Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2022 – 06:22 pm GMT

PDB ID	:	7BIX
Title	:	Crystal structure of UMPK from M. tuberculosis in complex with UDP and UTP (C2 form)
Authors	:	Labesse, G.; Walter, P.; Haouz, A.; Mechaly, A.E.; Munier-Lehmann, H.
Deposited on	:	2021-01-13
Resolution	:	3.12 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:

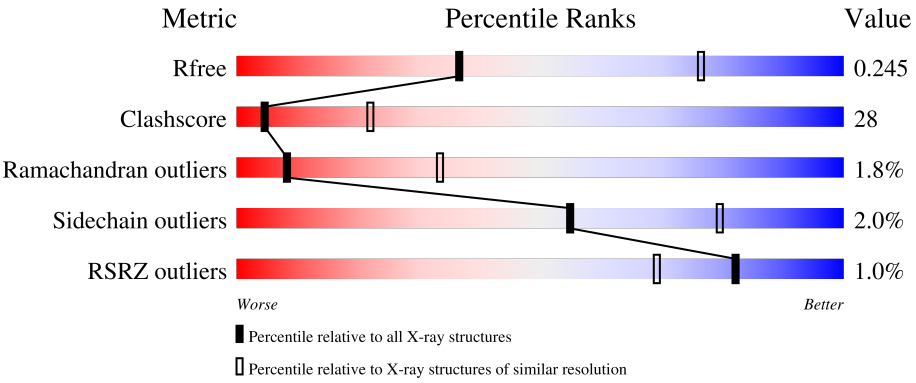
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.12 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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% 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	2% 44% 36% 20%
1	B	281	45% 34% • 20%
1	C	281	47% 33% • 19%
1	D	281	% 49% 30% • 20%
1	E	281	% 45% 32% • 20%

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Mol	Chain	Length	Quality of chain
1	F	281	2% 37% 38% 22%
1	G	281	2% 47% 30% 22%
1	H	281	47% 33% 20%
1	I	281	% 48% 31% 20%
1	J	281	46% 34% 19%
1	K	281	% 48% 32% 19%
1	L	281	43% 35% 19%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20295 atoms, of which 66 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	A	224	Total	C	N	O	S	0	0	0
			1625	1023	284	307	11			
1	B	226	Total	C	N	O	S	0	0	0
			1655	1040	291	313	11			
1	C	229	Total	C	N	O	S	0	0	0
			1694	1066	298	319	11			
1	D	225	Total	C	N	O	S	0	0	0
			1656	1042	294	309	11			
1	E	224	Total	C	N	O	S	0	0	0
			1652	1039	293	309	11			
1	F	220	Total	C	N	O	S	0	0	0
			1614	1021	281	301	11			
1	G	219	Total	C	N	O	S	0	0	0
			1584	1000	275	298	11			
1	H	225	Total	C	N	O	S	0	0	0
			1662	1046	294	311	11			
1	I	226	Total	C	N	O	S	0	0	0
			1656	1043	292	310	11			
1	J	228	Total	C	N	O	S	0	0	0
			1675	1056	294	314	11			
1	K	228	Total	C	N	O	S	0	0	0
			1673	1053	296	313	11			
1	L	227	Total	C	N	O	S	0	0	0
			1654	1040	291	313	10			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
I	-8	SER	-	expression tag	UNP P9WHK5
I	-7	GLY	-	expression tag	UNP P9WHK5

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Chain	Residue	Modelled	Actual	Comment	Reference
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
K	-6	LEU	-	expression tag	UNP P9WHK5
K	-5	VAL	-	expression tag	UNP P9WHK5

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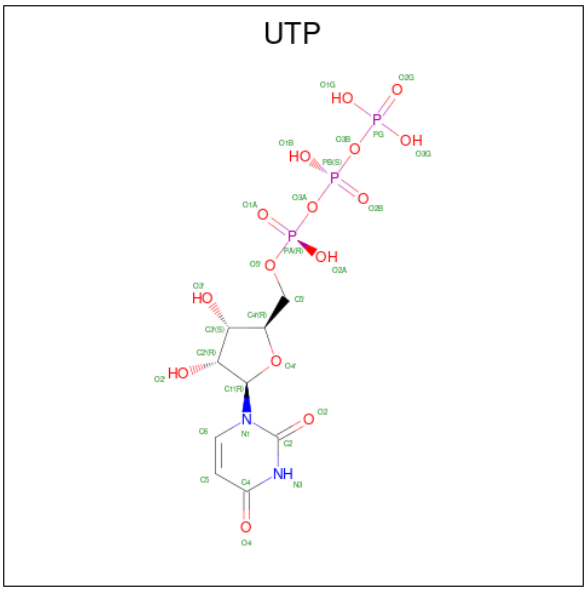
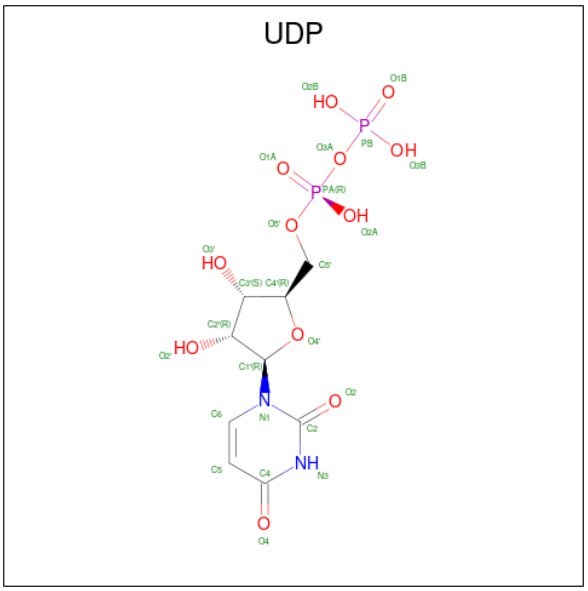
Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP P9WHK5
K	-3	ARG	-	expression tag	UNP P9WHK5
K	-2	GLY	-	expression tag	UNP P9WHK5
K	-1	SER	-	expression tag	UNP P9WHK5
K	0	HIS	-	expression tag	UNP P9WHK5
L	-19	MET	-	initiating methionine	UNP P9WHK5
L	-18	GLY	-	expression tag	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

- Molecule 2 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
2	A	1	Total	C	H	N	O	P	0	0
			40	9	11	2	15	3		
2	C	1	Total	C	H	N	O	P	0	0
			40	9	11	2	15	3		
2	D	1	Total	C	H	N	O	P	0	0
			40	9	11	2	15	3		
2	G	1	Total	C	H	N	O	P	0	0
			40	9	11	2	15	3		
2	I	1	Total	C	H	N	O	P	0	0
			40	9	11	2	15	3		
2	J	1	Total	C	H	N	O	P	0	0
			40	9	11	2	15	3		

- Molecule 3 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
3	B	1	Total C N O P 25 9 2 12 2	0	0
3	C	1	Total C N O P 25 9 2 12 2	0	0
3	D	1	Total C N O P 25 9 2 12 2	0	0
3	E	1	Total C N O P 25 9 2 12 2	0	0
3	H	1	Total C N O P 25 9 2 12 2	0	0
3	I	1	Total C N O P 25 9 2 12 2	0	0
3	J	1	Total C N O P 25 9 2 12 2	0	0
3	K	1	Total C N O P 25 9 2 12 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	2	Total O 2 2	0	0
4	C	4	Total O 4 4	0	0
4	D	5	Total O 5 5	0	0

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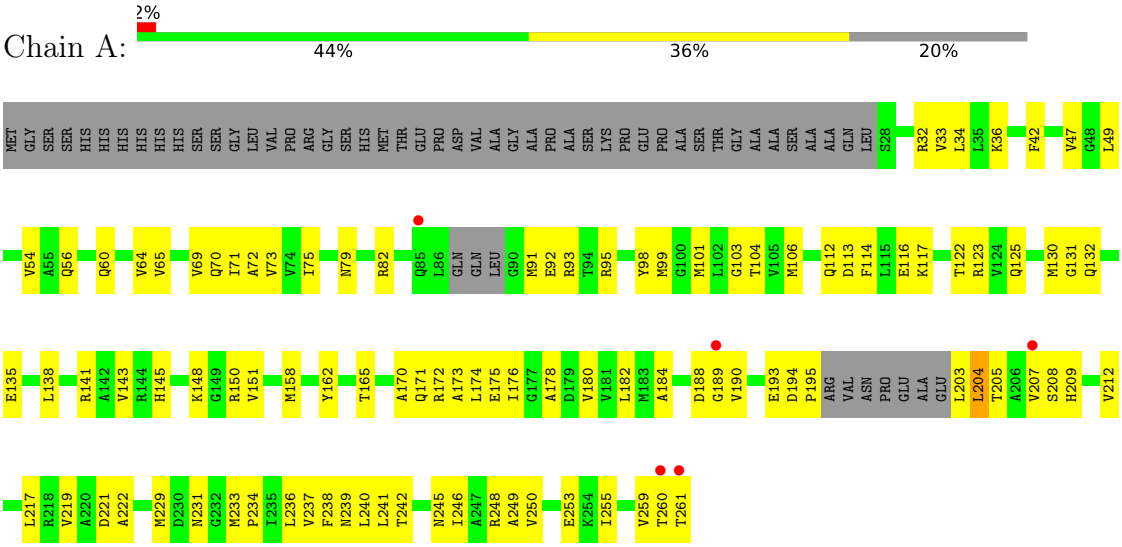
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	5	Total O 5 5	0	0
4	F	6	Total O 6 6	0	0
4	G	6	Total O 6 6	0	0
4	H	1	Total O 1 1	0	0
4	I	5	Total O 5 5	0	0
4	J	8	Total O 8 8	0	0
4	K	4	Total O 4 4	0	0
4	L	6	Total O 6 6	0	0

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.

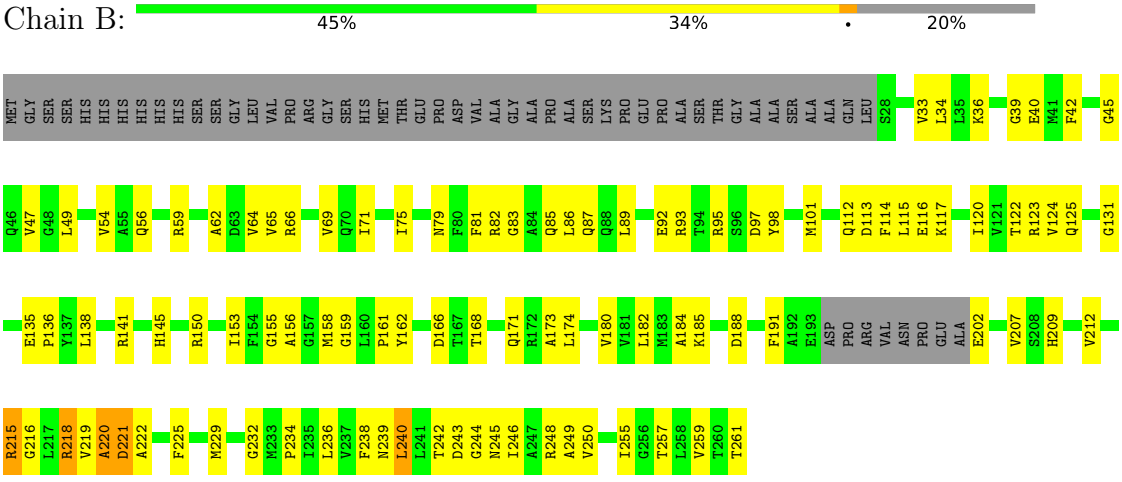
• Molecule 1: Uridylate kinase

Chain A:



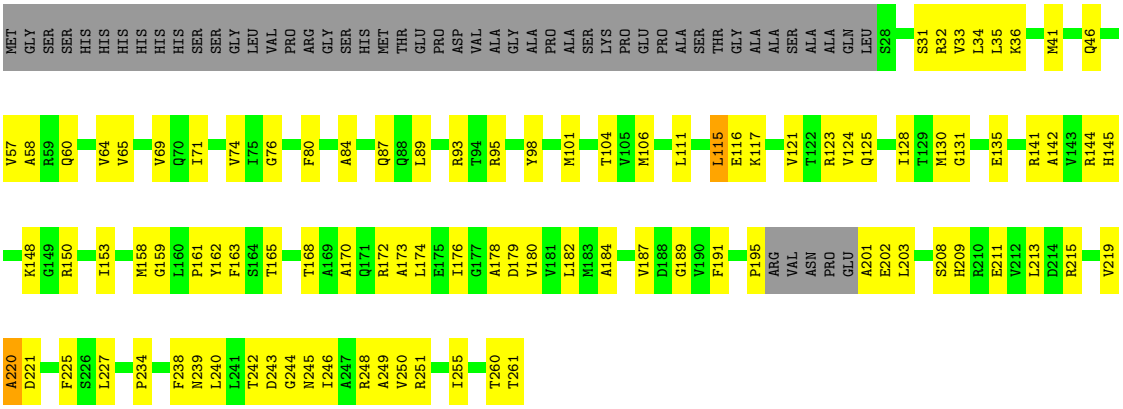
• Molecule 1: Uridylate kinase

Chain B:

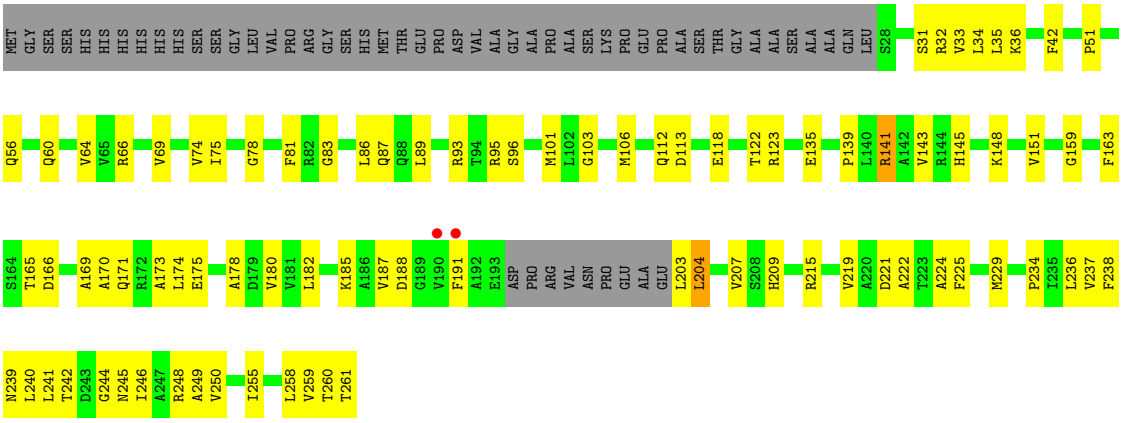


• Molecule 1: Uridylate kinase

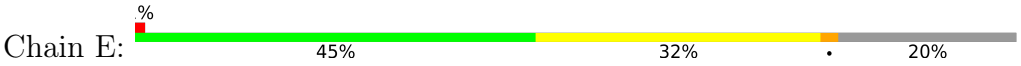
Chain C:

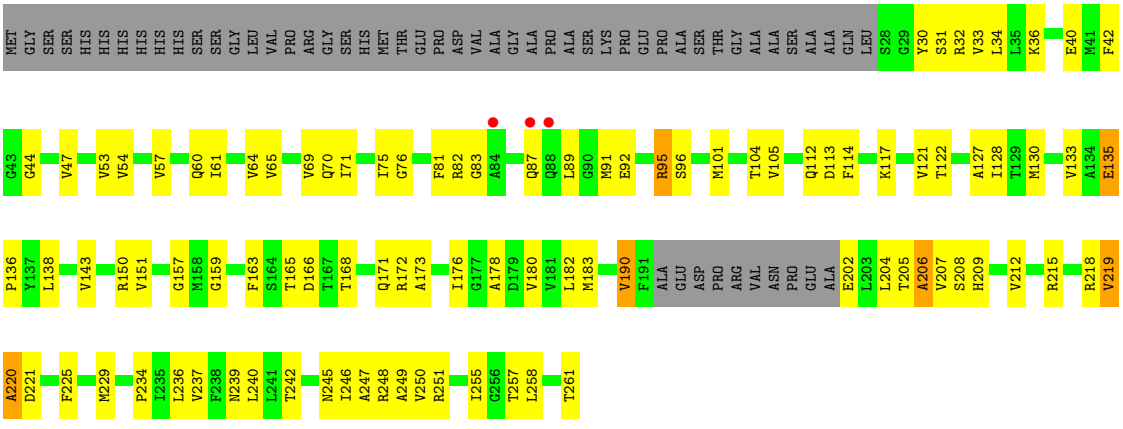


• Molecule 1: Uridylate kinase

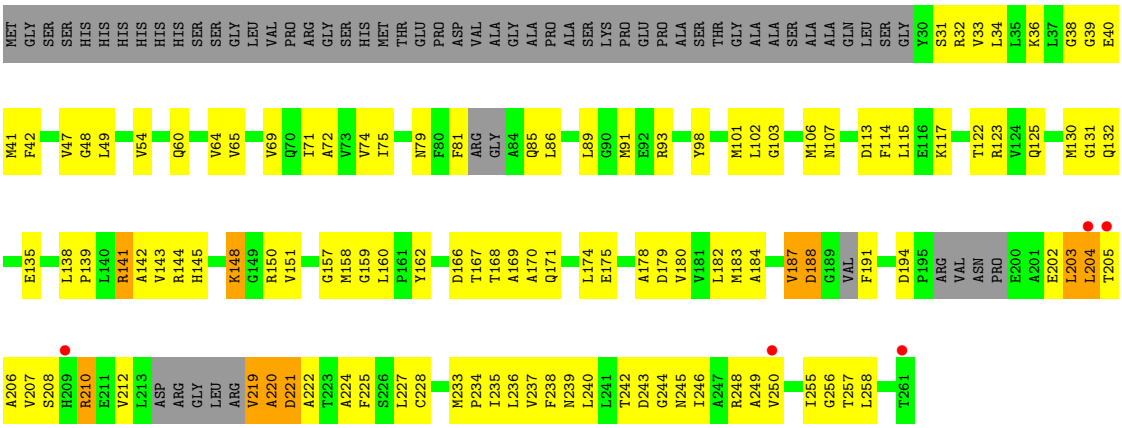


• Molecule 1: Uridylate kinase



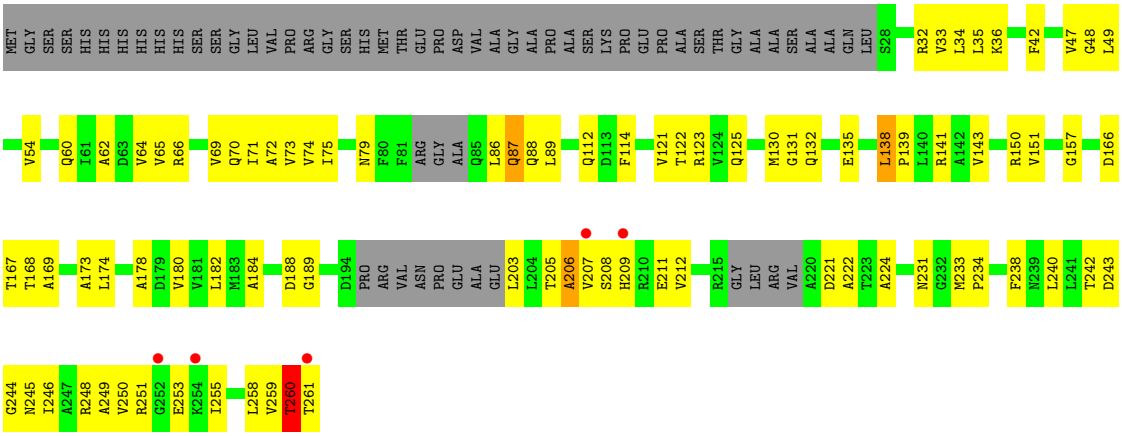


• Molecule 1: Uridylate kinase



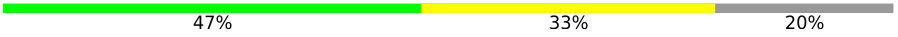
• Molecule 1: Uridylate kinase

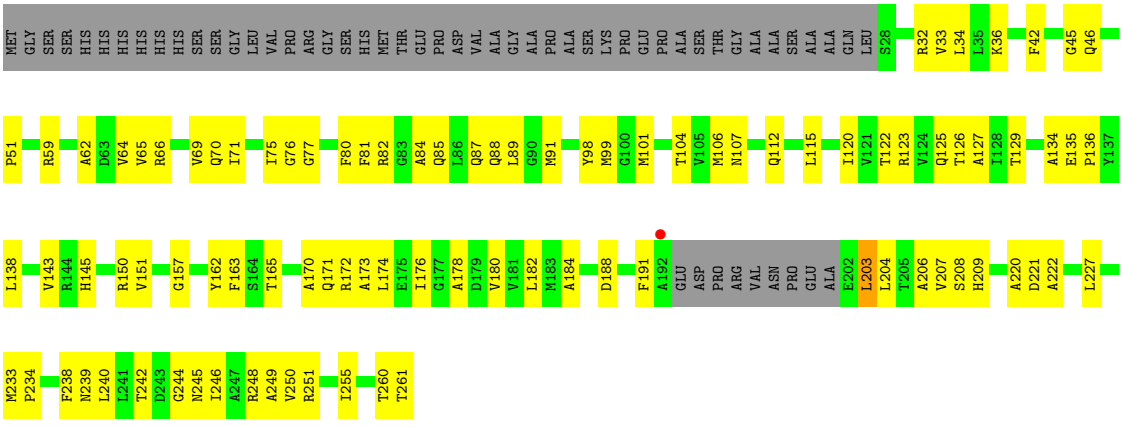
Chain G:



• Molecule 1: Uridylate kinase

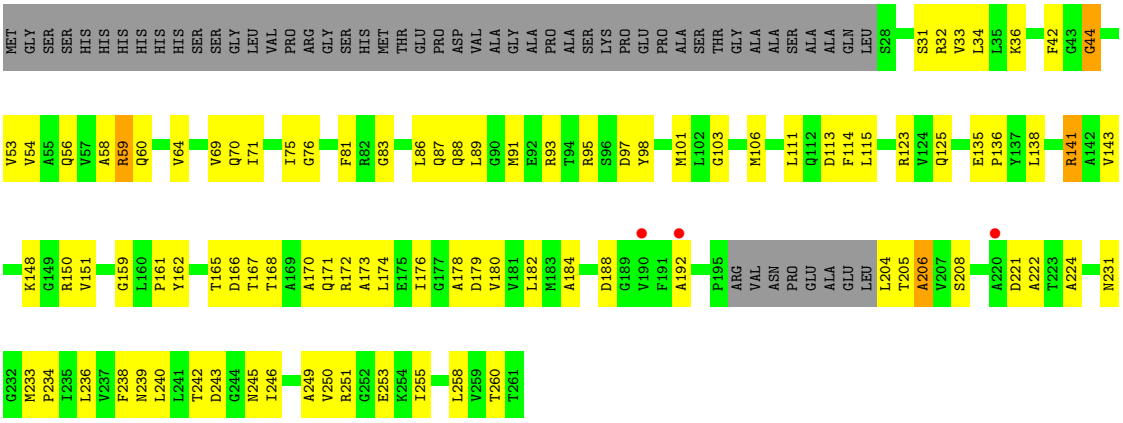
Chain H:





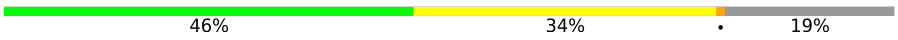
• Molecule 1: Uridylate kinase

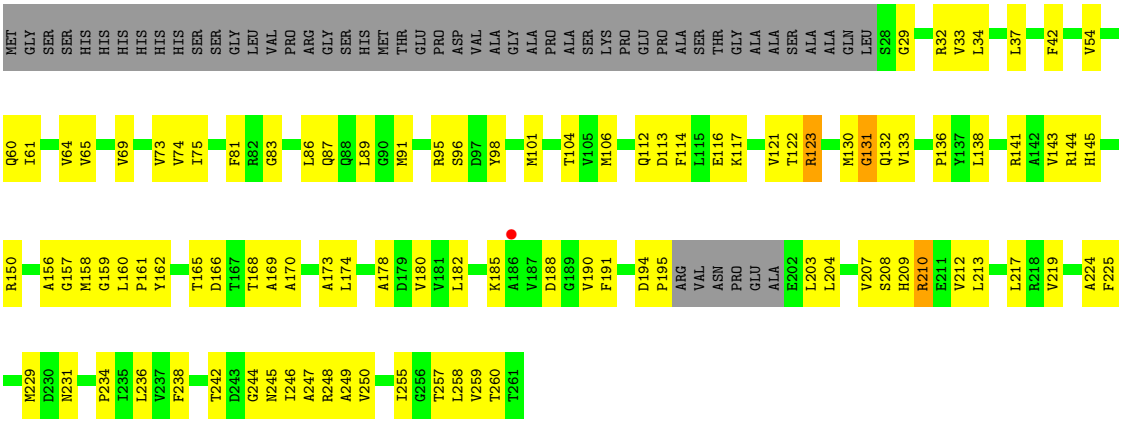
Chain I:



• Molecule 1: Uridylate kinase

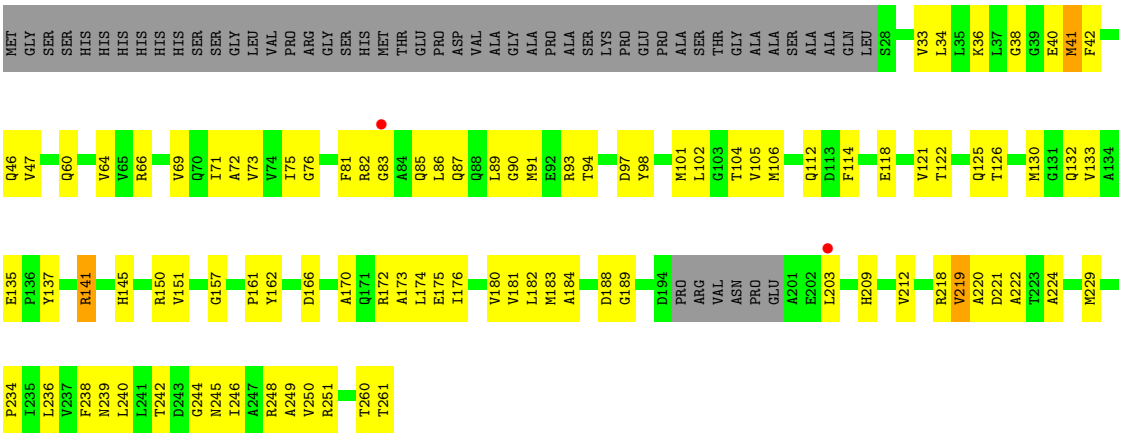
Chain J:





