



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:21 PM UTC

PDB ID : 5F9H / pdb_00005f9h
Title : Crystal structure of RIG-I helicase-RD in complex with 24-mer 5' triphosphate hairpin RNA
Authors : Wang, C.; Marcotrigiano, J.; Miller, M.; Jiang, F.
Deposited on : 2015-12-09
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

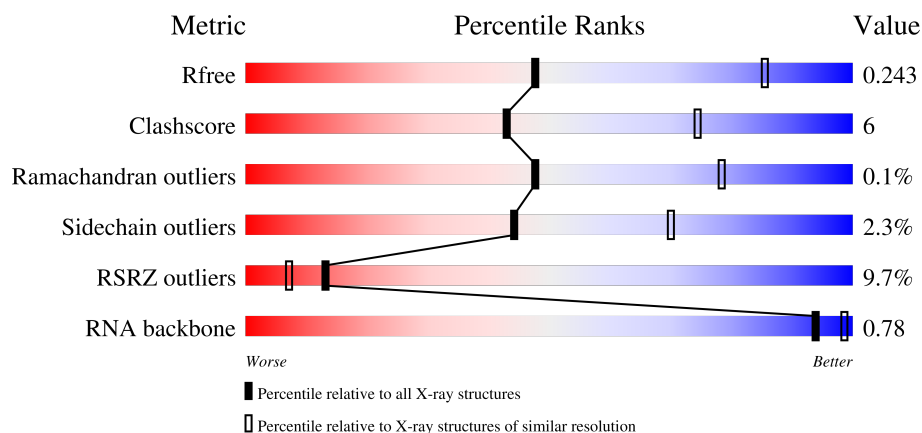
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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

Mol	Chain	Length	Quality of chain
1	A	695	 10% 78% 14% • 7%
1	C	695	 10% 81% 12% 7%
1	E	695	 8% 71% 18% • 8%
1	G	695	 6% 75% 17% • 6%

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Mol	Chain	Length	Quality of chain
1	I	695	
1	K	695	
2	B	23	
2	D	23	
2	F	23	
2	H	23	
2	J	23	
2	L	23	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33602 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 Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	646	Total	C	N	O	S	0	0	0
			5119	3272	865	951	31			
1	C	647	Total	C	N	O	S	0	0	0
			5083	3249	854	949	31			
1	E	638	Total	C	N	O	S	0	0	0
			5047	3234	847	935	31			
1	G	653	Total	C	N	O	S	0	0	0
			5168	3307	877	953	31			
1	I	644	Total	C	N	O	S	0	0	0
			5039	3229	846	932	32			
1	K	637	Total	C	N	O	S	0	0	0
			5024	3217	845	932	30			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	SER	-	expression tag	UNP O95786
C	231	SER	-	expression tag	UNP O95786
E	231	SER	-	expression tag	UNP O95786
G	231	SER	-	expression tag	UNP O95786
I	231	SER	-	expression tag	UNP O95786
K	231	SER	-	expression tag	UNP O95786

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	23	Total	C	N	O	P	0	0	0
			486	219	83	161	23			
2	D	23	Total	C	N	O	P	0	0	0
			486	219	83	161	23			
2	F	23	Total	C	N	O	P	0	0	0
			486	219	83	161	23			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	23	Total 486	C 219	N 83	O 161	P 23	0	0	0
2	J	23	Total 486	C 219	N 83	O 161	P 23	0	0	0
2	L	23	Total 486	C 219	N 83	O 161	P 23	0	0	0

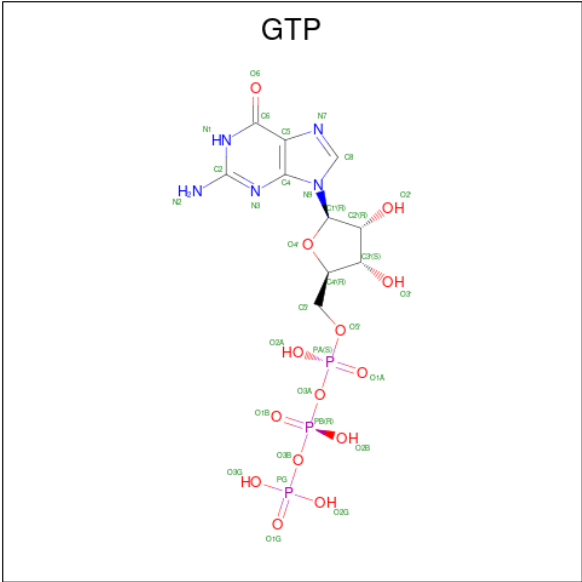
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	G	1	Total 1	Zn 1	0	0
3	I	1	Total 1	Zn 1	0	0
3	K	1	Total 1	Zn 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Mg 3	0	0
4	E	1	Total 1	Mg 1	0	0
4	G	2	Total 2	Mg 2	0	0
4	I	1	Total 1	Mg 1	0	0
4	K	1	Total 1	Mg 1	0	0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

