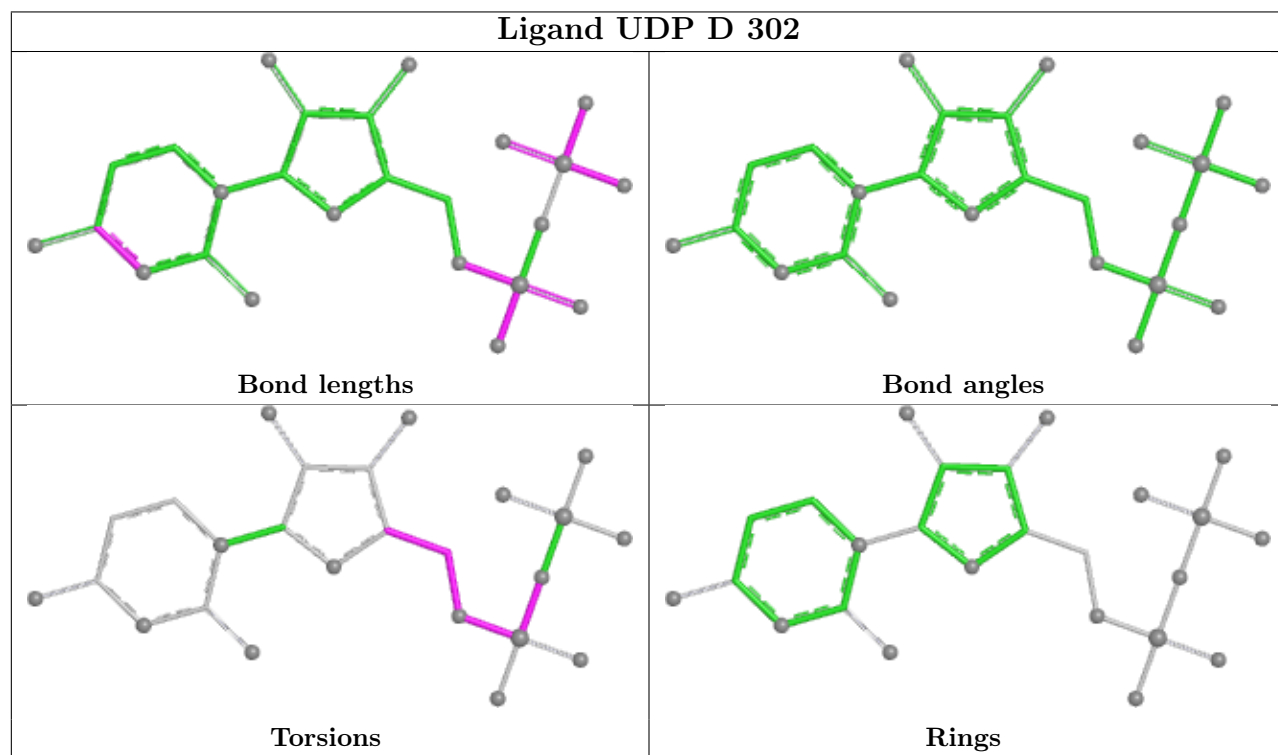
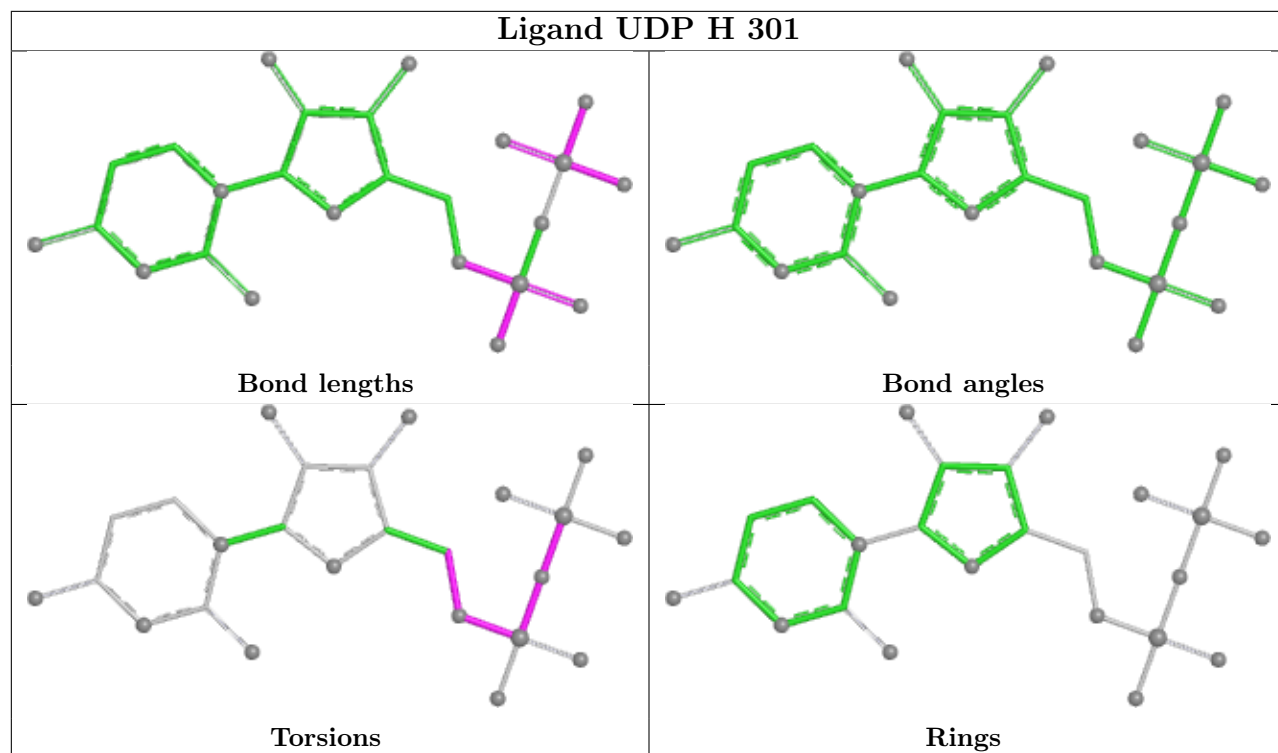