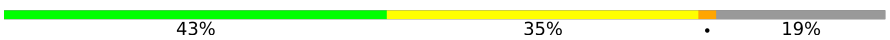
• Molecule 1: Uridylate kinase

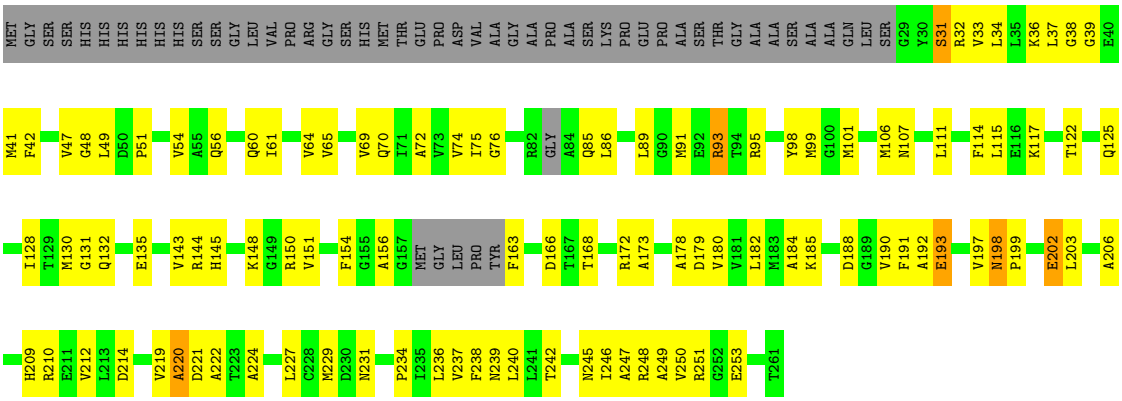
Chain K:



• Molecule 1: Uridylate kinase

Chain L:




MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET THR GLU PRO ASP VAL ALA GLY ALA PRO ALA SER LYS PRO GLU PRO ALA SER THR GLY ALA ALA SER ALA ALA GLN LEU SER G29 Y30 S31 R32 V33 L34 L35 K36 L37 G38 G39 E40
M41 F42 V47 G48 L49 D50 P51 V54 A55 Q56 Q60 I61 V64 V65 V69 Q70 I71 A72 V73 V74 I75 G76 R82 GLY A84 Q85 L86 L89 G90 M91 E92 R93 T94 R95 Y98 M99 G100 M101 M106 N107 L111 F114 L115 E116 K117 T122 Q125
I128 T129 M130 G131 Q132 E135 V143 R144 H145 K148 G149 R150 V151 F154 G155 A156 G157 MET GLY LEU PRO TYR F163 D166 T167 T168 R172 A173 A178 D179 V180 V181 L182 M183 A184 K185 D188 G189 V190 F191 A192 E193 V197 N198 P199 E202 L203 A206
H209 R210 E211 V212 L213 D214 V219 A220 D221 A222 T223 A224 L227 C228 M229 D230 N231 P234 I235 L236 V237 F238 N239 L240 L241 T242 N245 I246 A247 R248 A249 V250 R251 G252 E253 T261

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	197.47Å 152.82Å 125.11Å 90.00° 121.39° 90.00°	Depositor
Resolution (Å)	27.98 – 3.12 113.22 – 2.82	Depositor EDS
% Data completeness (in resolution range)	93.9 (27.98-3.12) 76.7 (113.22-2.82)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, R_{free}	0.191 , (Not available) 0.189 , 0.245	Depositor DCC
R_{free} test set	2651 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å^2)	57.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20295	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.32	0/1642	0.49	0/2220
1	B	0.32	0/1672	0.54	1/2259 (0.0%)
1	C	0.41	0/1713	0.52	0/2314
1	D	0.37	0/1674	0.50	0/2260
1	E	0.43	0/1670	0.54	0/2253
1	F	0.30	0/1629	0.51	0/2198
1	G	0.34	0/1599	0.48	1/2160 (0.0%)
1	H	0.25	0/1680	0.45	0/2268
1	I	0.31	0/1675	0.45	0/2264
1	J	0.37	0/1694	0.49	0/2290
1	K	0.34	0/1691	0.48	0/2284
1	L	0.37	0/1671	0.51	0/2260
All	All	0.35	0/20010	0.50	2/27030 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	218	ARG	N-CA-C	5.34	125.43	111.00
1	G	260	THR	N-CA-C	5.08	124.73	111.00

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	1625	0	1634	102	0
1	B	1655	0	1672	98	0
1	C	1694	0	1721	81	0
1	D	1656	0	1679	85	0
1	E	1652	0	1674	102	0
1	F	1614	0	1630	123	0
1	G	1584	0	1585	92	0
1	H	1662	0	1690	92	0
1	I	1656	0	1673	98	0
1	J	1675	0	1697	95	0
1	K	1673	0	1693	102	0
1	L	1654	0	1654	120	0
2	A	29	11	11	5	0
2	C	29	11	11	4	0
2	D	29	11	11	3	0
2	G	29	11	11	1	0
2	I	29	11	11	6	0
2	J	29	11	11	1	0
3	B	25	0	11	4	0
3	C	25	0	11	0	0
3	D	25	0	11	2	0
3	E	25	0	11	3	0
3	H	25	0	11	0	0
3	I	25	0	11	2	0
3	J	25	0	11	3	0
3	K	25	0	11	5	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	4	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	1	0
4	F	6	0	0	0	0
4	G	6	0	0	0	0
4	H	1	0	0	0	0
4	I	5	0	0	0	0
4	J	8	0	0	1	0
4	K	4	0	0	0	0
4	L	6	0	0	0	0
All	All	20229	66	20156	1136	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 28.