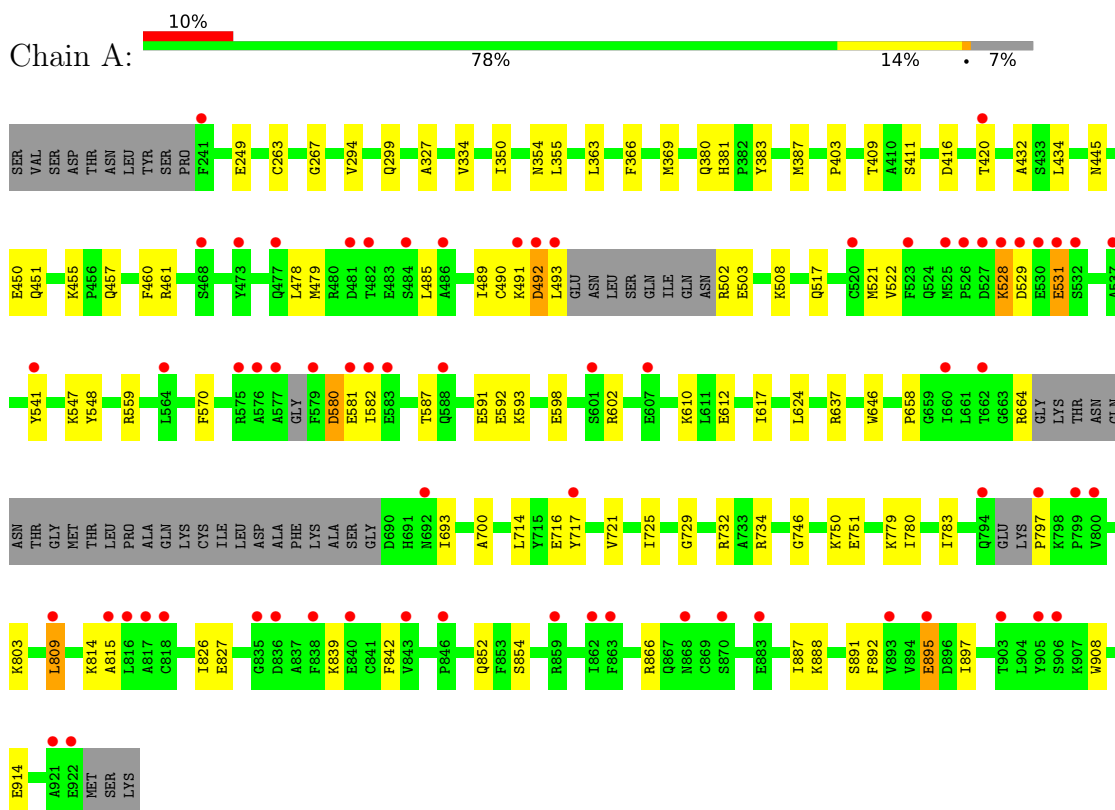


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	J	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	L	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

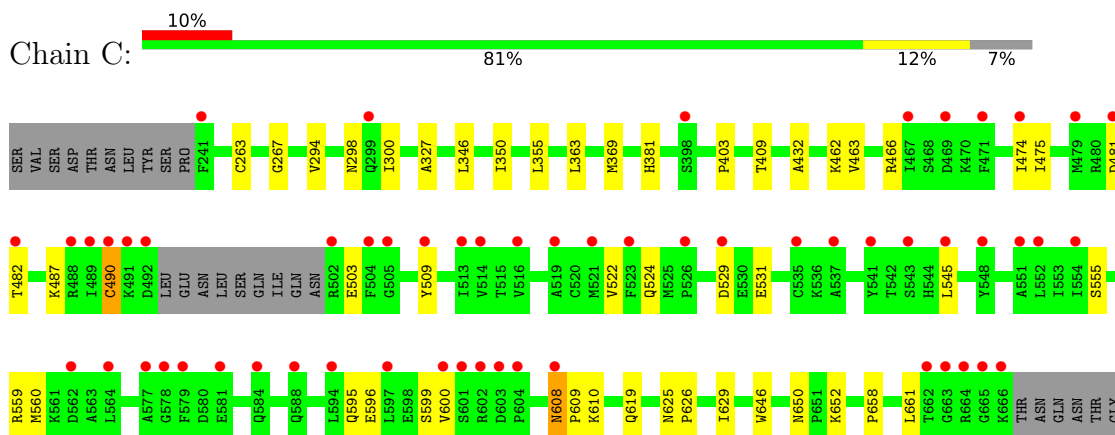
3 Residue-property plots [i](#)

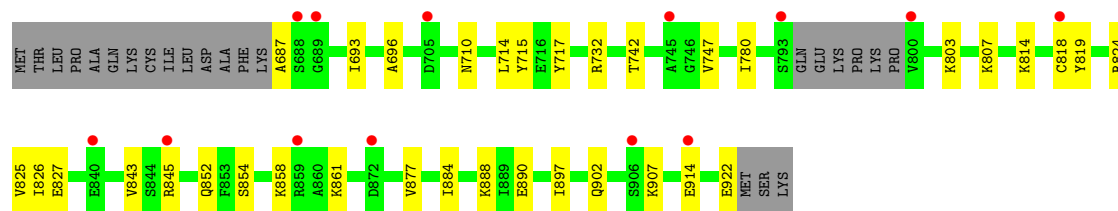
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Probable ATP-dependent RNA helicase DDX58

