Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 04:00 AM EST

PDB ID	:	3NWY
Title	:	Structure and allosteric regulation of the uridine monophosphate kinase from Mycobacterium tuberculosis
Authors	:	Labesse, G.; Munier-Lehmann, H.
Deposited on	:	2010-07-12
Resolution	:	2.54 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

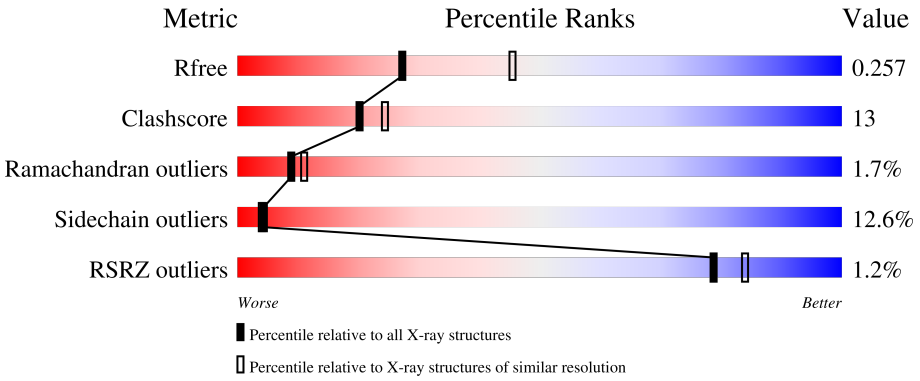
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	59% 17% • 19%
1	B	281	% 63% 16% • 18%
1	C	281	% 55% 21% 5% • 18%
1	D	281	64% 15% • 18%
1	E	281	55% 20% • 22%

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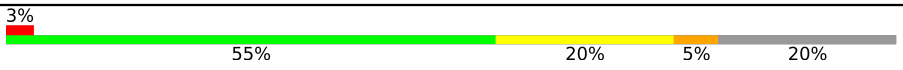
Mol	Chain	Length	Quality of chain
1	F	281	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10350 atoms, of which 0 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	227	Total	C	N	O	S	0	1	0
			1670	1055	292	312	11			
1	B	231	Total	C	N	O	S	0	0	0
			1695	1068	297	319	11			
1	C	230	Total	C	N	O	S	0	0	0
			1685	1059	298	317	11			
1	D	230	Total	C	N	O	S	0	0	0
			1703	1069	302	321	11			
1	E	220	Total	C	N	O	S	0	0	0
			1601	1004	283	303	11			
1	F	226	Total	C	N	O	S	0	0	0
			1637	1032	290	304	11			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P65929
A	-18	GLY	-	expression tag	UNP P65929
A	-17	SER	-	expression tag	UNP P65929
A	-16	SER	-	expression tag	UNP P65929
A	-15	HIS	-	expression tag	UNP P65929
A	-14	HIS	-	expression tag	UNP P65929
A	-13	HIS	-	expression tag	UNP P65929
A	-12	HIS	-	expression tag	UNP P65929
A	-11	HIS	-	expression tag	UNP P65929
A	-10	HIS	-	expression tag	UNP P65929
A	-9	SER	-	expression tag	UNP P65929
A	-8	SER	-	expression tag	UNP P65929
A	-7	GLY	-	expression tag	UNP P65929
A	-6	LEU	-	expression tag	UNP P65929
A	-5	VAL	-	expression tag	UNP P65929
A	-4	PRO	-	expression tag	UNP P65929
A	-3	ARG	-	expression tag	UNP P65929

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P65929
A	-1	SER	-	expression tag	UNP P65929
A	0	HIS	-	expression tag	UNP P65929
B	-19	MET	-	expression tag	UNP P65929
B	-18	GLY	-	expression tag	UNP P65929
B	-17	SER	-	expression tag	UNP P65929
B	-16	SER	-	expression tag	UNP P65929
B	-15	HIS	-	expression tag	UNP P65929
B	-14	HIS	-	expression tag	UNP P65929
B	-13	HIS	-	expression tag	UNP P65929
B	-12	HIS	-	expression tag	UNP P65929
B	-11	HIS	-	expression tag	UNP P65929
B	-10	HIS	-	expression tag	UNP P65929
B	-9	SER	-	expression tag	UNP P65929
B	-8	SER	-	expression tag	UNP P65929
B	-7	GLY	-	expression tag	UNP P65929
B	-6	LEU	-	expression tag	UNP P65929
B	-5	VAL	-	expression tag	UNP P65929
B	-4	PRO	-	expression tag	UNP P65929
B	-3	ARG	-	expression tag	UNP P65929
B	-2	GLY	-	expression tag	UNP P65929
B	-1	SER	-	expression tag	UNP P65929
B	0	HIS	-	expression tag	UNP P65929
C	-19	MET	-	expression tag	UNP P65929
C	-18	GLY	-	expression tag	UNP P65929
C	-17	SER	-	expression tag	UNP P65929
C	-16	SER	-	expression tag	UNP P65929
C	-15	HIS	-	expression tag	UNP P65929
C	-14	HIS	-	expression tag	UNP P65929
C	-13	HIS	-	expression tag	UNP P65929
C	-12	HIS	-	expression tag	UNP P65929
C	-11	HIS	-	expression tag	UNP P65929
C	-10	HIS	-	expression tag	UNP P65929
C	-9	SER	-	expression tag	UNP P65929
C	-8	SER	-	expression tag	UNP P65929
C	-7	GLY	-	expression tag	UNP P65929
C	-6	LEU	-	expression tag	UNP P65929
C	-5	VAL	-	expression tag	UNP P65929
C	-4	PRO	-	expression tag	UNP P65929
C	-3	ARG	-	expression tag	UNP P65929
C	-2	GLY	-	expression tag	UNP P65929
C	-1	SER	-	expression tag	UNP P65929

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP P65929
D	-19	MET	-	expression tag	UNP P65929
D	-18	GLY	-	expression tag	UNP P65929
D	-17	SER	-	expression tag	UNP P65929
D	-16	SER	-	expression tag	UNP P65929
D	-15	HIS	-	expression tag	UNP P65929
D	-14	HIS	-	expression tag	UNP P65929
D	-13	HIS	-	expression tag	UNP P65929
D	-12	HIS	-	expression tag	UNP P65929
D	-11	HIS	-	expression tag	UNP P65929
D	-10	HIS	-	expression tag	UNP P65929
D	-9	SER	-	expression tag	UNP P65929
D	-8	SER	-	expression tag	UNP P65929
D	-7	GLY	-	expression tag	UNP P65929
D	-6	LEU	-	expression tag	UNP P65929
D	-5	VAL	-	expression tag	UNP P65929
D	-4	PRO	-	expression tag	UNP P65929
D	-3	ARG	-	expression tag	UNP P65929
D	-2	GLY	-	expression tag	UNP P65929
D	-1	SER	-	expression tag	UNP P65929
D	0	HIS	-	expression tag	UNP P65929
E	-19	MET	-	expression tag	UNP P65929
E	-18	GLY	-	expression tag	UNP P65929
E	-17	SER	-	expression tag	UNP P65929
E	-16	SER	-	expression tag	UNP P65929
E	-15	HIS	-	expression tag	UNP P65929
E	-14	HIS	-	expression tag	UNP P65929
E	-13	HIS	-	expression tag	UNP P65929
E	-12	HIS	-	expression tag	UNP P65929
E	-11	HIS	-	expression tag	UNP P65929
E	-10	HIS	-	expression tag	UNP P65929
E	-9	SER	-	expression tag	UNP P65929
E	-8	SER	-	expression tag	UNP P65929
E	-7	GLY	-	expression tag	UNP P65929
E	-6	LEU	-	expression tag	UNP P65929
E	-5	VAL	-	expression tag	UNP P65929
E	-4	PRO	-	expression tag	UNP P65929
E	-3	ARG	-	expression tag	UNP P65929
E	-2	GLY	-	expression tag	UNP P65929
E	-1	SER	-	expression tag	UNP P65929
E	0	HIS	-	expression tag	UNP P65929
F	-19	MET	-	expression tag	UNP P65929

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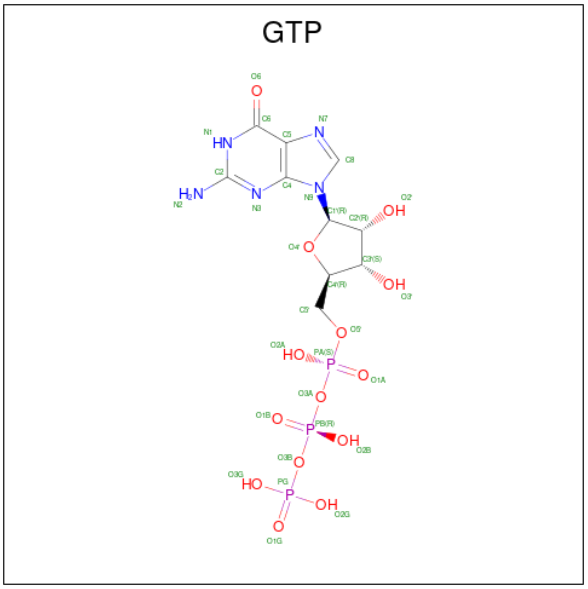
Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	expression tag	UNP P65929
F	-17	SER	-	expression tag	UNP P65929
F	-16	SER	-	expression tag	UNP P65929
F	-15	HIS	-	expression tag	UNP P65929
F	-14	HIS	-	expression tag	UNP P65929
F	-13	HIS	-	expression tag	UNP P65929
F	-12	HIS	-	expression tag	UNP P65929
F	-11	HIS	-	expression tag	UNP P65929
F	-10	HIS	-	expression tag	UNP P65929
F	-9	SER	-	expression tag	UNP P65929
F	-8	SER	-	expression tag	UNP P65929
F	-7	GLY	-	expression tag	UNP P65929
F	-6	LEU	-	expression tag	UNP P65929
F	-5	VAL	-	expression tag	UNP P65929
F	-4	PRO	-	expression tag	UNP P65929
F	-3	ARG	-	expression tag	UNP P65929
F	-2	GLY	-	expression tag	UNP P65929
F	-1	SER	-	expression tag	UNP P65929
F	0	HIS	-	expression tag	UNP P65929

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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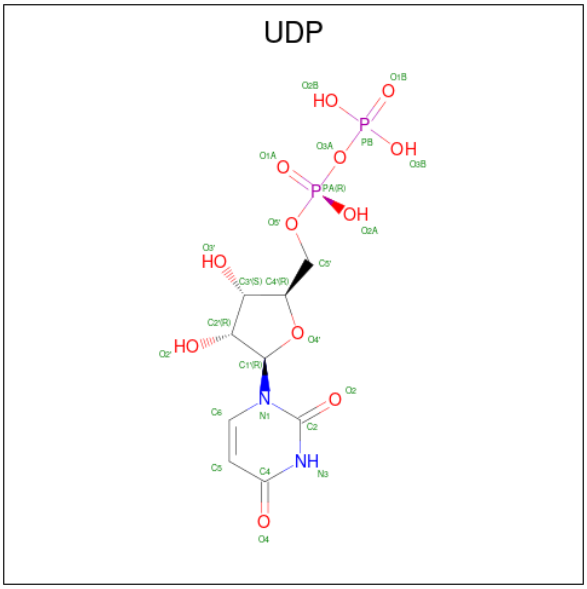
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	32	Total	O	0	0
			32	32		
4	C	23	Total	O	0	0
			23	23		

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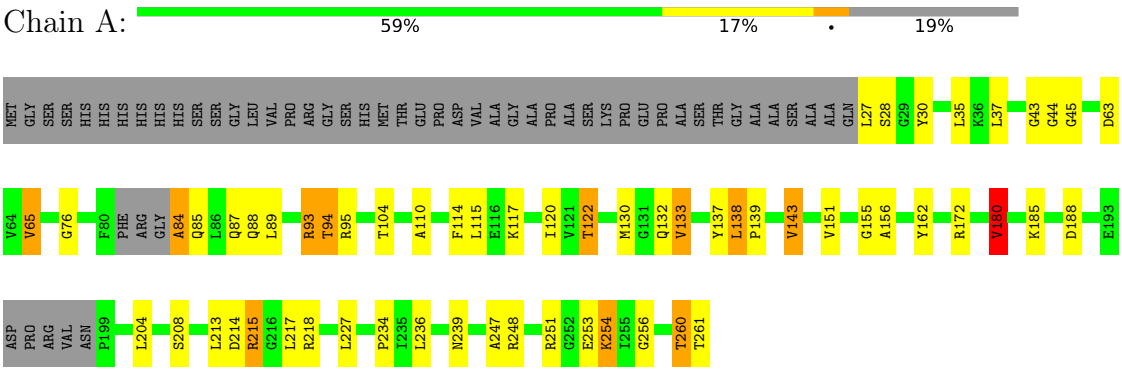
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	14	Total O 14 14	0	0
4	E	14	Total O 14 14	0	0
4	F	18	Total O 18 18	0	0

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.