All (1136) 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:184:ALA:HB1	1:I:240:LEU:HD22	1.28	1.16
1:L:122:THR:HG22	1:L:151:VAL:HB	1.27	1.12
1:L:191:PHE:CE1	1:L:203:LEU:HD13	1.84	1.12
1:E:190:VAL:HG23	1:E:257:THR:CB	1.83	1.09
1:H:69:VAL:HG21	1:H:250:VAL:HG11	1.35	1.09
1:A:249:ALA:HB2	1:A:255:ILE:HD11	1.31	1.08
1:C:65:VAL:HG22	1:C:71:ILE:HD13	1.35	1.06
1:J:69:VAL:HG21	1:J:250:VAL:HG11	1.37	1.06
1:L:32:ARG:HH22	1:L:143:VAL:HG13	1.21	1.05
1:G:69:VAL:HG21	1:G:250:VAL:HG11	1.34	1.05
1:J:136:PRO:HG2	1:J:138:LEU:HD21	1.39	1.03
1:F:204:LEU:HD21	1:F:207:VAL:CG1	1.87	1.03
1:F:184:ALA:HB1	1:F:240:LEU:HD23	1.41	1.02
1:D:170:ALA:O	1:D:174:LEU:HD12	1.60	1.01
1:A:188:ASP:HB2	1:A:239:ASN:HB2	1.42	1.01
1:G:184:ALA:HB1	1:G:240:LEU:HD23	1.44	1.00
1:G:122:THR:HG22	1:G:151:VAL:HB	1.44	0.98
1:B:240:LEU:HD12	1:B:240:LEU:H	1.28	0.98
1:E:190:VAL:HG23	1:E:257:THR:OG1	1.65	0.97
1:L:198:ASN:HB3	1:L:199:PRO:CD	1.94	0.97
1:L:191:PHE:HE1	1:L:203:LEU:HD13	1.28	0.96
1:F:69:VAL:HG21	1:F:250:VAL:HG11	1.47	0.95
1:G:64:VAL:HG21	1:G:246:ILE:HG22	1.46	0.95
1:A:69:VAL:HG21	1:A:250:VAL:HG11	1.47	0.94
1:J:64:VAL:HG21	1:J:246:ILE:HG13	1.48	0.94
1:C:69:VAL:HG21	1:C:250:VAL:HG11	1.49	0.94
1:A:60:GLN:HB3	1:A:246:ILE:HD12	1.48	0.94
1:J:32:ARG:HH22	1:J:143:VAL:HG13	1.31	0.93
1:I:240:LEU:HB2	1:I:246:ILE:HD11	1.51	0.92
1:K:69:VAL:HG21	1:K:250:VAL:HG11	1.52	0.90
1:L:93:ARG:HH21	1:L:93:ARG:HG2	1.33	0.89
1:I:64:VAL:HG21	1:I:246:ILE:HG22	1.53	0.89
1:G:89:LEU:HD21	1:H:51:PRO:HB3	1.55	0.89
1:G:249:ALA:HB2	1:G:255:ILE:HD11	1.53	0.88
1:I:192:ALA:HB2	1:I:204:LEU:HD21	1.53	0.88
1:K:219:VAL:HG13	1:K:220:ALA:H	1.39	0.88
1:J:194:ASP:HB3	1:J:195:PRO:HD2	1.53	0.88
1:D:242:THR:HB	1:D:245:ASN:ND2	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:VAL:HG21	1:E:246:ILE:HG22	1.57	0.86
1:L:198:ASN:HB3	1:L:199:PRO:HD2	1.55	0.85
1:A:180:VAL:HG23	1:A:234:PRO:HB2	1.60	0.84
1:E:190:VAL:CG2	1:E:257:THR:CB	2.55	0.84
1:L:192:ALA:HB2	1:L:202:GLU:HG2	1.59	0.83
1:K:242:THR:HB	1:K:245:ASN:ND2	1.93	0.83
1:L:198:ASN:CB	1:L:199:PRO:HD2	2.08	0.83
1:E:83:GLY:HA2	1:E:96:SER:HB3	1.59	0.83
1:I:32:ARG:HH22	1:I:143:VAL:HG13	1.43	0.83
1:B:249:ALA:HB2	1:B:255:ILE:HD11	1.59	0.83
1:B:184:ALA:HB1	1:B:240:LEU:HG	1.59	0.82
1:F:204:LEU:CD2	1:F:207:VAL:CG1	2.56	0.82
1:E:190:VAL:HG23	1:E:257:THR:HB	1.61	0.82
1:E:242:THR:HB	1:E:245:ASN:ND2	1.94	0.82
1:C:249:ALA:HB2	1:C:255:ILE:HD11	1.59	0.82
1:K:69:VAL:HG21	1:K:250:VAL:CG1	2.10	0.82
1:L:198:ASN:CB	1:L:199:PRO:CD	2.58	0.82
1:D:69:VAL:HG21	1:D:250:VAL:CG1	2.09	0.81
1:E:180:VAL:HG23	1:E:234:PRO:HB2	1.60	0.81
1:F:64:VAL:HG21	1:F:246:ILE:HG22	1.63	0.81
1:D:64:VAL:HG21	1:D:246:ILE:HG12	1.60	0.81
1:J:249:ALA:HB2	1:J:255:ILE:HD11	1.62	0.81
1:F:32:ARG:HG3	1:F:178:ALA:HA	1.63	0.81
1:J:242:THR:HB	1:J:245:ASN:ND2	1.95	0.80
1:F:184:ALA:CB	1:F:240:LEU:HD23	2.10	0.80
1:E:190:VAL:HG21	1:E:257:THR:HG21	1.64	0.80
1:I:69:VAL:HG21	1:I:250:VAL:HG11	1.62	0.80
1:A:138:LEU:HB2	1:A:141:ARG:HB3	1.62	0.80
1:A:242:THR:HB	1:A:245:ASN:HD22	1.47	0.80
1:L:192:ALA:CB	1:L:202:GLU:HG2	2.11	0.79
1:J:121:VAL:CG1	1:J:123:ARG:HH11	1.95	0.79
1:J:242:THR:HB	1:J:245:ASN:HD22	1.43	0.79
1:K:64:VAL:CG1	1:K:71:ILE:HD11	2.13	0.79
1:B:65:VAL:HG22	1:B:71:ILE:HD13	1.65	0.78
1:F:204:LEU:CD2	1:F:207:VAL:HG13	2.12	0.78
1:K:189:GLY:HA3	1:K:203:LEU:HD11	1.64	0.78
1:I:184:ALA:HB1	1:I:240:LEU:CD2	2.12	0.78
1:F:122:THR:HG22	1:F:151:VAL:HB	1.65	0.78
1:B:69:VAL:HG21	1:B:250:VAL:HG11	1.65	0.78
1:G:209:HIS:CE1	1:G:259:VAL:O	2.37	0.78
1:C:242:THR:HB	1:C:245:ASN:ND2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLN:HB3	1:A:246:ILE:CD1	2.12	0.77
1:A:221:ASP:OD1	1:A:222:ALA:N	2.18	0.77
1:D:204:LEU:HD21	1:D:215:ARG:NH1	2.00	0.77
1:E:190:VAL:CG2	1:E:257:THR:HB	2.14	0.77
1:K:64:VAL:HG21	1:K:246:ILE:HG22	1.65	0.77
1:J:113:ASP:OD2	1:J:117:LYS:HE2	1.84	0.77
1:H:249:ALA:HB2	1:H:255:ILE:HD11	1.66	0.76
1:G:184:ALA:CB	1:G:240:LEU:HD23	2.16	0.76
1:A:242:THR:HB	1:A:245:ASN:ND2	2.01	0.76
1:B:113:ASP:OD2	1:B:117:LYS:HE2	1.86	0.76
1:L:85:GLN:O	1:L:89:LEU:HD22	1.86	0.76
1:A:122:THR:HG22	1:A:151:VAL:HB	1.67	0.75
1:D:204:LEU:HG	1:D:207:VAL:CG1	2.16	0.75
1:F:65:VAL:HG22	1:F:71:ILE:HD13	1.67	0.75
1:G:65:VAL:HG22	1:G:71:ILE:HD13	1.67	0.75
1:B:182:LEU:HB3	1:B:238:PHE:HE1	1.51	0.75
1:E:64:VAL:HG21	1:E:246:ILE:CG2	2.16	0.75
1:G:89:LEU:O	1:G:89:LEU:HD23	1.85	0.75
1:A:69:VAL:HG21	1:A:250:VAL:CG1	2.16	0.75
1:L:193:GLU:HG2	1:L:199:PRO:HD2	1.69	0.75
1:I:95:ARG:HH22	1:J:116:GLU:CD	1.89	0.74
1:F:206:ALA:HA	1:F:258:LEU:O	1.85	0.74
1:B:124:VAL:HG22	1:B:153:ILE:HB	1.68	0.74
1:E:69:VAL:HG21	1:E:250:VAL:CG1	2.17	0.74
1:G:89:LEU:HD21	1:H:51:PRO:CB	2.18	0.74
1:J:136:PRO:HG2	1:J:138:LEU:CD2	2.16	0.74
1:C:64:VAL:HG21	1:C:246:ILE:HG12	1.69	0.74
1:H:65:VAL:HG22	1:H:71:ILE:HD13	1.69	0.74
1:F:182:LEU:HB3	1:F:238:PHE:HE1	1.52	0.74
1:K:180:VAL:HG23	1:K:234:PRO:HB2	1.69	0.74
1:E:249:ALA:HB2	1:E:255:ILE:HD11	1.68	0.73
1:G:32:ARG:HH22	1:G:143:VAL:HG13	1.51	0.73
1:J:194:ASP:HB3	1:J:195:PRO:CD	2.19	0.73
1:A:42:PHE:HB2	1:A:79:ASN:ND2	2.03	0.73
1:I:170:ALA:O	1:I:174:LEU:HD23	1.87	0.73
1:G:221:ASP:OD1	1:G:222:ALA:N	2.20	0.73
1:E:65:VAL:HG22	1:E:71:ILE:HD13	1.70	0.73
1:H:244:GLY:O	1:H:248:ARG:HG3	1.88	0.73
1:H:32:ARG:HH22	1:H:143:VAL:HG13	1.51	0.73
1:A:188:ASP:HB2	1:A:239:ASN:CB	2.16	0.72
1:C:32:ARG:HG3	1:C:178:ALA:HA	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:184:ALA:HB1	1:K:240:LEU:HD23	1.71	0.72
1:L:191:PHE:CD1	1:L:203:LEU:HD13	2.24	0.72
1:F:188:ASP:HB3	1:F:239:ASN:HB2	1.70	0.72
1:K:248:ARG:HG2	1:K:251:ARG:HH11	1.55	0.72
1:E:136:PRO:HG2	1:E:138:LEU:HD21	1.72	0.71
1:I:32:ARG:HG3	1:I:178:ALA:HA	1.72	0.71
1:I:135:GLU:HB3	2:I:301:UTP:C6	2.24	0.71
1:L:101:MET:CE	1:L:156:ALA:HB2	2.20	0.71
1:F:242:THR:HB	1:F:245:ASN:ND2	2.06	0.71
1:G:242:THR:HB	1:G:245:ASN:ND2	2.04	0.71
1:G:60:GLN:NE2	1:G:243:ASP:HA	2.05	0.71
1:B:69:VAL:HG21	1:B:250:VAL:CG1	2.21	0.71
1:H:64:VAL:HG21	1:H:246:ILE:HG22	1.72	0.71
1:I:141:ARG:NH2	2:I:301:UTP:O1A	2.24	0.71
1:E:32:ARG:HH22	1:E:143:VAL:HG13	1.56	0.71
1:E:32:ARG:HG3	1:E:178:ALA:HA	1.73	0.71
1:I:221:ASP:OD1	1:I:222:ALA:N	2.24	0.71
1:B:245:ASN:O	1:B:248:ARG:N	2.25	0.70
1:H:242:THR:HB	1:H:245:ASN:ND2	2.05	0.70
1:K:184:ALA:CB	1:K:240:LEU:HD23	2.21	0.70
1:J:69:VAL:HG21	1:J:250:VAL:CG1	2.17	0.70
1:H:163:PHE:HE2	1:I:171:GLN:HG3	1.57	0.70
1:I:148:LYS:NZ	2:I:301:UTP:O2G	2.25	0.70
1:C:208:SER:HA	1:C:260:THR:O	1.91	0.69
1:L:190:VAL:O	1:L:203:LEU:HD12	1.92	0.69
1:E:240:LEU:HD21	1:E:246:ILE:HD11	1.74	0.69
1:L:93:ARG:HG2	1:L:93:ARG:NH2	2.07	0.69
1:D:56:GLN:NE2	1:D:241:LEU:HD22	2.07	0.69
1:I:180:VAL:HG23	1:I:234:PRO:HB2	1.74	0.69
1:C:33:VAL:HG11	1:C:182:LEU:HD12	1.74	0.69
1:E:209:HIS:ND1	1:E:261:THR:O	2.23	0.69
1:G:208:SER:O	1:G:212:VAL:HG23	1.93	0.69
1:J:180:VAL:HG23	1:J:234:PRO:HB2	1.72	0.69
1:A:32:ARG:HG3	1:A:178:ALA:HA	1.75	0.69
1:A:240:LEU:HD11	1:A:246:ILE:HD11	1.73	0.69
1:I:184:ALA:CB	1:I:240:LEU:HD22	2.17	0.69
1:F:60:GLN:NE2	1:F:243:ASP:HA	2.07	0.69
1:E:190:VAL:CG2	1:E:257:THR:HG21	2.23	0.68
1:L:145:HIS:O	1:L:150:ARG:HG2	1.93	0.68
1:A:47:VAL:HG22	1:A:82:ARG:CB	2.22	0.68
1:B:145:HIS:ND1	1:B:150:ARG:HD2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLY:O	1:B:248:ARG:HG3	1.93	0.68
1:A:93:ARG:HD3	1:A:162:TYR:CE1	2.29	0.68
1:E:248:ARG:HG2	1:E:251:ARG:HH22	1.57	0.68
1:F:187:VAL:O	1:F:239:ASN:HB2	1.94	0.68
1:G:49:LEU:HD11	1:H:99:MET:HE1	1.74	0.68
1:C:69:VAL:CG2	1:C:250:VAL:HG11	2.24	0.68
1:L:89:LEU:HD21	1:L:91:MET:HB2	1.76	0.68
1:I:33:VAL:HG23	1:I:180:VAL:HG13	1.76	0.68
1:K:126:THR:HG21	1:K:130:MET:CE	2.24	0.67
1:K:209:HIS:ND1	1:K:261:THR:OXT	2.24	0.67
1:A:141:ARG:NH2	2:A:301:UTP:O2A	2.27	0.67
1:F:204:LEU:O	1:F:205:THR:HG23	1.93	0.67
1:I:60:GLN:HB3	1:I:246:ILE:HD12	1.76	0.67
1:B:64:VAL:HG12	1:B:71:ILE:HD11	1.75	0.67
1:G:189:GLY:HA3	1:G:203:LEU:HD11	1.76	0.67
1:I:64:VAL:HG21	1:I:246:ILE:CG2	2.25	0.67
1:A:135:GLU:HB3	2:A:301:UTP:C6	2.30	0.67
1:I:240:LEU:HB2	1:I:246:ILE:CD1	2.23	0.67
1:D:221:ASP:OD1	1:D:222:ALA:N	2.28	0.67
1:A:99:MET:HE3	1:B:49:LEU:HD11	1.77	0.66
1:G:69:VAL:HG21	1:G:250:VAL:CG1	2.18	0.66
1:H:69:VAL:HG21	1:H:250:VAL:CG1	2.21	0.66
1:F:40:GLU:N	1:F:40:GLU:OE1	2.29	0.66
1:K:133:VAL:HG22	1:L:98:TYR:CD1	2.31	0.66
1:F:204:LEU:HD21	1:F:207:VAL:HG13	1.72	0.66
1:E:69:VAL:HG21	1:E:250:VAL:HG11	1.78	0.66
1:K:89:LEU:HD21	1:L:51:PRO:HB3	1.76	0.66
1:L:209:HIS:HB3	1:L:229:MET:HG3	1.78	0.66
1:F:158:MET:O	1:F:160:LEU:N	2.24	0.66
1:I:136:PRO:HG2	1:I:138:LEU:HD21	1.78	0.66
1:F:204:LEU:HD21	1:F:207:VAL:HG11	1.75	0.65
1:B:207:VAL:CG2	1:B:259:VAL:HG22	2.26	0.65
1:C:33:VAL:HG11	1:C:182:LEU:CD1	2.25	0.65
1:B:40:GLU:OE1	1:B:40:GLU:N	2.28	0.65
1:B:145:HIS:HB3	1:B:150:ARG:HG3	1.78	0.65
1:H:204:LEU:HD23	1:H:204:LEU:H	1.60	0.65
1:H:184:ALA:HB1	1:H:240:LEU:HD23	1.77	0.65
1:C:35:LEU:HD11	1:C:184:ALA:HB2	1.77	0.65
1:D:204:LEU:HD21	1:D:215:ARG:HH12	1.60	0.65
1:L:145:HIS:ND1	1:L:150:ARG:HD2	2.12	0.65
1:C:209:HIS:ND1	1:C:261:THR:OG1	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:GLY:O	1:G:248:ARG:HG3	1.96	0.65
1:I:240:LEU:HD12	1:I:246:ILE:HD11	1.77	0.64
1:L:75:ILE:HD11	1:L:111:LEU:HD22	1.79	0.64
1:D:185:LYS:HD2	1:D:237:VAL:CG1	2.27	0.64
1:E:240:LEU:HD21	1:E:246:ILE:CD1	2.27	0.64
1:H:42:PHE:CZ	1:H:75:ILE:HD12	2.32	0.64
1:H:240:LEU:HB2	1:H:246:ILE:HD11	1.78	0.64
1:A:188:ASP:CB	1:A:239:ASN:HB2	2.23	0.64
1:D:83:GLY:HA2	1:D:96:SER:HB3	1.79	0.64
1:D:69:VAL:HG21	1:D:250:VAL:HG11	1.79	0.64
1:J:182:LEU:HB3	1:J:238:PHE:HE1	1.62	0.64
1:C:244:GLY:O	1:C:248:ARG:HD2	1.98	0.64
1:K:81:PHE:CD1	1:K:86:LEU:HD11	2.32	0.64
1:L:242:THR:HB	1:L:245:ASN:ND2	2.12	0.64
1:A:130:MET:O	1:A:132:GLN:N	2.30	0.64
1:I:242:THR:HB	1:I:245:ASN:ND2	2.13	0.64
1:D:249:ALA:HB2	1:D:255:ILE:HD11	1.81	0.63
1:H:136:PRO:HG2	1:H:138:LEU:HD21	1.80	0.63
1:D:32:ARG:HG3	1:D:178:ALA:HA	1.79	0.63
1:F:208:SER:O	1:F:212:VAL:HG23	1.99	0.63
1:J:157:GLY:HA3	3:J:302:UDP:C5	2.33	0.63
1:B:36:LYS:HE2	1:B:166:ASP:OD1	1.98	0.63
1:B:215:ARG:CG	1:B:215:ARG:HH21	2.11	0.63
1:F:81:PHE:CG	1:F:86:LEU:HD11	2.33	0.63
1:L:34:LEU:HD13	1:L:173:ALA:HB2	1.81	0.63
1:D:204:LEU:HG	1:D:207:VAL:HG13	1.79	0.63
1:D:242:THR:HB	1:D:245:ASN:HD22	1.62	0.63
1:A:240:LEU:CD1	1:A:246:ILE:HD11	2.28	0.63
1:L:101:MET:HE3	1:L:156:ALA:HB2	1.79	0.63
1:F:85:GLN:O	1:F:89:LEU:HD22	1.98	0.63
1:B:42:PHE:CZ	1:B:75:ILE:HD12	2.34	0.62
1:C:135:GLU:HB3	2:C:301:UTP:C6	2.33	0.62
1:I:234:PRO:HB3	1:I:260:THR:HG22	1.80	0.62
1:G:54:VAL:HG12	1:G:114:PHE:HD2	1.65	0.62
1:F:236:LEU:CD2	1:F:249:ALA:HB1	2.30	0.62
1:B:33:VAL:HG11	1:B:182:LEU:CD1	2.29	0.62
1:E:136:PRO:HG2	1:E:138:LEU:CD2	2.29	0.62
1:E:190:VAL:HG21	1:E:257:THR:CG2	2.29	0.62
1:B:97:ASP:HB3	3:B:300:UDP:O2	1.99	0.62
1:G:174:LEU:HD23	1:G:233:MET:CE	2.30	0.62
1:G:249:ALA:CB	1:G:255:ILE:HD11	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:LEU:HG	1:D:260:THR:HG23	1.82	0.62
1:J:145:HIS:O	1:J:150:ARG:HG2	2.00	0.62
1:A:64:VAL:HG21	1:A:246:ILE:HG22	1.82	0.61
1:C:65:VAL:HG22	1:C:71:ILE:CD1	2.22	0.61
1:H:184:ALA:CB	1:H:240:LEU:HD23	2.29	0.61
1:C:191:PHE:CE1	1:C:203:LEU:HD13	2.35	0.61
1:D:103:GLY:HA2	1:D:106:MET:HE3	1.80	0.61
1:F:125:GLN:HG2	1:F:135:GLU:HG3	1.83	0.61
1:D:163:PHE:HE2	1:E:171:GLN:HG3	1.65	0.61
1:E:113:ASP:OD1	1:E:117:LYS:NZ	2.33	0.61
1:J:32:ARG:HG3	1:J:178:ALA:HA	1.83	0.61
1:B:240:LEU:HD23	1:B:246:ILE:HD11	1.83	0.61
1:A:248:ARG:HB2	1:A:253:GLU:CD	2.21	0.61
1:A:91:MET:HA	1:B:113:ASP:OD2	2.01	0.60
1:B:64:VAL:HG21	1:B:246:ILE:HG22	1.82	0.60
1:F:113:ASP:OD1	1:F:117:LYS:HE2	2.01	0.60
1:G:242:THR:HB	1:G:245:ASN:HD22	1.64	0.60
1:J:204:LEU:HD12	1:J:207:VAL:CG1	2.31	0.60
1:E:248:ARG:HG2	1:E:251:ARG:NH2	2.16	0.60
1:E:82:ARG:HA	3:E:301:UDP:O3'	2.01	0.60
1:G:32:ARG:HG3	1:G:178:ALA:HA	1.83	0.60
1:E:112:GLN:HG3	1:E:122:THR:OG1	2.01	0.60
1:J:212:VAL:HG13	1:J:217:LEU:HB2	1.84	0.60
1:K:64:VAL:HG12	1:K:71:ILE:HD11	1.83	0.60
1:K:248:ARG:HG2	1:K:251:ARG:NH1	2.15	0.60
1:L:191:PHE:CD1	1:L:203:LEU:CD1	2.83	0.60
1:H:221:ASP:OD1	1:H:222:ALA:N	2.34	0.60
1:A:184:ALA:HB1	1:A:240:LEU:HB2	1.83	0.60
1:G:65:VAL:CG2	1:G:71:ILE:HD13	2.32	0.60
1:G:138:LEU:HD13	1:G:141:ARG:HD3	1.83	0.60
1:L:209:HIS:CB	1:L:229:MET:HG3	2.30	0.60
1:J:246:ILE:O	1:J:250:VAL:HG23	2.01	0.60
1:F:42:PHE:CD1	1:F:54:VAL:HG22	2.37	0.60
1:I:33:VAL:CG2	1:I:182:LEU:HG	2.32	0.60
1:C:125:GLN:HG2	1:C:135:GLU:HG3	1.84	0.60
1:E:190:VAL:CG2	1:E:257:THR:CG2	2.79	0.60
1:F:157:GLY:HA2	1:F:168:THR:HG21	1.83	0.60
1:I:89:LEU:O	1:I:89:LEU:HD23	2.02	0.60
1:C:170:ALA:O	1:C:174:LEU:HD23	2.02	0.59
1:H:248:ARG:HG2	1:H:251:ARG:NH1	2.16	0.59
1:I:188:ASP:HA	1:I:239:ASN:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:VAL:CG2	1:D:182:LEU:HG	2.32	0.59
1:F:38:GLY:O	1:F:41:MET:HB2	2.02	0.59
1:G:166:ASP:OD2	1:G:221:ASP:HB2	2.02	0.59
1:K:145:HIS:ND1	1:K:150:ARG:HD2	2.17	0.59
1:F:145:HIS:ND1	1:F:150:ARG:HD2	2.16	0.59
1:G:259:VAL:O	1:G:259:VAL:HG12	2.02	0.59
1:K:170:ALA:O	1:K:174:LEU:HD23	2.01	0.59
1:F:182:LEU:CD2	1:F:236:LEU:HD23	2.32	0.59
1:H:65:VAL:CG2	1:H:71:ILE:HD13	2.33	0.59
1:A:259:VAL:HG12	1:A:259:VAL:O	2.03	0.59
1:D:123:ARG:HG3	1:D:145:HIS:ND1	2.17	0.59
1:E:81:PHE:CE1	1:F:49:LEU:HD12	2.38	0.59
1:B:42:PHE:HZ	1:B:75:ILE:HD12	1.67	0.59
1:G:246:ILE:O	1:G:250:VAL:HG23	2.02	0.59
1:I:208:SER:HA	1:I:260:THR:O	2.03	0.59
1:F:33:VAL:HG21	1:F:182:LEU:CD1	2.32	0.59
1:D:139:PRO:HG3	1:D:175:GLU:OE2	2.02	0.59
1:F:115:LEU:HD13	1:F:122:THR:HG21	1.84	0.59
1:I:95:ARG:NH2	1:J:116:GLU:OE2	2.36	0.59
1:L:125:GLN:HG2	1:L:135:GLU:HG3	1.85	0.59
1:E:239:ASN:O	1:E:245:ASN:ND2	2.35	0.59
1:F:220:ALA:CB	1:F:225:PHE:HD1	2.16	0.59
1:I:135:GLU:HB3	2:I:301:UTP:C5	2.37	0.59
1:K:87:GLN:OE1	1:K:93:ARG:HD3	2.03	0.59
1:B:87:GLN:OE1	1:B:93:ARG:HB2	2.03	0.58
1:E:65:VAL:CG2	1:E:71:ILE:HD13	2.33	0.58
1:F:36:LYS:HE3	1:F:166:ASP:OD1	2.01	0.58
1:C:36:LYS:HE2	1:C:165:THR:CG2	2.33	0.58
1:G:33:VAL:HG21	1:G:182:LEU:HD11	1.86	0.58
2:G:301:UTP:O2A	1:I:141:ARG:HD2	2.02	0.58
1:I:103:GLY:HA2	1:I:106:MET:HE2	1.86	0.58
1:L:33:VAL:HG21	1:L:182:LEU:CD1	2.32	0.58
1:L:198:ASN:HB3	1:L:199:PRO:HD3	1.80	0.58
1:G:64:VAL:HG21	1:G:246:ILE:CG2	2.27	0.58
1:A:194:ASP:N	1:A:194:ASP:OD1	2.37	0.58
1:E:40:GLU:OE1	1:E:40:GLU:N	2.36	0.58
1:F:236:LEU:HD21	1:F:249:ALA:HB1	1.83	0.58
1:L:182:LEU:HB3	1:L:238:PHE:HE1	1.69	0.58
1:L:248:ARG:HD2	1:L:253:GLU:OE1	2.02	0.58
1:E:135:GLU:HG2	1:E:136:PRO:HD2	1.85	0.58
1:D:112:GLN:HG3	1:D:122:THR:OG1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:VAL:HG12	1:H:71:ILE:HD11	1.85	0.58
1:J:130:MET:O	1:J:132:GLN:N	2.37	0.58
1:L:56:GLN:O	1:L:60:GLN:HG3	2.03	0.58
1:L:221:ASP:OD1	1:L:222:ALA:N	2.35	0.58
1:A:249:ALA:CB	1:A:255:ILE:HD11	2.21	0.58
1:F:65:VAL:CG2	1:F:71:ILE:HD13	2.33	0.58
1:F:182:LEU:HD23	1:F:236:LEU:HB3	1.86	0.58
1:H:62:ALA:O	1:H:66:ARG:HG3	2.04	0.58
1:B:158:MET:HG3	1:B:168:THR:OG1	2.03	0.58
1:B:171:GLN:HG3	1:C:163:PHE:HE2	1.69	0.58
1:I:56:GLN:HG3	1:I:59:ARG:CZ	2.34	0.58
1:L:32:ARG:CB	1:L:70:GLN:HB2	2.34	0.58
1:C:135:GLU:HB3	2:C:301:UTP:C5	2.39	0.58
1:J:74:VAL:HG21	1:J:169:ALA:HA	1.86	0.58
1:L:101:MET:SD	1:L:128:ILE:HD12	2.44	0.58
1:J:34:LEU:HD13	1:J:173:ALA:N	2.19	0.58
1:K:112:GLN:HG3	1:K:122:THR:OG1	2.03	0.57
1:G:42:PHE:CE2	1:G:75:ILE:HG23	2.39	0.57
1:A:49:LEU:HD12	1:B:81:PHE:CE1	2.39	0.57
1:B:82:ARG:HB3	1:B:85:GLN:HB2	1.86	0.57
1:H:33:VAL:HG23	1:H:180:VAL:HG13	1.87	0.57
1:J:244:GLY:O	1:J:248:ARG:HG3	2.05	0.57
1:E:204:LEU:HD23	1:E:207:VAL:CG1	2.34	0.57
1:F:187:VAL:O	1:F:188:ASP:HB3	2.04	0.57
1:H:42:PHE:HZ	1:H:75:ILE:HD12	1.69	0.57
1:B:242:THR:HG22	1:B:242:THR:O	2.04	0.57
1:K:145:HIS:HB3	1:K:150:ARG:HG3	1.87	0.57
1:D:209:HIS:HA	1:D:225:PHE:HZ	1.69	0.57
1:H:80:PHE:CZ	1:H:106:MET:HE3	2.40	0.57
1:L:32:ARG:NH2	1:L:143:VAL:HG13	2.05	0.57
1:C:95:ARG:HD2	1:D:113:ASP:HB2	1.87	0.57
1:F:89:LEU:HD21	1:F:91:MET:HG3	1.85	0.57
1:H:82:ARG:HB2	1:H:85:GLN:CG	2.34	0.57
1:J:190:VAL:HG21	1:J:219:VAL:CG1	2.35	0.57
1:B:138:LEU:HD12	1:B:141:ARG:HD3	1.87	0.57
1:D:135:GLU:CG	2:D:301:UTP:H2'	2.35	0.57
1:K:219:VAL:HG13	1:K:220:ALA:N	2.14	0.57
1:A:209:HIS:HB3	1:A:229:MET:HG3	1.87	0.57
1:E:247:ALA:O	1:E:251:ARG:HB2	2.05	0.57
1:F:93:ARG:HG2	1:F:162:TYR:CE1	2.40	0.57
1:H:122:THR:HG22	1:H:151:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:145:HIS:HB3	1:L:150:ARG:HG3	1.87	0.57
1:J:258:LEU:HG	1:J:260:THR:HG23	1.87	0.56
1:B:115:LEU:O	1:B:120:ILE:HB	2.05	0.56
1:G:130:MET:O	1:G:132:GLN:N	2.38	0.56
1:K:60:GLN:HB3	1:K:246:ILE:HD12	1.86	0.56
1:A:112:GLN:HG3	1:A:122:THR:OG1	2.05	0.56
1:D:33:VAL:HG22	1:D:182:LEU:HG	1.87	0.56
1:F:139:PRO:HB3	1:F:175:GLU:HG3	1.86	0.56
1:G:89:LEU:HD11	1:H:51:PRO:HG3	1.87	0.56
1:H:82:ARG:HB2	1:H:85:GLN:HG2	1.86	0.56
1:A:42:PHE:HB2	1:A:79:ASN:HD21	1.70	0.56
1:A:125:GLN:HG2	1:A:135:GLU:HG3	1.86	0.56
1:E:61:ILE:O	1:E:65:VAL:HG23	2.05	0.56
1:J:33:VAL:CG2	1:J:182:LEU:HG	2.35	0.56
1:K:105:VAL:HG21	1:K:130:MET:HE1	1.86	0.56
1:A:65:VAL:HG22	1:A:71:ILE:HD13	1.86	0.56
1:D:56:GLN:O	1:D:60:GLN:HB2	2.04	0.56
1:E:32:ARG:CB	1:E:70:GLN:HB2	2.36	0.56
1:E:122:THR:HG22	1:E:151:VAL:HB	1.88	0.56
1:F:204:LEU:O	1:F:205:THR:CG2	2.53	0.56
1:J:69:VAL:CG2	1:J:250:VAL:HG11	2.24	0.56
1:G:180:VAL:HG23	1:G:234:PRO:HB2	1.87	0.56
1:J:89:LEU:HD23	1:J:89:LEU:O	2.06	0.56
1:B:47:VAL:HG13	1:B:79:ASN:O	2.06	0.56
1:C:58:ALA:HB1	1:C:115:LEU:HD23	1.88	0.56
1:I:174:LEU:HD22	1:I:233:MET:CE	2.35	0.56
1:J:174:LEU:HD11	1:J:231:ASN:HB3	1.87	0.56
1:K:172:ARG:O	1:K:176:ILE:HG12	2.06	0.56
1:L:242:THR:HB	1:L:245:ASN:HD21	1.70	0.56
1:F:42:PHE:HD1	1:F:54:VAL:HG22	1.68	0.56
1:H:64:VAL:HG21	1:H:246:ILE:CG2	2.36	0.56
1:E:89:LEU:HD23	1:E:89:LEU:O	2.06	0.55
1:E:114:PHE:HZ	1:F:89:LEU:HD12	1.71	0.55
1:H:191:PHE:HA	1:H:203:LEU:HA	1.88	0.55
1:K:42:PHE:CE2	1:K:75:ILE:HG23	2.41	0.55
1:B:240:LEU:HD12	1:B:240:LEU:N	2.01	0.55
1:G:54:VAL:HG12	1:G:114:PHE:CD2	2.40	0.55
1:G:87:GLN:O	1:G:89:LEU:N	2.37	0.55
1:A:54:VAL:HG12	1:A:114:PHE:CD2	2.41	0.55
1:A:123:ARG:NH1	2:A:301:UTP:O1B	2.39	0.55
1:E:33:VAL:CG2	1:E:182:LEU:HG	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:TYR:CE2	1:I:174:LEU:HB3	2.42	0.55
1:F:123:ARG:HG2	1:F:150:ARG:HD3	1.88	0.55
1:K:221:ASP:HB3	1:K:224:ALA:HB3	1.88	0.55
1:A:116:GLU:OE1	1:B:95:ARG:NH2	2.40	0.55
1:B:83:GLY:HA3	3:B:300:UDP:O2'	2.06	0.55
1:J:83:GLY:HA2	1:J:96:SER:HB3	1.89	0.55
1:K:212:VAL:HG11	1:K:219:VAL:HG11	1.89	0.55
1:A:236:LEU:HD21	1:A:249:ALA:HB1	1.89	0.55
1:G:74:VAL:HG21	1:G:169:ALA:HA	1.89	0.55
1:H:33:VAL:CG2	1:H:182:LEU:HG	2.36	0.55
1:J:60:GLN:NE2	1:J:246:ILE:HG22	2.22	0.55
1:J:174:LEU:HB3	1:K:162:TYR:CE2	2.41	0.55
1:L:86:LEU:O	1:L:91:MET:HB3	2.06	0.55
1:B:125:GLN:HG2	1:B:135:GLU:HG3	1.89	0.55
1:B:215:ARG:HG2	1:B:215:ARG:NH2	2.22	0.55
1:J:157:GLY:HA3	3:J:302:UDP:H5	1.72	0.55
1:K:83:GLY:HA3	1:K:97:ASP:OD1	2.06	0.55
1:B:39:GLY:N	3:B:300:UDP:O1B	2.33	0.55
1:E:33:VAL:HG21	1:E:182:LEU:HG	1.89	0.55
1:F:220:ALA:CB	1:F:225:PHE:CD1	2.90	0.55
1:K:132:GLN:HG3	1:L:98:TYR:OH	2.07	0.55
1:K:141:ARG:NH2	1:K:141:ARG:HG3	2.21	0.55
1:I:95:ARG:NH2	1:J:116:GLU:CD	2.59	0.55
1:J:87:GLN:HA	1:J:91:MET:O	2.07	0.55
1:B:174:LEU:HB3	1:C:162:TYR:CE2	2.41	0.55
1:L:240:LEU:HD22	1:L:240:LEU:O	2.06	0.55
1:E:42:PHE:CZ	1:E:75:ILE:HD12	2.42	0.54
1:F:64:VAL:HG12	1:F:71:ILE:HD11	1.88	0.54
1:K:141:ARG:HH21	1:K:141:ARG:CG	2.20	0.54
1:L:32:ARG:HG3	1:L:178:ALA:HA	1.89	0.54
1:B:62:ALA:O	1:B:66:ARG:HG3	2.07	0.54
1:H:46:GLN:OE1	1:H:46:GLN:N	2.40	0.54
1:I:188:ASP:CA	1:I:239:ASN:HB2	2.37	0.54
1:C:93:ARG:HG2	1:C:162:TYR:CE1	2.43	0.54
1:D:182:LEU:HB3	1:D:238:PHE:HE1	1.70	0.54
1:H:89:LEU:HD23	1:H:89:LEU:O	2.08	0.54
1:I:34:LEU:HD13	1:I:173:ALA:N	2.22	0.54
1:K:38:GLY:O	1:K:41:MET:HB3	2.07	0.54
1:L:191:PHE:CE1	1:L:203:LEU:CD1	2.75	0.54
1:B:65:VAL:CG2	1:B:71:ILE:HD13	2.36	0.54
1:H:208:SER:HA	1:H:260:THR:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:165:THR:HB	3:J:302:UDP:O2A	2.07	0.54
1:H:77:GLY:N	1:H:104:THR:HG22	2.23	0.54
1:H:115:LEU:O	1:H:120:ILE:HB	2.08	0.54
1:J:121:VAL:HG13	1:J:123:ARG:HH11	1.72	0.54
1:J:236:LEU:HD12	1:J:257:THR:O	2.07	0.54
1:K:221:ASP:OD1	1:K:222:ALA:N	2.40	0.54
1:B:238:PHE:CZ	1:B:246:ILE:HG12	2.43	0.54
1:B:245:ASN:O	1:B:246:ILE:C	2.44	0.54
1:H:209:HIS:CG	1:H:261:THR:HG1	2.24	0.54
1:K:240:LEU:HD22	1:K:246:ILE:HD11	1.90	0.54
1:C:34:LEU:HD13	1:C:173:ALA:N	2.22	0.54
1:F:220:ALA:HB3	1:F:225:PHE:CD1	2.43	0.54
1:H:123:ARG:HG3	1:H:145:HIS:CE1	2.43	0.54
1:H:249:ALA:CB	1:H:255:ILE:HD11	2.36	0.54
1:I:33:VAL:HG21	1:I:182:LEU:HG	1.88	0.54
1:J:209:HIS:HB3	1:J:229:MET:HG3	1.89	0.54
1:C:123:ARG:NH1	2:C:301:UTP:O2B	2.37	0.53
1:E:240:LEU:HD13	1:E:240:LEU:O	2.08	0.53
1:F:182:LEU:HB3	1:F:238:PHE:CE1	2.40	0.53
1:K:86:LEU:O	1:K:91:MET:HB2	2.08	0.53
1:A:36:LYS:HE2	1:A:165:THR:CG2	2.38	0.53
1:J:207:VAL:O	1:J:259:VAL:HA	2.09	0.53
1:L:166:ASP:HB3	1:L:224:ALA:CB	2.38	0.53
1:H:170:ALA:O	1:H:174:LEU:HD23	2.07	0.53
1:I:174:LEU:HD22	1:I:233:MET:HE3	1.89	0.53
1:L:33:VAL:HG21	1:L:182:LEU:HG	1.91	0.53
1:A:42:PHE:HB3	1:A:49:LEU:HD23	1.90	0.53
1:A:171:GLN:O	1:A:175:GLU:HG2	2.09	0.53
1:F:69:VAL:HG21	1:F:250:VAL:CG1	2.28	0.53
1:L:91:MET:HE3	1:L:95:ARG:CB	2.39	0.53
1:B:69:VAL:HG11	1:B:250:VAL:HG11	1.90	0.53
1:H:191:PHE:CE2	1:H:203:LEU:HB2	2.43	0.53
1:I:249:ALA:HB2	1:I:255:ILE:HD11	1.91	0.53
1:I:258:LEU:HD13	1:I:260:THR:HG23	1.91	0.53
1:L:182:LEU:HD23	1:L:236:LEU:HB3	1.91	0.53
1:C:32:ARG:CG	1:C:178:ALA:HA	2.38	0.53
1:J:190:VAL:CG1	1:J:217:LEU:HD12	2.39	0.53
1:L:32:ARG:HB3	1:L:70:GLN:HB2	1.90	0.53
1:A:101:MET:O	1:A:104:THR:OG1	2.22	0.53
1:E:64:VAL:HG12	1:E:71:ILE:HD11	1.91	0.53
1:E:133:VAL:HG22	1:F:98:TYR:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:PHE:HE1	1:I:111:LEU:HB2	1.74	0.53
1:L:180:VAL:HG23	1:L:234:PRO:HB2	1.91	0.53
1:L:188:ASP:CA	1:L:239:ASN:HB2	2.39	0.53
1:L:198:ASN:HB2	1:L:199:PRO:HD2	1.89	0.53
1:J:219:VAL:HG23	1:J:219:VAL:O	2.08	0.53
1:K:238:PHE:HZ	1:K:246:ILE:HG12	1.74	0.53
1:L:210:ARG:NH2	1:L:214:ASP:OD2	2.42	0.53
1:B:54:VAL:HG12	1:B:114:PHE:HD2	1.73	0.53
1:C:158:MET:HG3	1:C:168:THR:OG1	2.10	0.53
1:K:97:ASP:HB3	3:K:301:UDP:O2	2.08	0.53
1:K:238:PHE:CZ	1:K:246:ILE:HG12	2.44	0.53
1:L:166:ASP:OD2	1:L:221:ASP:HB2	2.09	0.53
1:A:42:PHE:HB3	1:A:49:LEU:CD2	2.39	0.52
1:A:170:ALA:O	1:A:174:LEU:HD23	2.09	0.52
1:G:174:LEU:HD23	1:G:233:MET:HE3	1.90	0.52
1:K:82:ARG:HG3	3:K:301:UDP:O3'	2.09	0.52
1:K:209:HIS:HB3	1:K:229:MET:HG3	1.91	0.52
1:B:209:HIS:HB3	1:B:229:MET:HG3	1.89	0.52
1:A:174:LEU:HD22	1:A:233:MET:HE3	1.91	0.52
1:L:240:LEU:HD21	1:L:246:ILE:HD11	1.91	0.52
1:D:66:ARG:NH2	1:D:118:GLU:O	2.43	0.52
1:E:32:ARG:HB3	1:E:70:GLN:HB2	1.90	0.52
1:H:76:GLY:C	1:H:104:THR:HG22	2.30	0.52
1:I:101:MET:SD	1:I:159:GLY:HA2	2.50	0.52
1:F:81:PHE:CD2	1:F:86:LEU:HD11	2.45	0.52
1:G:62:ALA:O	1:G:66:ARG:HG3	2.09	0.52
1:G:121:VAL:CG1	1:G:123:ARG:NH2	2.73	0.52
1:C:111:LEU:O	1:C:115:LEU:HB2	2.10	0.52
1:E:42:PHE:HZ	1:E:75:ILE:HD12	1.73	0.52
1:H:234:PRO:HB3	1:H:260:THR:HG22	1.91	0.52
1:I:240:LEU:HB2	1:I:246:ILE:CG1	2.40	0.52
1:L:89:LEU:CD2	1:L:91:MET:HB2	2.39	0.52
1:A:240:LEU:HD11	1:A:246:ILE:CD1	2.38	0.52
1:B:185:LYS:HE2	1:B:219:VAL:HG11	1.92	0.52
1:F:145:HIS:HB3	1:F:150:ARG:HG3	1.91	0.52
1:F:248:ARG:HB2	1:F:255:ILE:HD13	1.90	0.52
1:H:172:ARG:O	1:H:176:ILE:HG12	2.10	0.52
1:I:33:VAL:HG23	1:I:180:VAL:CG1	2.39	0.52
1:K:89:LEU:HD21	1:L:51:PRO:CB	2.40	0.52
1:L:33:VAL:CG2	1:L:182:LEU:HG	2.40	0.52
1:B:220:ALA:O	1:B:221:ASP:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ALA:O	1:C:87:GLN:HG2	2.08	0.52
1:E:172:ARG:O	1:E:176:ILE:HG12	2.10	0.52
1:E:209:HIS:HA	1:E:225:PHE:HZ	1.75	0.52
1:E:242:THR:HB	1:E:245:ASN:HD21	1.69	0.52
1:F:54:VAL:HG12	1:F:114:PHE:HD2	1.75	0.52
1:I:42:PHE:CE1	1:I:111:LEU:HB2	2.45	0.52
1:J:158:MET:HG3	1:J:168:THR:OG1	2.10	0.52
1:A:189:GLY:HA2	1:A:203:LEU:CD1	2.40	0.52
1:L:188:ASP:HB3	1:L:239:ASN:HB2	1.91	0.52
1:A:32:ARG:HA	1:A:70:GLN:O	2.10	0.52
1:J:74:VAL:HG12	1:J:165:THR:HG23	1.90	0.52
1:K:188:ASP:HB3	1:K:239:ASN:HB3	1.92	0.52
1:L:122:THR:HA	1:L:151:VAL:O	2.10	0.52
1:D:33:VAL:HG23	1:D:180:VAL:HG13	1.91	0.51
1:L:184:ALA:HB1	1:L:240:LEU:HB2	1.91	0.51
1:A:36:LYS:HE2	1:A:165:THR:HG22	1.92	0.51
1:A:92:GLU:HG3	1:A:95:ARG:NH1	2.24	0.51
1:B:215:ARG:HH21	1:B:215:ARG:HG2	1.75	0.51
1:D:171:GLN:HG3	1:E:163:PHE:HE2	1.75	0.51
1:E:157:GLY:HA2	1:E:168:THR:HG21	1.92	0.51
1:F:74:VAL:HG21	1:F:169:ALA:HA	1.93	0.51
1:A:145:HIS:O	1:A:150:ARG:HB2	2.10	0.51
1:C:69:VAL:HG21	1:C:250:VAL:CG1	2.30	0.51
1:D:34:LEU:HD13	1:D:173:ALA:CA	2.41	0.51
1:E:240:LEU:CD2	1:E:246:ILE:HG13	2.41	0.51
1:D:34:LEU:HD13	1:D:173:ALA:N	2.25	0.51
2:D:301:UTP:H6	2:D:301:UTP:H5'2	1.75	0.51
1:F:47:VAL:HG12	1:F:48:GLY:N	2.25	0.51
1:I:174:LEU:HD11	1:I:231:ASN:HB3	1.92	0.51
1:K:76:GLY:HA3	3:K:301:UDP:O1B	2.10	0.51
1:L:89:LEU:O	1:L:89:LEU:HG	2.10	0.51
1:A:33:VAL:CG2	1:A:182:LEU:HG	2.39	0.51
1:B:98:TYR:HA	1:B:101:MET:HE3	1.92	0.51
1:B:145:HIS:O	1:B:150:ARG:HG2	2.09	0.51
1:L:93:ARG:NH2	1:L:93:ARG:CG	2.73	0.51
1:C:33:VAL:HG13	1:C:182:LEU:HG	1.92	0.51
1:F:171:GLN:HG2	1:F:227:LEU:HD21	1.91	0.51
1:K:182:LEU:HB3	1:K:238:PHE:HE1	1.76	0.51
1:L:41:MET:HE1	1:L:184:ALA:O	2.11	0.51
1:L:192:ALA:HB3	1:L:202:GLU:HG2	1.90	0.51
1:B:39:GLY:O	1:B:79:ASN:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:GLY:HA2	1:F:106:MET:HE3	1.92	0.51
1:F:205:THR:O	1:F:206:ALA:HB3	2.11	0.51