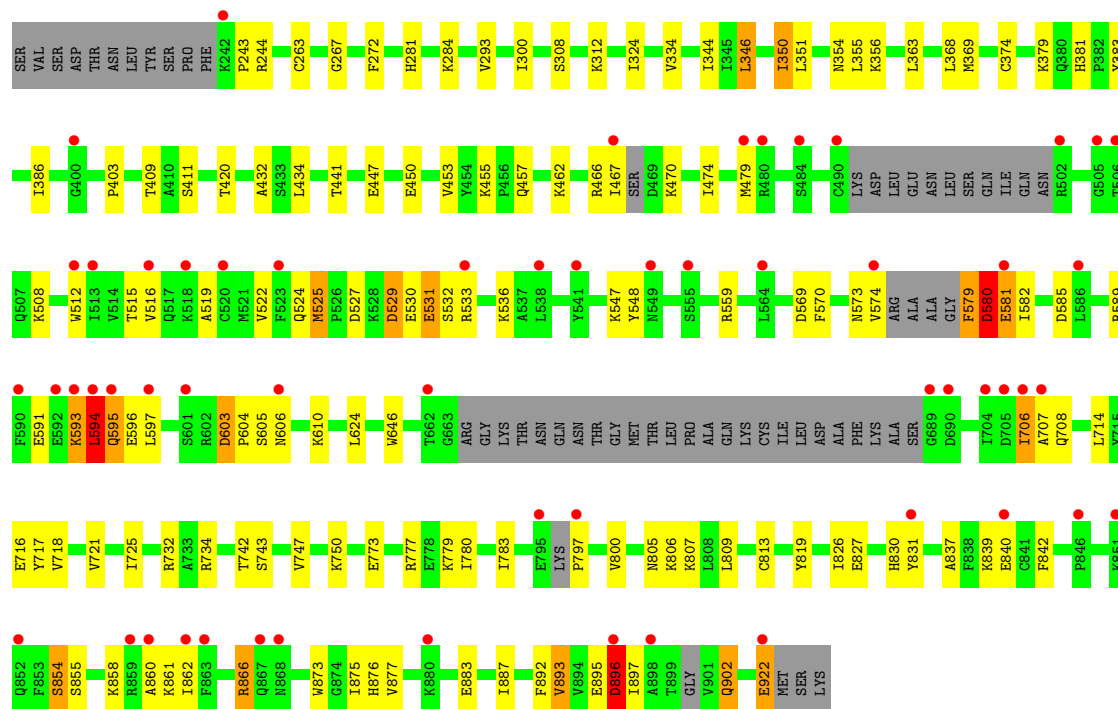
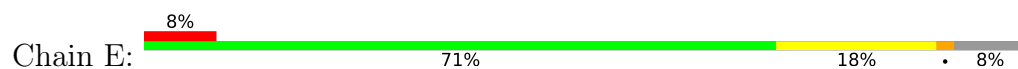


- Molecule 1: Probable ATP-dependent RNA helicase DDX58

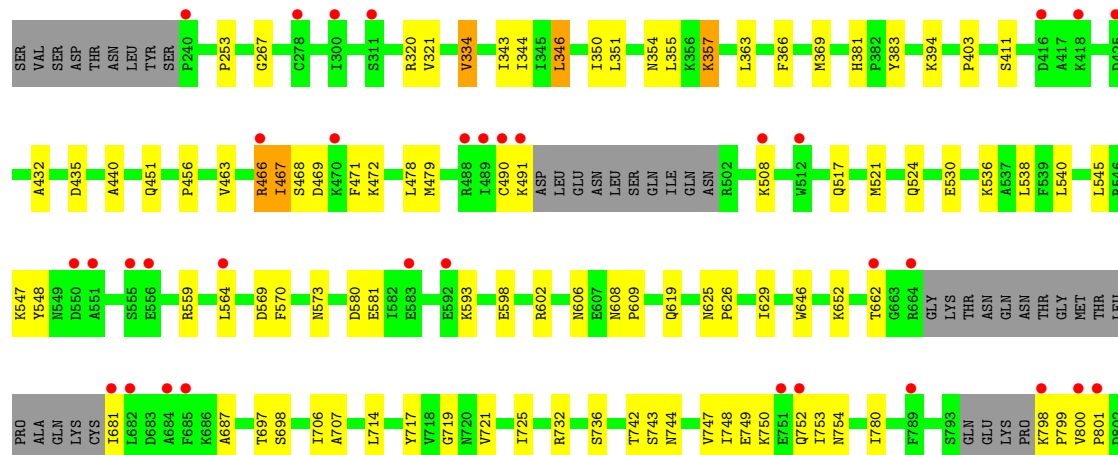
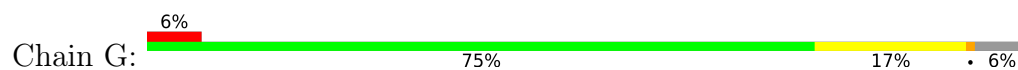