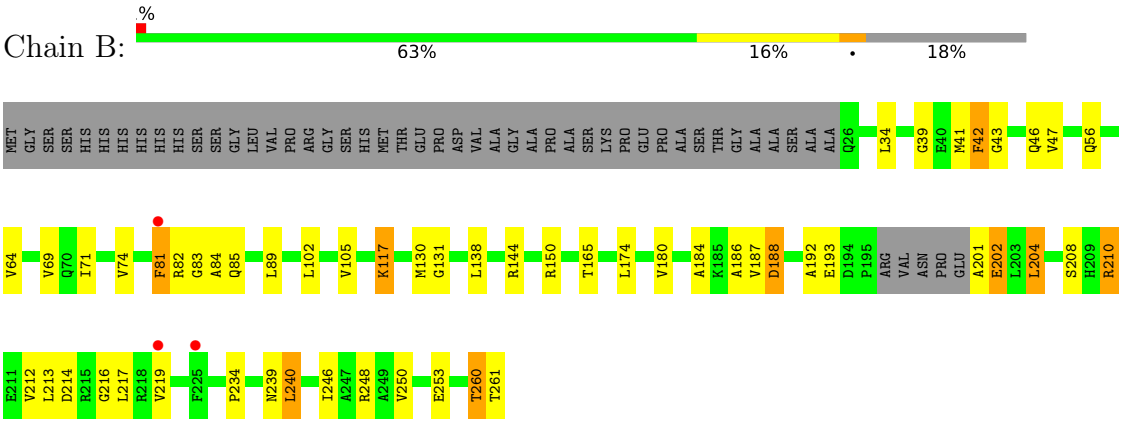
• Molecule 1: Uridylate kinase

Chain A:



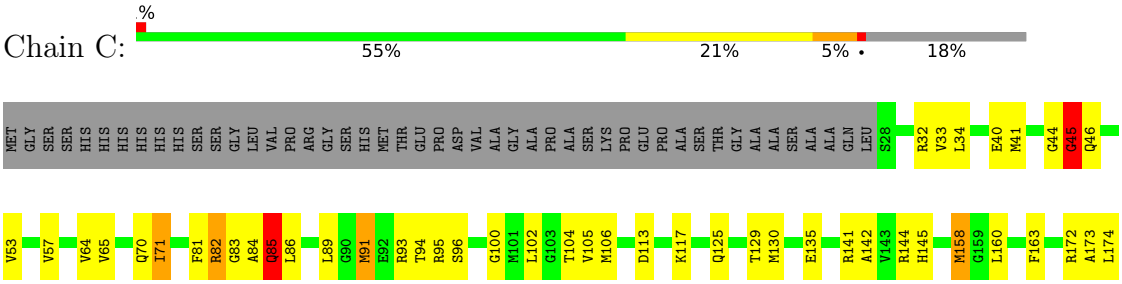
• Molecule 1: Uridylate kinase

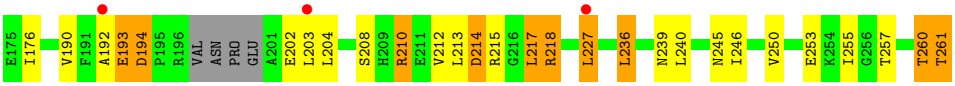
Chain B:



• Molecule 1: Uridylate kinase

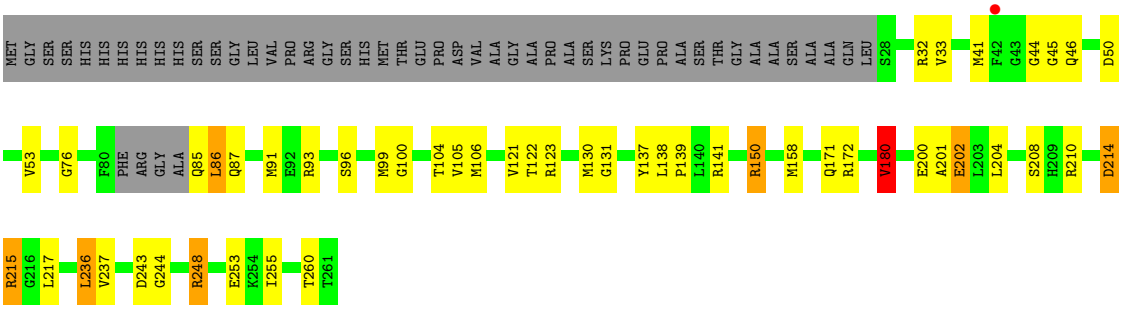
Chain C:





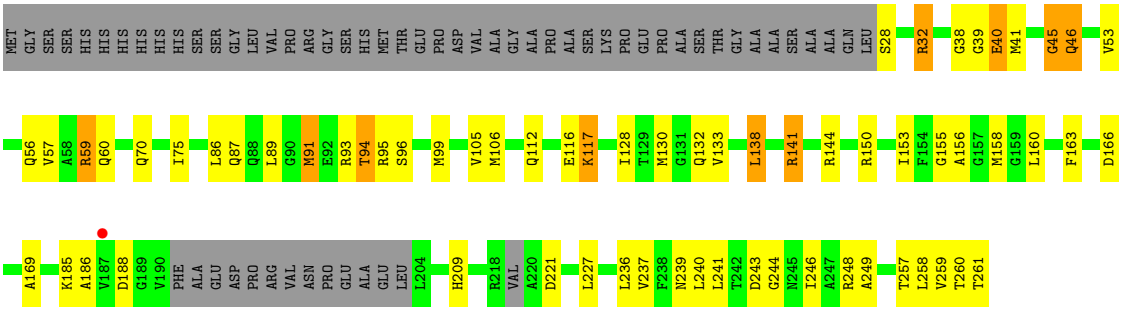
• Molecule 1: Uridylate kinase

Chain D:



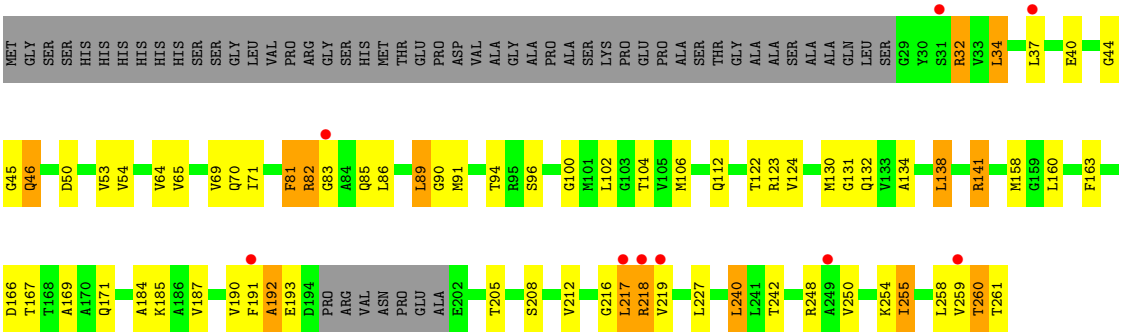
• Molecule 1: Uridylate kinase

Chain E:



• Molecule 1: Uridylate kinase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	136.71Å 175.48Å 65.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.70 – 2.54 87.74 – 2.54	Depositor EDS
% Data completeness (in resolution range)	86.1 (87.70-2.54) 86.1 (87.74-2.54)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.205 , 0.269 0.203 , 0.257	Depositor DCC
R_{free} test set	2372 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10350	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: GTP, 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	0.54	0/1692	0.74	1/2285 (0.0%)
1	B	0.51	0/1714	0.76	1/2317 (0.0%)
1	C	0.51	0/1704	0.68	0/2303
1	D	0.49	0/1722	0.71	1/2329 (0.0%)
1	E	0.50	0/1617	0.67	2/2183 (0.1%)
1	F	0.47	0/1655	0.67	0/2239
All	All	0.50	0/10104	0.71	5/13656 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	1
1	E	0	1
1	F	0	1
All	All	0	7

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	180	VAL	CB-CA-C	-7.35	97.44	111.40
1	E	46	GLN	N-CA-C	5.88	126.88	111.00
1	D	180	VAL	CB-CA-C	-5.58	100.81	111.40
1	B	82	ARG	N-CA-C	-5.50	96.15	111.00
1	E	45	GLY	N-CA-C	-5.15	100.22	113.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	GLY	Peptide
1	A	84	ALA	Peptide
1	B	260	THR	Peptide
1	B	81	PHE	Peptide
1	C	45	GLY	Peptide
1	E	45	GLY	Peptide
1	F	44	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1670	0	1710	30	0
1	B	1695	0	1712	46	0
1	C	1685	0	1694	61	0
1	D	1703	0	1728	45	0
1	E	1601	0	1607	44	0
1	F	1637	0	1640	58	0
2	A	32	0	12	0	0
2	B	32	0	12	1	0
2	C	32	0	12	1	0
2	D	32	0	12	1	0
2	E	32	0	12	0	0
2	F	32	0	12	1	0
3	B	25	0	11	0	0
4	A	41	0	0	0	0
4	B	32	0	0	0	0
4	C	23	0	0	0	0
4	D	14	0	0	0	0
4	E	14	0	0	1	0
4	F	18	0	0	0	0
All	All	10350	0	10174	255	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 13.