1:L:219:VAL:HG13	1:L:219:VAL:O	2.10	0.51
1:E:30:TYR:OH	1:E:258:LEU:HD11	2.11	0.51
1:F:204:LEU:CD2	1:F:207:VAL:HG11	2.35	0.51
1:G:249:ALA:HB2	1:G:255:ILE:CD1	2.34	0.51
1:K:105:VAL:HG11	1:K:130:MET:CE	2.41	0.51
1:B:34:LEU:HD13	1:B:173:ALA:N	2.25	0.51
1:C:144:ARG:HG3	1:C:148:LYS:HE3	1.92	0.51
1:D:244:GLY:HA3	1:D:248:ARG:NH2	2.26	0.51
1:E:34:LEU:HD13	1:E:173:ALA:N	2.26	0.51
1:E:113:ASP:OD2	1:F:91:MET:HG2	2.11	0.51
1:I:71:ILE:HG23	1:I:151:VAL:HG13	1.92	0.51
1:I:165:THR:HB	3:I:302:UDP:O1A	2.11	0.51
1:B:34:LEU:HD13	1:B:173:ALA:CA	2.41	0.51
1:H:33:VAL:HG23	1:H:180:VAL:CG1	2.41	0.51
1:K:81:PHE:CZ	1:L:49:LEU:HD12	2.46	0.51
1:C:219:VAL:HG11	1:C:225:PHE:CD1	2.46	0.50
1:D:209:HIS:CB	1:D:229:MET:HG3	2.42	0.50
1:E:166:ASP:CB	1:E:221:ASP:HB2	2.41	0.50
1:J:213:LEU:HD21	1:J:225:PHE:HE2	1.76	0.50
1:L:251:ARG:NH2	1:L:253:GLU:OE2	2.44	0.50
1:B:180:VAL:HG23	1:B:234:PRO:HB2	1.94	0.50
1:J:81:PHE:CD1	1:J:86:LEU:HD11	2.46	0.50
1:B:64:VAL:HG21	1:B:246:ILE:CG2	2.41	0.50
1:C:36:LYS:HE2	1:C:165:THR:HG22	1.93	0.50
1:I:56:GLN:HG3	1:I:59:ARG:NH2	2.27	0.50
1:I:69:VAL:CG2	1:I:250:VAL:HG11	2.37	0.50
1:K:189:GLY:HA3	1:K:203:LEU:CD1	2.40	0.50
1:C:219:VAL:HG11	1:C:225:PHE:CE1	2.46	0.50
1:D:69:VAL:HG21	1:D:250:VAL:HG12	1.91	0.50
1:K:98:TYR:HA	1:K:101:MET:HE3	1.92	0.50
1:C:74:VAL:HG12	1:C:165:THR:HG23	1.94	0.50
1:E:54:VAL:HG12	1:E:114:PHE:CD2	2.46	0.50
1:G:34:LEU:HA	1:G:72:ALA:O	2.12	0.50
1:A:174:LEU:HD22	1:A:233:MET:CE	2.42	0.50
1:C:64:VAL:HG23	1:C:246:ILE:HG23	1.94	0.50
1:E:36:LYS:HE3	1:E:166:ASP:OD1	2.12	0.50
1:G:209:HIS:CE1	1:G:260:THR:O	2.65	0.50
1:I:234:PRO:HB3	1:I:260:THR:CG2	2.42	0.50
1:I:251:ARG:NH2	1:I:253:GLU:OE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:213:LEU:CD2	1:J:225:PHE:HE2	2.25	0.50
1:A:56:GLN:NE2	1:A:241:LEU:O	2.44	0.50
1:B:182:LEU:HB3	1:B:238:PHE:CE1	2.39	0.50
1:C:195:PRO:HG3	1:C:201:ALA:HB3	1.93	0.50
1:F:180:VAL:HG23	1:F:234:PRO:HB2	1.93	0.50
1:G:166:ASP:HB2	1:G:221:ASP:CB	2.41	0.50
1:K:106:MET:HE2	1:L:99:MET:O	2.12	0.50
1:L:248:ARG:HG2	1:L:251:ARG:CZ	2.42	0.50
1:A:95:ARG:NH2	1:B:116:GLU:OE1	2.45	0.50
1:L:36:LYS:HE2	1:L:166:ASP:OD1	2.12	0.50
1:B:123:ARG:HG3	1:B:145:HIS:CE1	2.47	0.49
1:F:33:VAL:CG2	1:F:182:LEU:HG	2.42	0.49
1:H:182:LEU:HB3	1:H:238:PHE:HE1	1.77	0.49
1:H:188:ASP:HA	1:H:239:ASN:HB2	1.93	0.49
1:K:126:THR:HG21	1:K:130:MET:HE1	1.93	0.49
1:K:209:HIS:CB	1:K:229:MET:HG3	2.40	0.49
1:A:208:SER:O	1:A:212:VAL:HG23	2.11	0.49
1:C:148:LYS:HD2	1:C:150:ARG:NH2	2.27	0.49
1:E:240:LEU:O	1:E:240:LEU:HD22	2.13	0.49
1:H:188:ASP:N	1:H:188:ASP:OD1	2.44	0.49
1:B:81:PHE:HB3	1:B:86:LEU:HD11	1.93	0.49
1:E:60:GLN:HB3	1:E:246:ILE:HD12	1.94	0.49
1:G:207:VAL:CG2	1:G:259:VAL:HG22	2.42	0.49
1:J:190:VAL:HG21	1:J:219:VAL:HG12	1.94	0.49
1:K:102:LEU:HD21	1:L:130:MET:HE1	1.94	0.49
1:L:42:PHE:HB3	1:L:49:LEU:HD23	1.94	0.49
1:B:33:VAL:CG1	1:B:182:LEU:HG	2.43	0.49
1:C:41:MET:HB3	1:C:57:VAL:HG21	1.94	0.49
1:C:60:GLN:NE2	1:C:243:ASP:HA	2.27	0.49
1:G:123:ARG:HD3	1:G:150:ARG:HD2	1.93	0.49
1:I:172:ARG:O	1:I:176:ILE:HG12	2.13	0.49
1:J:188:ASP:OD1	1:J:188:ASP:N	2.42	0.49
1:A:113:ASP:OD1	1:A:117:LYS:HE2	2.13	0.49
1:D:33:VAL:HG21	1:D:182:LEU:HD11	1.92	0.49
1:F:220:ALA:O	1:F:221:ASP:HB3	2.12	0.49
1:J:236:LEU:HA	1:J:257:THR:O	2.12	0.49
1:A:98:TYR:HA	1:A:101:MET:HE3	1.93	0.49
1:D:33:VAL:HG23	1:D:180:VAL:CG1	2.42	0.49
1:D:191:PHE:CZ	1:D:203:LEU:HD13	2.48	0.49
1:F:81:PHE:CE2	1:F:86:LEU:HD21	2.47	0.49
1:F:167:THR:O	1:F:171:GLN:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:130:MET:O	1:L:132:GLN:N	2.43	0.49
1:A:33:VAL:HG21	1:A:182:LEU:HD11	1.94	0.49
1:C:170:ALA:HB3	1:C:227:LEU:HD23	1.95	0.49
1:I:87:GLN:HA	1:I:91:MET:O	2.13	0.49
1:L:219:VAL:HG23	1:L:237:VAL:HG21	1.95	0.49
1:L:248:ARG:HG2	1:L:251:ARG:NH2	2.28	0.49
1:D:89:LEU:O	1:D:89:LEU:HD23	2.12	0.49
1:L:188:ASP:HA	1:L:239:ASN:HB2	1.94	0.49
1:D:87:GLN:OE1	1:D:93:ARG:HB2	2.12	0.49
1:G:112:GLN:HG3	1:G:122:THR:OG1	2.13	0.49
1:I:87:GLN:HG3	1:I:88:GLN:N	2.28	0.49
1:I:125:GLN:HG2	1:I:135:GLU:HG3	1.95	0.49
1:J:61:ILE:O	1:J:65:VAL:HG23	2.13	0.49
1:K:34:LEU:HD12	1:K:72:ALA:HB3	1.95	0.49
1:L:64:VAL:HG21	1:L:246:ILE:HG22	1.94	0.49
1:L:101:MET:HE2	1:L:156:ALA:HB2	1.95	0.49
1:B:246:ILE:O	1:B:250:VAL:HG23	2.12	0.49
1:F:123:ARG:HG3	1:F:145:HIS:CE1	2.48	0.49
1:F:144:ARG:O	1:F:148:LYS:HE3	2.13	0.49
1:G:258:LEU:HG	1:G:260:THR:CG2	2.42	0.49
1:J:112:GLN:HG3	1:J:122:THR:OG1	2.12	0.49
1:D:185:LYS:HD2	1:D:237:VAL:HG13	1.95	0.48
1:D:244:GLY:HA3	1:D:248:ARG:HH22	1.78	0.48
1:B:215:ARG:CG	1:B:215:ARG:NH2	2.72	0.48
1:C:211:GLU:HG2	1:C:215:ARG:HD2	1.94	0.48
1:D:236:LEU:HD21	1:D:249:ALA:HB1	1.94	0.48
1:F:31:SER:HB2	1:F:179:ASP:OD2	2.13	0.48
1:F:39:GLY:O	1:F:79:ASN:HB3	2.13	0.48
1:L:219:VAL:O	1:L:220:ALA:HB3	2.12	0.48
1:B:145:HIS:HB3	1:B:150:ARG:CG	2.43	0.48
1:D:64:VAL:HG23	1:D:246:ILE:HG23	1.93	0.48
1:D:180:VAL:HG23	1:D:234:PRO:HB2	1.95	0.48
1:F:86:LEU:O	1:F:89:LEU:HD23	2.14	0.48
1:G:89:LEU:CD2	1:H:51:PRO:HB3	2.36	0.48
1:H:64:VAL:CG2	1:H:246:ILE:HG22	2.42	0.48
1:I:240:LEU:CD1	1:I:246:ILE:HD11	2.43	0.48
1:L:209:HIS:HB3	1:L:229:MET:CG	2.40	0.48
1:G:167:THR:N	1:G:224:ALA:HB2	2.27	0.48
1:B:220:ALA:O	1:B:221:ASP:CB	2.61	0.48
1:D:31:SER:O	1:D:69:VAL:HG13	2.13	0.48
1:D:209:HIS:ND1	1:D:261:THR:O	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:GLY:HA2	1:G:168:THR:HG21	1.94	0.48
1:H:125:GLN:HG2	1:H:135:GLU:HG3	1.95	0.48
1:H:126:THR:HG23	1:H:134:ALA:HB3	1.95	0.48
1:G:49:LEU:HD12	1:H:81:PHE:CE1	2.49	0.48
1:H:136:PRO:HG2	1:H:138:LEU:CD2	2.44	0.48
1:H:184:ALA:HB1	1:H:240:LEU:CD2	2.44	0.48
1:K:89:LEU:HG	1:K:89:LEU:O	2.12	0.48
1:G:209:HIS:N	1:G:261:THR:O	2.45	0.48
1:I:258:LEU:CD1	1:I:260:THR:HG23	2.43	0.48
1:K:121:VAL:O	1:K:150:ARG:HB2	2.13	0.48
1:K:218:ARG:O	1:K:220:ALA:N	2.47	0.48
1:A:182:LEU:HB3	1:A:238:PHE:HE1	1.79	0.48
1:E:40:GLU:HB2	4:E:403:HOH:O	2.14	0.48
1:G:174:LEU:HD11	1:G:231:ASN:HD22	1.79	0.48
1:A:95:ARG:NH1	1:B:113:ASP:OD1	2.46	0.48
1:C:46:GLN:HA	1:J:194:ASP:OD2	2.12	0.48
1:D:74:VAL:HG21	1:D:169:ALA:HA	1.94	0.48
1:C:101:MET:SD	1:C:159:GLY:HA2	2.54	0.48
1:D:36:LYS:HE2	1:D:165:THR:HG22	1.95	0.48
1:F:139:PRO:CB	1:F:175:GLU:HG3	2.43	0.48
1:G:42:PHE:HB2	1:G:79:ASN:ND2	2.29	0.48
1:H:98:TYR:CD1	1:H:101:MET:HE3	2.49	0.48
1:L:74:VAL:HG22	1:L:154:PHE:HB2	1.96	0.48
1:A:219:VAL:CG2	1:A:237:VAL:HG21	2.42	0.47
1:B:56:GLN:HG3	1:B:59:ARG:NH1	2.30	0.47
1:B:188:ASP:HB3	1:B:239:ASN:CB	2.44	0.47
1:C:170:ALA:CB	1:C:227:LEU:HD23	2.44	0.47
1:C:172:ARG:O	1:C:176:ILE:HG12	2.14	0.47
1:E:101:MET:SD	1:E:128:ILE:HD11	2.54	0.47
1:F:158:MET:C	1:F:160:LEU:H	2.15	0.47
1:F:228:CYS:SG	1:F:235:ILE:HD11	2.54	0.47
1:G:34:LEU:HD21	1:G:74:VAL:CG2	2.44	0.47
1:H:87:GLN:HA	1:H:91:MET:O	2.14	0.47
1:H:84:ALA:HA	1:H:87:GLN:HG2	1.95	0.47
1:K:94:THR:HG23	1:K:161:PRO:HG2	1.95	0.47
1:E:208:SER:O	1:E:212:VAL:HG23	2.14	0.47
1:J:42:PHE:CE2	1:J:75:ILE:HG23	2.48	0.47
1:J:101:MET:O	1:J:104:THR:OG1	2.26	0.47
1:K:122:THR:HG22	1:K:151:VAL:HB	1.96	0.47
1:B:236:LEU:HD12	1:B:257:THR:O	2.14	0.47
1:H:170:ALA:HB3	1:H:227:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:ARG:NH2	1:I:143:VAL:HG13	2.21	0.47
1:I:33:VAL:HG21	1:I:182:LEU:CD1	2.44	0.47
1:K:40:GLU:O	1:K:41:MET:HB2	2.13	0.47
1:K:137:TYR:OH	1:K:175:GLU:OE1	2.29	0.47
1:L:227:LEU:O	1:L:231:ASN:ND2	2.44	0.47
1:E:33:VAL:HG21	1:E:182:LEU:CD1	2.43	0.47
1:E:183:MET:HB2	1:E:237:VAL:HG22	1.97	0.47
1:H:34:LEU:HD13	1:H:173:ALA:N	2.30	0.47
1:L:64:VAL:HG12	1:L:69:VAL:HB	1.97	0.47
1:A:172:ARG:O	1:A:176:ILE:HG12	2.13	0.47
1:B:240:LEU:N	1:B:240:LEU:CD1	2.73	0.47
1:I:93:ARG:HG2	1:I:162:TYR:CE1	2.50	0.47
1:I:141:ARG:NH2	2:I:301:UTP:O1B	2.43	0.47
1:J:33:VAL:HG21	1:J:182:LEU:CD1	2.45	0.47
1:B:56:GLN:HG3	1:B:59:ARG:HH12	1.80	0.47
1:E:101:MET:HE3	3:E:301:UDP:C2	2.50	0.47
1:G:32:ARG:HA	1:G:70:GLN:O	2.15	0.47
1:G:248:ARG:HB3	1:G:253:GLU:OE1	2.13	0.47
1:H:249:ALA:N	1:H:255:ILE:HD11	2.29	0.47
1:I:60:GLN:NE2	1:I:243:ASP:OD1	2.48	0.47
1:I:103:GLY:HA2	1:I:106:MET:CE	2.44	0.47
1:L:202:GLU:HG3	1:L:203:LEU:N	2.27	0.47
1:B:221:ASP:OD1	1:B:222:ALA:N	2.48	0.47
1:D:165:THR:HB	3:D:302:UDP:O2A	2.15	0.47
1:G:240:LEU:HB2	1:G:246:ILE:HD11	1.95	0.47
1:K:33:VAL:CG2	1:K:182:LEU:HG	2.45	0.47
1:C:80:PHE:CZ	1:C:106:MET:HE3	2.50	0.47
1:C:184:ALA:CB	1:C:240:LEU:HD23	2.45	0.47
1:H:32:ARG:HG3	1:H:178:ALA:HA	1.96	0.47
1:H:163:PHE:CE2	1:I:171:GLN:HG3	2.43	0.47
1:F:79:ASN:HD21	1:F:107:ASN:CG	2.18	0.47
1:G:33:VAL:HG21	1:G:182:LEU:CD1	2.44	0.47
1:I:44:GLY:HA2	1:I:53:VAL:HG21	1.96	0.47
1:B:212:VAL:O	1:B:216:GLY:N	2.46	0.46
1:E:92:GLU:HB2	1:E:95:ARG:HD3	1.97	0.46
1:G:32:ARG:HB3	1:G:70:GLN:HB2	1.97	0.46
1:G:89:LEU:HD11	1:H:51:PRO:CG	2.45	0.46
1:H:33:VAL:HG21	1:H:182:LEU:HG	1.96	0.46
1:K:64:VAL:HG11	1:K:71:ILE:HD11	1.95	0.46
1:A:34:LEU:HD13	1:A:173:ALA:N	2.30	0.46
1:A:65:VAL:CG2	1:A:71:ILE:HD13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:THR:OXT	1:A:261:THR:OG1	2.23	0.46
1:K:121:VAL:HG11	1:K:150:ARG:HE	1.79	0.46
1:L:240:LEU:CD2	1:L:246:ILE:HD11	2.45	0.46
1:C:187:VAL:O	1:C:239:ASN:HB2	2.16	0.46
1:F:219:VAL:O	1:F:220:ALA:HB2	2.15	0.46
3:K:301:UDP:O2A	3:K:301:UDP:H3'	2.15	0.46
1:D:64:VAL:CG2	1:D:246:ILE:HG23	2.45	0.46
1:D:236:LEU:CD2	1:D:249:ALA:HB1	2.46	0.46
1:F:248:ARG:CB	1:F:255:ILE:HD13	2.44	0.46
1:L:31:SER:HB2	1:L:179:ASP:OD2	2.15	0.46
1:A:193:GLU:O	1:A:195:PRO:HD3	2.16	0.46
1:F:236:LEU:HD12	1:F:257:THR:O	2.15	0.46
1:J:170:ALA:O	1:J:174:LEU:HD23	2.16	0.46
1:L:47:VAL:HG12	1:L:48:GLY:N	2.31	0.46
1:L:193:GLU:HB3	1:L:199:PRO:HG2	1.97	0.46
1:E:209:HIS:HB3	1:E:229:MET:SD	2.56	0.46
1:E:219:VAL:O	1:E:220:ALA:HB3	2.16	0.46
1:L:54:VAL:HG12	1:L:114:PHE:HD2	1.81	0.46
1:L:91:MET:HE3	1:L:95:ARG:HB3	1.97	0.46
1:F:139:PRO:O	1:F:143:VAL:HG23	2.15	0.46
1:I:167:THR:N	1:I:224:ALA:HB2	2.30	0.46
1:E:166:ASP:HB2	1:E:221:ASP:HB2	1.98	0.46
1:F:240:LEU:HD12	1:F:240:LEU:C	2.36	0.46
1:G:249:ALA:CA	1:G:255:ILE:HD11	2.45	0.46
1:I:205:THR:O	1:I:206:ALA:HB2	2.15	0.46
1:D:185:LYS:O	1:D:239:ASN:HA	2.15	0.46
1:E:76:GLY:C	1:E:104:THR:HG22	2.37	0.46
1:E:182:LEU:HD23	1:E:236:LEU:HB3	1.98	0.46
1:F:205:THR:HG22	1:F:256:GLY:O	2.15	0.46
1:G:34:LEU:HD13	1:G:173:ALA:N	2.31	0.46
1:J:60:GLN:HE22	1:J:244:GLY:H	1.64	0.46
1:L:93:ARG:O	1:L:93:ARG:HG3	2.14	0.46
1:A:174:LEU:HD11	1:A:231:ASN:HB3	1.97	0.46
1:C:189:GLY:HA3	1:C:203:LEU:HD11	1.98	0.46
1:E:31:SER:O	1:E:69:VAL:HG13	2.16	0.46
1:I:81:PHE:CD1	1:I:86:LEU:HD11	2.51	0.46
1:J:174:LEU:HD11	1:J:231:ASN:CB	2.45	0.46
1:K:73:VAL:HG12	1:K:75:ILE:CD1	2.46	0.46
1:A:54:VAL:HG12	1:A:114:PHE:HD2	1.80	0.45
1:J:34:LEU:HD13	1:J:173:ALA:CA	2.45	0.45
1:D:207:VAL:O	1:D:259:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:VAL:HG12	1:F:102:LEU:HD11	1.97	0.45
1:F:191:PHE:CE2	1:F:203:LEU:HD23	2.51	0.45
1:J:86:LEU:O	1:J:89:LEU:HB3	2.16	0.45
1:D:33:VAL:HG21	1:D:182:LEU:CD1	2.47	0.45
1:D:36:LYS:HE2	1:D:165:THR:CG2	2.47	0.45
1:G:205:THR:O	1:G:206:ALA:HB2	2.17	0.45
1:J:37:LEU:HD12	1:J:73:VAL:HG11	1.98	0.45
1:A:34:LEU:HA	1:A:72:ALA:O	2.16	0.45
1:A:182:LEU:HD22	1:A:236:LEU:HD23	1.98	0.45
1:B:191:PHE:HA	1:B:202:GLU:O	2.15	0.45
1:E:127:ALA:HB2	1:E:157:GLY:O	2.17	0.45
1:E:180:VAL:CG2	1:E:234:PRO:HB2	2.39	0.45
1:F:98:TYR:HA	1:F:101:MET:HE3	1.99	0.45
1:F:130:MET:O	1:F:132:GLN:N	2.48	0.45
1:F:166:ASP:OD2	1:F:221:ASP:HB2	2.16	0.45
1:H:248:ARG:HB2	1:H:255:ILE:HD13	1.97	0.45
1:L:61:ILE:O	1:L:65:VAL:HG23	2.16	0.45
1:D:141:ARG:O	1:D:145:HIS:CD2	2.69	0.45
1:G:261:THR:OXT	1:G:261:THR:HG22	2.16	0.45
1:A:138:LEU:HB2	1:A:141:ARG:CB	2.42	0.45
1:B:33:VAL:HG13	1:B:182:LEU:HG	1.99	0.45
1:B:54:VAL:HG12	1:B:114:PHE:CD2	2.50	0.45
1:C:238:PHE:CE2	1:C:240:LEU:HB3	2.51	0.45
1:E:218:ARG:O	1:E:219:VAL:O	2.34	0.45
1:F:86:LEU:HD12	1:F:86:LEU:H	1.82	0.45
1:G:167:THR:HA	1:G:224:ALA:HB2	1.98	0.45
1:L:91:MET:HE3	1:L:95:ARG:HB2	1.98	0.45
1:I:42:PHE:CZ	1:I:75:ILE:HD12	2.52	0.45
1:I:192:ALA:CB	1:I:204:LEU:HD21	2.36	0.45
1:J:54:VAL:HG12	1:J:114:PHE:CD2	2.52	0.45
1:J:145:HIS:HB3	1:J:150:ARG:HG3	1.97	0.45
1:L:69:VAL:HG11	1:L:250:VAL:HG11	1.99	0.45
1:C:213:LEU:CD2	1:C:225:PHE:HE2	2.29	0.45
1:F:64:VAL:CG2	1:F:246:ILE:HG22	2.40	0.45
1:F:115:LEU:CD1	1:F:122:THR:HG21	2.46	0.45
1:G:182:LEU:HB3	1:G:238:PHE:HE1	1.82	0.45
1:J:33:VAL:HG21	1:J:182:LEU:HD11	1.98	0.45
1:J:161:PRO:HB2	1:J:162:TYR:HD1	1.80	0.45
1:A:73:VAL:HG12	1:A:75:ILE:CD1	2.47	0.45
1:B:207:VAL:HG23	1:B:259:VAL:HG22	1.96	0.45
1:C:76:GLY:C	1:C:104:THR:HG22	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ILE:O	1:C:130:MET:HG3	2.17	0.45
1:F:187:VAL:O	1:F:188:ASP:CB	2.65	0.45
1:H:209:HIS:HB2	1:H:261:THR:OG1	2.17	0.45
1:H:248:ARG:HG2	1:H:251:ARG:HH11	1.79	0.45
1:J:208:SER:O	1:J:212:VAL:HG23	2.17	0.45
1:A:141:ARG:NH2	2:A:301:UTP:O2B	2.47	0.45
1:A:158:MET:CE	1:A:171:GLN:HG2	2.46	0.45
1:C:60:GLN:HG3	1:C:246:ILE:CG2	2.47	0.45
1:H:87:GLN:HG3	1:H:88:GLN:N	2.31	0.45
1:J:246:ILE:HG23	1:J:247:ALA:N	2.32	0.45
1:A:64:VAL:CG2	1:A:246:ILE:HG22	2.46	0.44
1:C:161:PRO:O	1:C:162:TYR:HB2	2.17	0.44
1:B:188:ASP:OD1	1:B:188:ASP:N	2.45	0.44
1:C:31:SER:HB2	1:C:179:ASP:OD2	2.16	0.44
1:C:116:GLU:CD	1:D:95:ARG:HH22	2.20	0.44
1:E:87:GLN:HA	1:E:91:MET:O	2.17	0.44
1:K:73:VAL:HG12	1:K:75:ILE:HD13	1.99	0.44
1:L:220:ALA:O	1:L:224:ALA:HB3	2.17	0.44
1:C:60:GLN:HG3	1:C:246:ILE:HG22	1.97	0.44
1:F:148:LYS:HE2	1:F:148:LYS:CA	2.47	0.44
1:A:209:HIS:ND1	1:A:261:THR:HA	2.32	0.44
1:C:148:LYS:NZ	2:C:301:UTP:O1G	2.50	0.44
1:F:123:ARG:HG3	1:F:145:HIS:ND1	2.32	0.44
2:I:301:UTP:O2A	1:K:141:ARG:NH2	2.50	0.44
1:K:36:LYS:HE2	1:K:166:ASP:OD1	2.17	0.44
1:K:260:THR:O	1:K:261:THR:HG22	2.17	0.44
1:L:168:THR:O	1:L:172:ARG:HG2	2.17	0.44
1:A:103:GLY:HA2	1:A:106:MET:HE2	1.99	0.44
1:H:120:ILE:HG21	1:H:151:VAL:HG21	2.00	0.44
1:I:31:SER:N	1:I:179:ASP:OD2	2.49	0.44
1:I:161:PRO:O	1:I:162:TYR:HB2	2.17	0.44
1:I:242:THR:HB	1:I:245:ASN:HD22	1.79	0.44
1:A:64:VAL:HG21	1:A:246:ILE:CG2	2.46	0.44
1:F:183:MET:HB2	1:F:237:VAL:HG22	2.00	0.44
1:K:240:LEU:HD12	1:K:240:LEU:C	2.37	0.44
1:D:122:THR:HG22	1:D:151:VAL:HB	2.00	0.44
1:E:205:THR:O	1:E:206:ALA:HB2	2.18	0.44
1:F:187:VAL:HG12	1:F:188:ASP:N	2.33	0.44
1:G:32:ARG:CB	1:G:70:GLN:HB2	2.48	0.44
1:I:76:GLY:HA3	3:I:302:UDP:O1B	2.18	0.44
1:I:182:LEU:HB3	1:I:238:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:188:ASP:OD1	1:I:188:ASP:N	2.50	0.44
1:J:209:HIS:CB	1:J:229:MET:HG3	2.47	0.44
1:A:190:VAL:O	1:A:204:LEU:N	2.51	0.44
1:B:155:GLY:O	1:B:156:ALA:HB3	2.18	0.44
1:C:180:VAL:HG23	1:C:234:PRO:HB2	1.99	0.44
1:F:69:VAL:O	1:F:71:ILE:HD12	2.18	0.44
1:F:174:LEU:HD22	1:F:233:MET:CE	2.47	0.44
1:H:249:ALA:CA	1:H:255:ILE:HD11	2.47	0.44
1:I:36:LYS:HE3	1:I:166:ASP:OD1	2.17	0.44
1:I:98:TYR:CD1	1:J:133:VAL:HG22	2.52	0.44
1:K:34:LEU:HD22	1:K:173:ALA:HB2	1.99	0.44
1:K:90:GLY:O	1:L:117:LYS:HE2	2.18	0.44
1:B:232:GLY:HA2	1:B:261:THR:HG22	1.98	0.43
1:D:35:LEU:HA	1:D:182:LEU:HB2	2.00	0.43
1:D:135:GLU:HG2	2:D:301:UTP:H2'	2.00	0.43
1:D:187:VAL:HG22	1:D:188:ASP:H	1.83	0.43
1:F:242:THR:HB	1:F:245:ASN:HD22	1.78	0.43
1:J:64:VAL:HG22	1:J:247:ALA:HA	2.00	0.43
1:K:126:THR:HG21	1:K:130:MET:HE2	1.98	0.43
1:A:33:VAL:HG21	1:A:182:LEU:CD1	2.49	0.43
1:E:53:VAL:O	1:E:57:VAL:HG23	2.18	0.43
1:F:86:LEU:HD12	1:F:86:LEU:N	2.34	0.43
1:G:33:VAL:CG2	1:G:182:LEU:HG	2.48	0.43
1:K:209:HIS:HB3	1:K:229:MET:CG	2.48	0.43
1:C:131:GLY:O	1:E:138:LEU:HD12	2.18	0.43
1:E:121:VAL:CG1	1:E:150:ARG:HG2	2.47	0.43
1:E:209:HIS:CB	1:E:229:MET:HG3	2.48	0.43
1:J:162:TYR:CE2	1:K:174:LEU:HD12	2.53	0.43
1:B:161:PRO:O	1:B:162:TYR:HB2	2.18	0.43
1:C:60:GLN:HE22	1:C:243:ASP:HA	1.82	0.43
1:D:209:HIS:HB3	1:D:229:MET:HG3	2.01	0.43
1:D:240:LEU:HD12	1:D:240:LEU:C	2.39	0.43
1:E:190:VAL:O	1:E:204:LEU:HD13	2.17	0.43
1:E:204:LEU:HD21	1:E:215:ARG:NH1	2.33	0.43
1:F:166:ASP:HB2	1:F:221:ASP:OD2	2.18	0.43
1:F:166:ASP:HB3	1:F:224:ALA:CB	2.48	0.43
1:F:170:ALA:O	1:F:174:LEU:HD23	2.18	0.43
1:H:75:ILE:HG21	1:H:107:ASN:HB2	2.00	0.43
1:H:171:GLN:NE2	1:I:161:PRO:HD2	2.33	0.43
1:H:174:LEU:HD22	1:H:233:MET:CE	2.48	0.43
1:L:91:MET:CE	1:L:95:ARG:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:GLN:HG3	1:C:163:PHE:CE2	2.51	0.43
1:E:204:LEU:CD2	1:E:207:VAL:HG11	2.49	0.43
1:F:244:GLY:O	1:F:248:ARG:HG3	2.19	0.43
1:H:129:THR:HG23	1:H:136:PRO:HB3	2.00	0.43
1:K:47:VAL:HG12	1:L:47:VAL:HG12	2.01	0.43
1:K:106:MET:SD	1:L:106:MET:HE1	2.59	0.43
1:L:39:GLY:HA3	1:L:76:GLY:C	2.38	0.43
1:L:41:MET:HE2	1:L:185:LYS:HA	2.00	0.43
1:C:106:MET:SD	1:D:106:MET:HE2	2.59	0.43
1:G:166:ASP:HB2	1:G:221:ASP:HB3	2.01	0.43
1:A:65:VAL:HG22	1:A:71:ILE:CD1	2.48	0.43
1:E:69:VAL:HG21	1:E:250:VAL:HG12	1.99	0.43
1:K:76:GLY:C	1:K:104:THR:HG22	2.39	0.43
1:K:180:VAL:HG23	1:K:234:PRO:O	2.18	0.43
1:L:145:HIS:HB3	1:L:150:ARG:CG	2.47	0.43
1:A:32:ARG:NH2	1:A:143:VAL:HG22	2.33	0.43
1:A:64:VAL:HG12	1:A:71:ILE:HD11	2.01	0.43
1:B:182:LEU:HD22	1:B:236:LEU:HD23	2.01	0.43
1:C:124:VAL:HG22	1:C:153:ILE:HB	2.00	0.43
1:C:234:PRO:HB3	1:C:260:THR:HG22	2.00	0.43
1:C:240:LEU:C	1:C:240:LEU:HD12	2.39	0.43
1:G:139:PRO:O	1:G:143:VAL:HG23	2.19	0.43
1:I:182:LEU:HD23	1:I:236:LEU:HB3	2.00	0.43
1:K:87:GLN:HA	1:K:91:MET:O	2.19	0.43
1:A:240:LEU:CD1	1:A:246:ILE:CD1	2.95	0.43
1:B:92:GLU:HG3	1:B:95:ARG:HH12	1.84	0.43
1:C:89:LEU:HD21	1:D:51:PRO:HG3	2.00	0.43
1:D:187:VAL:HG22	1:D:188:ASP:N	2.33	0.43
1:D:209:HIS:HB3	1:D:229:MET:CG	2.49	0.43
1:G:174:LEU:HD13	1:G:231:ASN:ND2	2.34	0.43
1:G:248:ARG:HG2	1:G:251:ARG:NH1	2.34	0.43
1:H:32:ARG:CB	1:H:70:GLN:HB2	2.48	0.43
1:B:212:VAL:HB	1:B:225:PHE:CZ	2.54	0.43
1:C:248:ARG:HA	1:C:251:ARG:NH2	2.33	0.43
1:K:66:ARG:NH1	1:K:118:GLU:O	2.48	0.43
1:K:114:PHE:O	1:K:118:GLU:HG2	2.18	0.43
1:L:76:GLY:O	1:L:107:ASN:ND2	2.48	0.43
1:L:144:ARG:O	1:L:148:LYS:HG3	2.18	0.43
1:L:245:ASN:O	1:L:249:ALA:N	2.48	0.43
1:B:83:GLY:HA3	3:B:300:UDP:HO2'	1.83	0.42
1:B:180:VAL:HG23	1:B:234:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:ARG:NH2	1:E:143:VAL:HG13	2.30	0.42
1:E:212:VAL:HB	1:E:225:PHE:CZ	2.53	0.42
1:G:33:VAL:HG23	1:G:180:VAL:HG13	2.01	0.42
1:G:64:VAL:HG12	1:G:69:VAL:HB	2.01	0.42
1:I:123:ARG:HG2	1:I:150:ARG:HD2	2.00	0.42
4:J:403:HOH:O	1:K:94:THR:HG21	2.18	0.42
1:K:157:GLY:HA3	3:K:301:UDP:C5	2.53	0.42
1:D:74:VAL:HG12	1:D:165:THR:HG23	1.99	0.42
1:F:34:LEU:HA	1:F:72:ALA:O	2.19	0.42
1:F:188:ASP:HB3	1:F:239:ASN:CB	2.46	0.42
1:H:65:VAL:HG21	1:H:151:VAL:CG2	2.49	0.42
1:I:106:MET:CE	1:J:106:MET:HE2	2.50	0.42
1:B:238:PHE:HZ	1:B:246:ILE:HG12	1.83	0.42
1:F:141:ARG:O	1:F:142:ALA:C	2.57	0.42
1:A:64:VAL:CG1	1:A:69:VAL:HB	2.48	0.42
1:D:74:VAL:CG1	1:D:165:THR:HG23	2.50	0.42
1:H:240:LEU:HB2	1:H:246:ILE:CD1	2.49	0.42
1:J:145:HIS:ND1	1:J:150:ARG:HD2	2.35	0.42
1:L:212:VAL:HG11	1:L:219:VAL:CG1	2.49	0.42
1:C:36:LYS:HE2	1:C:165:THR:HG21	2.01	0.42
1:E:33:VAL:HG21	1:E:182:LEU:CG	2.48	0.42
1:A:255:ILE:HD12	1:A:255:ILE:O	2.19	0.42
1:D:166:ASP:OD2	1:D:221:ASP:HB2	2.19	0.42
1:F:42:PHE:CE2	1:F:75:ILE:HD12	2.55	0.42
1:H:204:LEU:HD12	1:H:207:VAL:HG11	2.02	0.42
1:I:83:GLY:HA3	1:I:97:ASP:OD1	2.19	0.42
1:I:165:THR:O	1:I:168:THR:HB	2.20	0.42
1:K:105:VAL:CG2	1:K:130:MET:HE1	2.49	0.42
1:L:115:LEU:CD1	1:L:122:THR:HG21	2.50	0.42
1:A:246:ILE:O	1:A:250:VAL:HG23	2.20	0.42
1:C:98:TYR:HA	1:C:101:MET:HE3	2.00	0.42
1:I:54:VAL:HG12	1:I:114:PHE:CD2	2.55	0.42
1:K:33:VAL:HG21	1:K:182:LEU:HD11	2.02	0.42
1:K:161:PRO:O	1:K:162:TYR:HB2	2.20	0.42
1:B:33:VAL:HG11	1:B:182:LEU:HD12	2.00	0.42
1:C:142:ALA:HA	1:C:145:HIS:HD2	1.85	0.42
1:D:34:LEU:HD13	1:D:173:ALA:HB2	2.02	0.42
1:F:75:ILE:HG21	1:F:107:ASN:HB2	2.02	0.42
1:G:166:ASP:HB2	1:G:221:ASP:HB2	2.02	0.42
1:G:174:LEU:CD1	1:G:231:ASN:HD22	2.32	0.42
1:H:112:GLN:HG3	1:H:122:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:102:LEU:HD21	1:L:130:MET:CE	2.49	0.42
1:L:33:VAL:HG21	1:L:182:LEU:CG	2.50	0.42
1:B:112:GLN:HG3	1:B:122:THR:OG1	2.20	0.42
1:E:40:GLU:O	1:E:44:GLY:N	2.50	0.42
1:G:125:GLN:HG2	1:G:135:GLU:HG3	2.02	0.42
1:I:69:VAL:HG21	1:I:250:VAL:CG1	2.43	0.42
1:A:209:HIS:CE1	1:A:261:THR:HA	2.54	0.41
1:D:81:PHE:HB3	1:D:86:LEU:HD11	2.02	0.41
1:F:123:ARG:CG	1:F:150:ARG:HD3	2.50	0.41
1:H:242:THR:HB	1:H:245:ASN:HD21	1.83	0.41
1:K:238:PHE:CE2	1:K:240:LEU:HB3	2.55	0.41
1:B:188:ASP:HB3	1:B:239:ASN:HB3	2.01	0.41
1:C:121:VAL:CG1	1:C:150:ARG:HG2	2.50	0.41
1:D:78:GLY:N	3:D:302:UDP:O3B	2.52	0.41
1:F:47:VAL:HG12	1:F:48:GLY:H	1.85	0.41
1:G:36:LYS:HE3	1:G:166:ASP:OD1	2.20	0.41
1:H:238:PHE:CE2	1:H:246:ILE:HG12	2.56	0.41
1:L:34:LEU:HA	1:L:72:ALA:O	2.20	0.41
1:A:209:HIS:CB	1:A:229:MET:HG3	2.49	0.41
1:B:64:VAL:HG11	1:B:71:ILE:HG12	2.02	0.41
1:D:166:ASP:C	1:D:224:ALA:HB2	2.41	0.41
1:E:113:ASP:OD2	1:F:91:MET:HA	2.19	0.41
1:G:65:VAL:HG22	1:G:71:ILE:CD1	2.45	0.41
1:G:188:ASP:OD1	1:G:189:GLY:N	2.53	0.41
1:I:182:LEU:CD2	1:I:236:LEU:HD23	2.50	0.41
1:K:219:VAL:CG1	1:K:220:ALA:H	2.20	0.41
1:K:236:LEU:CD2	1:K:249:ALA:HB1	2.50	0.41
1:L:72:ALA:HB1	1:L:154:PHE:HE2	1.85	0.41
1:A:207:VAL:CG1	1:A:259:VAL:HG22	2.50	0.41
1:F:54:VAL:CG1	1:F:114:PHE:HD2	2.34	0.41
1:G:89:LEU:HD11	1:H:51:PRO:HB3	2.02	0.41
1:G:240:LEU:HD12	1:G:240:LEU:C	2.41	0.41
1:I:148:LYS:HD2	1:I:150:ARG:NH1	2.36	0.41
1:K:93:ARG:HG2	1:K:162:TYR:CE1	2.54	0.41
1:A:64:VAL:HG12	1:A:69:VAL:HB	2.02	0.41
1:D:42:PHE:CE2	1:D:75:ILE:HG23	2.55	0.41
1:F:98:TYR:O	1:F:102:LEU:HG	2.20	0.41
1:I:58:ALA:HB1	1:I:115:LEU:HD23	2.03	0.41
1:J:166:ASP:HB3	1:J:224:ALA:CB	2.50	0.41
1:J:209:HIS:HA	1:J:225:PHE:HZ	1.86	0.41
1:K:137:TYR:CE1	1:K:172:ARG:NE	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:HB2	1:A:253:GLU:OE1	2.21	0.41
1:E:204:LEU:HD23	1:E:207:VAL:HG11	2.01	0.41
1:E:209:HIS:HB3	1:E:229:MET:CG	2.51	0.41
1:G:33:VAL:HG23	1:G:180:VAL:CG1	2.51	0.41
1:H:191:PHE:CD1	1:H:191:PHE:N	2.88	0.41
1:H:240:LEU:HD12	1:H:240:LEU:C	2.40	0.41
1:J:34:LEU:HD13	1:J:173:ALA:HB2	2.02	0.41
1:L:166:ASP:HB3	1:L:224:ALA:HB2	2.03	0.41
1:D:209:HIS:HA	1:D:225:PHE:CZ	2.54	0.41
1:F:240:LEU:HB2	1:F:246:ILE:HD11	2.03	0.41
1:G:73:VAL:HG12	1:G:75:ILE:CD1	2.50	0.41
1:H:36:LYS:HZ3	1:H:165:THR:HG22	1.86	0.41
1:H:204:LEU:CD1	1:H:207:VAL:HG11	2.50	0.41
1:A:73:VAL:HG12	1:A:75:ILE:HD13	2.01	0.41
1:D:32:ARG:HH22	1:D:143:VAL:HG13	1.85	0.41
1:D:74:VAL:HG12	1:D:165:THR:CG2	2.51	0.41
1:F:183:MET:O	1:F:237:VAL:HA	2.21	0.41
1:G:258:LEU:HG	1:G:260:THR:HG22	2.03	0.41
1:K:242:THR:HB	1:K:245:ASN:HD21	1.76	0.41
1:A:188:ASP:OD1	1:A:189:GLY:N	2.54	0.41
1:B:101:MET:SD	1:B:159:GLY:HA2	2.60	0.41
1:C:184:ALA:HB1	1:C:240:LEU:HD23	2.03	0.41
1:F:33:VAL:HG21	1:F:182:LEU:HG	2.02	0.41
1:J:29:GLY:HA2	1:J:250:VAL:O	2.21	0.41
1:J:131:GLY:O	2:J:301:UTP:N3	2.43	0.41
1:J:159:GLY:O	1:J:160:LEU:HD23	2.21	0.41
1:K:125:GLN:HA	1:K:135:GLU:O	2.21	0.41
1:K:180:VAL:HG22	1:K:181:VAL:N	2.36	0.41
1:K:239:ASN:O	1:K:245:ASN:ND2	2.53	0.41
1:L:64:VAL:HG22	1:L:247:ALA:HA	2.02	0.41
1:L:240:LEU:O	1:L:240:LEU:HD13	2.21	0.41
1:A:209:HIS:HB3	1:A:229:MET:CG	2.50	0.41
1:B:82:ARG:HD2	1:B:82:ARG:HA	1.94	0.41
1:A:32:ARG:CG	1:A:178:ALA:HA	2.49	0.40
1:B:123:ARG:HG3	1:B:145:HIS:ND1	2.36	0.40
1:E:81:PHE:HE1	1:F:49:LEU:HD12	1.85	0.40
1:F:42:PHE:CE2	1:F:75:ILE:HG23	2.56	0.40
1:G:35:LEU:HD11	1:G:184:ALA:HB2	2.02	0.40
1:G:167:THR:CA	1:G:224:ALA:HB2	2.51	0.40
1:I:113:ASP:HA	1:J:95:ARG:NH1	2.35	0.40
1:J:104:THR:OG1	1:J:156:ALA:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:244:GLY:O	1:K:248:ARG:HG3	2.21	0.40
1:K:260:THR:HG22	1:K:261:THR:N	2.36	0.40
1:L:37:LEU:HD23	1:L:38:GLY:O	2.22	0.40
1:C:106:MET:CE	1:D:106:MET:CE	3.00	0.40
1:D:191:PHE:CE1	1:D:203:LEU:HD13	2.56	0.40
1:E:165:THR:HB	3:E:301:UDP:O1A	2.22	0.40
1:G:47:VAL:HG12	1:G:48:GLY:N	2.37	0.40
1:H:145:HIS:CE1	1:H:150:ARG:HH11	2.39	0.40
1:I:36:LYS:C	1:I:36:LYS:HD3	2.42	0.40
1:J:98:TYR:HA	1:J:101:MET:HE3	2.03	0.40
1:J:210:ARG:HD2	1:J:210:ARG:HA	1.81	0.40
1:L:188:ASP:CB	1:L:239:ASN:HB2	2.52	0.40
1:A:148:LYS:NZ	2:A:301:UTP:O2G	2.54	0.40
1:D:204:LEU:HG	1:D:207:VAL:HG11	1.99	0.40
1:J:64:VAL:HG21	1:J:246:ILE:CG1	2.34	0.40
1:J:74:VAL:CG1	1:J:165:THR:HG23	2.52	0.40
1:J:138:LEU:N	1:J:138:LEU:HD22	2.36	0.40
1:J:191:PHE:HE1	1:J:203:LEU:HD13	1.86	0.40
1:A:32:ARG:HH22	1:A:143:VAL:HG22	1.85	0.40
1:C:202:GLU:HG2	1:C:203:LEU:N	2.36	0.40
1:C:219:VAL:O	1:C:220:ALA:HB2	2.21	0.40
1:D:101:MET:SD	1:D:159:GLY:HA2	2.61	0.40
1:E:101:MET:SD	1:E:159:GLY:HA2	2.62	0.40
1:F:148:LYS:HE2	1:F:148:LYS:HA	2.02	0.40
1:F:210:ARG:O	1:F:210:ARG:HG2	2.21	0.40
1:H:127:ALA:HB2	1:H:157:GLY:O	2.21	0.40
1:I:32:ARG:CB	1:I:70:GLN:HB2	2.51	0.40
1:I:174:LEU:HD22	1:I:233:MET:HE2	2.03	0.40
1:I:188:ASP:N	1:I:239:ASN:HB2	2.37	0.40
1:J:73:VAL:HG12	1:J:75:ILE:HD13	2.04	0.40
1:J:180:VAL:HG23	1:J:234:PRO:C	2.41	0.40
1:J:74:VAL:HG12	1:J:165:THR:CG2	2.52	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	218/281 (78%)	205 (94%)	12 (6%)	1 (0%)	29 63
1	B	222/281 (79%)	199 (90%)	16 (7%)	7 (3%)	4 21
1	C	225/281 (80%)	212 (94%)	11 (5%)	2 (1%)	17 51
1	D	221/281 (79%)	211 (96%)	9 (4%)	1 (0%)	29 63
1	E	220/281 (78%)	203 (92%)	14 (6%)	3 (1%)	11 39
1	F	210/281 (75%)	186 (89%)	15 (7%)	9 (4%)	2 15
1	G	211/281 (75%)	196 (93%)	9 (4%)	6 (3%)	5 24
1	H	221/281 (79%)	211 (96%)	6 (3%)	4 (2%)	8 33
1	I	222/281 (79%)	203 (91%)	17 (8%)	2 (1%)	17 51
1	J	224/281 (80%)	211 (94%)	12 (5%)	1 (0%)	34 68
1	K	224/281 (80%)	202 (90%)	18 (8%)	4 (2%)	8 33
1	L	221/281 (79%)	204 (92%)	10 (4%)	7 (3%)	4 21
All	All	2639/3372 (78%)	2443 (93%)	149 (6%)	47 (2%)	8 33