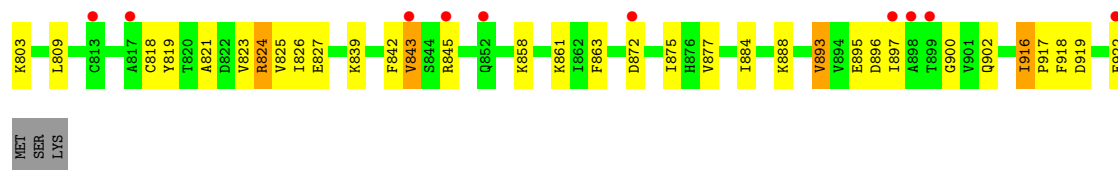


• Molecule 1: Probable ATP-dependent RNA helicase DDX58

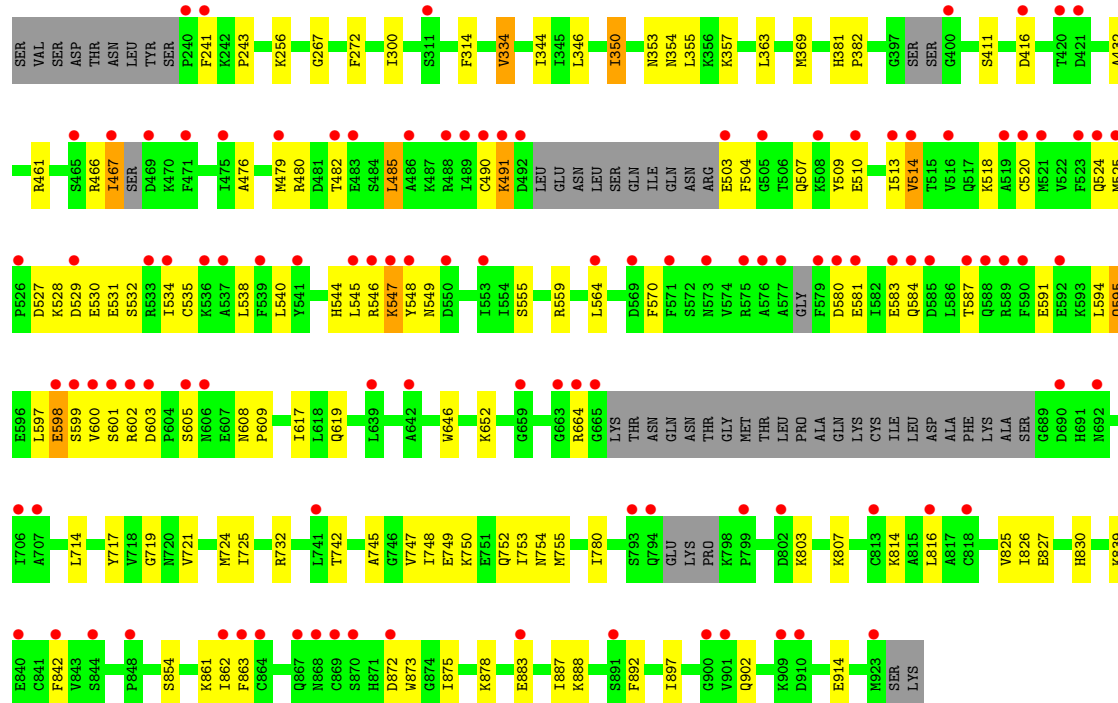
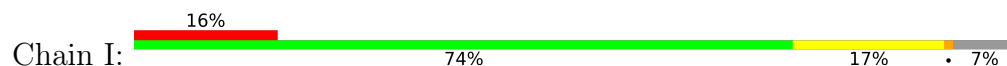


• Molecule 1: Probable ATP-dependent RNA helicase DDX58

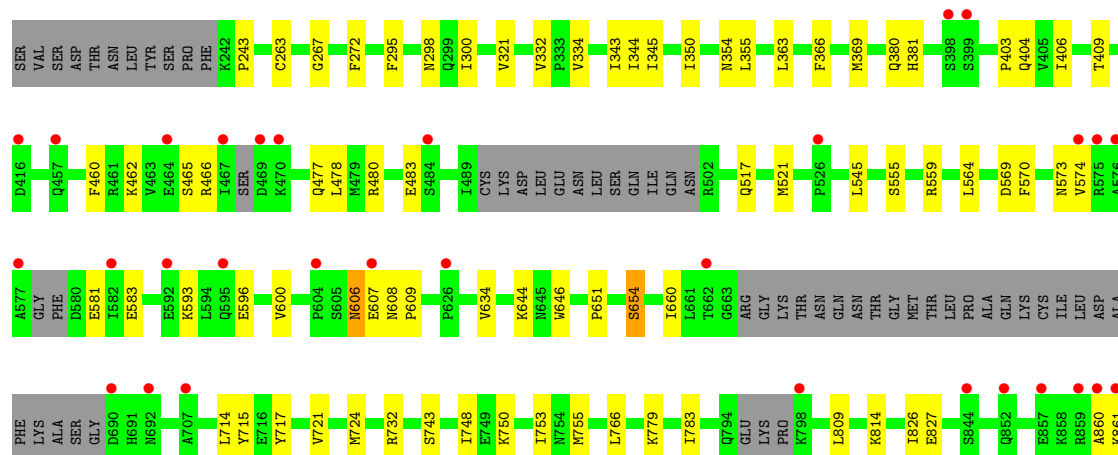
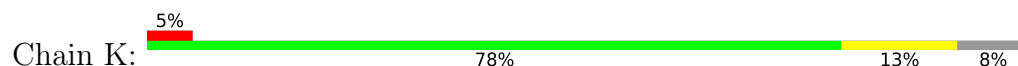