Ligand UTP C 301

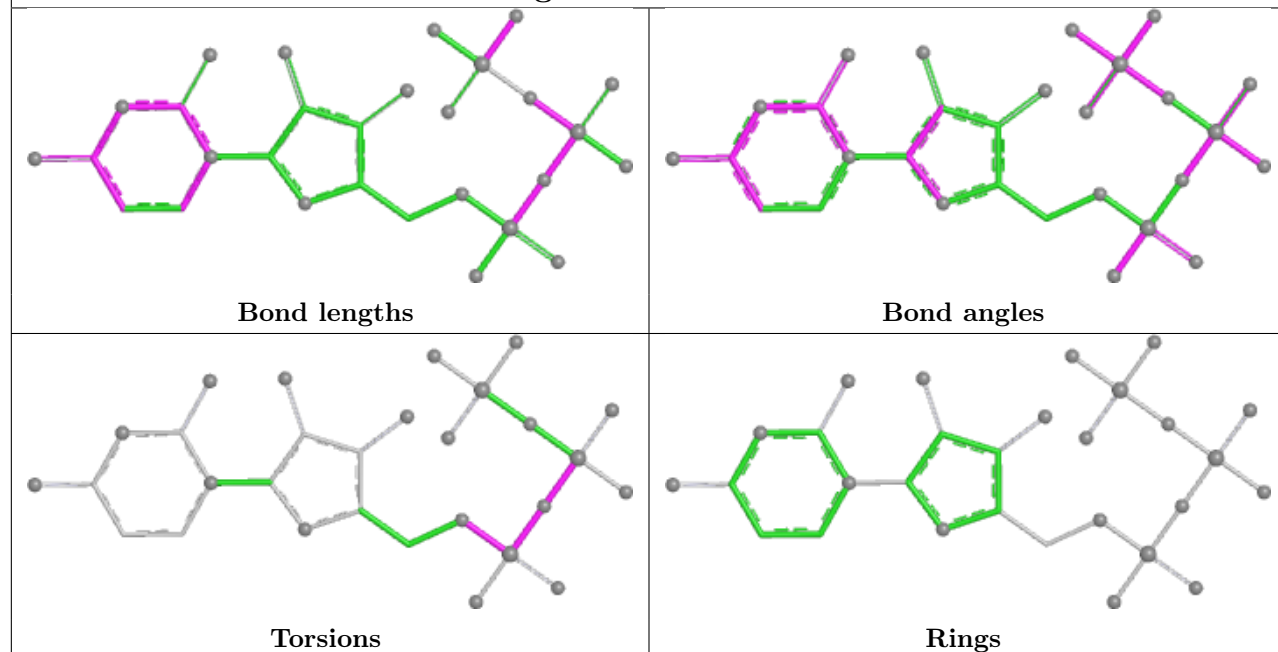


Ligand UDP I 302

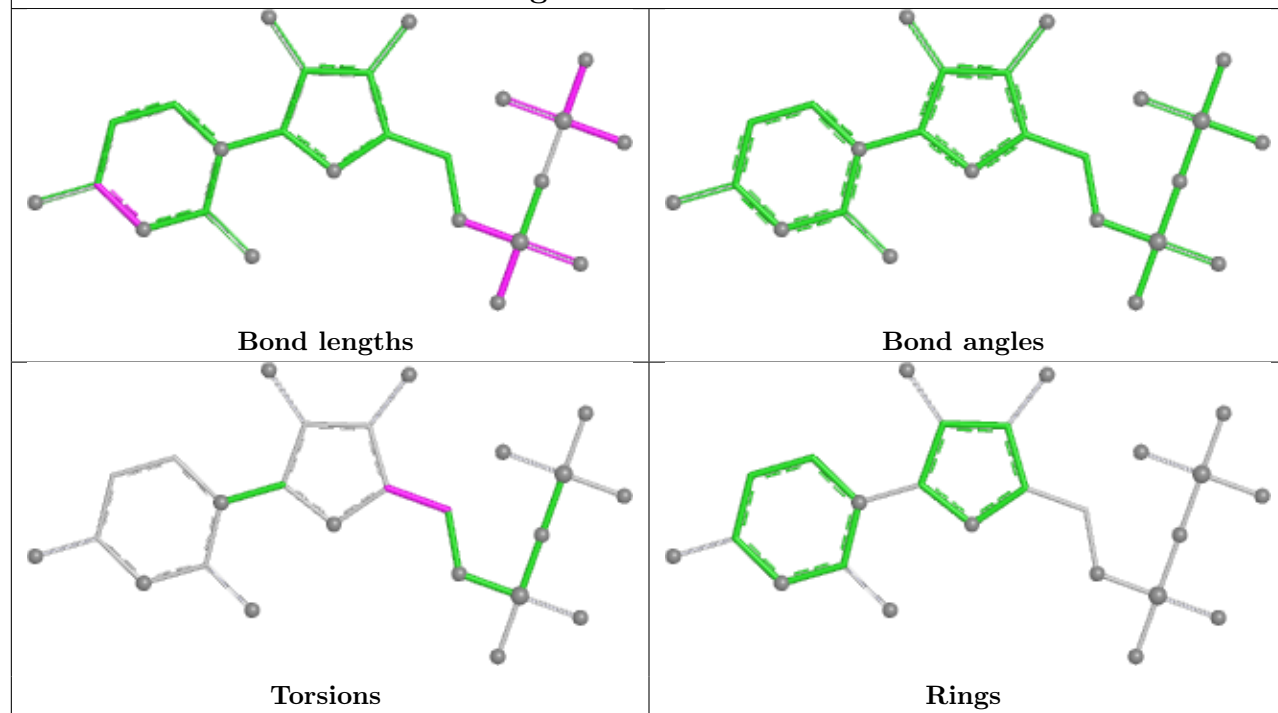


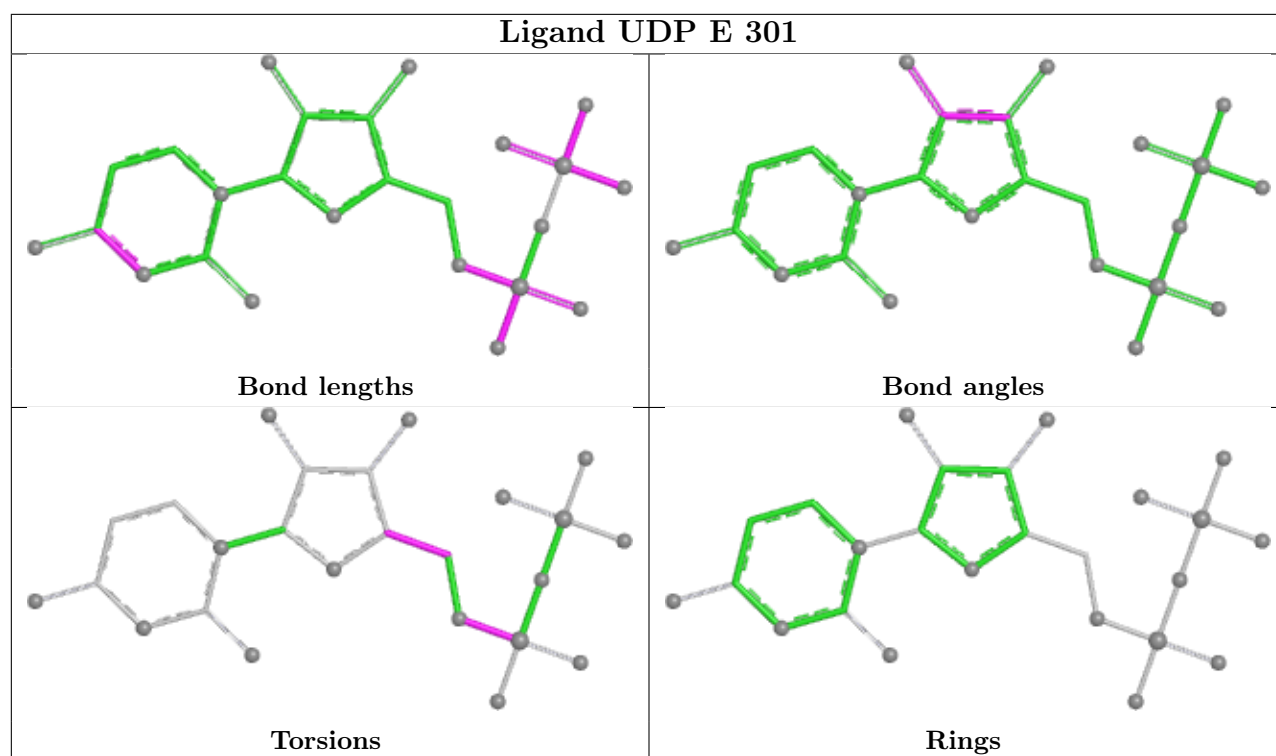


Ligand UTP J 301



Ligand UDP B 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	226/281 (80%)	-0.22	1 (0%) 88 80	20, 50, 77, 106	0
1	B	227/281 (80%)	-0.40	0 100 100	7, 31, 62, 88	0
1	C	230/281 (81%)	-0.32	2 (0%) 81 67	13, 32, 65, 85	1 (0%)
1	D	228/281 (81%)	-0.46	1 (0%) 88 80	13, 29, 57, 81	1 (0%)
1	E	222/281 (79%)	-0.35	0 100 100	17, 39, 65, 85	0
1	F	216/281 (76%)	0.02	7 (3%) 50 34	23, 48, 86, 116	3 (1%)
1	G	169/281 (60%)	0.48	12 (7%) 22 15	39, 77, 124, 141	4 (2%)
1	H	222/281 (79%)	-0.08	1 (0%) 87 77	32, 57, 82, 107	1 (0%)
1	I	225/281 (80%)	-0.29	2 (0%) 81 67	22, 43, 92, 115	0
1	J	227/281 (80%)	-0.29	1 (0%) 88 80	20, 40, 73, 95	0
1	K	224/281 (79%)	-0.20	0 100 100	24, 40, 76, 111	0
1	L	158/281 (56%)	0.49	7 (4%) 39 26	41, 84, 110, 125	3 (1%)
All	All	2574/3372 (76%)	-0.16	34 (1%) 75 57	7, 44, 90, 141	13 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	85	GLN	9.9
1	F	209	HIS	9.3
1	G	83	GLY	8.8
1	G	84	ALA	8.7
1	L	85	GLN	8.2
1	G	82	ARG	6.2
1	F	210	ARG	5.5
1	C	195	PRO	5.5
1	G	85	GLN	3.4
1	L	157	GLY	3.3
1	G	238	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	196	ARG	3.2