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	GLY
1	B	220	ALA
1	B	243	ASP
1	E	219	VAL
1	F	188	ASP
1	F	220	ALA
1	G	86	LEU
1	G	87	GLN
1	G	260	THR
1	K	41	MET
1	B	218	ARG
1	C	220	ALA
1	D	219	VAL
1	F	159	GLY
1	F	187	VAL
1	G	88	GLN
1	G	131	GLY
1	H	203	LEU

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Mol	Chain	Res	Type
1	I	44	GLY
1	J	131	GLY
1	K	219	VAL
1	L	131	GLY
1	L	198	ASN
1	B	221	ASP
1	E	206	ALA
1	E	220	ALA
1	F	131	GLY
1	F	202	GLU
1	K	46	GLN
1	L	31	SER
1	L	220	ALA
1	C	221	ASP
1	F	221	ASP
1	G	206	ALA
1	H	206	ALA
1	H	220	ALA
1	I	206	ALA
1	L	202	GLU
1	L	206	ALA
1	F	222	ALA
1	K	183	MET
1	F	194	ASP
1	B	45	GLY
1	B	136	PRO
1	H	45	GLY
1	L	197	VAL
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	164/215 (76%)	160 (98%)	4 (2%)	49 75
1	B	168/215 (78%)	165 (98%)	3 (2%)	59 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	174/215 (81%)	171 (98%)	3 (2%)	60 83
1	D	168/215 (78%)	165 (98%)	3 (2%)	59 82
1	E	168/215 (78%)	162 (96%)	6 (4%)	35 66
1	F	163/215 (76%)	156 (96%)	7 (4%)	29 61
1	G	158/215 (74%)	156 (99%)	2 (1%)	69 86
1	H	170/215 (79%)	169 (99%)	1 (1%)	86 93
1	I	168/215 (78%)	166 (99%)	2 (1%)	71 87
1	J	171/215 (80%)	166 (97%)	5 (3%)	42 71
1	K	169/215 (79%)	167 (99%)	2 (1%)	71 87
1	L	166/215 (77%)	163 (98%)	3 (2%)	59 82
All	All	2007/2580 (78%)	1966 (98%)	41 (2%)	55 79

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	LEU
1	A	205	THR
1	A	217	LEU
1	A	260	THR
1	B	89	LEU
1	B	215	ARG
1	B	240	LEU
1	C	115	LEU
1	C	117	LYS
1	C	141	ARG
1	D	141	ARG
1	D	148	LYS
1	D	204	LEU
1	E	47	VAL
1	E	95	ARG
1	E	130	MET
1	E	135	GLU
1	E	190	VAL
1	E	202	GLU
1	F	138	LEU
1	F	141	ARG
1	F	148	LYS
1	F	203	LEU

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Mol	Chain	Res	Type
1	F	204	LEU
1	F	210	ARG
1	F	219	VAL
1	G	138	LEU
1	G	211	GLU
1	H	59	ARG
1	I	59	ARG
1	I	141	ARG
1	J	123	ARG
1	J	141	ARG
1	J	144	ARG
1	J	185	LYS
1	J	210	ARG
1	K	85	GLN
1	K	141	ARG
1	L	93	ARG
1	L	163	PHE
1	L	193	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	C	60	GLN
1	D	245	ASN
1	G	209	HIS
1	G	231	ASN
1	G	245	ASN
1	I	245	ASN
1	J	60	GLN
1	J	245	ASN
1	K	245	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
3	UDP	I	302	-	20,26,26	1.01	1 (5%)	25,40,40	1.17	3 (12%)
2	UTP	G	301	-	26,30,30	2.42	10 (38%)	34,47,47	2.14	12 (35%)
2	UTP	I	301	-	26,30,30	2.66	13 (50%)	34,47,47	2.25	14 (41%)
3	UDP	H	301	-	20,26,26	0.93	1 (5%)	25,40,40	1.02	2 (8%)
3	UDP	E	301	-	20,26,26	1.05	1 (5%)	25,40,40	1.20	3 (12%)
3	UDP	C	302	-	20,26,26	1.01	1 (5%)	25,40,40	1.15	2 (8%)
2	UTP	J	301	-	26,30,30	2.83	16 (61%)	34,47,47	2.38	15 (44%)
2	UTP	A	301	-	26,30,30	2.42	8 (30%)	34,47,47	2.16	13 (38%)
3	UDP	J	302	-	20,26,26	1.00	1 (5%)	25,40,40	1.11	2 (8%)
3	UDP	K	301	-	20,26,26	1.02	1 (5%)	25,40,40	1.16	3 (12%)
3	UDP	D	302	-	20,26,26	0.93	1 (5%)	25,40,40	1.02	2 (8%)
2	UTP	D	301	-	26,30,30	2.47	8 (30%)	34,47,47	2.04	10 (29%)
3	UDP	B	300	-	20,26,26	0.97	1 (5%)	25,40,40	1.14	2 (8%)
2	UTP	C	301	-	26,30,30	2.37	8 (30%)	34,47,47	2.11	13 (38%)

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
3	UDP	I	302	-	-	1/14/32/32	0/2/2/2
2	UTP	G	301	-	-	8/22/38/38	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UTP	I	301	-	-	7/22/38/38	0/2/2/2
3	UDP	H	301	-	-	4/14/32/32	0/2/2/2
3	UDP	E	301	-	-	1/14/32/32	0/2/2/2
3	UDP	C	302	-	-	1/14/32/32	0/2/2/2
2	UTP	J	301	-	-	1/22/38/38	0/2/2/2
2	UTP	A	301	-	-	5/22/38/38	0/2/2/2
3	UDP	J	302	-	-	4/14/32/32	0/2/2/2
3	UDP	K	301	-	-	2/14/32/32	0/2/2/2
3	UDP	D	302	-	-	2/14/32/32	0/2/2/2
2	UTP	D	301	-	-	2/22/38/38	0/2/2/2
3	UDP	B	300	-	-	3/14/32/32	0/2/2/2
2	UTP	C	301	-	-	8/22/38/38	0/2/2/2

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	301	UTP	C6-C5	-7.84	1.31	1.52
2	D	301	UTP	C2-N1	7.27	1.46	1.35
2	I	301	UTP	C6-C5	-7.25	1.33	1.52
2	A	301	UTP	C2-N1	6.92	1.45	1.35
2	G	301	UTP	C2-N1	6.83	1.45	1.35
2	D	301	UTP	C6-C5	-6.58	1.35	1.52
2	C	301	UTP	C6-C5	-6.55	1.35	1.52
2	C	301	UTP	C2-N1	6.51	1.44	1.35
2	A	301	UTP	C6-C5	-6.38	1.35	1.52
2	G	301	UTP	C6-C5	-6.31	1.35	1.52
2	J	301	UTP	C2-N1	5.10	1.42	1.35
2	I	301	UTP	C2-N1	4.52	1.42	1.35
2	J	301	UTP	PG-O1G	-3.59	1.41	1.54
2	J	301	UTP	PG-O3G	-3.48	1.41	1.54
2	I	301	UTP	PG-O1G	-3.46	1.41	1.54
2	I	301	UTP	PG-O3G	-3.40	1.41	1.54
2	I	301	UTP	O4-C4	-3.30	1.16	1.23
2	J	301	UTP	C1'-N1	-3.27	1.40	1.46
3	D	302	UDP	C4-N3	3.20	1.38	1.33
3	E	301	UDP	C4-N3	3.17	1.38	1.33
3	B	300	UDP	C4-N3	3.15	1.38	1.33
3	J	302	UDP	C4-N3	3.14	1.38	1.33
3	H	301	UDP	C4-N3	3.14	1.38	1.33
2	I	301	UTP	C1'-N1	-3.13	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	302	UDP	C4-N3	3.12	1.38	1.33
2	J	301	UTP	PA-O2A	-3.11	1.40	1.55
3	C	302	UDP	C4-N3	3.09	1.38	1.33
3	K	301	UDP	C4-N3	3.08	1.38	1.33
2	I	301	UTP	O2-C2	-3.05	1.17	1.23
2	J	301	UTP	O2-C2	-2.95	1.17	1.23
2	I	301	UTP	PB-O1B	-2.95	1.41	1.55
2	I	301	UTP	PA-O2A	-2.91	1.41	1.55
2	J	301	UTP	PA-O1A	-2.88	1.40	1.50
2	J	301	UTP	PG-O2G	-2.86	1.41	1.50
2	J	301	UTP	PB-O1B	-2.83	1.42	1.55
2	I	301	UTP	PA-O1A	-2.78	1.41	1.50
2	A	301	UTP	C4-N3	2.75	1.42	1.37
2	G	301	UTP	C4-N3	2.74	1.42	1.37
2	I	301	UTP	PG-O2G	-2.64	1.42	1.50
2	J	301	UTP	PB-O2B	-2.58	1.41	1.50
2	J	301	UTP	O4-C4	-2.53	1.18	1.23
2	D	301	UTP	C4-N3	2.50	1.41	1.37
2	G	301	UTP	C2-N3	2.47	1.42	1.38
2	A	301	UTP	C2-N3	2.46	1.42	1.38
2	D	301	UTP	O4'-C1'	2.45	1.47	1.42
2	C	301	UTP	C2-N3	2.43	1.42	1.38
2	C	301	UTP	C4-N3	2.42	1.41	1.37
2	C	301	UTP	O4-C4	-2.31	1.18	1.23
2	J	301	UTP	C3'-C4'	-2.25	1.47	1.53
2	I	301	UTP	C3'-C4'	-2.25	1.47	1.53
2	I	301	UTP	PB-O2B	-2.24	1.43	1.50
2	A	301	UTP	O4-C4	-2.23	1.18	1.23
2	D	301	UTP	O4-C4	-2.20	1.18	1.23
2	A	301	UTP	O2-C2	-2.20	1.19	1.23
2	G	301	UTP	C1'-N1	-2.19	1.42	1.46
2	G	301	UTP	O2-C2	-2.18	1.19	1.23
2	G	301	UTP	O4-C4	-2.18	1.18	1.23
2	C	301	UTP	PG-O3G	-2.15	1.46	1.54
2	C	301	UTP	PG-O1G	-2.13	1.46	1.54
2	D	301	UTP	O2-C2	-2.13	1.19	1.23
2	G	301	UTP	PG-O3G	-2.12	1.46	1.54
2	A	301	UTP	PG-O3G	-2.12	1.46	1.54
2	G	301	UTP	PG-O1G	-2.12	1.46	1.54
2	D	301	UTP	C2-N3	2.12	1.41	1.38
2	A	301	UTP	PG-O1G	-2.11	1.46	1.54
2	D	301	UTP	PG-O3G	-2.10	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	301	UTP	C3'-C2'	-2.09	1.47	1.53
2	C	301	UTP	O2-C2	-2.07	1.19	1.23
2	J	301	UTP	C2-N3	2.06	1.41	1.38
2	J	301	UTP	O5'-C5'	-2.02	1.37	1.44
2	G	301	UTP	O4'-C1'	2.02	1.46	1.42