- Molecule 1: Probable ATP-dependent RNA helicase DDX58

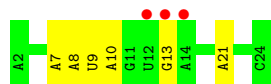
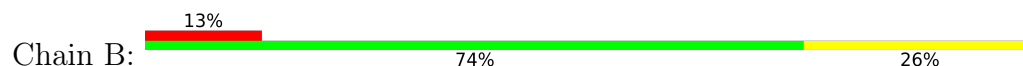


- Molecule 1: Probable ATP-dependent RNA helicase DDX58





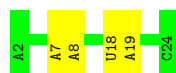
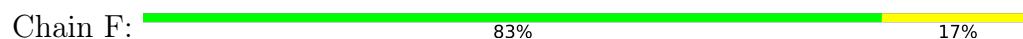
- Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3')



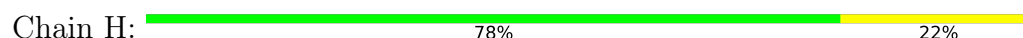
- Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3')



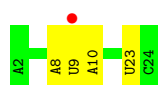
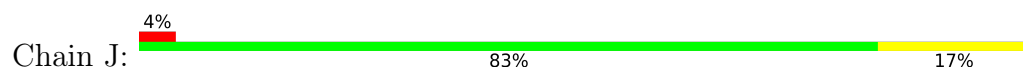
- Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3')



- Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3')



- Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3')



- Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3')



A2	U9	A10	G11	U12	G13	A14	U18	A19	C24
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.18Å 174.81Å 309.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.44 – 3.10 49.44 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.44-3.10) 93.1 (49.44-3.10)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1690	Depositor
R, R_{free}	0.213 , 0.266 (Not available) , 0.243	Depositor DCC
R_{free} test set	5452 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	33602	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GTP, MG

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	0.30	0/5220	0.73	3/7052 (0.0%)
1	C	0.31	0/5184	0.75	5/7008 (0.1%)
1	E	0.40	1/5148 (0.0%)	0.85	17/6957 (0.2%)
1	G	0.29	0/5273	0.73	1/7124 (0.0%)
1	I	0.33	1/5138 (0.0%)	0.77	8/6943 (0.1%)
1	K	0.30	0/5125	0.76	7/6930 (0.1%)
2	B	0.08	0/543	0.15	0/842
2	D	0.08	0/543	0.15	0/842
2	F	0.07	0/543	0.12	0/842
2	H	0.08	0/543	0.16	0/842
2	J	0.08	0/543	0.14	0/842
2	L	0.07	0/543	0.11	0/842
All	All	0.31	2/34346 (0.0%)	0.73	41/47066 (0.1%)

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	1
1	E	0	4
1	G	0	1
1	K	0	1
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	580	ASP	CA-C	8.15	1.63	1.52
1	I	595	GLN	C-O	5.10	1.29	1.24

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	896	ASP	N-CA-C	11.37	126.84	108.99
1	K	581	GLU	CB-CA-C	-8.65	106.59	116.54
1	E	596	GLU	N-CA-C	-8.58	101.84	111.71
1	E	595	GLN	N-CA-C	8.11	119.75	111.07
1	E	580	ASP	N-CA-C	7.89	127.61	110.80

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	580	ASP	Peptide
1	E	579	PHE	Peptide
1	E	580	ASP	Peptide
1	E	593	LYS	Peptide
1	E	896	ASP	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	5119	0	5077	60	0
1	C	5083	0	5012	43	0
1	E	5047	0	4975	91	0
1	G	5168	0	5132	79	0
1	I	5039	0	4966	78	0
1	K	5024	0	4950	52	0
2	B	486	0	244	4	0
2	D	486	0	244	1	0
2	F	486	0	244	3	0
2	H	486	0	244	3	0
2	J	486	0	244	4	0
2	L	486	0	244	5	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1	0	0	0	0
3	K	1	0	0	0	0
4	A	3	0	0	0	0
4	E	1	0	0	0	0
4	G	2	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	B	32	0	11	1	0
5	D	32	0	11	2	0
5	F	32	0	11	0	0
5	H	32	0	11	2	0
5	J	32	0	11	3	0
5	L	32	0	11	1	0
All	All	33602	0	31642	406	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 6.