1	G	87	GLN	3.0
1	J	201	ALA	2.8
1	L	164	SER	2.7
1	L	161	PRO	2.7
1	D	194	ASP	2.7
1	I	192	ALA	2.7
1	F	86	LEU	2.5
1	G	162	TYR	2.5
1	G	256	GLY	2.5
1	F	92	GLU	2.4
1	G	157	GLY	2.4
1	L	87	GLN	2.3
1	H	46	GLN	2.3
1	I	189	GLY	2.3
1	L	119	GLY	2.2
1	F	87	GLN	2.2
1	G	234	PRO	2.2
1	F	89	LEU	2.1
1	L	86	LEU	2.1
1	A	86	LEU	2.1
1	G	240	LEU	2.1
1	G	92	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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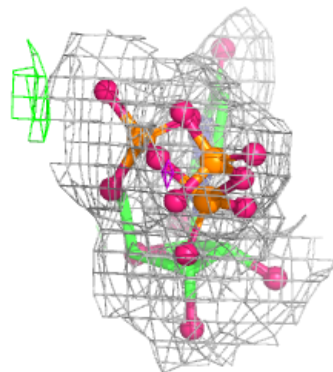
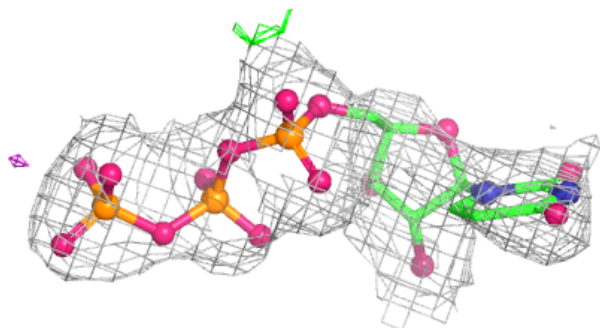
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UTP	L	301	29/29	0.88	0.10	51,68,92,97	0
3	UTP	A	301	29/29	0.91	0.09	47,58,99,102	0
2	UDP	H	301	25/25	0.91	0.10	23,44,62,73	0
2	UDP	K	301	25/25	0.94	0.09	23,49,86,95	0
2	UDP	B	301	25/25	0.94	0.09	23,46,72,78	0
3	UTP	G	301	29/29	0.94	0.08	21,45,72,79	0
2	UDP	D	302	25/25	0.95	0.08	23,31,59,71	0
2	UDP	C	302	25/25	0.95	0.08	23,28,45,78	0
3	UTP	J	301	29/29	0.95	0.07	24,37,72,74	0
2	UDP	J	302	25/25	0.95	0.07	23,39,51,57	0
2	UDP	E	301	25/25	0.95	0.08	23,44,79,90	0
3	UTP	I	301	29/29	0.96	0.06	10,31,54,67	0
2	UDP	I	302	25/25	0.96	0.08	23,38,52,66	0
3	UTP	F	301	29/29	0.96	0.07	2,26,63,68	0
3	UTP	D	301	29/29	0.96	0.07	9,21,44,52	0
3	UTP	C	301	29/29	0.97	0.06	8,25,36,45	0