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	UTP	C4-N3-C2	-7.34	119.70	125.79
2	D	301	UTP	C4-N3-C2	-7.34	119.70	125.79
2	I	301	UTP	C4-N3-C2	-7.20	119.82	125.79
2	A	301	UTP	C4-N3-C2	-7.15	119.86	125.79
2	J	301	UTP	C4-N3-C2	-7.06	119.94	125.79
2	C	301	UTP	C4-N3-C2	-6.88	120.09	125.79
2	I	301	UTP	N3-C2-N1	4.38	121.28	116.65
3	E	301	UDP	C5-C4-N3	-3.91	114.70	123.31
3	J	302	UDP	C5-C4-N3	-3.91	114.72	123.31
3	C	302	UDP	C5-C4-N3	-3.90	114.73	123.31
3	D	302	UDP	C5-C4-N3	-3.90	114.73	123.31
3	B	300	UDP	C5-C4-N3	-3.89	114.74	123.31
3	I	302	UDP	C5-C4-N3	-3.89	114.76	123.31
3	H	301	UDP	C5-C4-N3	-3.89	114.76	123.31
3	K	301	UDP	C5-C4-N3	-3.89	114.76	123.31
2	J	301	UTP	PB-O3A-PA	-3.85	119.61	132.83
2	J	301	UTP	O1G-PG-O3B	3.57	116.61	104.64
2	A	301	UTP	N3-C2-N1	3.48	120.34	116.65
2	G	301	UTP	N3-C2-N1	3.37	120.21	116.65
2	I	301	UTP	O1G-PG-O3B	3.36	115.91	104.64
2	D	301	UTP	C5-C4-N3	3.36	120.42	116.65
2	J	301	UTP	PB-O3B-PG	-3.32	121.43	132.83
2	A	301	UTP	C5-C4-N3	3.26	120.31	116.65
2	D	301	UTP	N3-C2-N1	3.24	120.08	116.65
2	G	301	UTP	C5-C4-N3	3.22	120.26	116.65
2	J	301	UTP	O2-C2-N1	-3.19	119.10	123.11
2	G	301	UTP	PB-O3B-PG	-3.17	121.94	132.83
2	C	301	UTP	C5-C4-N3	3.17	120.21	116.65
2	C	301	UTP	N3-C2-N1	3.11	119.94	116.65
2	C	301	UTP	PB-O3B-PG	-3.05	122.36	132.83
2	J	301	UTP	N3-C2-N1	3.00	119.82	116.65
2	I	301	UTP	O3G-PG-O3B	2.99	114.66	104.64
2	J	301	UTP	O3G-PG-O3B	2.99	114.66	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	UTP	O2-C2-N1	-2.98	119.36	123.11
2	G	301	UTP	O2-C2-N1	-2.97	119.38	123.11
2	J	301	UTP	O2A-PA-O1A	-2.95	97.66	112.24
2	C	301	UTP	O3G-PG-O3B	2.89	114.33	104.64
2	C	301	UTP	C2'-C3'-C4'	2.86	108.20	102.64
2	A	301	UTP	O3G-PG-O3B	2.86	114.22	104.64
2	D	301	UTP	O1G-PG-O3B	2.85	114.18	104.64
2	J	301	UTP	O4'-C1'-N1	-2.82	105.45	109.30
2	J	301	UTP	C5-C6-N1	2.81	120.87	111.61
2	I	301	UTP	O2-C2-N1	-2.81	119.58	123.11
2	G	301	UTP	O1G-PG-O3B	2.81	114.05	104.64
2	I	301	UTP	O3G-PG-O2G	-2.80	99.73	110.68
2	A	301	UTP	O2-C2-N1	-2.79	119.61	123.11
2	A	301	UTP	O1G-PG-O3B	2.76	113.89	104.64
2	G	301	UTP	C2'-C3'-C4'	2.71	107.91	102.64
2	D	301	UTP	O3G-PG-O3B	2.69	113.66	104.64
2	C	301	UTP	C5-C6-N1	2.66	120.39	111.61
2	G	301	UTP	O3G-PG-O3B	2.65	113.53	104.64
2	I	301	UTP	O2A-PA-O1A	-2.65	99.15	112.24
2	D	301	UTP	PB-O3B-PG	-2.65	123.75	132.83
2	A	301	UTP	PB-O3B-PG	-2.64	123.77	132.83
2	D	301	UTP	PB-O3A-PA	-2.62	123.82	132.83
2	A	301	UTP	C5-C6-N1	2.62	120.26	111.61
2	I	301	UTP	C5-C6-N1	2.62	120.24	111.61
2	A	301	UTP	C2'-C3'-C4'	2.56	107.62	102.64
2	D	301	UTP	C5-C6-N1	2.53	119.95	111.61
2	I	301	UTP	C3'-C2'-C1'	2.50	106.18	101.43
2	G	301	UTP	C5-C6-N1	2.44	119.67	111.61
2	C	301	UTP	O1G-PG-O3B	2.44	112.82	104.64
2	J	301	UTP	O4'-C1'-C2'	-2.43	101.33	106.64
2	J	301	UTP	O1G-PG-O2G	-2.43	101.19	110.68
2	I	301	UTP	C5-C4-N3	2.36	119.30	116.65
2	I	301	UTP	C2'-C3'-C4'	2.36	107.22	102.64
2	G	301	UTP	O2A-PA-O1A	-2.35	100.63	112.24
2	A	301	UTP	C3'-C2'-C1'	2.31	105.82	101.43
2	G	301	UTP	O1B-PB-O2B	-2.30	100.86	112.24
2	A	301	UTP	O1B-PB-O2B	-2.30	100.87	112.24
3	B	300	UDP	O3B-PB-O3A	2.30	112.34	104.64
2	C	301	UTP	C3'-C2'-C1'	2.29	105.78	101.43
3	H	301	UDP	PA-O3A-PB	-2.29	124.97	132.83
2	I	301	UTP	O1B-PB-O2B	-2.29	100.94	112.24
3	C	302	UDP	O3B-PB-O3A	2.29	112.30	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	302	UDP	O3B-PB-O3A	2.28	112.28	104.64
2	I	301	UTP	PB-O3B-PG	-2.28	125.01	132.83
3	E	301	UDP	PA-O3A-PB	-2.27	125.05	132.83
2	I	301	UTP	O4'-C1'-N1	-2.26	106.22	109.30
3	E	301	UDP	O3B-PB-O3A	2.25	112.17	104.64
2	J	301	UTP	O1B-PB-O2B	-2.24	101.18	112.24
3	K	301	UDP	O3B-PB-O3A	2.23	112.13	104.64
3	D	302	UDP	PA-O3A-PB	-2.23	125.17	132.83
2	C	301	UTP	O3'-C3'-C4'	-2.22	104.64	111.05
3	J	302	UDP	O3B-PB-O3A	2.19	111.99	104.64
2	D	301	UTP	O2A-PA-O1A	-2.18	101.44	112.24
2	A	301	UTP	O4'-C1'-N1	2.18	112.27	109.30
2	G	301	UTP	PB-O3A-PA	-2.16	125.40	132.83
2	C	301	UTP	O2A-PA-O1A	-2.12	101.74	112.24
2	C	301	UTP	PB-O3A-PA	-2.11	125.58	132.83
2	A	301	UTP	O2A-PA-O1A	-2.10	101.88	112.24
2	J	301	UTP	C2'-C3'-C4'	2.07	106.67	102.64
3	K	301	UDP	PA-O3A-PB	-2.04	125.84	132.83
3	I	302	UDP	PA-O3A-PB	-2.02	125.89	132.83
2	J	301	UTP	O3'-C3'-C4'	-2.02	105.21	111.05
2	D	301	UTP	O1B-PB-O2B	-2.02	102.26	112.24

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	UTP	C5'-O5'-PA-O2A
2	A	301	UTP	C5'-O5'-PA-O3A
2	A	301	UTP	O4'-C4'-C5'-O5'
2	C	301	UTP	C5'-O5'-PA-O3A
2	D	301	UTP	PB-O3B-PG-O1G
2	G	301	UTP	C5'-O5'-PA-O3A
2	G	301	UTP	PB-O3B-PG-O1G
2	G	301	UTP	O4'-C4'-C5'-O5'
2	G	301	UTP	C3'-C4'-C5'-O5'
2	I	301	UTP	PB-O3B-PG-O1G
2	I	301	UTP	PB-O3B-PG-O3G
3	H	301	UDP	C5'-O5'-PA-O1A
2	A	301	UTP	C3'-C4'-C5'-O5'
3	K	301	UDP	C4'-C5'-O5'-PA
3	H	301	UDP	C5'-O5'-PA-O3A
2	C	301	UTP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	C	301	UTP	PG-O3B-PB-O1B
2	C	301	UTP	C5'-O5'-PA-O1A
2	C	301	UTP	C5'-O5'-PA-O2A
2	D	301	UTP	C5'-O5'-PA-O2A
2	G	301	UTP	C5'-O5'-PA-O1A
2	G	301	UTP	C5'-O5'-PA-O2A
3	B	300	UDP	O4'-C4'-C5'-O5'
3	C	302	UDP	C4'-C5'-O5'-PA
2	A	301	UTP	PB-O3A-PA-O1A
2	C	301	UTP	PB-O3A-PA-O2A
2	I	301	UTP	PG-O3B-PB-O1B
3	B	300	UDP	C4'-C5'-O5'-PA
3	E	301	UDP	C4'-C5'-O5'-PA
3	J	302	UDP	C4'-C5'-O5'-PA
3	B	300	UDP	C3'-C4'-C5'-O5'
2	I	301	UTP	PB-O3B-PG-O2G
2	I	301	UTP	PA-O3A-PB-O1B
2	C	301	UTP	O4'-C4'-C5'-O5'
2	I	301	UTP	C2'-C1'-N1-C6
3	D	302	UDP	C4'-C5'-O5'-PA
2	G	301	UTP	PB-O3B-PG-O3G
2	I	301	UTP	C2'-C1'-N1-C2
3	I	302	UDP	C4'-C5'-O5'-PA
2	C	301	UTP	PB-O3A-PA-O1A
2	G	301	UTP	PA-O3A-PB-O2B
2	J	301	UTP	PG-O3B-PB-O1B
3	J	302	UDP	PB-O3A-PA-O1A
3	J	302	UDP	PB-O3A-PA-O2A
3	K	301	UDP	PB-O3A-PA-O2A
3	H	301	UDP	C4'-C5'-O5'-PA
3	D	302	UDP	C5'-O5'-PA-O1A
3	H	301	UDP	C5'-O5'-PA-O2A
3	J	302	UDP	C5'-O5'-PA-O1A

There are no ring outliers.

12 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	302	UDP	2	0
2	G	301	UTP	1	0
2	I	301	UTP	6	0
3	E	301	UDP	3	0

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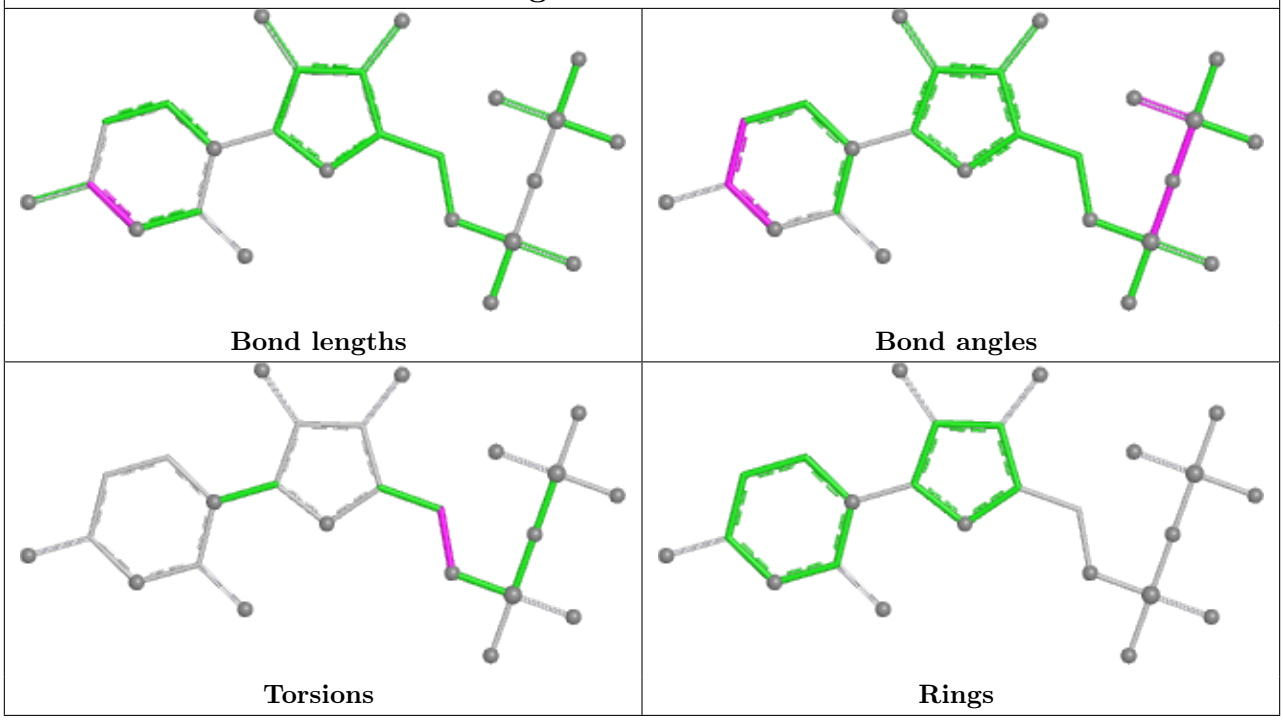
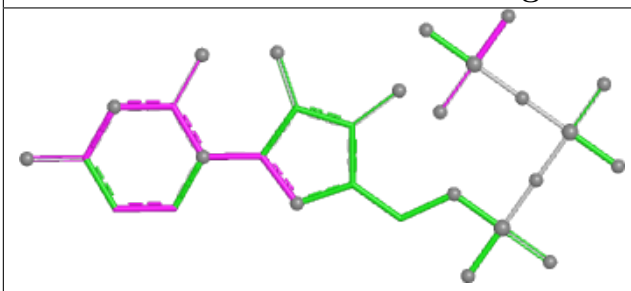
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	301	UTP	1	0
2	A	301	UTP	5	0
3	J	302	UDP	3	0
3	K	301	UDP	5	0
3	D	302	UDP	2	0
2	D	301	UTP	3	0
3	B	300	UDP	4	0
2	C	301	UTP	4	0

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 I 302



Ligand UTP G 301



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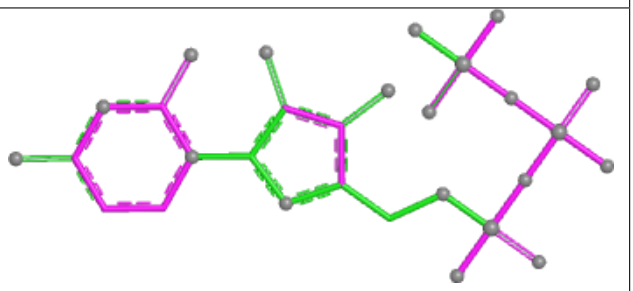
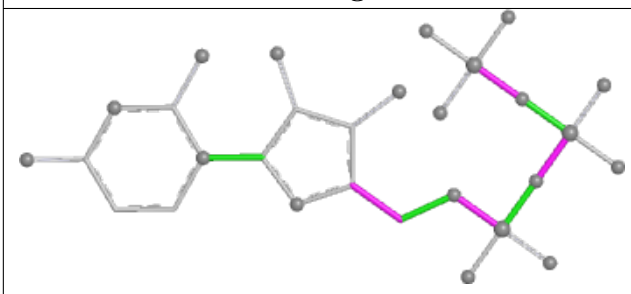
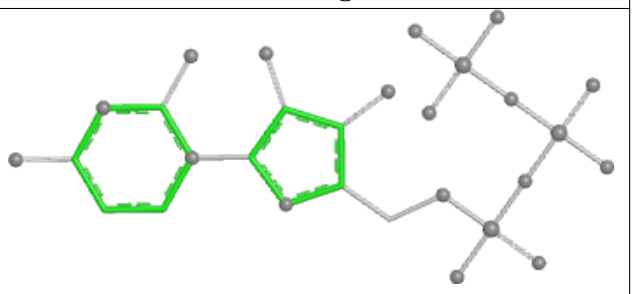


Bond angles

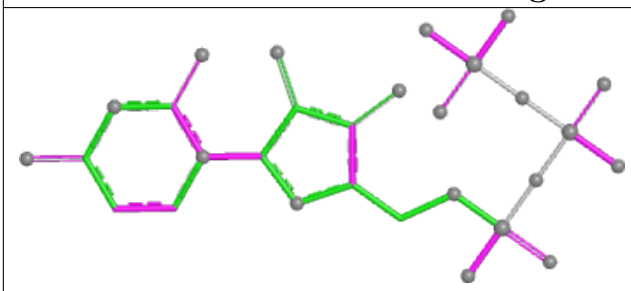


Torsions



Rings

Ligand UTP I 301



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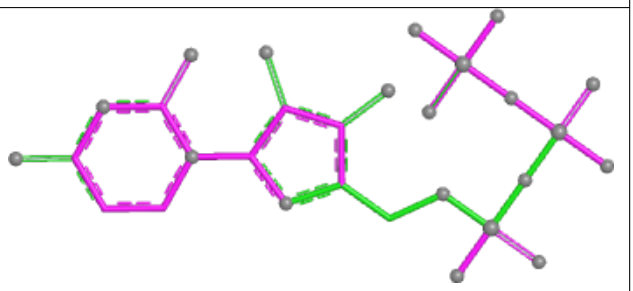
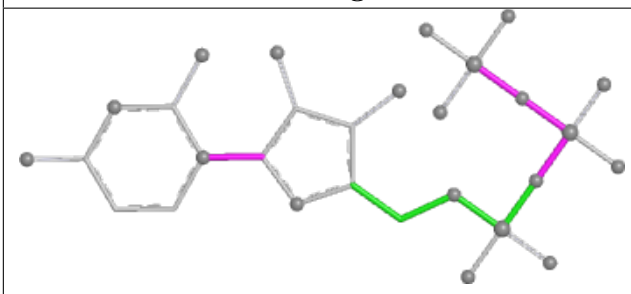
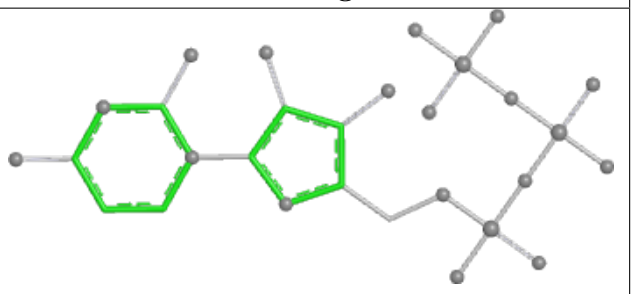


Bond angles



Torsions



Rings

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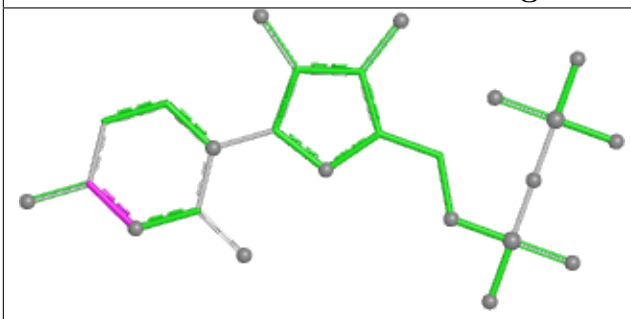
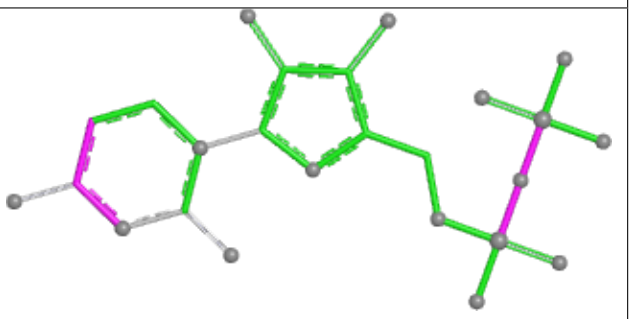
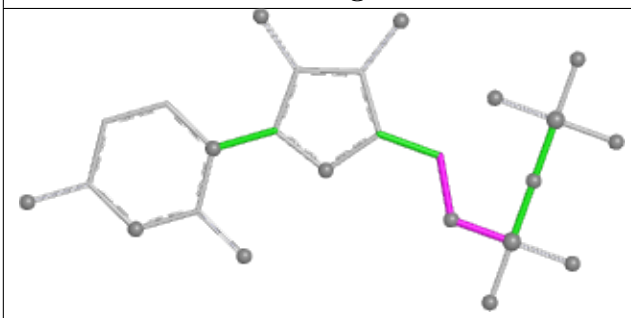
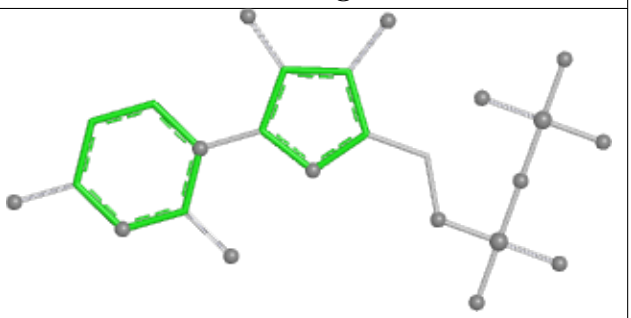
 Bond lengths	 Bond angles
 Torsions	 Rings

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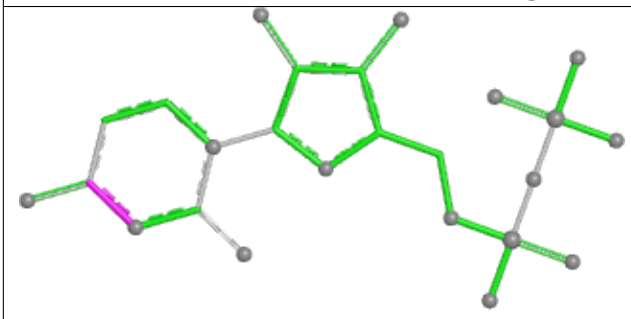
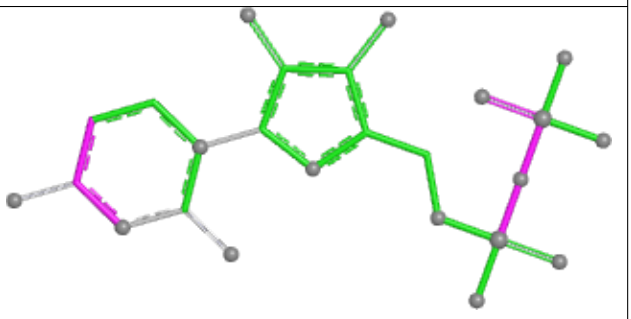
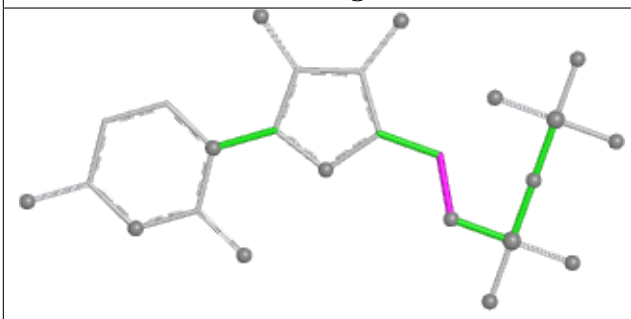
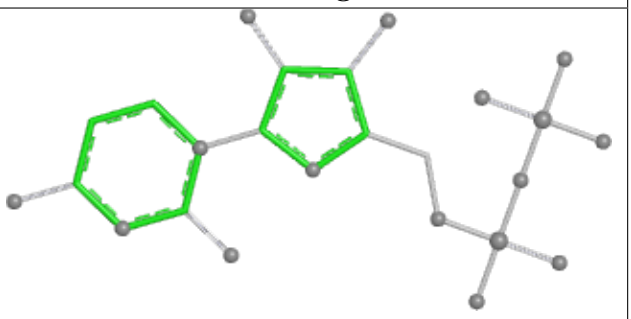
 Bond lengths	 Bond angles
 Torsions	 Rings