The worst 5 of 406 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:E:594:LEU:O	1:E:597:LEU:HB2	1.80	0.81
1:K:466:ARG:NH2	1:K:555:SER:O	2.16	0.78
1:G:267:GLY:HA3	1:G:732:ARG:HD3	1.66	0.78
1:A:478:LEU:HD11	1:A:593:LYS:HG3	1.67	0.77
1:I:591:GLU:HA	1:I:594:LEU:HB2	1.69	0.74

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	636/695 (92%)	618 (97%)	18 (3%)	0	100	100
1	C	639/695 (92%)	621 (97%)	18 (3%)	0	100	100
1	E	624/695 (90%)	602 (96%)	19 (3%)	3 (0%)	24	57
1	G	645/695 (93%)	628 (97%)	16 (2%)	1 (0%)	43	73
1	I	630/695 (91%)	611 (97%)	19 (3%)	0	100	100
1	K	625/695 (90%)	607 (97%)	18 (3%)	0	100	100
All	All	3799/4170 (91%)	3687 (97%)	108 (3%)	4 (0%)	48	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	580	ASP
1	G	467	ILE
1	E	581	GLU
1	E	594	LEU

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	559/623 (90%)	544 (97%)	15 (3%)	39	67
1	C	551/623 (88%)	539 (98%)	12 (2%)	45	71
1	E	549/623 (88%)	531 (97%)	18 (3%)	33	63
1	G	562/623 (90%)	548 (98%)	14 (2%)	42	69
1	I	542/623 (87%)	532 (98%)	10 (2%)	51	73
1	K	545/623 (88%)	537 (98%)	8 (2%)	57	75
All	All	3308/3738 (88%)	3231 (98%)	77 (2%)	44	70

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	893	VAL

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Mol	Chain	Res	Type
1	K	545	LEU
1	I	256	LYS
1	I	547	LYS
1	K	766	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	511	GLN
1	I	349	GLN
1	G	549	ASN
1	G	902	GLN
1	I	619	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	22/23 (95%)	1 (4%)	0
2	D	22/23 (95%)	0	0
2	F	22/23 (95%)	0	0
2	H	22/23 (95%)	0	0
2	J	22/23 (95%)	0	0
2	L	22/23 (95%)	0	0
All	All	132/138 (95%)	1 (0%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	13	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 14 are monoatomic - leaving 6 for Mogul analysis.

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
5	GTP	H	101	2	33,34,34	0.95	1 (3%)	50,54,54	1.60	8 (16%)
5	GTP	L	101	2	33,34,34	0.95	1 (3%)	50,54,54	1.57	8 (16%)
5	GTP	D	101	2	33,34,34	0.96	1 (3%)	50,54,54	1.61	8 (16%)
5	GTP	F	101	2	33,34,34	0.96	1 (3%)	50,54,54	1.65	8 (16%)
5	GTP	J	101	2	33,34,34	1.02	2 (6%)	50,54,54	1.61	8 (16%)
5	GTP	B	101	2	33,34,34	1.02	3 (9%)	50,54,54	1.63	8 (16%)

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
5	GTP	H	101	2	-	5/22/38/38	0/3/3/3
5	GTP	L	101	2	-	7/22/38/38	0/3/3/3
5	GTP	D	101	2	-	5/22/38/38	0/3/3/3
5	GTP	F	101	2	-	8/22/38/38	0/3/3/3
5	GTP	J	101	2	-	5/22/38/38	0/3/3/3
5	GTP	B	101	2	-	11/22/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	101	GTP	PB-O3A	2.32	1.62	1.59
5	D	101	GTP	C2-N3	2.29	1.38	1.33
5	F	101	GTP	C2-N3	2.29	1.38	1.33
5	H	101	GTP	C2-N3	2.28	1.38	1.33
5	J	101	GTP	C2-N3	2.28	1.38	1.33

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	101	GTP	C5-C4-N3	-5.70	119.31	128.39
5	D	101	GTP	C5-C4-N3	-5.54	119.57	128.39
5	J	101	GTP	C5-C4-N3	-5.52	119.60	128.39
5	B	101	GTP	C5-C4-N3	-5.52	119.61	128.39
5	L	101	GTP	C5-C4-N3	-5.44	119.73	128.39

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	101	GTP	C5'-O5'-PA-O3A
5	B	101	GTP	C5'-O5'-PA-O1A
5	D	101	GTP	C5'-O5'-PA-O3A
5	D	101	GTP	C5'-O5'-PA-O1A
5	D	101	GTP	C5'-O5'-PA-O2A