All (255) 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:B:41:MET:CE	1:B:186:ALA:HB2	1.83	1.07
1:B:201:ALA:HB1	1:B:202:GLU:HA	1.15	1.07
1:B:83:GLY:HA3	1:B:84:ALA:HB3	1.42	1.02
1:E:188:ASP:HA	1:E:239:ASN:HB2	1.46	0.98
1:C:106:MET:HE3	1:D:106:MET:HE1	1.50	0.94
1:B:201:ALA:CB	1:B:202:GLU:HA	1.98	0.93
1:C:160:LEU:HD13	1:F:158:MET:CE	1.99	0.93
1:C:84:ALA:HA	1:C:85:GLN:CB	1.99	0.92
1:E:240:LEU:HD11	1:E:246:ILE:HD11	1.50	0.90
1:E:86:LEU:HD13	1:E:91:MET:HE2	1.55	0.89
1:E:236:LEU:HD13	1:E:258:LEU:HD13	1.56	0.88
1:E:40:GLU:OE2	4:E:392:HOH:O	1.92	0.86
1:C:84:ALA:HA	1:C:85:GLN:HB2	1.58	0.84
1:B:208:SER:HA	1:B:260:THR:O	1.78	0.84
1:B:41:MET:HE1	1:B:186:ALA:HB2	1.57	0.84
1:D:123:ARG:NH1	2:D:262:GTP:O2B	2.11	0.83
1:A:260:THR:HA	1:A:261:THR:HB	1.62	0.82
1:F:205:THR:HG23	1:F:255:ILE:HG21	1.61	0.82
1:C:105:VAL:HG11	1:C:130:MET:HE1	1.62	0.82
1:A:208:SER:HA	1:A:260:THR:O	1.80	0.79
1:B:201:ALA:HB1	1:B:202:GLU:CA	2.06	0.79
1:F:65:VAL:HG22	1:F:71:ILE:HD13	1.64	0.79
1:C:192:ALA:O	1:C:193:GLU:HG2	1.83	0.78
1:B:41:MET:CE	1:B:186:ALA:CB	2.61	0.78
1:D:201:ALA:HA	1:D:202:GLU:HB2	1.66	0.78
1:D:201:ALA:HA	1:D:202:GLU:CB	2.15	0.76
1:E:209:HIS:ND1	1:E:261:THR:HB	2.00	0.76
1:E:240:LEU:CD1	1:E:246:ILE:HD11	2.14	0.76
1:C:106:MET:CE	1:D:106:MET:HE1	2.13	0.76
1:C:160:LEU:HD13	1:F:158:MET:HE1	1.68	0.74
1:B:42:PHE:H	1:B:43:GLY:HA3	1.53	0.74
1:E:105:VAL:HG11	1:E:130:MET:CE	2.18	0.73
1:C:106:MET:HG2	1:D:99:MET:HE2	1.72	0.71
1:E:105:VAL:HG11	1:E:130:MET:HE1	1.72	0.70
1:B:41:MET:HE3	1:B:186:ALA:HB2	1.72	0.70
1:A:130:MET:O	1:A:133:VAL:HG13	1.91	0.70
1:B:102:LEU:HD21	1:F:130:MET:CE	2.21	0.70
1:F:254:LYS:HA	1:F:255:ILE:HB	1.72	0.70
1:B:41:MET:HE2	1:B:186:ALA:HA	1.74	0.69
1:C:106:MET:CE	1:D:106:MET:CE	2.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LEU:HD13	1:F:158:MET:HE2	1.75	0.68
1:B:41:MET:HE2	1:B:186:ALA:CA	2.23	0.68
1:E:236:LEU:HD13	1:E:258:LEU:CD1	2.24	0.66
1:F:205:THR:HG23	1:F:255:ILE:CG2	2.26	0.65
1:E:32:ARG:NH1	1:E:70:GLN:OE1	2.29	0.65
1:E:128:ILE:HD12	1:E:156:ALA:HB1	1.79	0.65
1:F:216:GLY:H	1:F:217:LEU:HD13	1.62	0.64
1:E:186:ALA:HA	1:E:241:LEU:HD13	1.78	0.64
1:A:260:THR:CA	1:A:261:THR:HB	2.26	0.64
1:C:105:VAL:HG11	1:C:130:MET:CE	2.28	0.64
1:A:30:TYR:CD2	1:A:180:VAL:HG22	2.32	0.64
1:C:84:ALA:HA	1:C:85:GLN:HB3	1.79	0.64
1:C:82:ARG:HH22	1:D:46:GLN:HG3	1.63	0.63
1:B:102:LEU:HD21	1:F:130:MET:HE1	1.79	0.63
1:B:47:VAL:O	1:F:82:ARG:NH2	2.31	0.63
1:D:105:VAL:HG11	1:D:130:MET:HE1	1.80	0.63
1:A:65:VAL:HG21	1:A:120:ILE:HD12	1.80	0.61
1:D:86:LEU:HD23	1:D:87:GLN:H	1.64	0.61
1:F:65:VAL:CG2	1:F:71:ILE:HD13	2.30	0.61
1:C:210:ARG:NH1	1:C:213:LEU:HD23	2.15	0.61
1:F:255:ILE:HD11	1:F:258:LEU:HB2	1.83	0.61
1:B:83:GLY:HA3	1:B:84:ALA:CB	2.24	0.60
1:B:192:ALA:HB2	1:B:204:LEU:HD11	1.84	0.60
1:C:41:MET:O	1:C:53:VAL:HG11	2.01	0.60
1:F:254:LYS:CA	1:F:255:ILE:HB	2.31	0.60
1:C:106:MET:HE3	1:D:106:MET:CE	2.29	0.59
1:C:194:ASP:OD1	1:C:194:ASP:C	2.40	0.59
1:B:41:MET:CE	1:B:186:ALA:CA	2.81	0.59
1:E:185:LYS:HG3	1:E:237:VAL:HG13	1.84	0.59
1:A:260:THR:HA	1:A:261:THR:CB	2.33	0.58
1:D:215:ARG:HD2	1:D:217:LEU:CD1	2.34	0.58
1:E:60:GLN:HB3	1:E:246:ILE:HD12	1.84	0.57
1:B:89:LEU:O	1:B:89:LEU:HD23	2.04	0.57
1:C:158:MET:HG2	1:F:160:LEU:HD13	1.86	0.57
1:B:102:LEU:HD21	1:F:130:MET:HE3	1.87	0.57
1:D:87:GLN:HE22	1:D:93:ARG:HD2	1.70	0.57
1:D:248:ARG:HB3	1:D:255:ILE:HG13	1.86	0.57
1:D:158:MET:HE2	1:E:163:PHE:HE1	1.70	0.56
1:F:37:LEU:HD23	1:F:184:ALA:HB3	1.86	0.56
1:C:32:ARG:HB3	1:C:70:GLN:HB2	1.87	0.56
1:D:214:ASP:O	1:D:215:ARG:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:HG13	1:A:234:PRO:HB2	1.86	0.56
1:C:84:ALA:HB1	1:C:86:LEU:H	1.70	0.56
1:C:192:ALA:C	1:C:193:GLU:HG2	2.26	0.56
1:C:102:LEU:HD21	1:D:130:MET:HE1	1.87	0.56
1:D:50:ASP:OD2	1:D:53:VAL:HG23	2.06	0.55
1:C:84:ALA:CA	1:C:85:GLN:CB	2.80	0.55
1:F:71:ILE:N	1:F:71:ILE:HD12	2.21	0.55
1:B:69:VAL:HG12	1:B:71:ILE:CD1	2.37	0.55
1:A:213:LEU:O	1:A:215:ARG:N	2.33	0.55
1:E:94:THR:HG22	1:E:95:ARG:N	2.22	0.55
1:D:214:ASP:O	1:D:215:ARG:HB2	2.07	0.54
1:E:86:LEU:CD1	1:E:91:MET:HE2	2.35	0.54
1:F:184:ALA:HB1	1:F:240:LEU:HD23	1.89	0.54
1:F:138:LEU:HB3	1:F:141:ARG:HB2	1.90	0.54
1:B:41:MET:HE1	1:B:186:ALA:CB	2.33	0.54
1:D:158:MET:CE	1:E:163:PHE:HE1	2.21	0.54
1:F:124:VAL:O	1:F:134:ALA:HB1	2.08	0.54
1:D:158:MET:CE	1:D:171:GLN:HG3	2.37	0.54
1:C:174:LEU:CD1	1:C:227:LEU:HD22	2.38	0.53
1:A:260:THR:HG22	1:A:261:THR:HB	1.91	0.53
1:E:155:GLY:O	1:E:156:ALA:HB3	2.09	0.53
1:E:105:VAL:HG11	1:E:130:MET:HE3	1.90	0.52
1:F:65:VAL:HG22	1:F:71:ILE:CD1	2.37	0.52
1:C:33:VAL:CG2	1:C:71:ILE:HG23	2.40	0.52
1:E:236:LEU:HD12	1:E:257:THR:O	2.08	0.52
1:F:191:PHE:O	1:F:192:ALA:CB	2.56	0.52
1:C:208:SER:O	1:C:212:VAL:HG23	2.10	0.52
1:D:158:MET:HE1	1:D:171:GLN:HG3	1.91	0.52
1:A:122:THR:HB	1:A:151:VAL:HB	1.92	0.51
1:C:208:SER:HA	1:C:260:THR:O	2.10	0.51
1:F:208:SER:HA	1:F:260:THR:O	2.10	0.51
1:C:163:PHE:HE1	1:F:158:MET:CE	2.24	0.51
1:D:105:VAL:HG11	1:D:130:MET:CE	2.39	0.51
1:B:83:GLY:CA	1:B:84:ALA:HB3	2.28	0.51
1:B:74:VAL:CG1	1:B:165:THR:CG2	2.89	0.51
1:B:130:MET:CE	1:F:102:LEU:HD21	2.41	0.51
1:C:174:LEU:HD11	1:C:227:LEU:HD22	1.93	0.50
1:C:82:ARG:CB	1:C:83:GLY:CA	2.90	0.50
1:E:94:THR:CG2	1:E:95:ARG:N	2.74	0.50
1:C:65:VAL:CG2	1:C:71:ILE:HD11	2.41	0.50
1:F:50:ASP:OD2	1:F:53:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:PHE:O	1:F:192:ALA:HB3	2.10	0.50
1:F:123:ARG:NH1	2:F:262:GTP:O1B	2.43	0.50
1:F:185:LYS:NZ	1:F:218:ARG:NH1	2.60	0.50
1:D:215:ARG:HD2	1:D:217:LEU:HD11	1.93	0.49
1:E:138:LEU:HB3	1:E:141:ARG:HG3	1.95	0.49
1:C:106:MET:HE1	1:D:106:MET:CE	2.40	0.49
1:A:115:LEU:HB2	1:A:122:THR:HG21	1.95	0.49
1:A:188:ASP:HA	1:A:239:ASN:HB2	1.95	0.48
1:A:76:GLY:C	1:A:104:THR:HG22	2.33	0.48
1:B:184:ALA:HB1	1:B:240:LEU:HB3	1.94	0.48
1:D:248:ARG:HG3	1:D:253:GLU:OE1	2.13	0.48
1:A:139:PRO:O	1:A:143:VAL:HG13	2.14	0.48
1:C:106:MET:HE1	1:D:106:MET:HE2	1.95	0.48
1:E:75:ILE:HD11	1:E:153:ILE:HG21	1.96	0.48
1:F:192:ALA:HA	1:F:193:GLU:CB	2.44	0.48
1:C:44:GLY:O	1:C:45:GLY:O	2.30	0.48
1:F:32:ARG:NH1	1:F:70:GLN:OE1	2.45	0.48
1:E:259:VAL:HG12	1:E:259:VAL:O	2.13	0.48
1:A:93:ARG:HD2	1:A:162:TYR:CE2	2.48	0.48
1:A:94:THR:HG22	1:A:95:ARG:N	2.28	0.48
1:A:213:LEU:C	1:A:215:ARG:H	2.17	0.48
1:C:106:MET:HA	1:D:99:MET:HE1	1.96	0.47
1:B:69:VAL:HG12	1:B:71:ILE:HD12	1.96	0.47
1:C:172:ARG:O	1:C:176:ILE:HG12	2.14	0.47
1:F:112:GLN:HA	1:F:122:THR:HG21	1.96	0.47
1:B:105:VAL:HG11	1:B:130:MET:HE1	1.97	0.47
1:C:239:ASN:O	1:C:245:ASN:ND2	2.47	0.47
1:E:39:GLY:C	1:E:41:MET:H	2.17	0.47
1:E:53:VAL:O	1:E:57:VAL:HG23	2.15	0.47
1:F:190:VAL:HG21	1:F:219:VAL:HG22	1.96	0.47
1:C:236:LEU:C	1:C:236:LEU:HD12	2.34	0.47
1:B:130:MET:HE1	1:F:102:LEU:HD21	1.97	0.47
1:C:64:VAL:HG21	1:C:246:ILE:HG12	1.97	0.47
1:C:65:VAL:HG22	1:C:71:ILE:HD11	1.97	0.47
1:C:163:PHE:HE1	1:F:158:MET:HE1	1.79	0.46
1:B:210:ARG:HG3	1:B:214:ASP:OD1	2.15	0.46
1:F:163:PHE:CD2	1:F:167:THR:HG21	2.51	0.46
1:F:50:ASP:O	1:F:54:VAL:HG23	2.16	0.46
1:F:158:MET:HE3	1:F:171:GLN:HG3	1.98	0.46
1:B:192:ALA:O	1:B:193:GLU:CB	2.64	0.45
1:F:81:PHE:N	1:F:81:PHE:CD1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:LEU:HD21	1:D:130:MET:CE	2.47	0.45
1:C:190:VAL:HG23	1:C:257:THR:HB	1.99	0.45
1:C:160:LEU:CD1	1:F:158:MET:HE2	2.46	0.45
1:B:180:VAL:HG23	1:B:234:PRO:HB2	1.98	0.45
1:F:34:LEU:HD22	1:F:169:ALA:O	2.17	0.45
1:B:74:VAL:HG12	1:B:165:THR:CG2	2.47	0.45
1:B:212:VAL:O	1:B:217:LEU:N	2.43	0.45
1:B:117:LYS:HE2	1:F:90:GLY:O	2.16	0.45
1:E:243:ASP:OD2	1:E:244:GLY:N	2.50	0.45
1:A:137:TYR:O	1:A:138:LEU:HD13	2.17	0.45
1:B:64:VAL:HG12	1:B:71:ILE:HD11	1.98	0.45
1:D:44:GLY:N	1:D:45:GLY:HA2	2.31	0.45
1:B:39:GLY:O	1:B:42:PHE:HB2	2.17	0.45
1:B:188:ASP:HA	1:B:239:ASN:HB2	1.99	0.45
1:D:201:ALA:HA	1:D:202:GLU:HB3	1.97	0.45
1:E:75:ILE:HD11	1:E:153:ILE:CG2	2.47	0.45
1:E:117:LYS:HE3	1:E:117:LYS:HB3	1.85	0.45
1:E:128:ILE:O	1:E:130:MET:HG3	2.17	0.45
1:F:64:VAL:HG12	1:F:69:VAL:HB	1.99	0.45
1:E:236:LEU:HD23	1:E:249:ALA:HB1	1.99	0.45
1:F:258:LEU:HD12	1:F:259:VAL:H	1.82	0.45
1:D:121:VAL:HG12	1:D:150:ARG:HD2	1.98	0.44
1:E:105:VAL:CG1	1:E:130:MET:HE1	2.45	0.44
1:E:209:HIS:CE1	1:E:259:VAL:O	2.70	0.44
1:D:87:GLN:NE2	1:D:93:ARG:HD2	2.30	0.44
1:A:44:GLY:HA2	1:A:45:GLY:HA2	1.71	0.44
1:C:91:MET:SD	1:C:95:ARG:HG2	2.57	0.44
1:F:64:VAL:HG13	1:F:250:VAL:HG21	1.99	0.44
1:A:35:LEU:HD21	1:A:37:LEU:HD21	1.99	0.44
1:D:201:ALA:CA	1:D:202:GLU:CB	2.91	0.44
2:B:262:GTP:O1A	2:B:262:GTP:H8	2.01	0.44
1:E:112:GLN:O	1:E:116:GLU:HG3	2.17	0.44
1:F:81:PHE:N	1:F:81:PHE:HD1	2.16	0.44
1:A:30:TYR:CD2	1:A:180:VAL:CG2	2.98	0.43
1:F:45:GLY:CA	1:F:46:GLN:O	2.66	0.43
1:C:246:ILE:O	1:C:250:VAL:HG22	2.18	0.43
1:C:210:ARG:O	1:C:214:ASP:HB2	2.18	0.43
1:A:94:THR:CG2	1:A:95:ARG:N	2.80	0.43
1:D:158:MET:HE2	1:E:160:LEU:HD13	2.00	0.43
1:C:34:LEU:HD13	1:C:173:ALA:N	2.34	0.43
1:C:192:ALA:O	1:C:193:GLU:CG	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:MET:CE	1:F:96:SER:HA	2.48	0.43
1:C:217:LEU:C	1:C:218:ARG:HG3	2.38	0.43
1:D:236:LEU:HD12	1:D:237:VAL:N	2.34	0.43
1:A:115:LEU:CB	1:A:122:THR:HG21	2.49	0.43
1:C:82:ARG:HH22	1:D:46:GLN:CG	2.29	0.43
1:B:248:ARG:HG2	1:B:253:GLU:OE2	2.19	0.42
1:F:40:GLU:CD	1:F:40:GLU:H	2.23	0.42
1:A:247:ALA:O	1:A:251:ARG:HG3	2.19	0.42
1:F:100:GLY:O	1:F:104:THR:HG23	2.19	0.42
1:D:76:GLY:C	1:D:104:THR:HG22	2.40	0.42
1:D:208:SER:HA	1:D:260:THR:O	2.19	0.42
1:F:86:LEU:HA	1:F:89:LEU:HB2	2.01	0.42
1:B:192:ALA:O	1:B:193:GLU:HB3	2.20	0.42
1:C:253:GLU:O	1:C:255:ILE:HG23	2.19	0.42
1:C:260:THR:HG23	1:C:261:THR:N	2.34	0.42
1:D:85:GLN:HG2	1:D:85:GLN:O	2.20	0.42
1:C:113:ASP:O	1:C:117:LYS:HG2	2.20	0.42
2:C:262:GTP:O1A	1:E:141:ARG:NH1	2.53	0.42
1:D:244:GLY:O	1:D:248:ARG:HD3	2.20	0.42
1:E:95:ARG:O	1:E:99:MET:HG3	2.20	0.42
1:A:155:GLY:O	1:A:156:ALA:HB3	2.19	0.42
1:B:81:PHE:HE1	1:F:106:MET:SD	2.43	0.42
1:C:125:GLN:HA	1:C:135:GLU:O	2.20	0.42
1:A:188:ASP:O	1:A:256:GLY:HA2	2.20	0.42
1:C:217:LEU:HD13	1:C:217:LEU:HA	1.88	0.42
1:E:38:GLY:O	1:E:41:MET:HG2	2.20	0.42
1:D:33:VAL:HG12	1:D:180:VAL:HG23	2.02	0.41
1:D:137:TYR:CZ	1:D:139:PRO:HG3	2.55	0.41
1:C:64:VAL:CG2	1:C:246:ILE:HG12	2.50	0.41
1:A:254:LYS:HA	1:A:254:LYS:HE2	2.03	0.41
1:F:184:ALA:HB1	1:F:240:LEU:HB3	2.03	0.41
1:A:84:ALA:HA	1:A:87:GLN:HG3	2.03	0.41
1:C:142:ALA:O	1:C:145:HIS:HB2	2.20	0.41
1:D:100:GLY:O	1:D:104:THR:HG23	2.20	0.41
1:A:110:ALA:O	1:A:114:PHE:HD1	2.04	0.41
1:B:42:PHE:N	1:B:43:GLY:HA3	2.25	0.41
1:B:69:VAL:HG12	1:B:71:ILE:HD11	2.02	0.41
1:B:246:ILE:O	1:B:250:VAL:HG23	2.21	0.41
1:C:53:VAL:O	1:C:57:VAL:HG23	2.20	0.41
1:E:130:MET:HE3	1:E:133:VAL:HG11	2.03	0.41
1:B:74:VAL:CG1	1:B:165:THR:HG22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ARG:HD2	1:B:144:ARG:HA	1.83	0.41
1:C:100:GLY:O	1:C:104:THR:HG23	2.21	0.41
1:E:59:ARG:HE	1:E:59:ARG:HB3	1.56	0.41
1:F:255:ILE:HD11	1:F:258:LEU:CB	2.50	0.40
1:F:240:LEU:HD12	1:F:240:LEU:O	2.22	0.40
1:E:60:GLN:CB	1:E:246:ILE:HD12	2.51	0.40
1:F:208:SER:O	1:F:212:VAL:HG23	2.22	0.40
1:D:215:ARG:HD2	1:D:217:LEU:HD13	2.03	0.40
1:E:166:ASP:O	1:E:169:ALA:HB3	2.20	0.40
1:F:205:THR:CG2	1:F:255:ILE:HG21	2.42	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	222/281 (79%)	207 (93%)	13 (6%)	2 (1%)	17 24
1	B	227/281 (81%)	210 (92%)	15 (7%)	2 (1%)	17 24
1	C	226/281 (80%)	204 (90%)	15 (7%)	7 (3%)	4 3
1	D	226/281 (80%)	212 (94%)	10 (4%)	4 (2%)	8 10
1	E	214/281 (76%)	198 (92%)	13 (6%)	3 (1%)	11 15
1	F	222/281 (79%)	204 (92%)	13 (6%)	5 (2%)	6 6
All	All	1337/1686 (79%)	1235 (92%)	79 (6%)	23 (2%)	9 11