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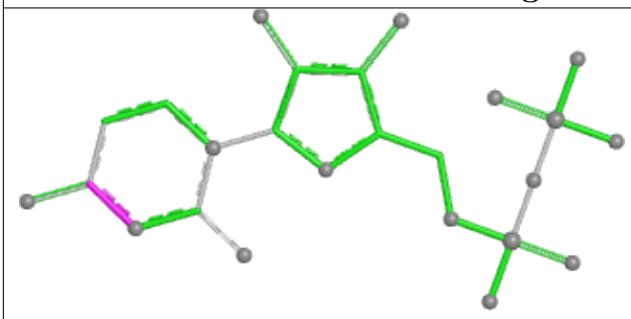
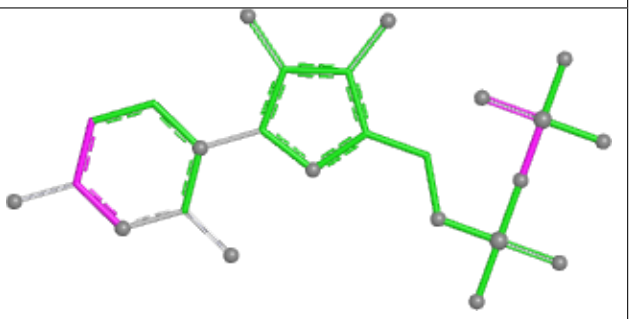
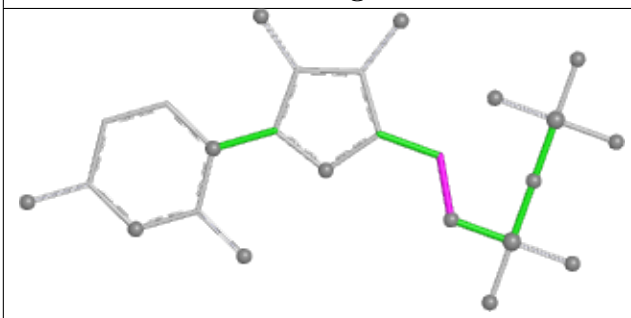
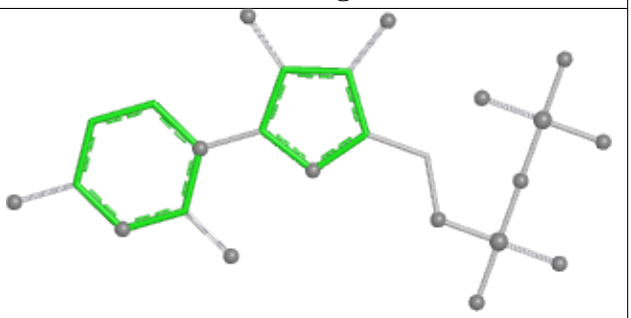
 Bond lengths	 Bond angles
 Torsions	 Rings

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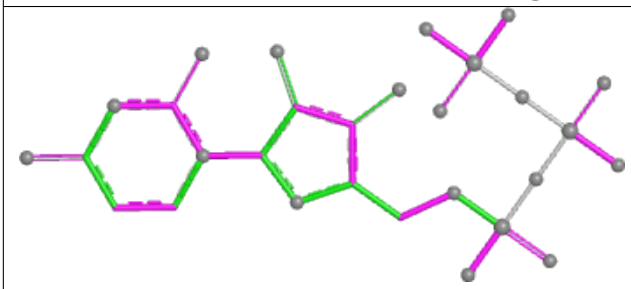
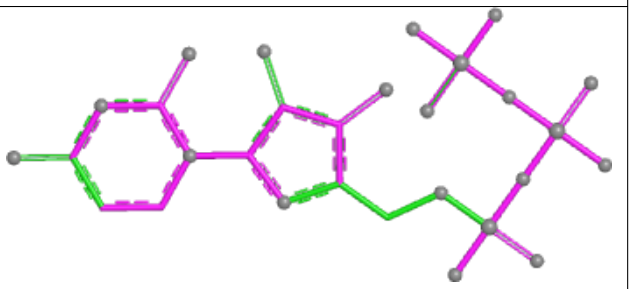
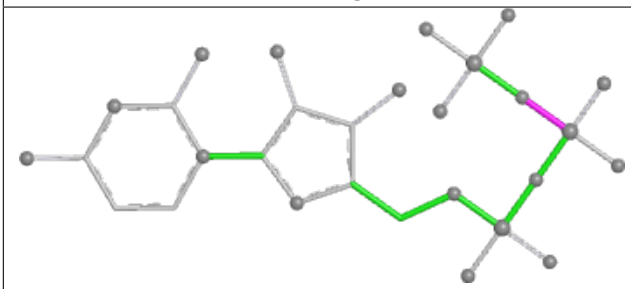
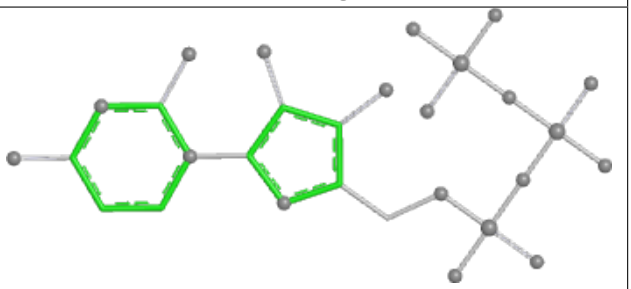
 Bond lengths	 Bond angles
 Torsions	 Rings

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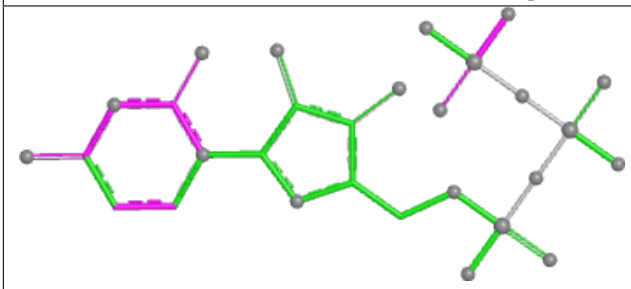
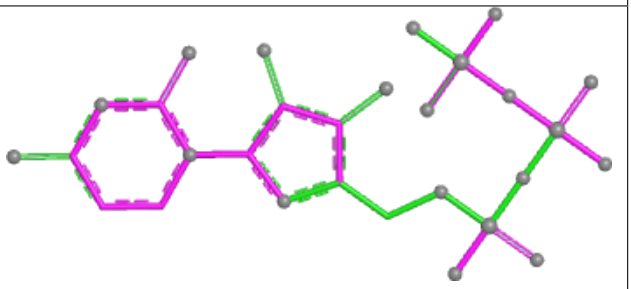
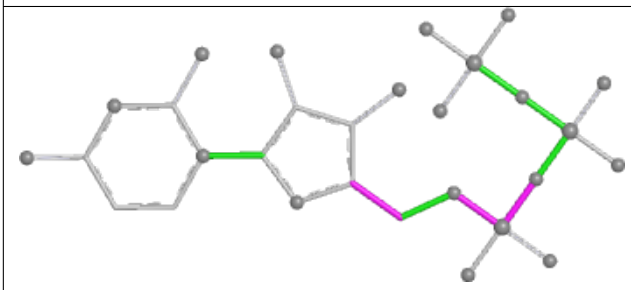
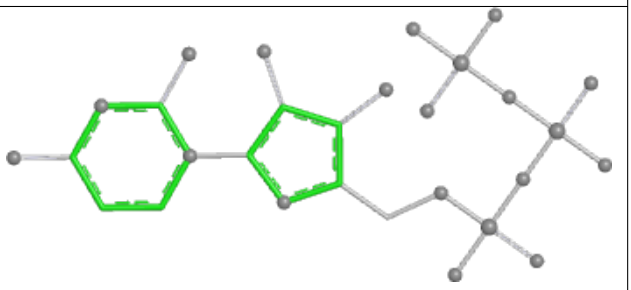
 Bond lengths	 Bond angles
 Torsions	 Rings

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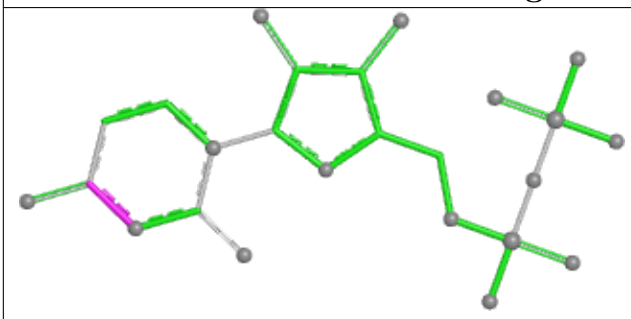
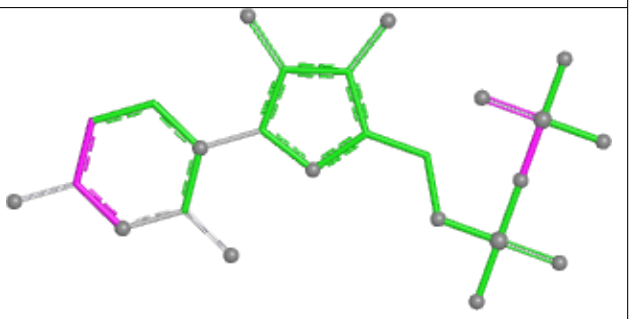
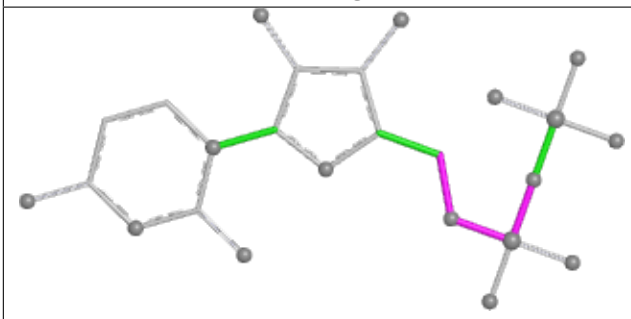
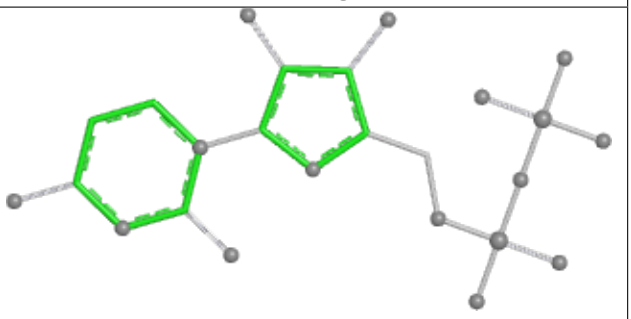
 Bond lengths	 Bond angles
 Torsions	 Rings

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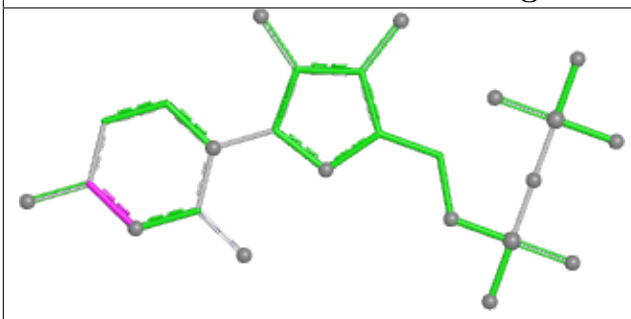
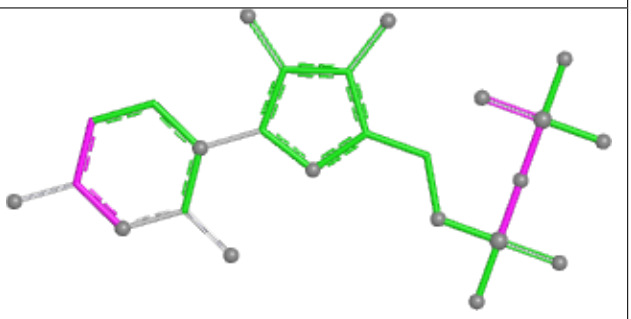
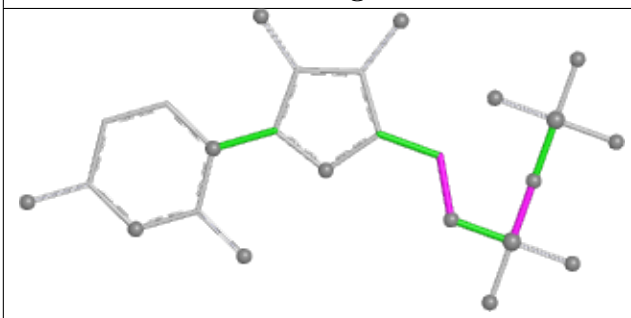
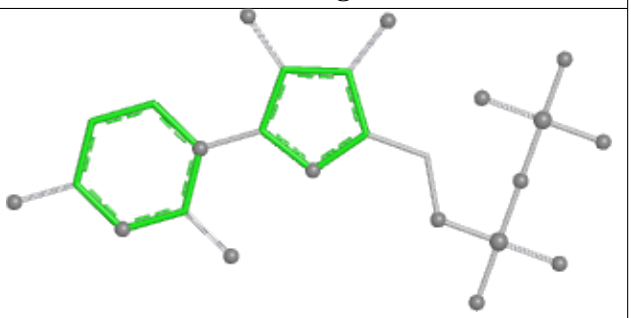
 Bond lengths	 Bond angles
 Torsions	 Rings

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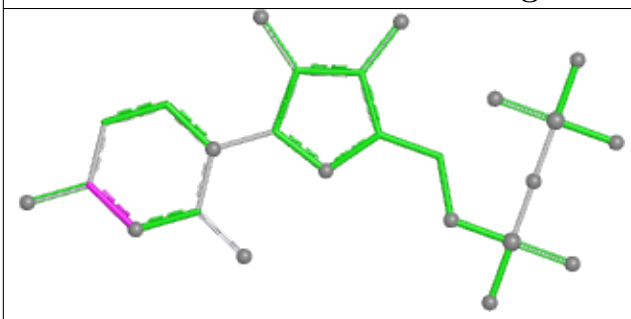
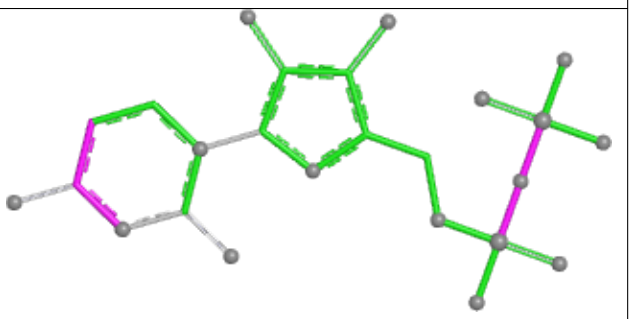
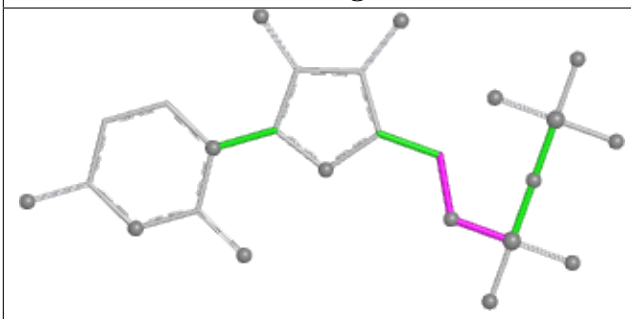
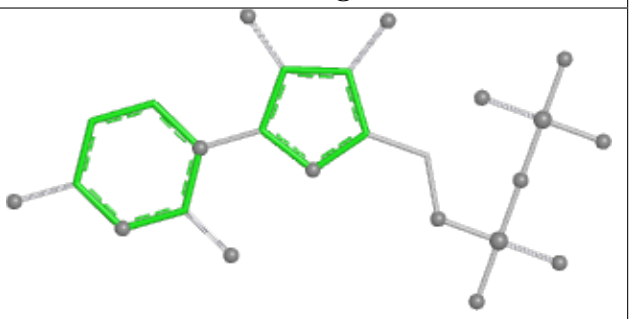
 Bond lengths	 Bond angles
 Torsions	 Rings

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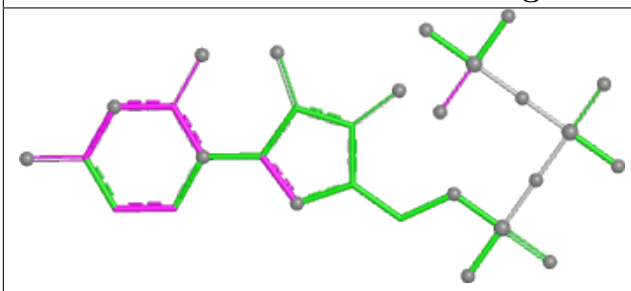
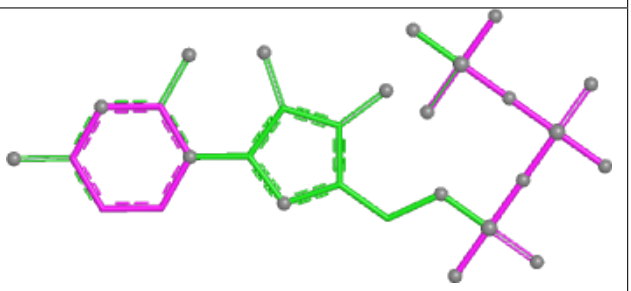
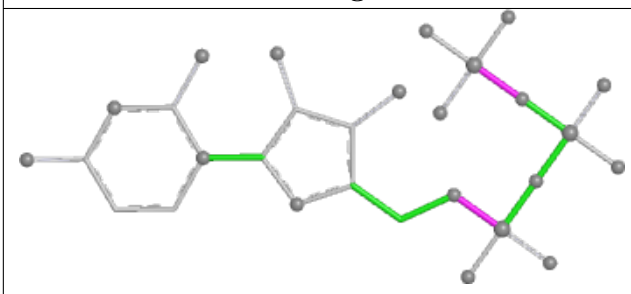
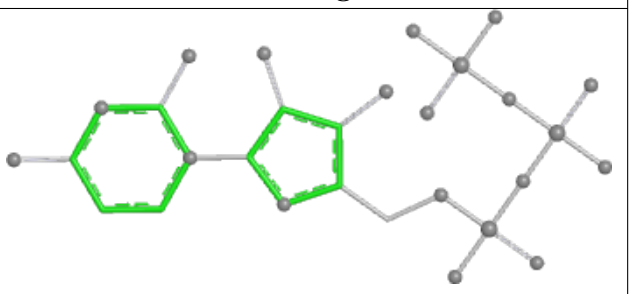
 Bond lengths	 Bond angles
 Torsions	 Rings

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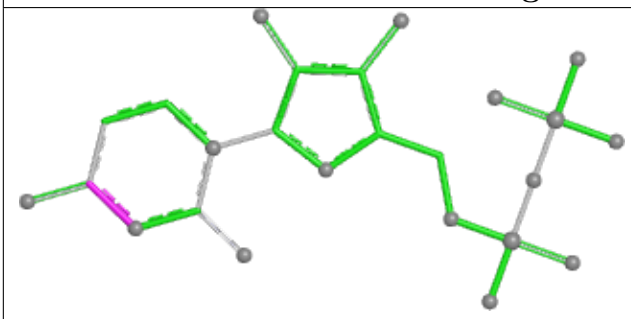
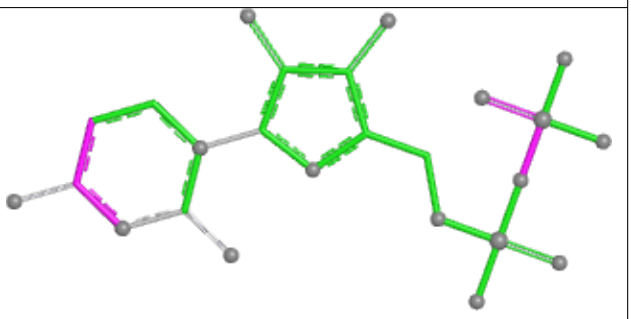
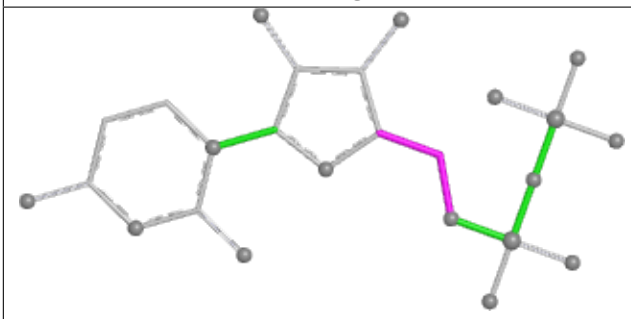
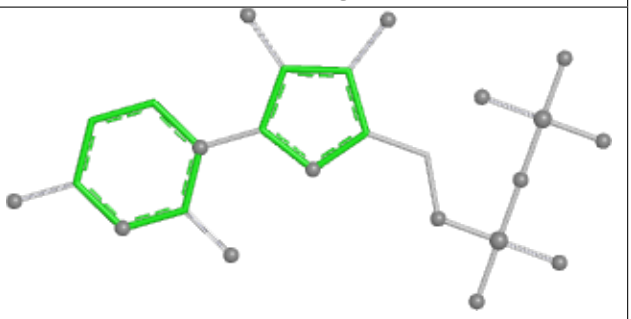
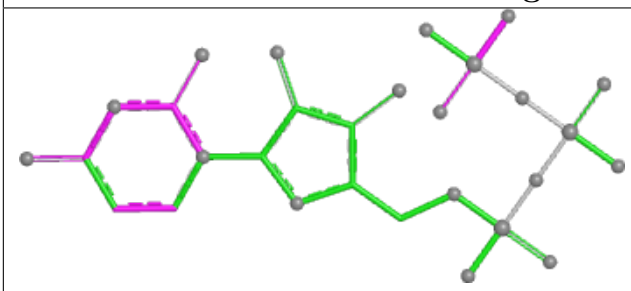
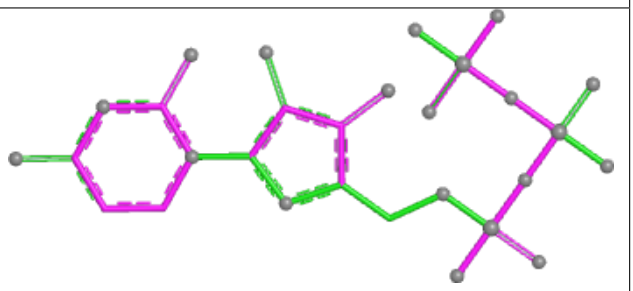
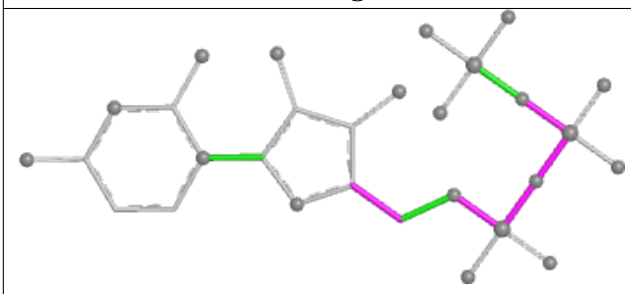
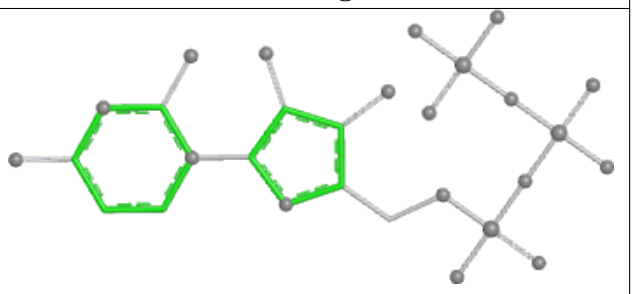
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UTP C 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

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, 95^{th} 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	224/281 (79%)	-0.03	5 (2%) 62 41	30, 64, 105, 134	13 (5%)
1	B	226/281 (80%)	-0.20	0 100 100	29, 63, 114, 135	9 (3%)
1	C	229/281 (81%)	-0.27	0 100 100	22, 40, 95, 144	6 (2%)
1	D	225/281 (80%)	-0.18	2 (0%) 84 71	21, 50, 99, 131	4 (1%)
1	E	224/281 (79%)	-0.13	3 (1%) 77 60	20, 51, 104, 133	5 (2%)
1	F	220/281 (78%)	-0.01	5 (2%) 60 39	43, 96, 138, 157	8 (3%)
1	G	219/281 (77%)	-0.10	5 (2%) 60 39	34, 75, 120, 145	10 (4%)
1	H	225/281 (80%)	-0.05	1 (0%) 92 85	33, 61, 106, 130	5 (2%)
1	I	226/281 (80%)	-0.22	3 (1%) 77 60	26, 55, 119, 143	7 (3%)
1	J	228/281 (81%)	-0.16	1 (0%) 92 85	23, 49, 104, 135	13 (5%)
1	K	228/281 (81%)	-0.16	2 (0%) 84 71	22, 49, 98, 124	8 (3%)
1	L	227/281 (80%)	-0.25	0 100 100	22, 69, 108, 141	8 (3%)
All	All	2701/3372 (80%)	-0.15	27 (0%) 82 69	20, 60, 116, 157	96 (3%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	261	THR	4.3
1	A	189	GLY	3.0
1	H	192	ALA	2.7
1	G	252	GLY	2.6
1	F	205	THR	2.6
1	F	209	HIS	2.5
1	F	250	VAL	2.5
1	A	260	THR	2.5
1	I	192	ALA	2.5
1	G	209	HIS	2.4
1	J	186	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	261	THR	2.4
1	G	261	THR	2.4
1	K	83	GLY	2.3
1	A	207	VAL	2.2
1	D	190	VAL	2.2
1	I	190	VAL	2.2
1	G	254	LYS	2.1
1	G	207	VAL	2.1
1	D	191	PHE	2.1
1	F	204	LEU	2.1
1	E	84	ALA	2.1
1	E	88	GLN	2.1
1	I	220	ALA	2.0
1	K	203	LEU	2.0
1	E	87	GLN	2.0
1	A	85	GLN	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 monosaccharides 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, 95^{th} 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	UDP	K	301	25/25	0.90	0.32	55,81,90,93	0
2	UTP	A	301	29/29	0.91	0.28	38,73,97,101	0
3	UDP	H	301	25/25	0.92	0.23	50,66,78,83	0
3	UDP	E	301	25/25	0.93	0.25	57,64,79,80	0
2	UTP	I	301	29/29	0.93	0.29	43,68,82,82	0
2	UTP	J	301	29/29	0.93	0.20	44,55,78,79	0
2	UTP	C	301	29/29	0.94	0.26	27,43,69,73	0

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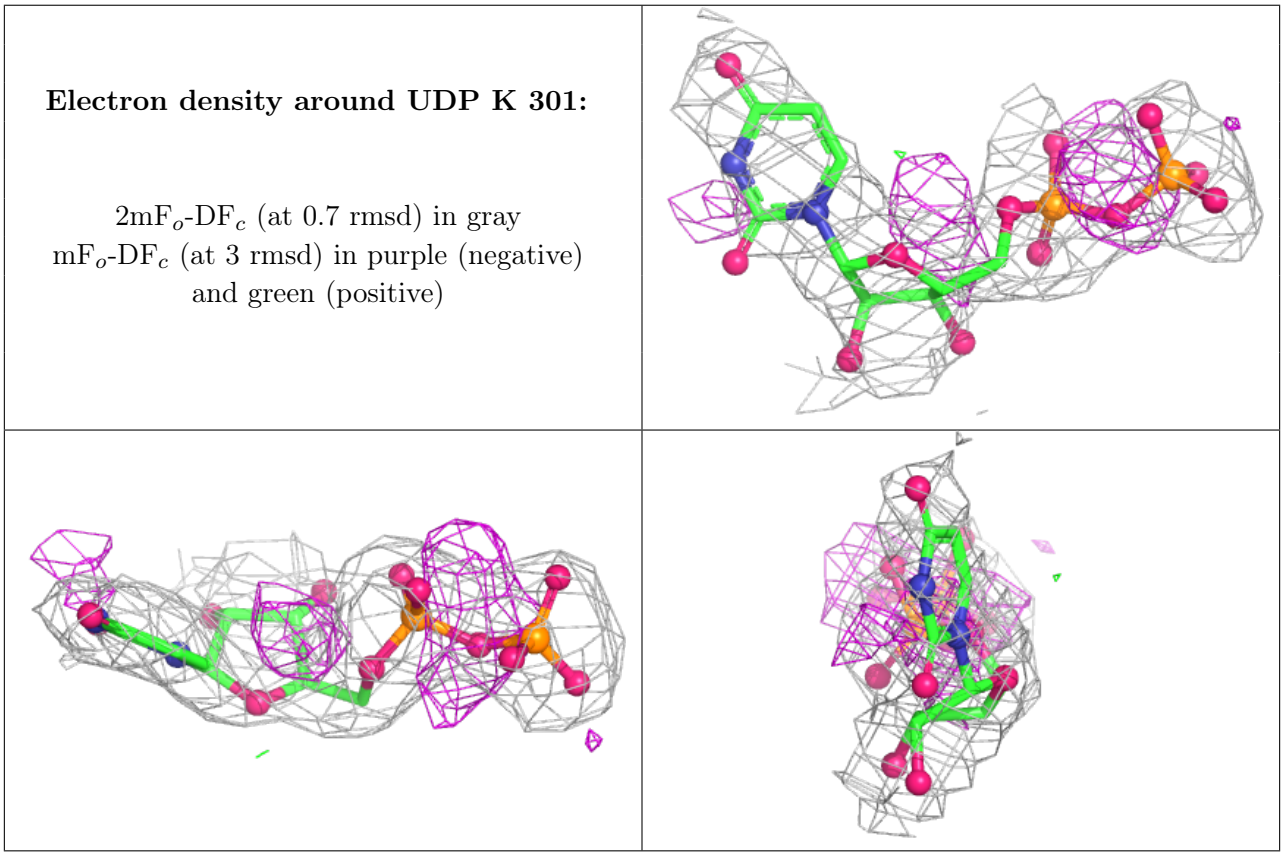
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UTP	G	301	29/29	0.94	0.20	53,69,79,84	0
3	UDP	B	300	25/25	0.94	0.20	39,52,61,62	0
3	UDP	J	302	25/25	0.95	0.19	38,56,66,72	0
3	UDP	D	302	25/25	0.95	0.19	36,48,58,62	0
2	UTP	D	301	29/29	0.96	0.22	2,13,31,38	40
3	UDP	I	302	25/25	0.96	0.21	28,38,54,61	0
3	UDP	C	302	25/25	0.97	0.20	24,32,47,57	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.