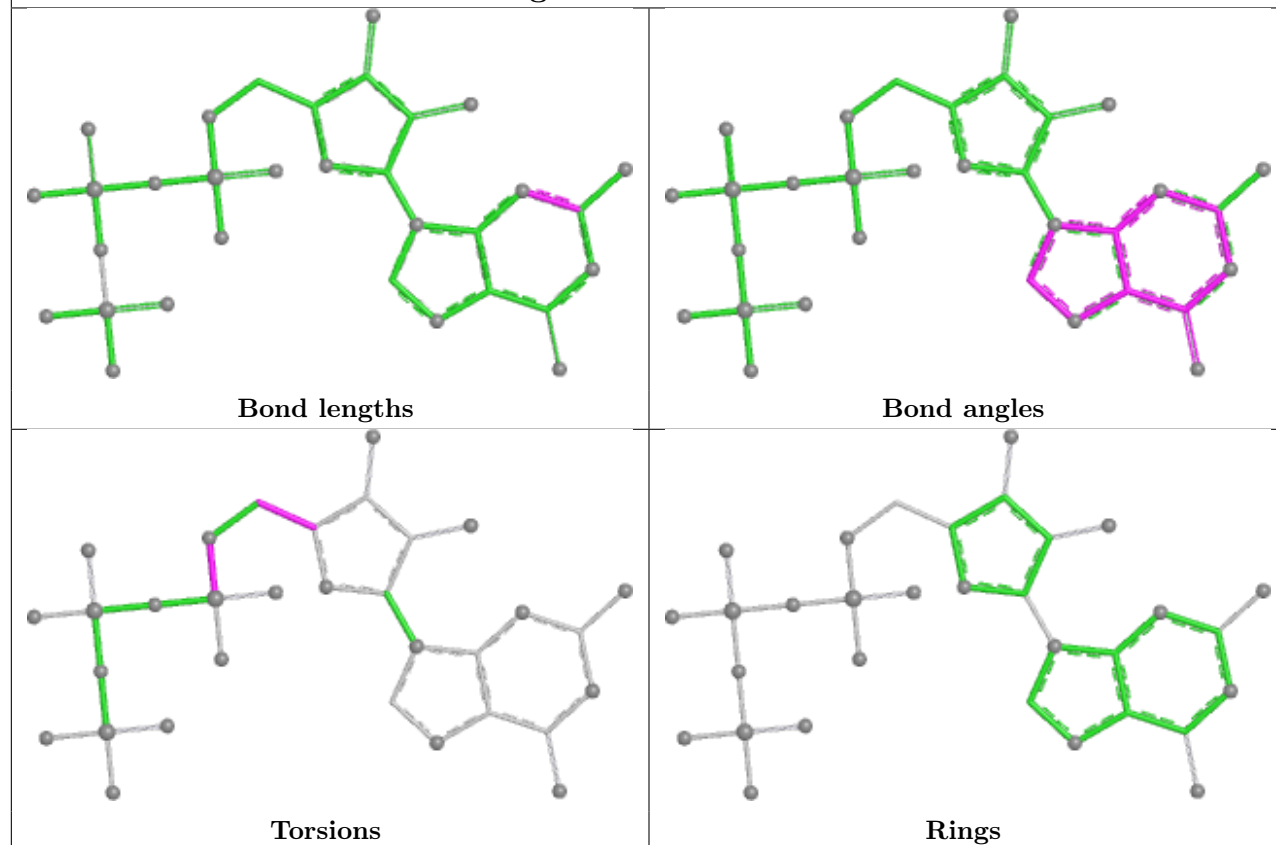
There are no ring outliers.

5 monomers are involved in 9 short contacts:

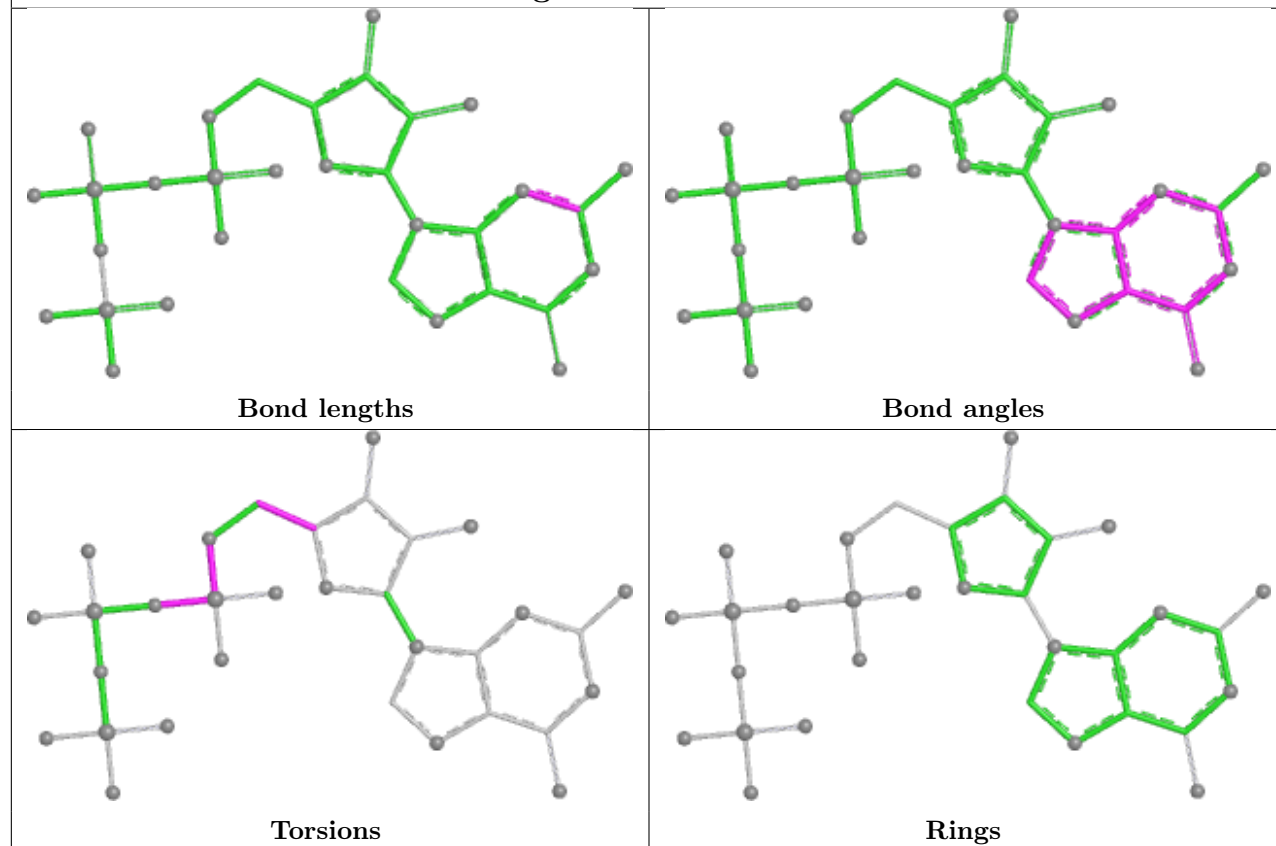
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	101	GTP	2	0
5	L	101	GTP	1	0
5	D	101	GTP	2	0
5	J	101	GTP	3	0
5	B	101	GTP	1	0