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ASP
1	C	82	ARG

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Mol	Chain	Res	Type
1	C	85	GLN
1	C	89	LEU
1	D	86	LEU
1	D	202	GLU
1	F	255	ILE
1	C	45	GLY
1	C	193	GLU
1	C	214	ASP
1	D	131	GLY
1	D	215	ARG
1	F	131	GLY
1	F	192	ALA
1	B	216	GLY
1	C	215	ARG
1	E	40	GLU
1	E	46	GLN
1	E	221	ASP
1	A	215	ARG
1	F	46	GLN
1	F	83	GLY
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	172/215 (80%)	144 (84%)	28 (16%)	2	2
1	B	172/215 (80%)	154 (90%)	18 (10%)	7	7
1	C	170/215 (79%)	145 (85%)	25 (15%)	3	2
1	D	176/215 (82%)	159 (90%)	17 (10%)	8	9
1	E	162/215 (75%)	141 (87%)	21 (13%)	4	3
1	F	162/215 (75%)	142 (88%)	20 (12%)	4	4
All	All	1014/1290 (79%)	885 (87%)	129 (13%)	4	4

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	28	SER
1	A	63	ASP
1	A	65	VAL
1	A	85	GLN
1	A	88	GLN
1	A	89	LEU
1	A	93	ARG
1	A	94	THR
1	A	117[A]	LYS
1	A	117[B]	LYS
1	A	122	THR
1	A	132	GLN
1	A	133	VAL
1	A	138	LEU
1	A	143	VAL
1	A	172	ARG
1	A	180	VAL
1	A	185	LYS
1	A	204	LEU
1	A	217	LEU
1	A	218	ARG
1	A	227	LEU
1	A	236	LEU
1	A	248	ARG
1	A	253	GLU
1	A	254	LYS
1	A	260	THR
1	B	34	LEU
1	B	42	PHE
1	B	46	GLN
1	B	56	GLN
1	B	85	GLN
1	B	117	LYS
1	B	138	LEU
1	B	150	ARG
1	B	174	LEU
1	B	187	VAL
1	B	188	ASP
1	B	202	GLU
1	B	204	LEU
1	B	210	ARG

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Mol	Chain	Res	Type
1	B	213	LEU
1	B	219	VAL
1	B	240	LEU
1	B	261	THR
1	C	40	GLU
1	C	46	GLN
1	C	71	ILE
1	C	81	PHE
1	C	85	GLN
1	C	91	MET
1	C	93	ARG
1	C	94	THR
1	C	96	SER
1	C	129	THR
1	C	141	ARG
1	C	144	ARG
1	C	158	MET
1	C	194	ASP
1	C	202	GLU
1	C	203	LEU
1	C	204	LEU
1	C	210	ARG
1	C	217	LEU
1	C	218	ARG
1	C	227	LEU
1	C	236	LEU
1	C	240	LEU
1	C	260	THR
1	C	261	THR
1	D	32	ARG
1	D	41	MET
1	D	91	MET
1	D	96	SER
1	D	122	THR
1	D	138	LEU
1	D	141	ARG
1	D	150	ARG
1	D	172	ARG
1	D	180	VAL
1	D	200	GLU
1	D	204	LEU
1	D	210	ARG

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Mol	Chain	Res	Type
1	D	214	ASP
1	D	236	LEU
1	D	243	ASP
1	D	248	ARG
1	E	28	SER
1	E	32	ARG
1	E	56	GLN
1	E	59	ARG
1	E	87	GLN
1	E	89	LEU
1	E	91	MET
1	E	93	ARG
1	E	94	THR
1	E	96	SER
1	E	106	MET
1	E	117	LYS
1	E	132	GLN
1	E	138	LEU
1	E	141	ARG
1	E	144	ARG
1	E	150	ARG
1	E	158	MET
1	E	227	LEU
1	E	248	ARG
1	E	260	THR
1	F	32	ARG
1	F	34	LEU
1	F	81	PHE
1	F	82	ARG
1	F	85	GLN
1	F	89	LEU
1	F	94	THR
1	F	132	GLN
1	F	138	LEU
1	F	141	ARG
1	F	166	ASP
1	F	187	VAL
1	F	217	LEU
1	F	218	ARG
1	F	227	LEU
1	F	240	LEU
1	F	242	THR