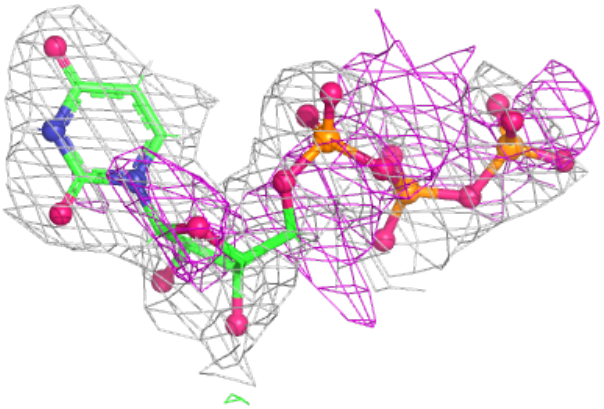
Electron density around UDP K 301:

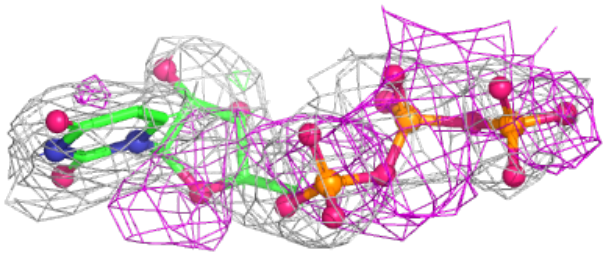
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

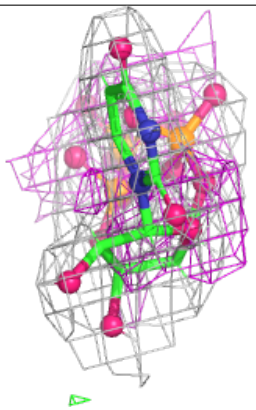


Electron density around UTP A 301:

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

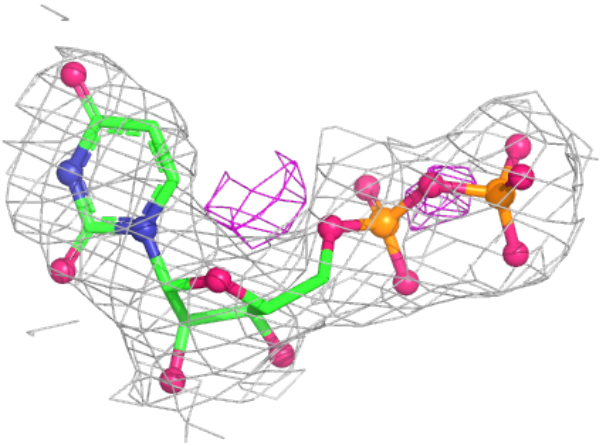


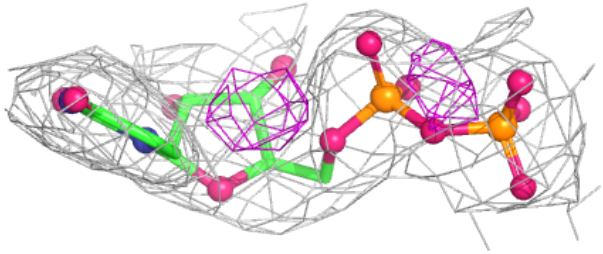


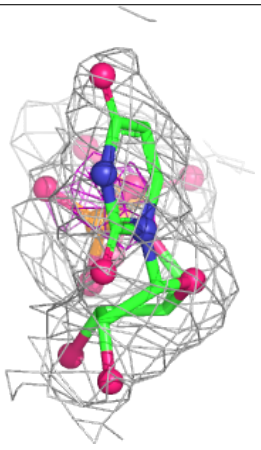


Electron density around UDP H 301:

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

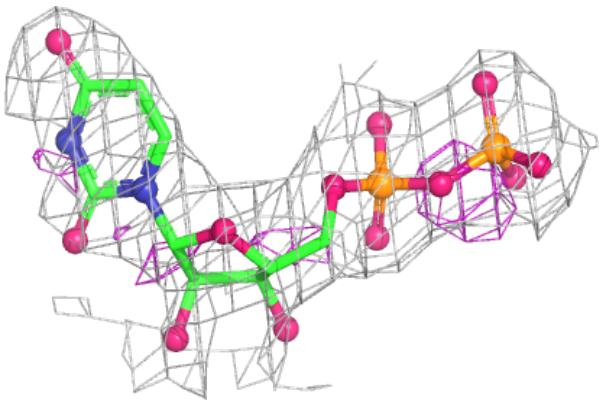


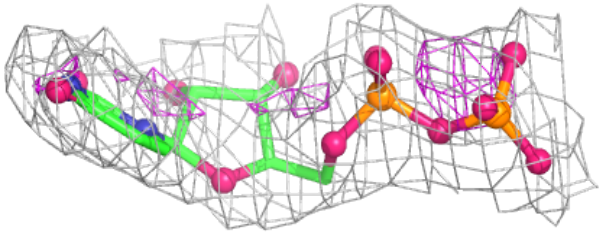


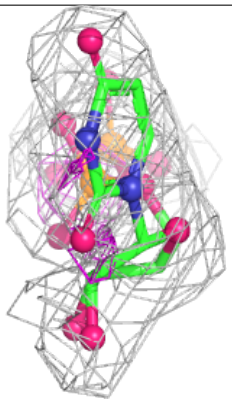


Electron density around UDP E 301:

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

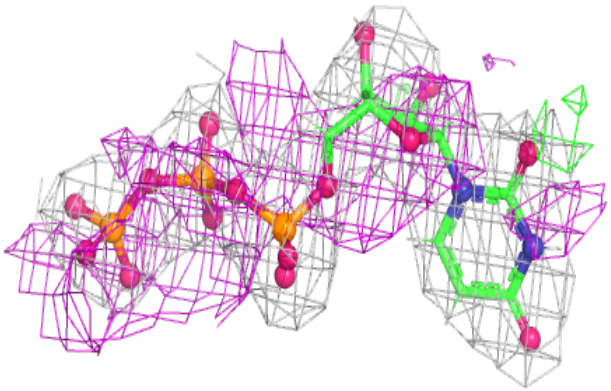


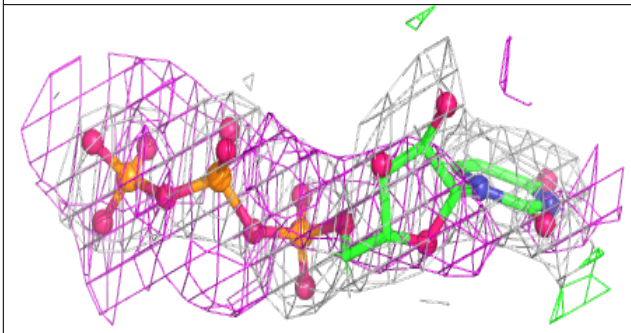


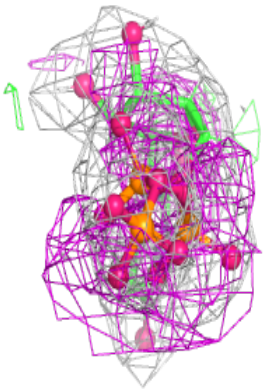


Electron density around UTP I 301:

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

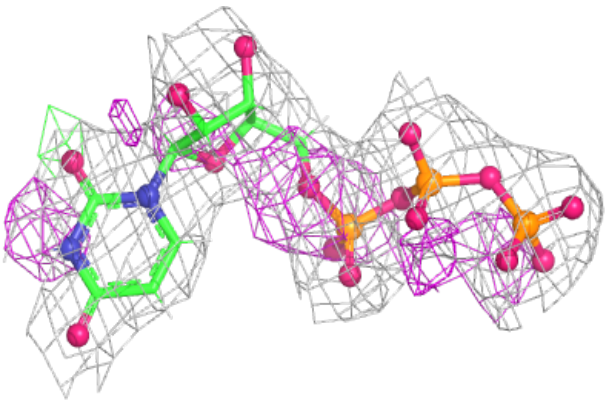


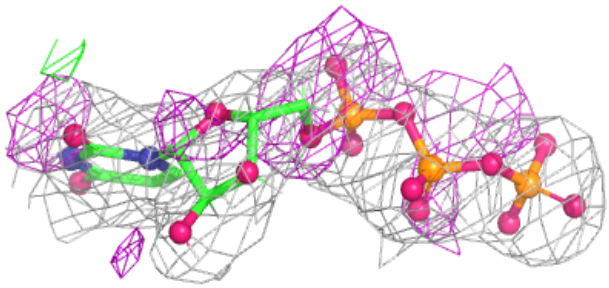


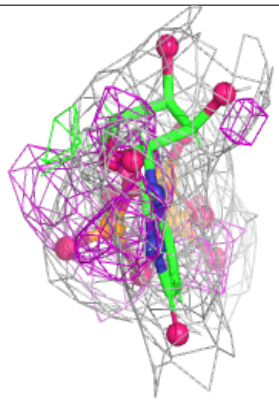


Electron density around UTP J 301:

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

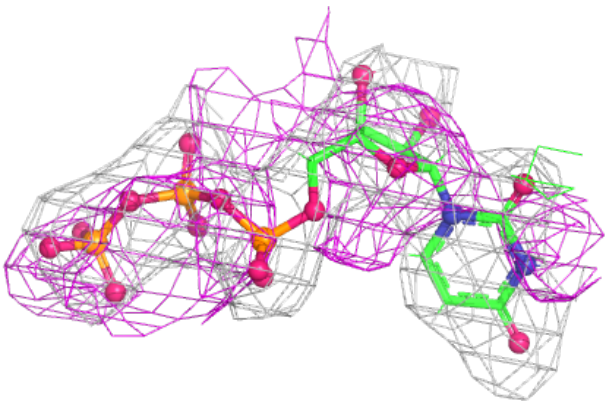


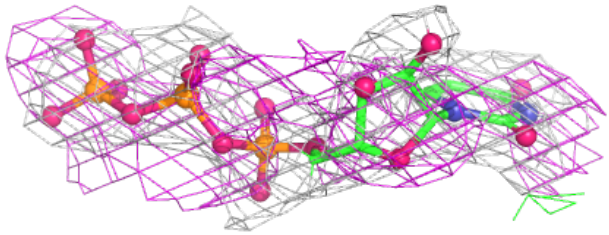


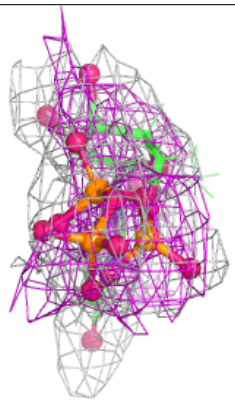


Electron density around UTP C 301:

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

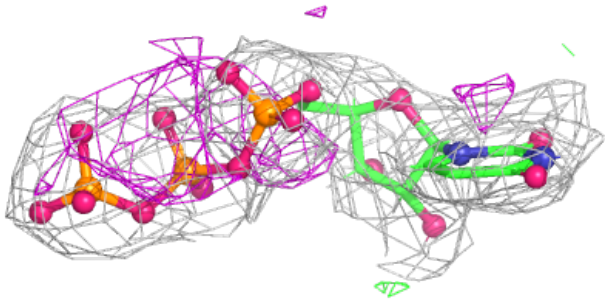


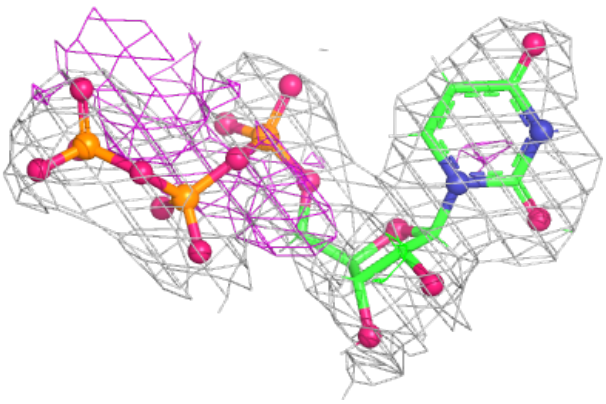


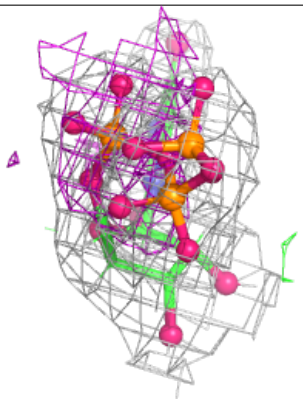


Electron density around UTP G 301:

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

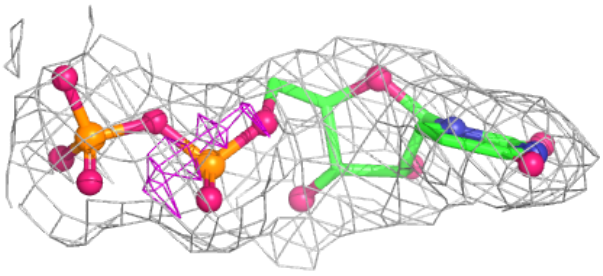


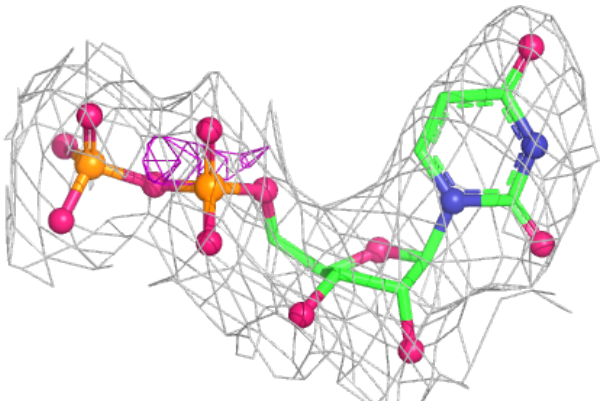


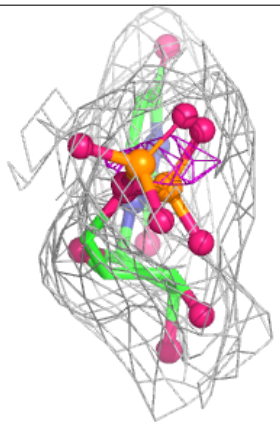


Electron density around UDP B 300:

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

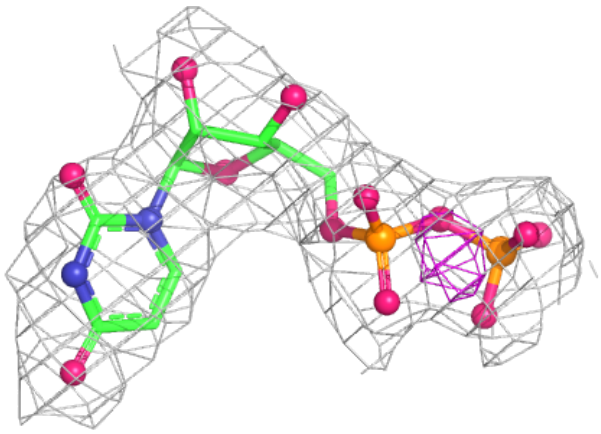


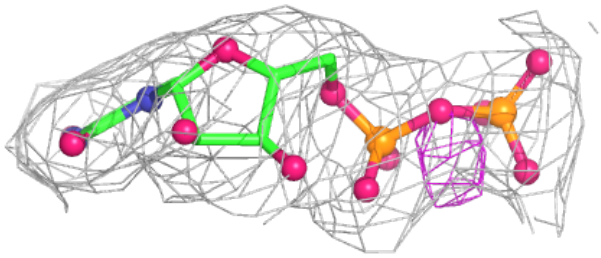


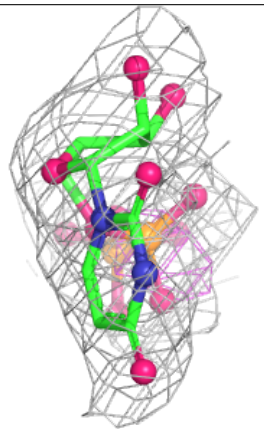


Electron density around UDP J 302:

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

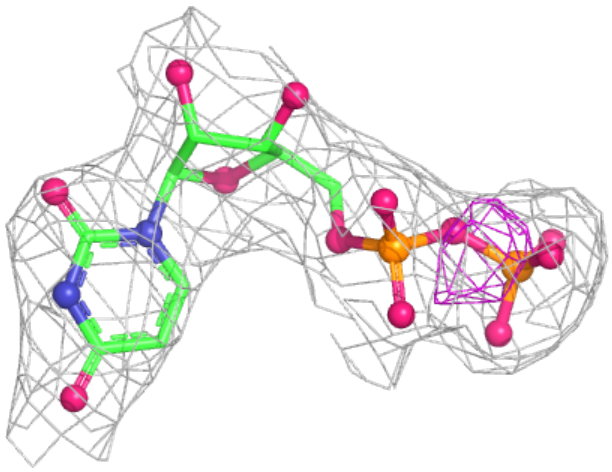


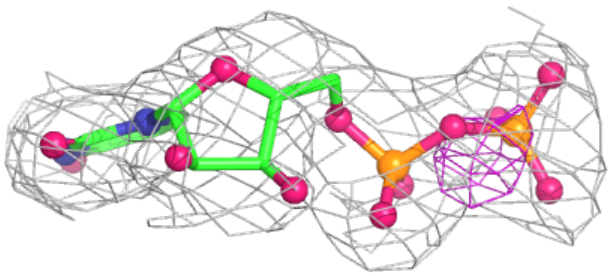


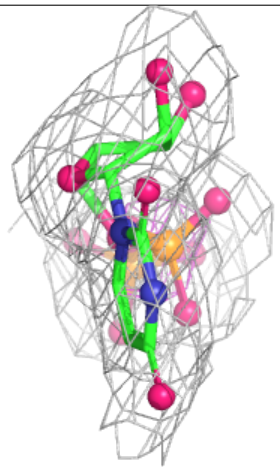


Electron density around UDP D 302:

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

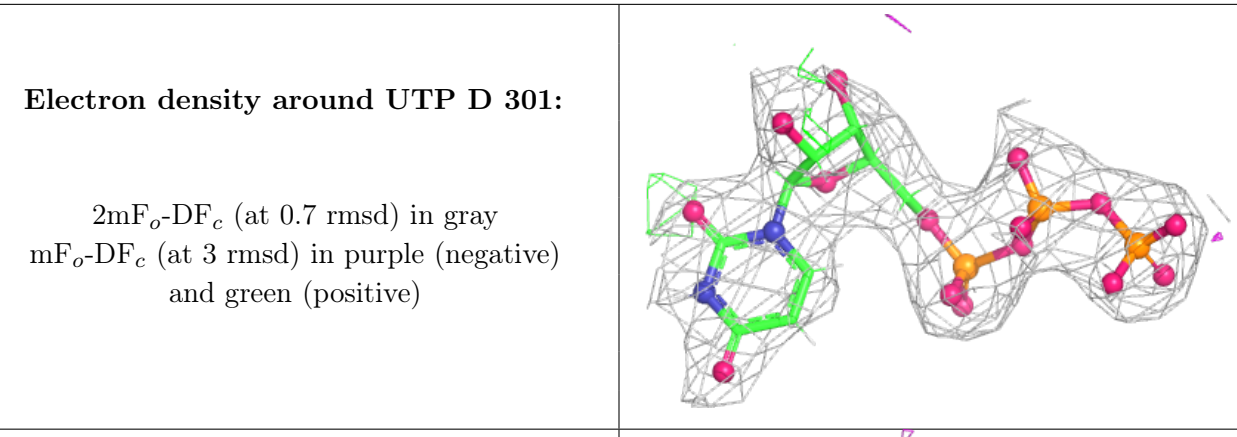






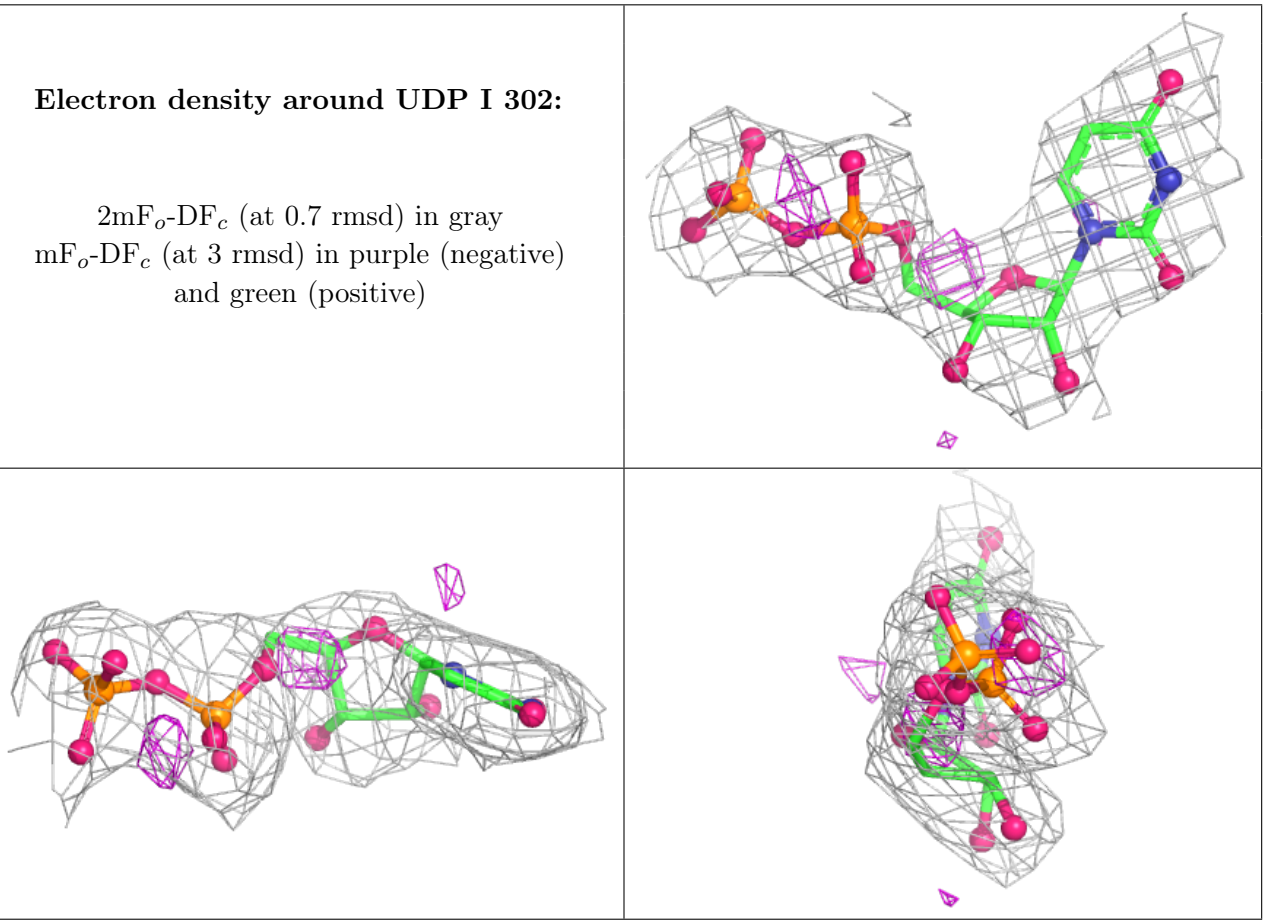
Electron density around UTP D 301:

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



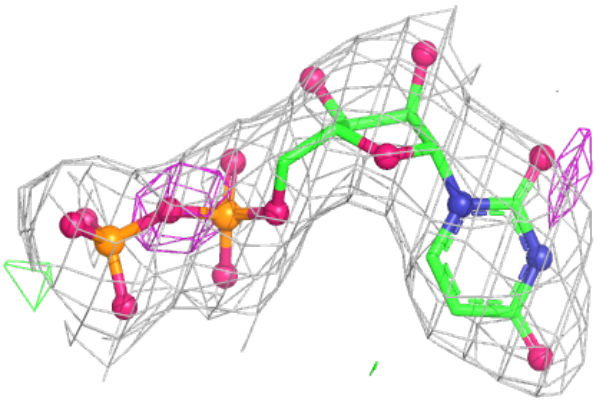
Electron density around UDP I 302:

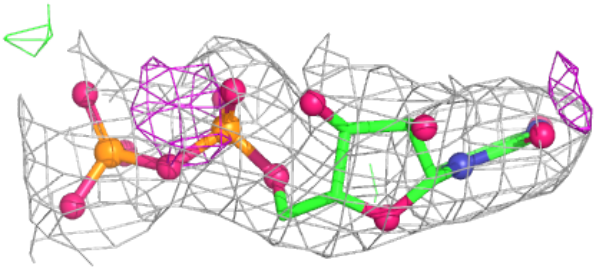
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

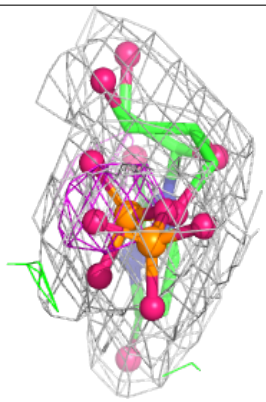


Electron density around UDP C 302:

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







6.5 Other polymers

There are no such residues in this entry.