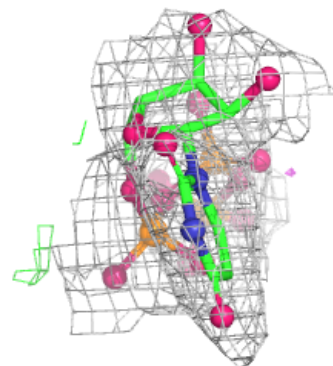
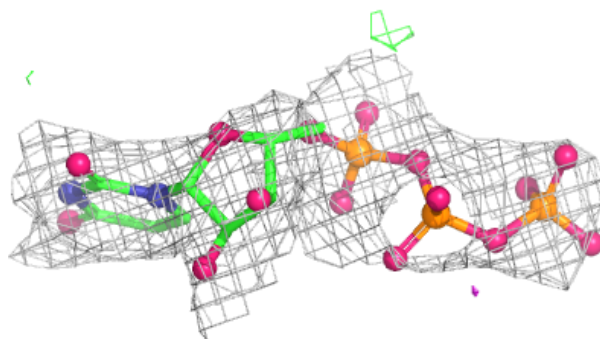
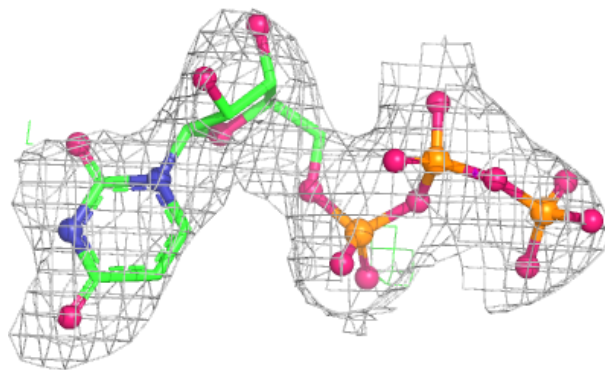
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

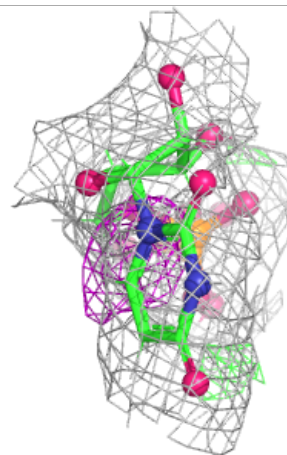
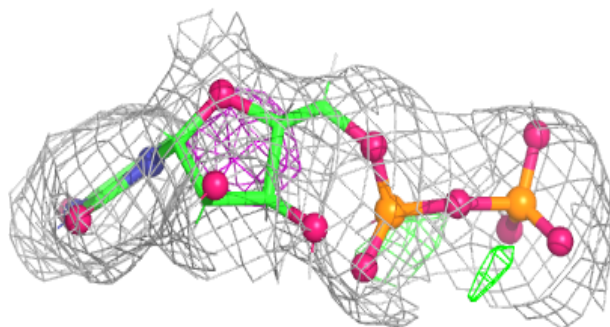
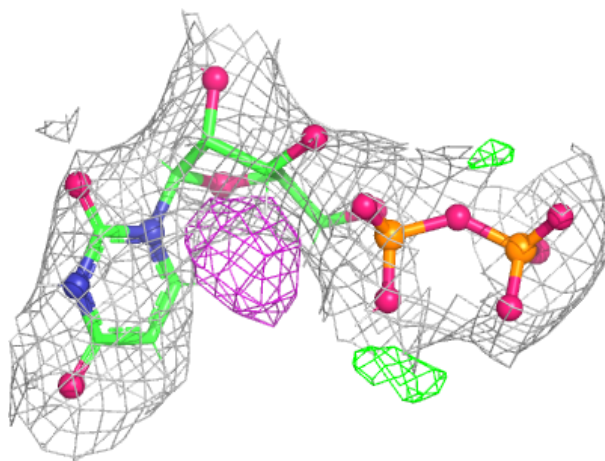
**Electron density around UTP A 301:**

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



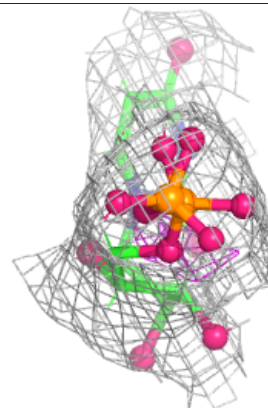
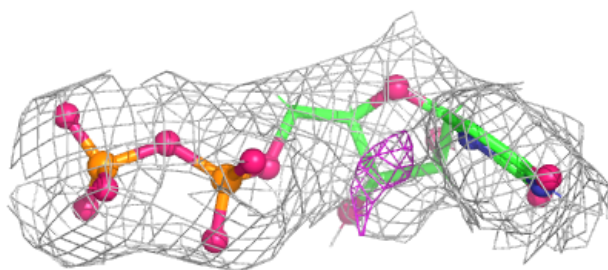
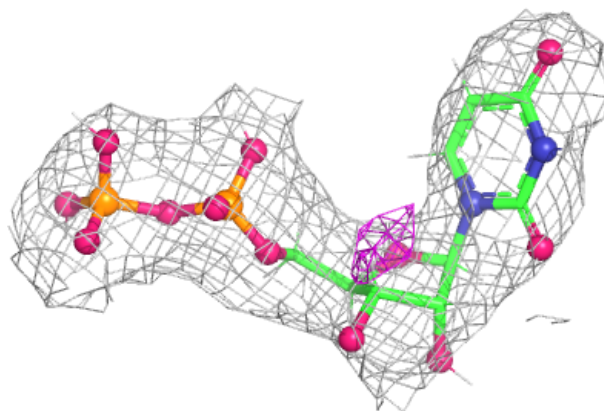
Electron density around UDP H 301:

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



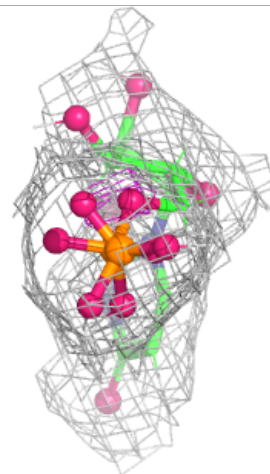
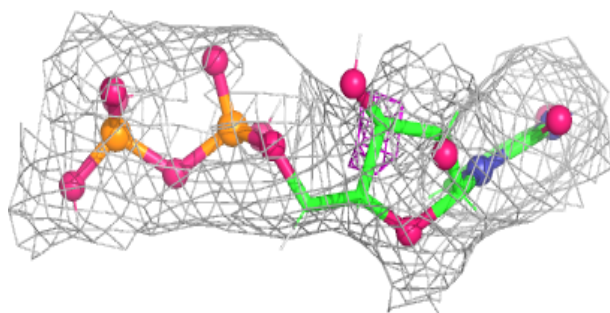
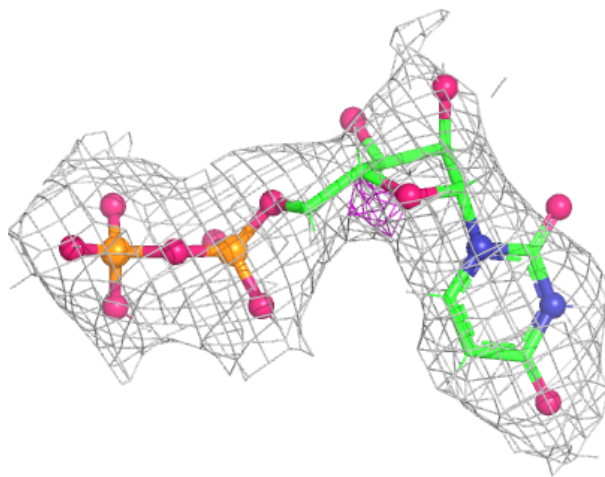
Electron density around UDP K 301:

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



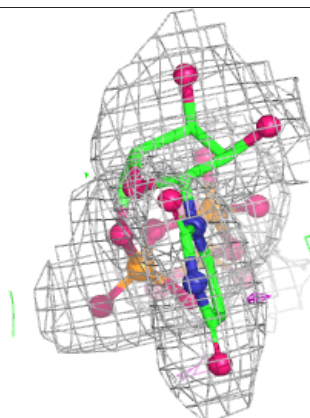
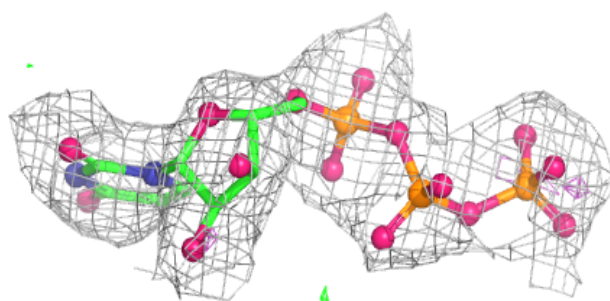
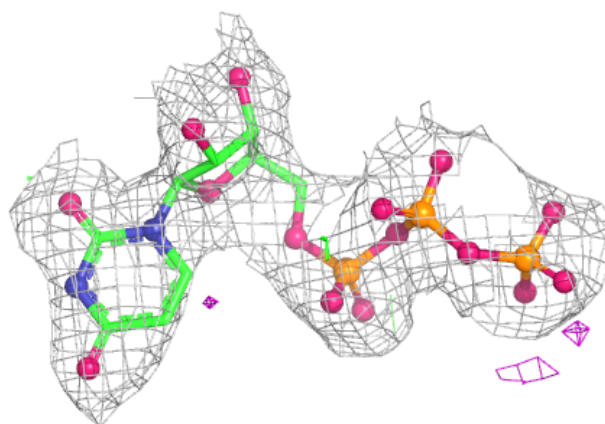
Electron density around UDP B 301:

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



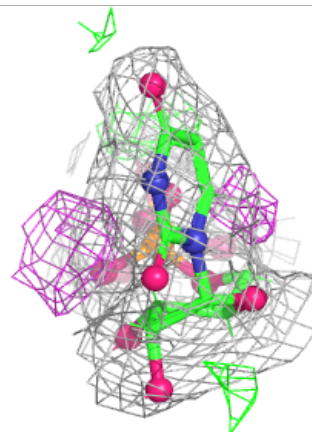
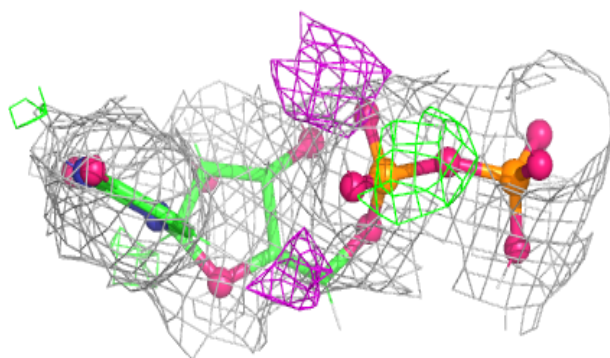
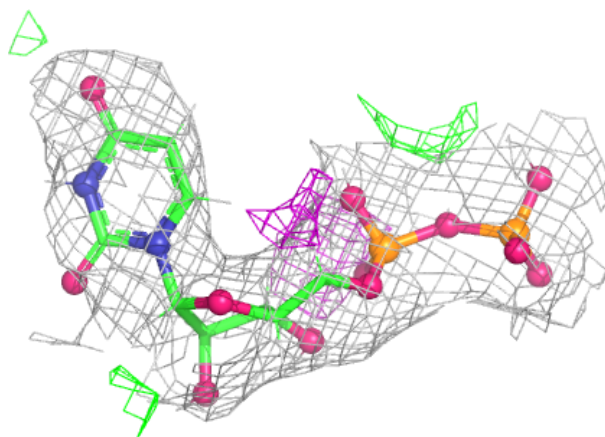
Electron density around UTP G 301:

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



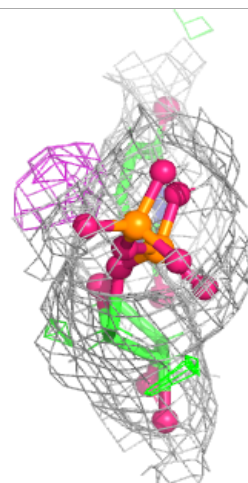
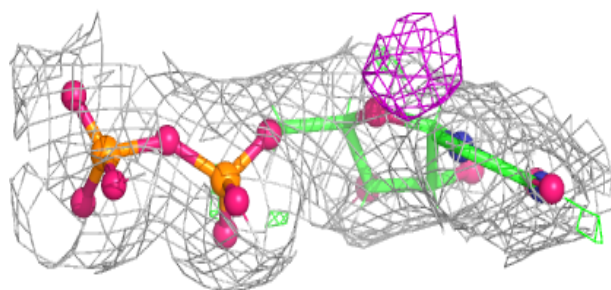
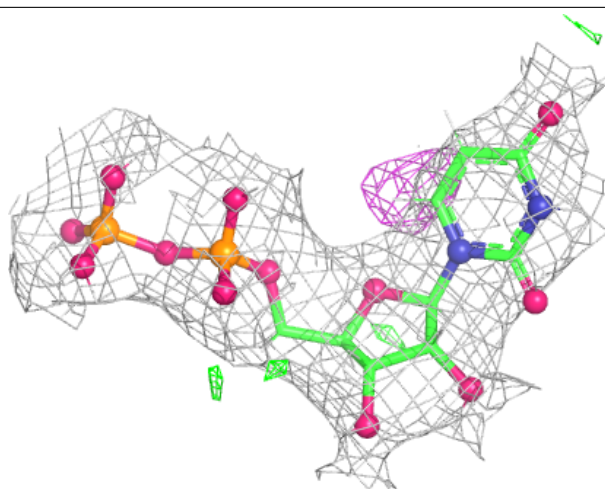
Electron density around UDP D 302:

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



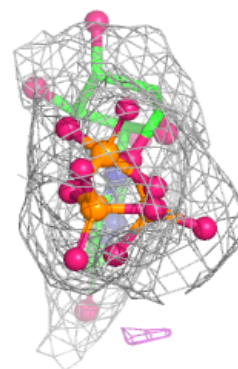
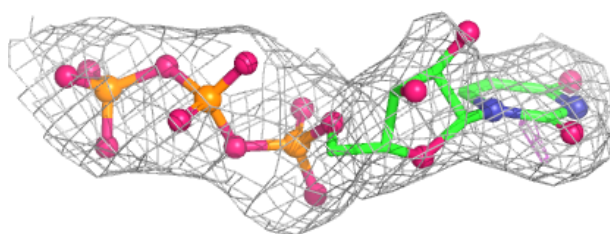
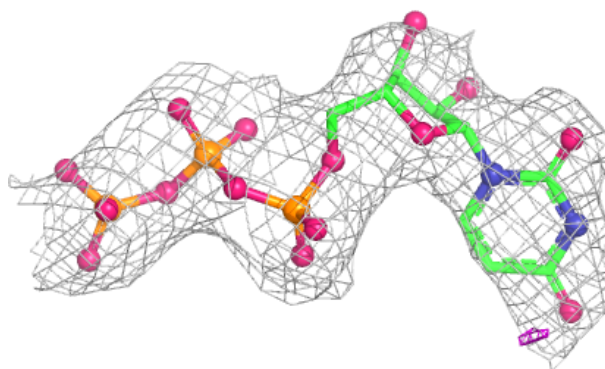
Electron density around UDP C 302:

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

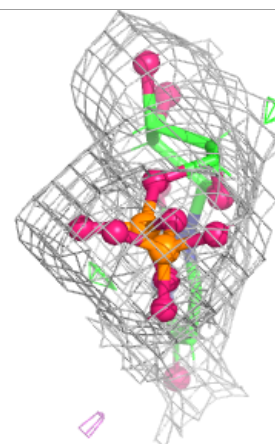
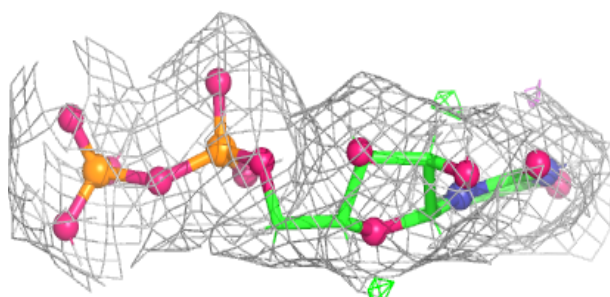
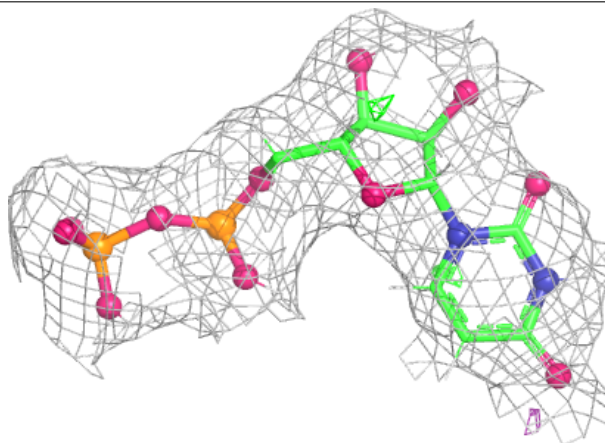


Electron density around UTP J 301:

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

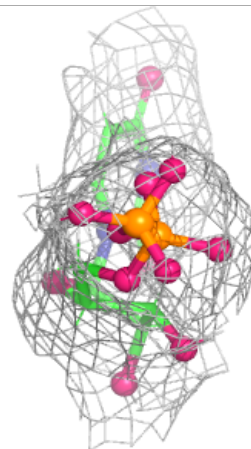
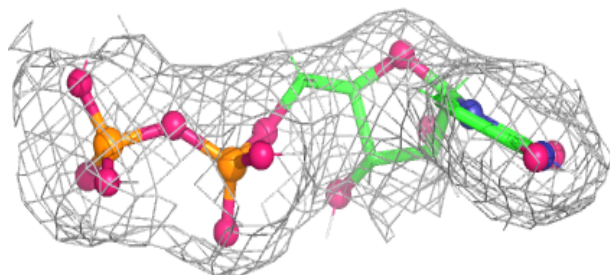
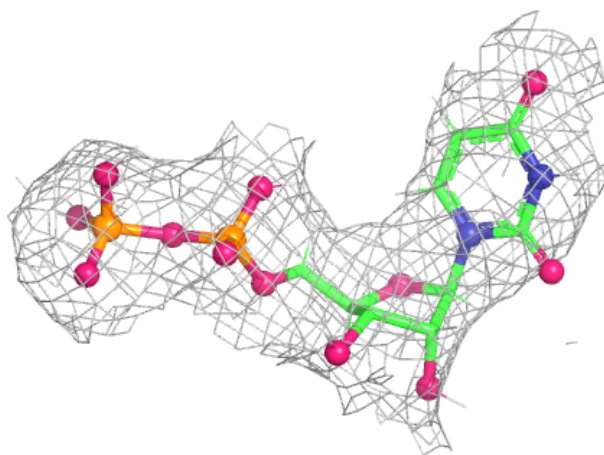
**Electron density around UDP J 302:**

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



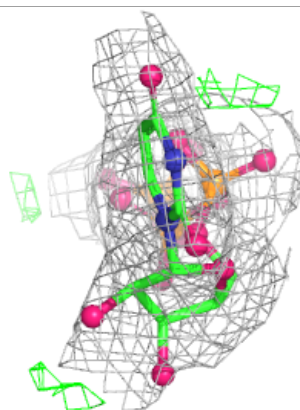
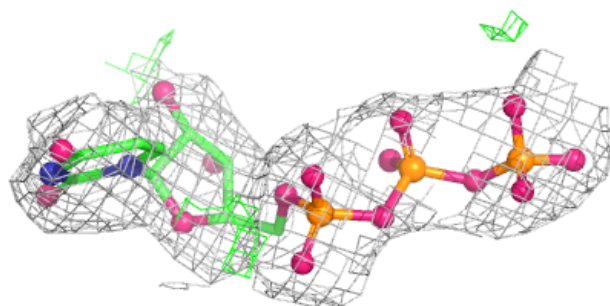
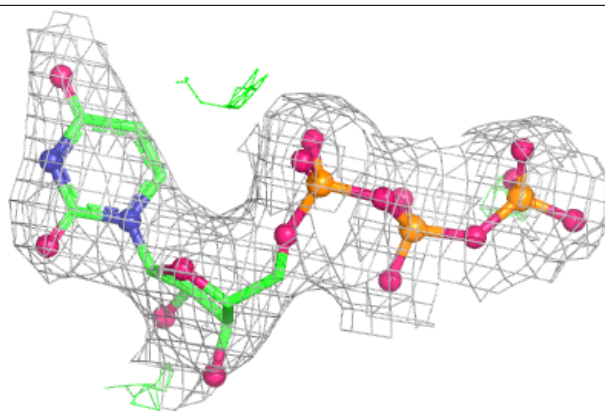
Electron density around UDP E 301:

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

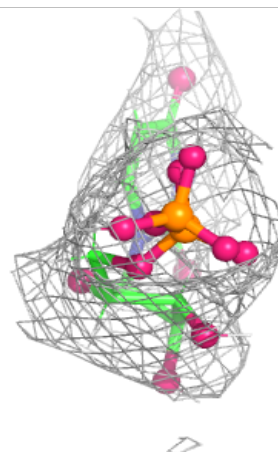
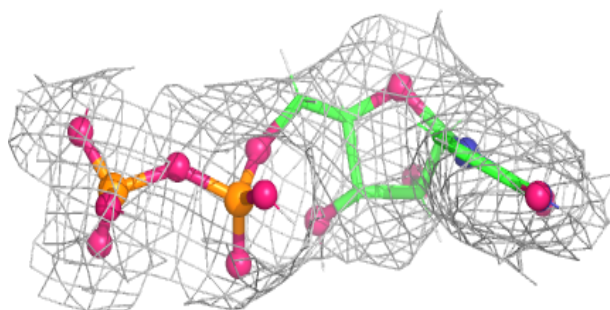
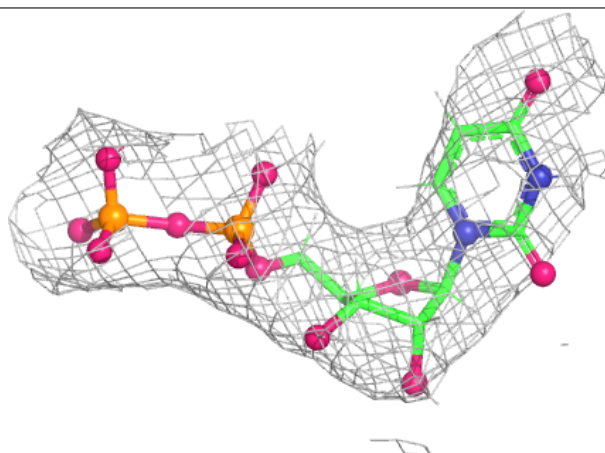


Electron density around UTP I 301:

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

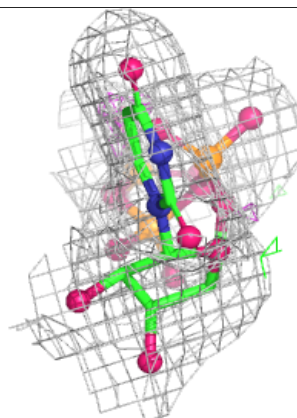
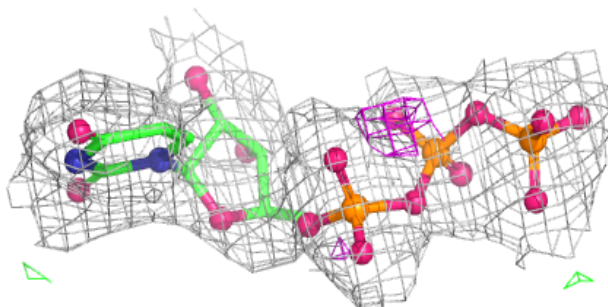
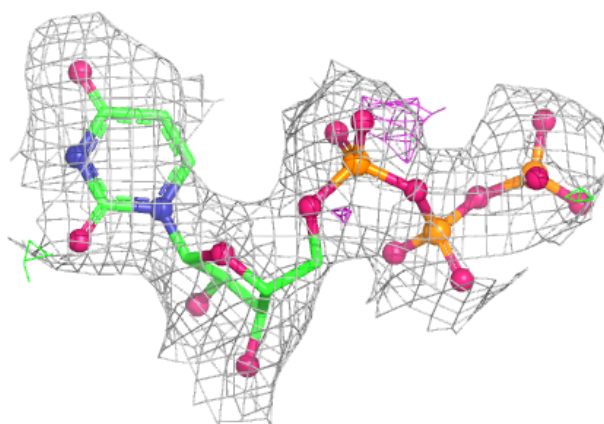
**Electron density around UDP I 302:**

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

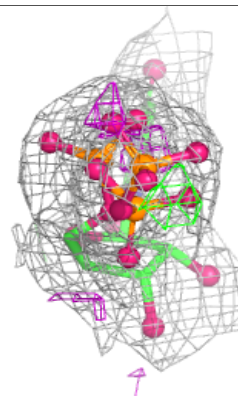
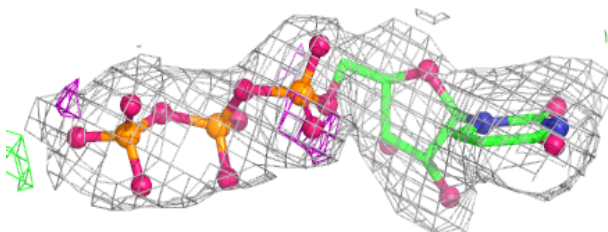
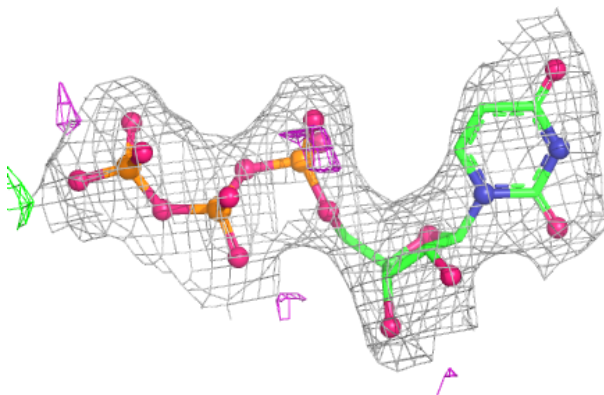


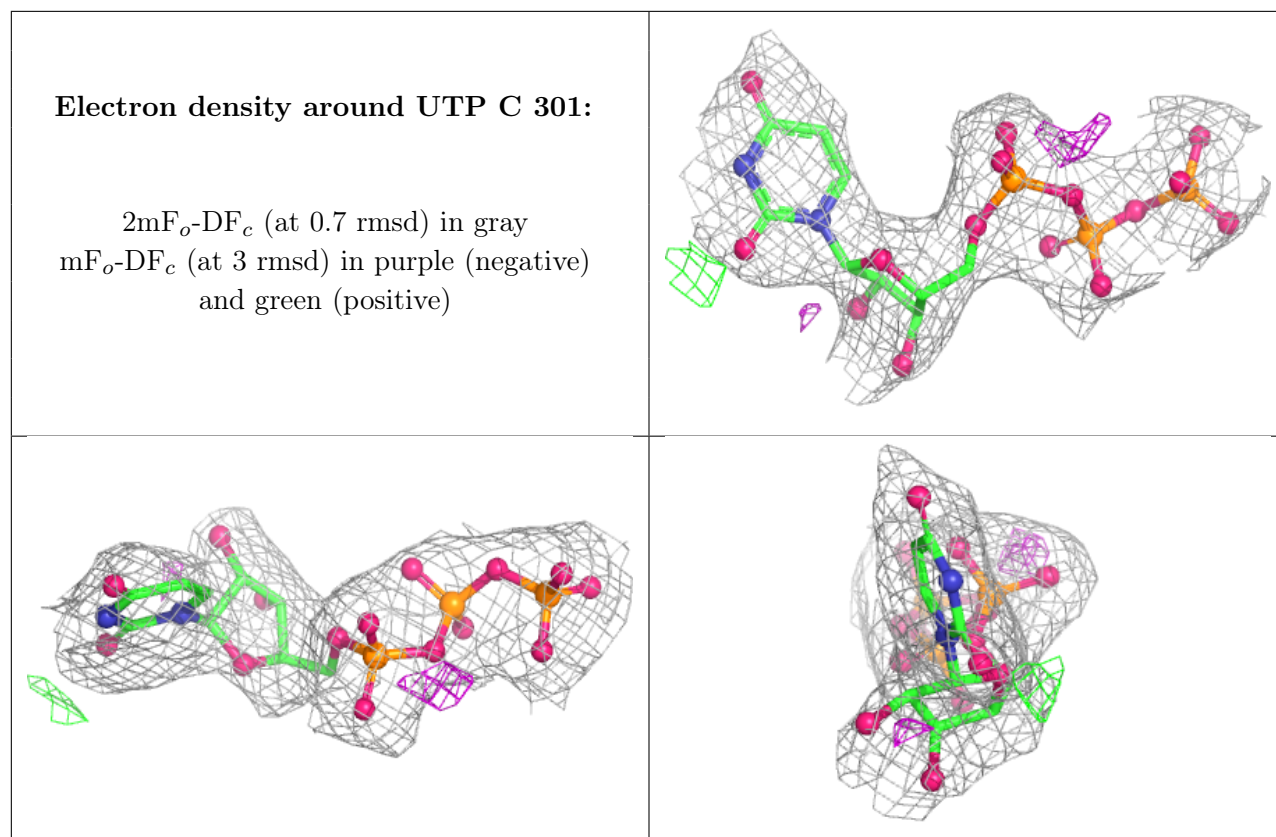
Electron density around UTP F 301:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.