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Mol	Chain	Res	Type
1	F	248	ARG
1	F	260	THR
1	F	261	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	B	56	GLN
1	C	85	GLN
1	D	56	GLN
1	D	87	GLN
1	E	56	GLN
1	E	85	GLN
1	F	132	GLN
1	F	245	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GTP	E	262	-	26,34,34	1.13	2 (7%)	32,54,54	1.53	5 (15%)
2	GTP	B	262	-	26,34,34	1.16	2 (7%)	32,54,54	1.59	6 (18%)
2	GTP	F	262	-	26,34,34	1.17	2 (7%)	32,54,54	1.58	6 (18%)
3	UDP	B	263	-	24,26,26	0.96	1 (4%)	37,40,40	1.56	7 (18%)
2	GTP	C	262	-	26,34,34	1.12	1 (3%)	32,54,54	1.46	6 (18%)
2	GTP	A	262	-	26,34,34	1.03	1 (3%)	32,54,54	1.54	5 (15%)
2	GTP	D	262	-	26,34,34	1.11	2 (7%)	32,54,54	1.61	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	E	262	-	-	4/18/38/38	0/3/3/3
2	GTP	B	262	-	-	6/18/38/38	0/3/3/3
2	GTP	F	262	-	-	4/18/38/38	0/3/3/3
3	UDP	B	263	-	-	1/16/32/32	0/2/2/2
2	GTP	C	262	-	-	4/18/38/38	0/3/3/3
2	GTP	A	262	-	-	6/18/38/38	0/3/3/3
2	GTP	D	262	-	-	5/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	262	GTP	C5-C6	-4.19	1.38	1.47
2	C	262	GTP	C5-C6	-4.13	1.39	1.47
2	B	262	GTP	C5-C6	-4.07	1.39	1.47
2	D	262	GTP	C5-C6	-3.72	1.39	1.47
2	A	262	GTP	C5-C6	-3.56	1.40	1.47
2	E	262	GTP	C5-C6	-3.43	1.40	1.47
2	B	262	GTP	C2-N3	2.75	1.39	1.33
2	D	262	GTP	C2-N3	2.69	1.39	1.33
2	E	262	GTP	C2-N3	2.60	1.39	1.33
2	F	262	GTP	C2-N3	2.57	1.39	1.33
3	B	263	UDP	C5-C4	-2.05	1.39	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	262	GTP	PB-O3B-PG	-4.47	117.50	132.83
3	B	263	UDP	C4-N3-C2	-4.32	120.88	126.58
2	A	262	GTP	PB-O3B-PG	-4.30	118.08	132.83
3	B	263	UDP	N3-C2-N1	4.11	120.34	114.89
2	E	262	GTP	PB-O3B-PG	-4.01	119.08	132.83
2	B	262	GTP	PB-O3B-PG	-3.74	119.98	132.83
2	B	262	GTP	PA-O3A-PB	-3.65	120.31	132.83
2	F	262	GTP	C5-C6-N1	3.53	120.18	113.95
2	F	262	GTP	PB-O3B-PG	-3.49	120.85	132.83
2	C	262	GTP	PA-O3A-PB	-3.44	121.01	132.83
2	E	262	GTP	C8-N7-C5	3.33	109.33	102.99
2	B	262	GTP	C5-C6-N1	3.25	119.69	113.95
2	F	262	GTP	PA-O3A-PB	-3.22	121.79	132.83
2	A	262	GTP	PA-O3A-PB	-3.16	121.98	132.83
2	E	262	GTP	C5-C6-N1	3.11	119.44	113.95
2	A	262	GTP	C8-N7-C5	3.10	108.89	102.99
2	D	262	GTP	C8-N7-C5	3.09	108.87	102.99
2	D	262	GTP	C5-C6-N1	3.06	119.35	113.95
2	F	262	GTP	C2-N1-C6	-3.05	119.48	125.10
3	B	263	UDP	C6-N1-C2	-3.04	117.10	120.99
3	B	263	UDP	PA-O3A-PB	-2.99	122.55	132.83
2	F	262	GTP	O6-C6-C5	-2.97	118.56	124.37
2	D	262	GTP	PA-O3A-PB	-2.93	122.76	132.83
2	C	262	GTP	C8-N7-C5	2.91	108.53	102.99
2	B	262	GTP	C2-N1-C6	-2.90	119.75	125.10
2	D	262	GTP	C2-N1-C6	-2.90	119.75	125.10
2	F	262	GTP	C8-N7-C5	2.90	108.50	102.99
2	A	262	GTP	C5-C6-N1	2.87	119.01	113.95
2	B	262	GTP	C8-N7-C5	2.86	108.43	102.99
2	D	262	GTP	C3'-C2'-C1'	2.84	105.26	100.98
2	C	262	GTP	O3G-PG-O3B	2.83	114.12	104.64
2	A	262	GTP	C2-N1-C6	-2.76	120.01	125.10
2	E	262	GTP	C2-N1-C6	-2.71	120.10	125.10
2	C	262	GTP	C5-C6-N1	2.61	118.55	113.95
3	B	263	UDP	C5-C4-N3	2.50	118.58	114.84
2	C	262	GTP	C2-N1-C6	-2.38	120.72	125.10
3	B	263	UDP	O3B-PB-O3A	2.26	112.22	104.64
2	C	262	GTP	PB-O3B-PG	-2.20	125.27	132.83
3	B	263	UDP	O4-C4-C5	-2.17	121.34	125.16
2	E	262	GTP	C5'-C4'-C3'	-2.15	107.11	115.18
2	B	262	GTP	O6-C6-C5	-2.08	120.30	124.37

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	262	GTP	C5'-O5'-PA-O1A
2	A	262	GTP	C5'-O5'-PA-O2A
2	B	262	GTP	C5'-O5'-PA-O3A
2	C	262	GTP	PB-O3B-PG-O2G
2	C	262	GTP	PB-O3B-PG-O3G
2	D	262	GTP	C5'-O5'-PA-O1A
2	D	262	GTP	C5'-O5'-PA-O2A
2	E	262	GTP	PB-O3B-PG-O2G
2	E	262	GTP	PB-O3B-PG-O3G
2	E	262	GTP	C5'-O5'-PA-O1A
2	F	262	GTP	C5'-O5'-PA-O1A
2	F	262	GTP	C5'-O5'-PA-O2A
2	B	262	GTP	PG-O3B-PB-O1B
2	C	262	GTP	PG-O3B-PB-O1B
2	A	262	GTP	PB-O3A-PA-O5'
2	A	262	GTP	C5'-O5'-PA-O3A
2	D	262	GTP	PA-O3A-PB-O2B
2	B	262	GTP	C5'-O5'-PA-O1A
2	B	262	GTP	C4'-C5'-O5'-PA
2	A	262	GTP	PG-O3B-PB-O1B
2	A	262	GTP	PG-O3B-PB-O2B
2	B	262	GTP	PG-O3B-PB-O2B
2	F	262	GTP	C4'-C5'-O5'-PA
3	B	263	UDP	C4'-C5'-O5'-PA
2	B	262	GTP	PB-O3A-PA-O5'
2	D	262	GTP	PB-O3A-PA-O5'
2	D	262	GTP	C5'-O5'-PA-O3A
2	F	262	GTP	C5'-O5'-PA-O3A
2	C	262	GTP	PB-O3B-PG-O1G
2	E	262	GTP	PB-O3B-PG-O1G

There are no ring outliers.

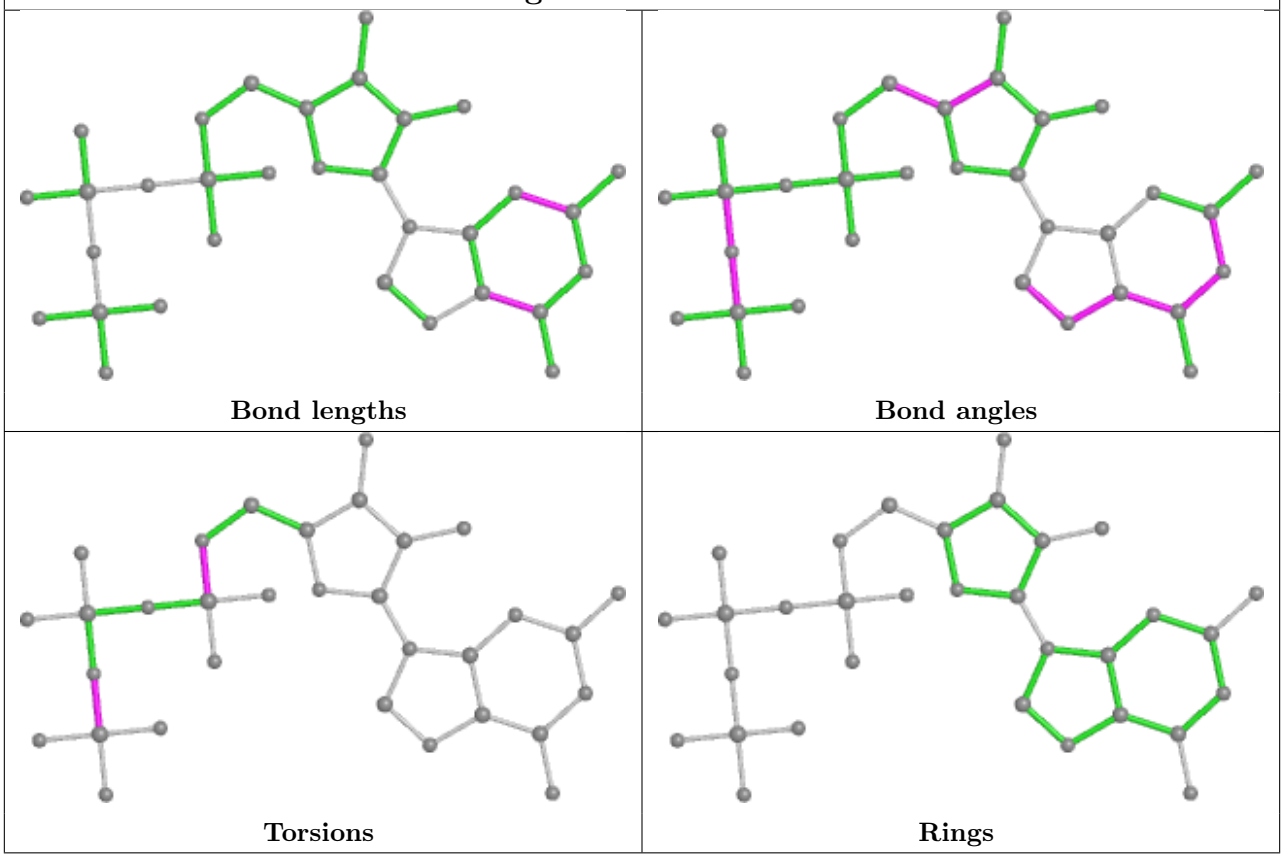
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	262	GTP	1	0
2	F	262	GTP	1	0
2	C	262	GTP	1	0
2	D	262	GTP	1	0

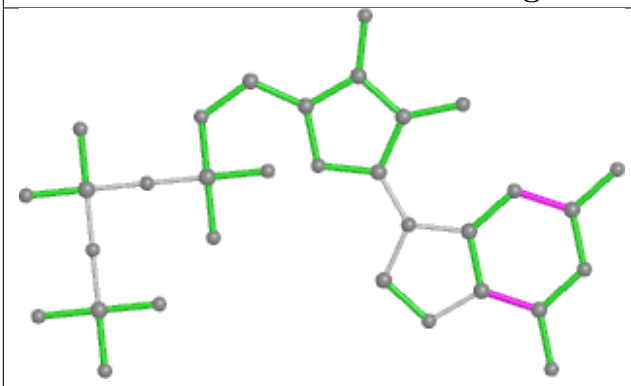
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

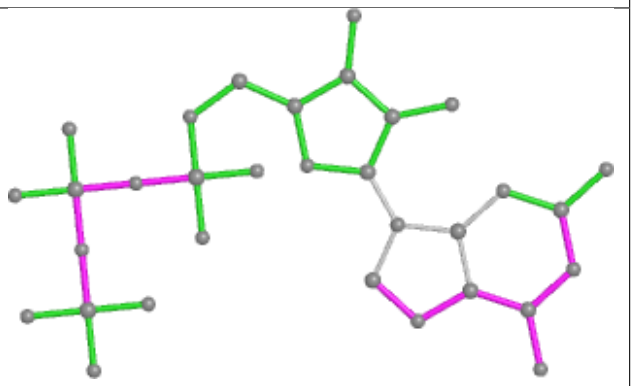
Ligand GTP E 262



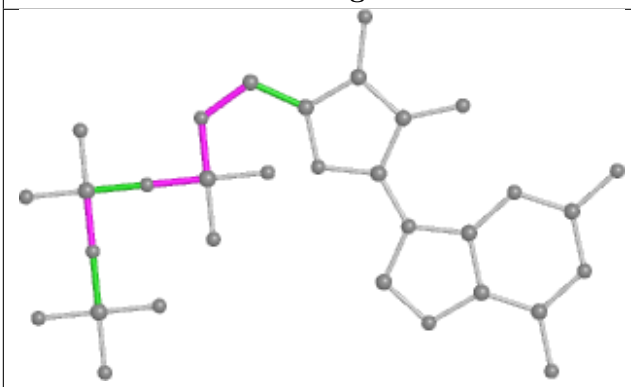
Ligand GTP B 262



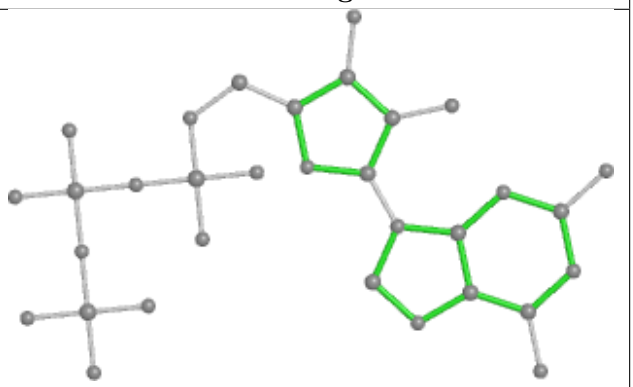
Bond lengths



Bond angles

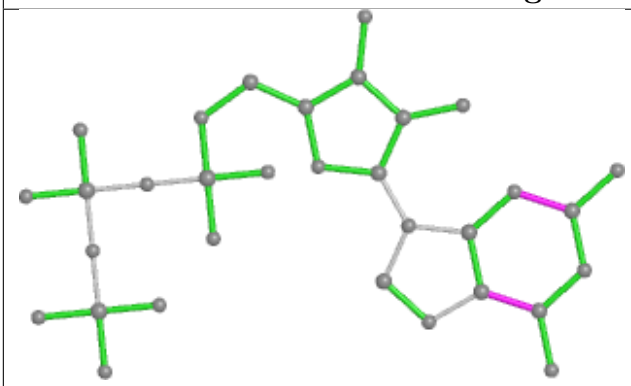


Torsions

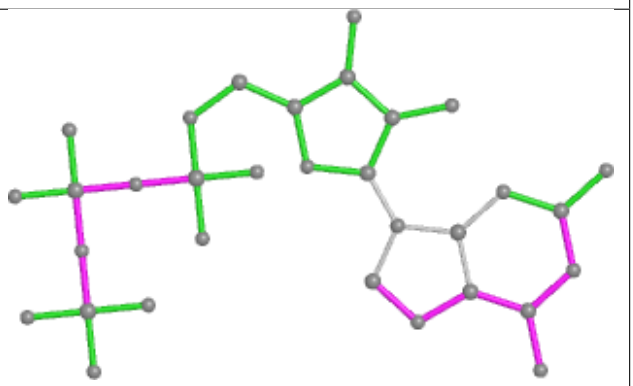


Rings

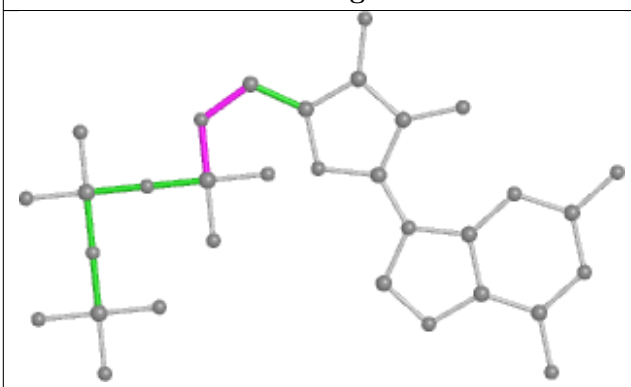
Ligand GTP F 262



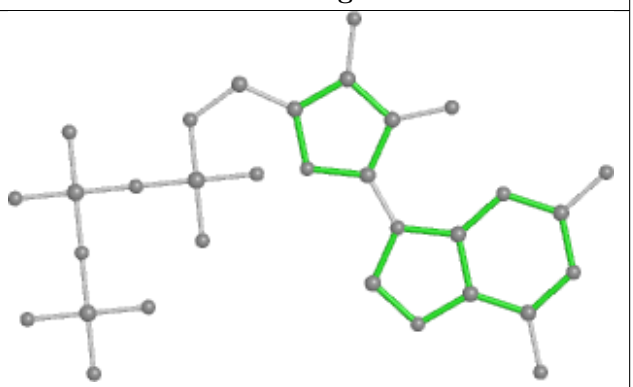
Bond lengths



Bond angles

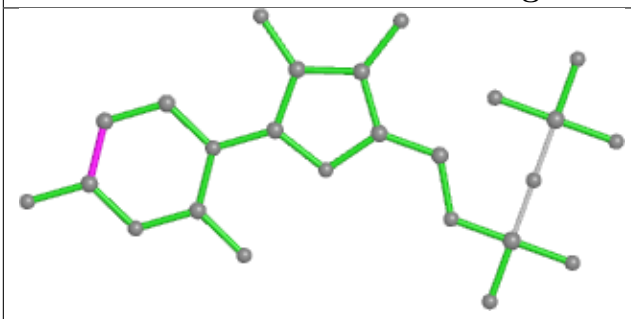


Torsions

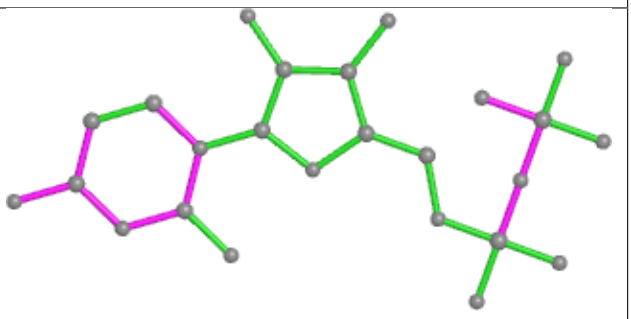


Rings

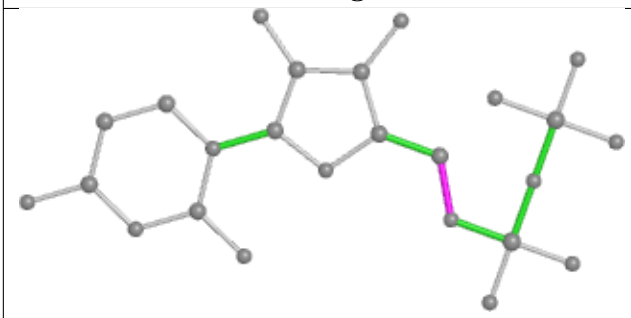
Ligand UDP B 263



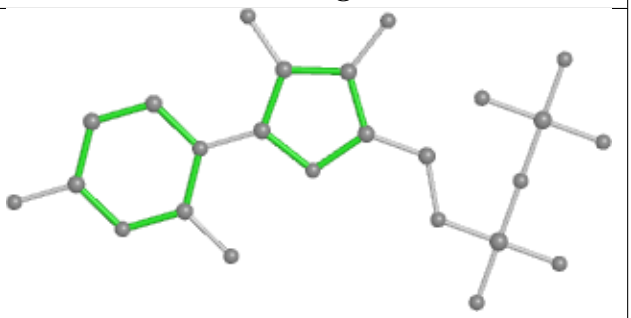
Bond lengths



Bond angles

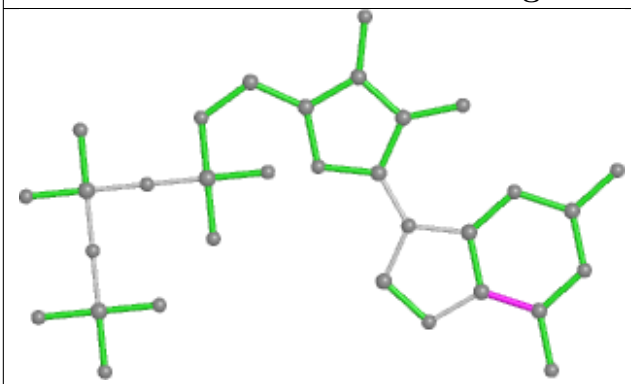


Torsions

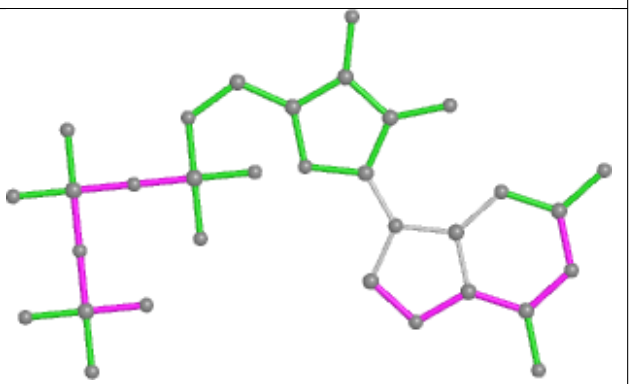


Rings

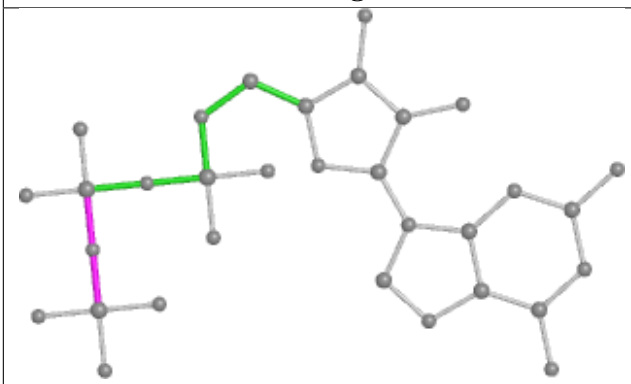
Ligand GTP C 262



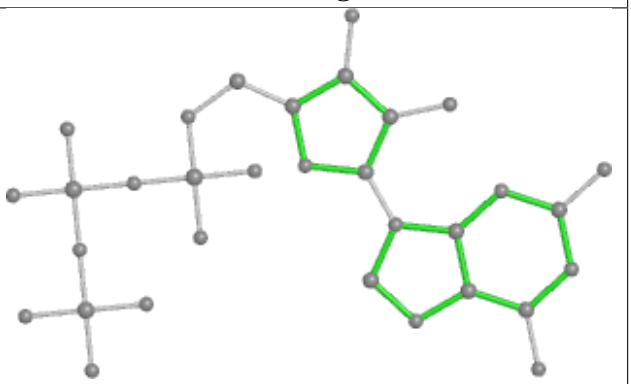
Bond lengths



Bond angles

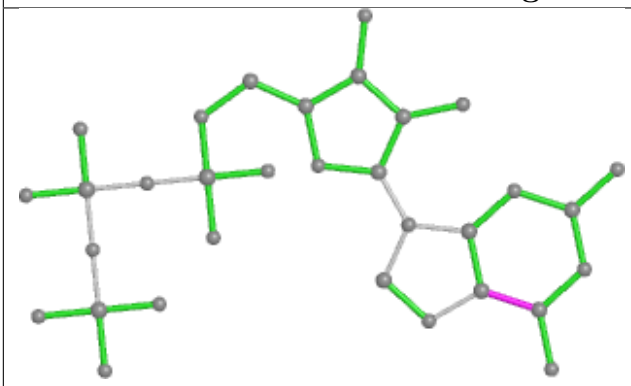


Torsions

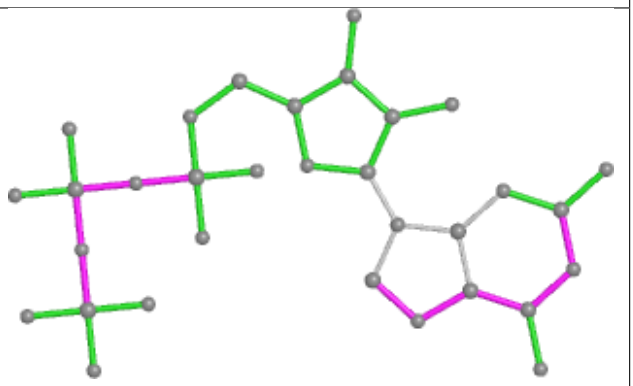


Rings

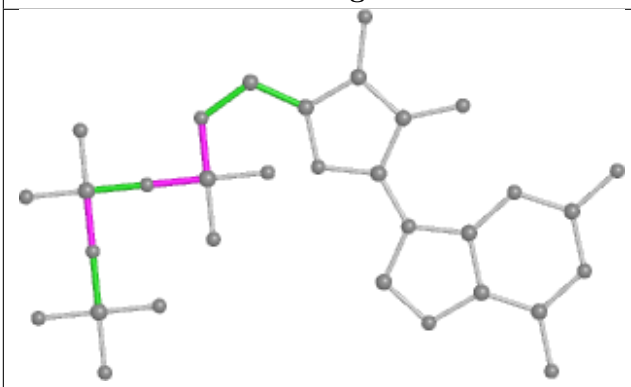
Ligand GTP A 262



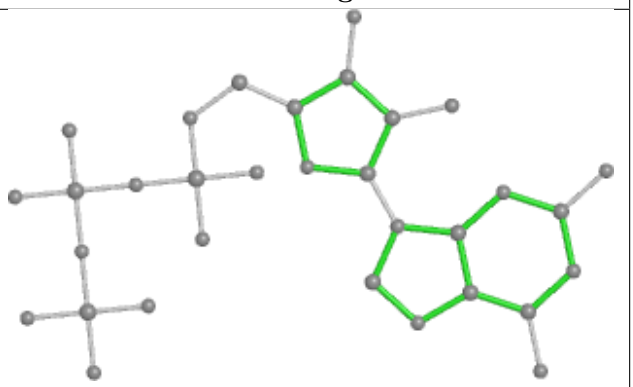
Bond lengths



Bond angles

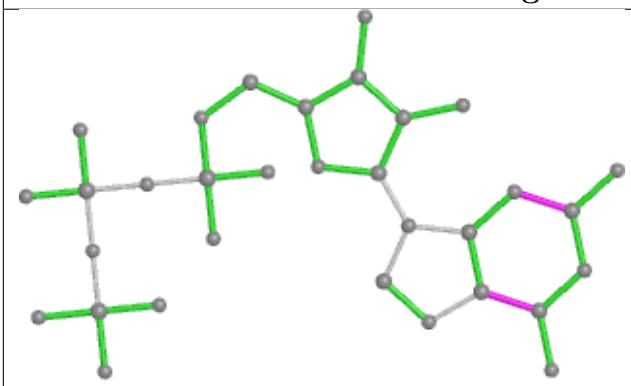


Torsions

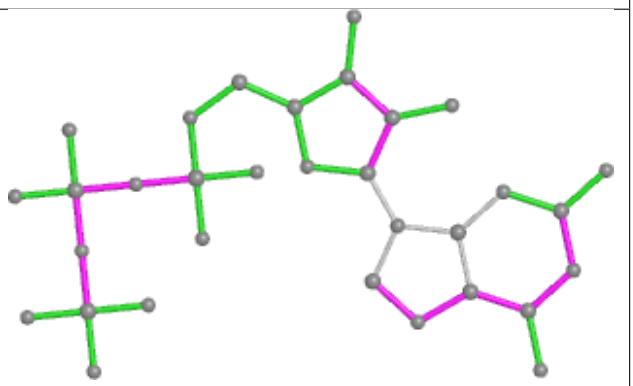


Rings

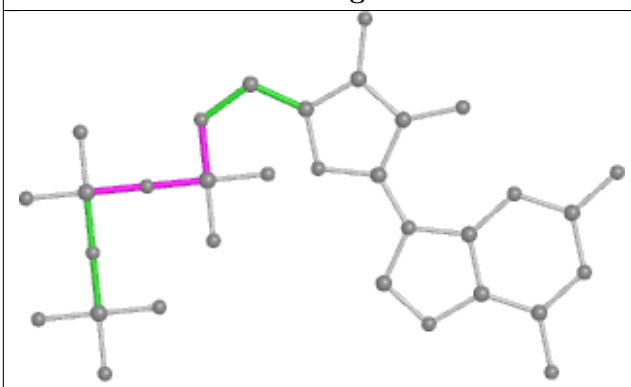
Ligand GTP D 262



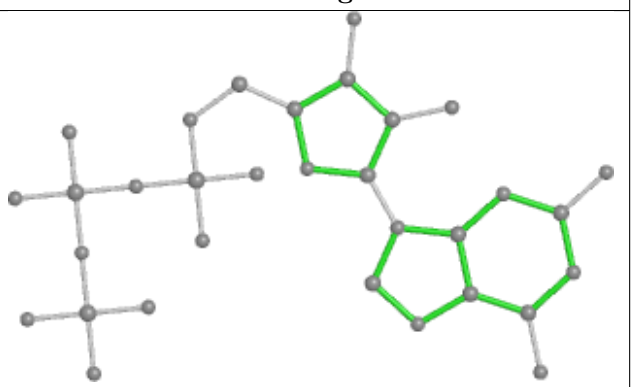
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	227/281 (80%)	-0.21	0 100 100	19, 31, 68, 99	10 (4%)
1	B	231/281 (82%)	-0.15	3 (1%) 77 82	19, 38, 70, 81	7 (3%)
1	C	230/281 (81%)	-0.19	3 (1%) 77 82	21, 40, 77, 98	6 (2%)
1	D	230/281 (81%)	-0.19	1 (0%) 92 96	24, 42, 60, 67	7 (3%)
1	E	220/281 (78%)	-0.12	1 (0%) 91 94	21, 45, 103, 119	3 (1%)
1	F	226/281 (80%)	0.10	9 (3%) 38 45	22, 44, 76, 93	12 (5%)
All	All	1364/1686 (80%)	-0.13	17 (1%) 79 84	19, 39, 78, 119	45 (3%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	187	VAL	2.9
1	F	191	PHE	2.8
1	F	259	VAL	2.7
1	F	217	LEU	2.7
1	D	42	PHE	2.5
1	F	83	GLY	2.5
1	C	227	LEU	2.4
1	C	192	ALA	2.4
1	C	203	LEU	2.2
1	F	31	SER	2.1
1	F	219	VAL	2.1
1	B	81	PHE	2.1
1	F	37	LEU	2.1
1	F	218	ARG	2.1
1	F	249	ALA	2.0
1	B	219	VAL	2.0
1	B	225	PHE	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)

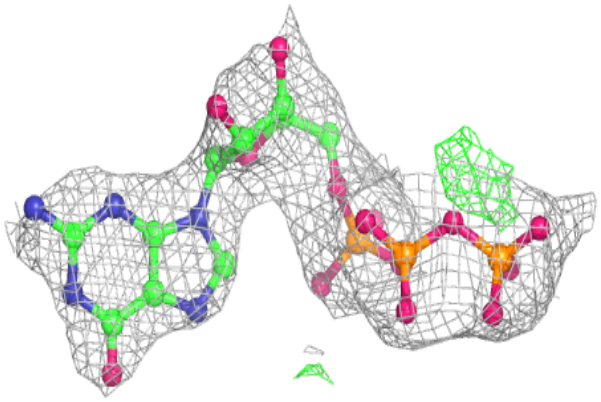
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

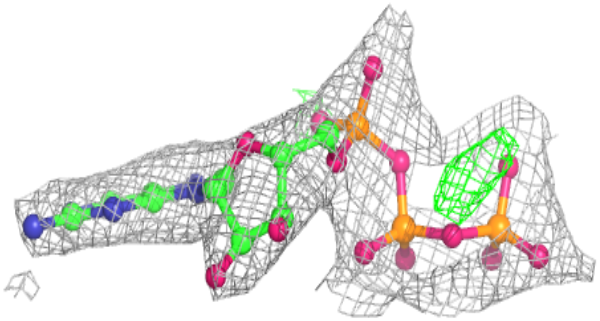
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GTP	D	262	32/32	0.90	0.18	45,53,64,65	32
2	GTP	F	262	32/32	0.90	0.16	52,58,71,72	32
2	GTP	E	262	32/32	0.92	0.16	61,66,72,73	0
2	GTP	C	262	32/32	0.95	0.11	38,45,56,56	0
2	GTP	A	262	32/32	0.95	0.12	42,46,61,62	0
2	GTP	B	262	32/32	0.96	0.11	37,47,66,67	0
3	UDP	B	263	25/25	0.96	0.14	35,42,49,50	0

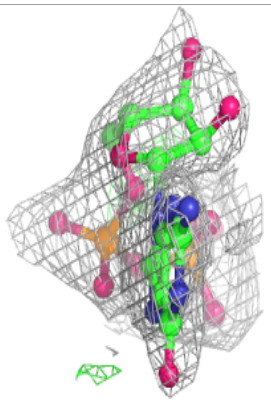
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP D 262:

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

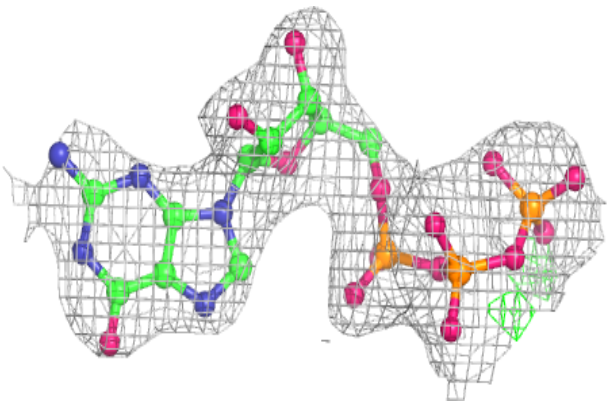


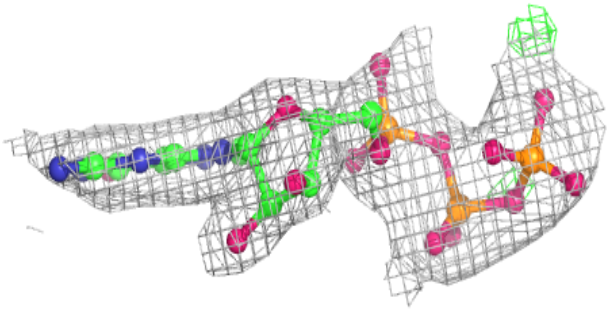


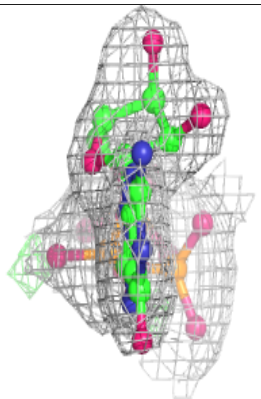


Electron density around GTP F 262:

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

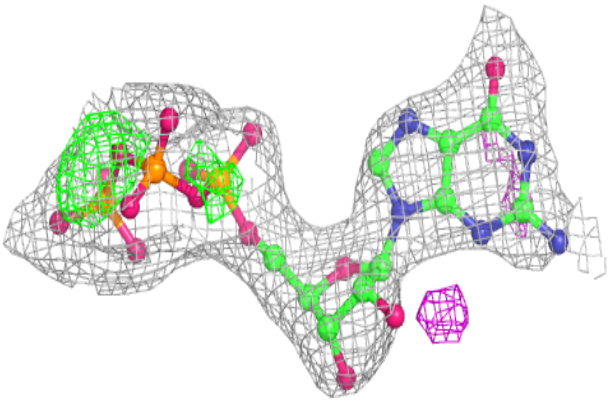


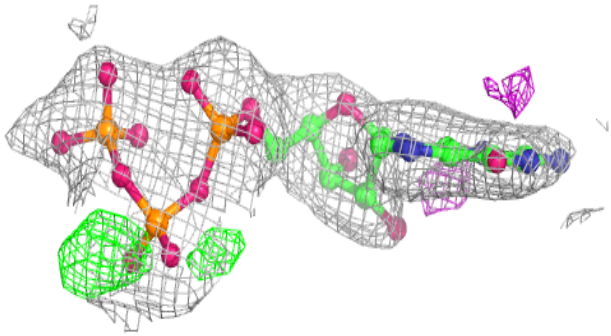


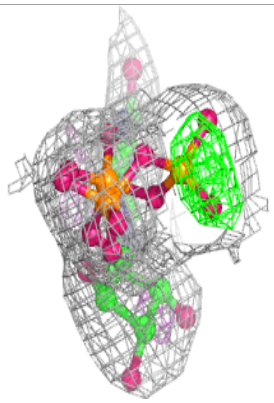


Electron density around GTP E 262:

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

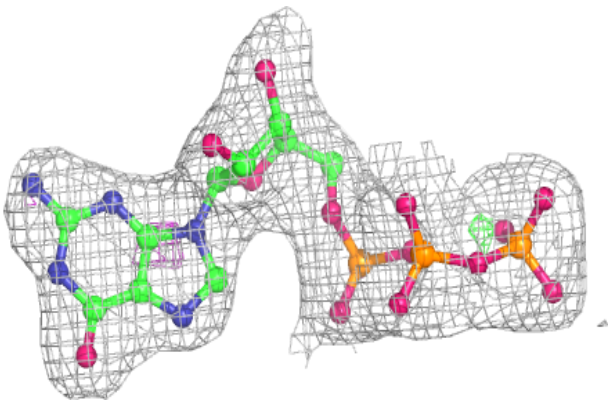


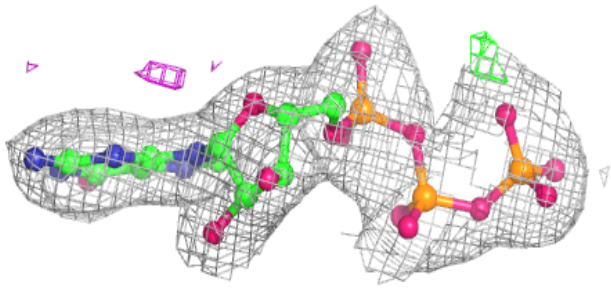


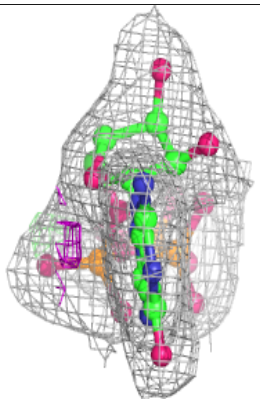


Electron density around GTP C 262:

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

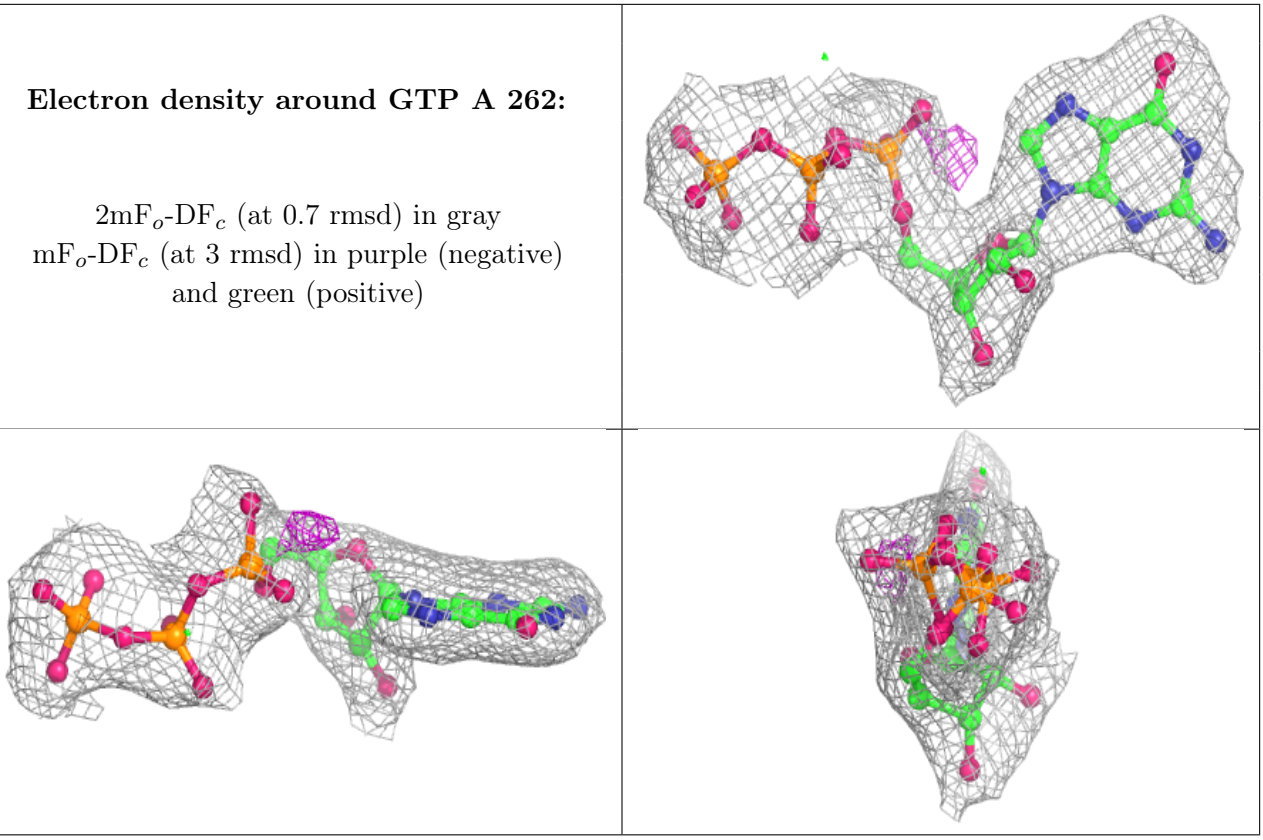






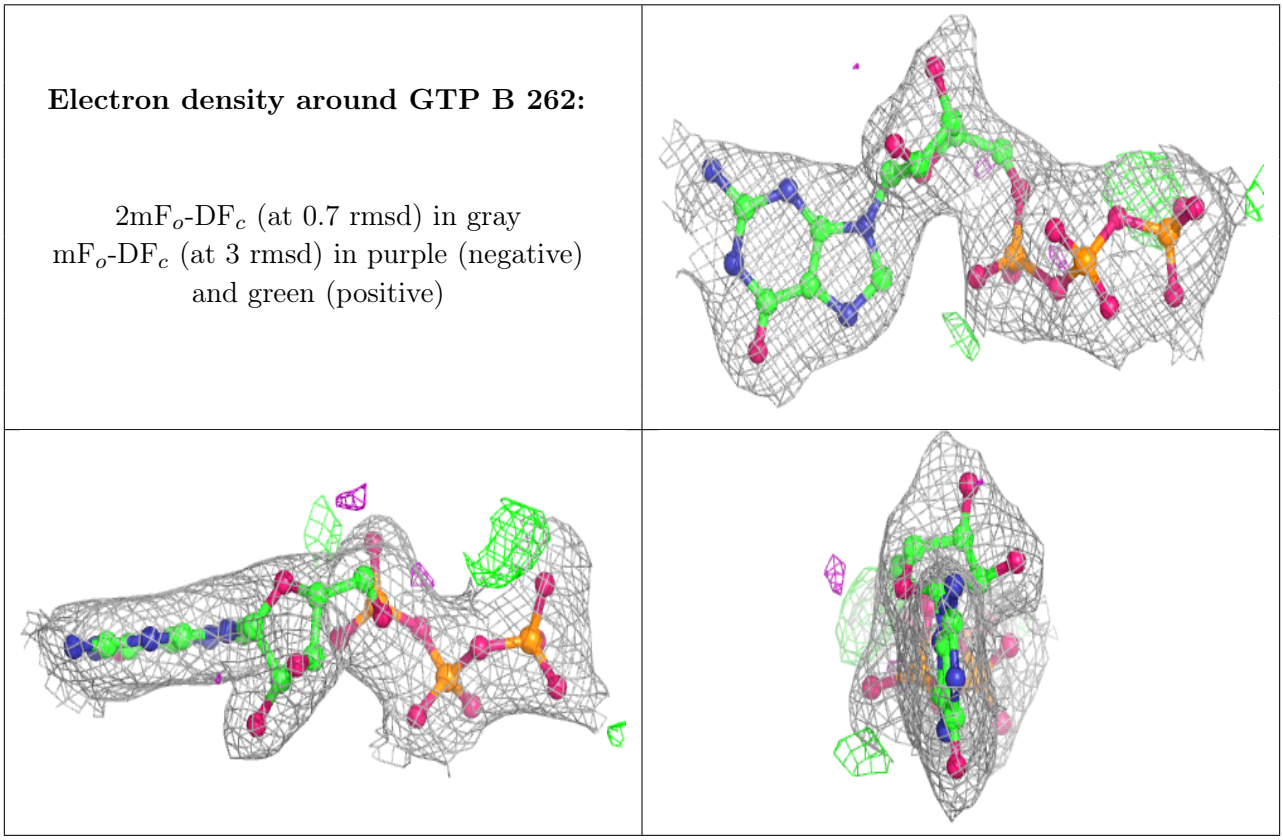
Electron density around GTP A 262:

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



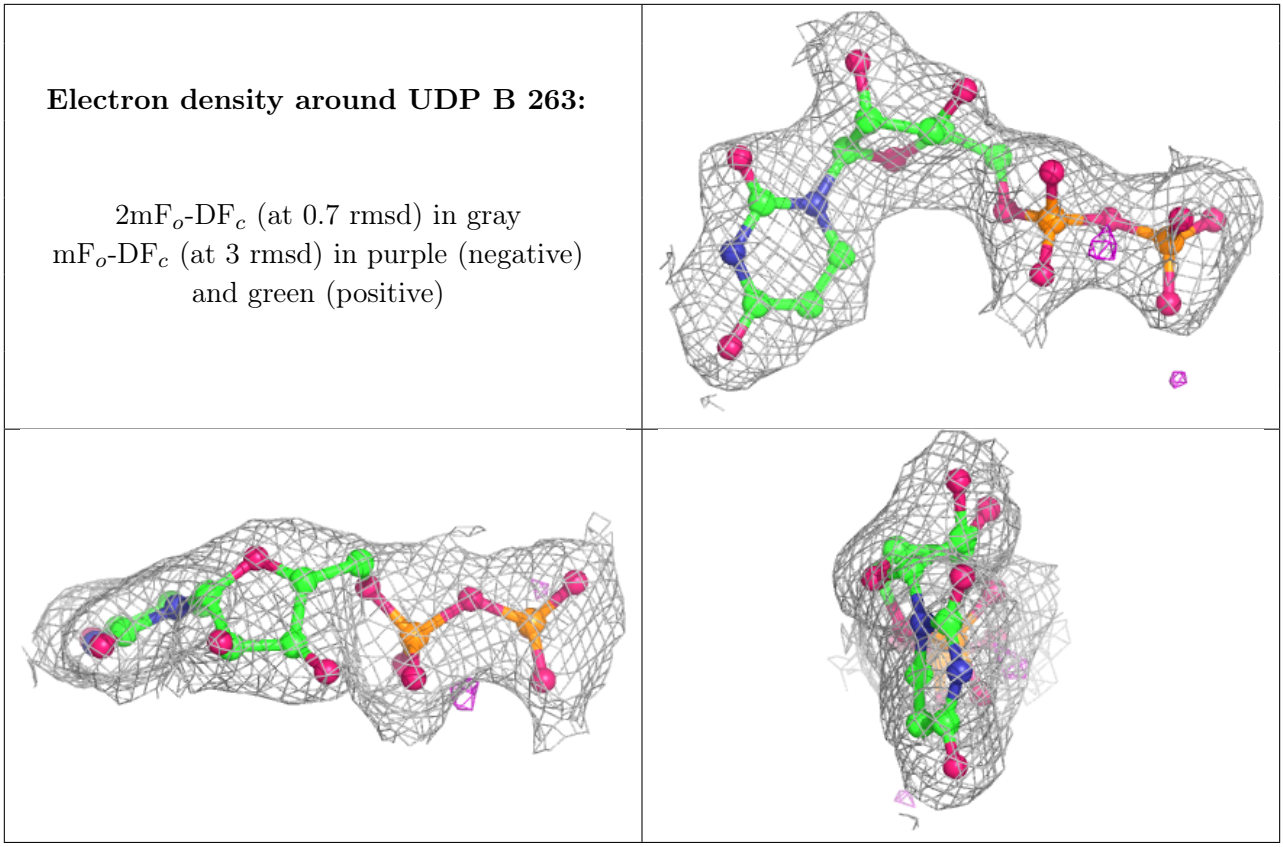
Electron density around GTP B 262:

$2mF_o$-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 263:

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



6.5 Other polymers (i)

There are no such residues in this entry.