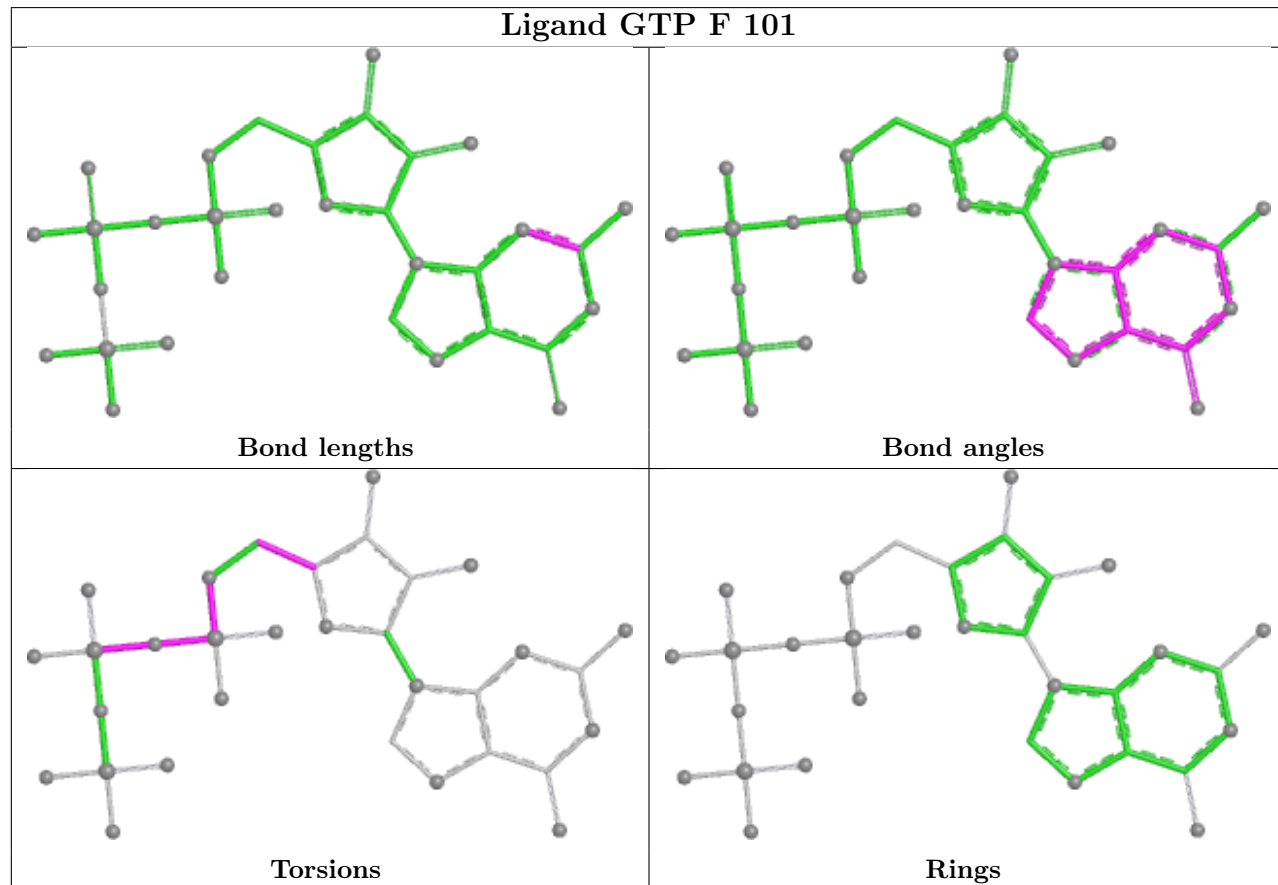
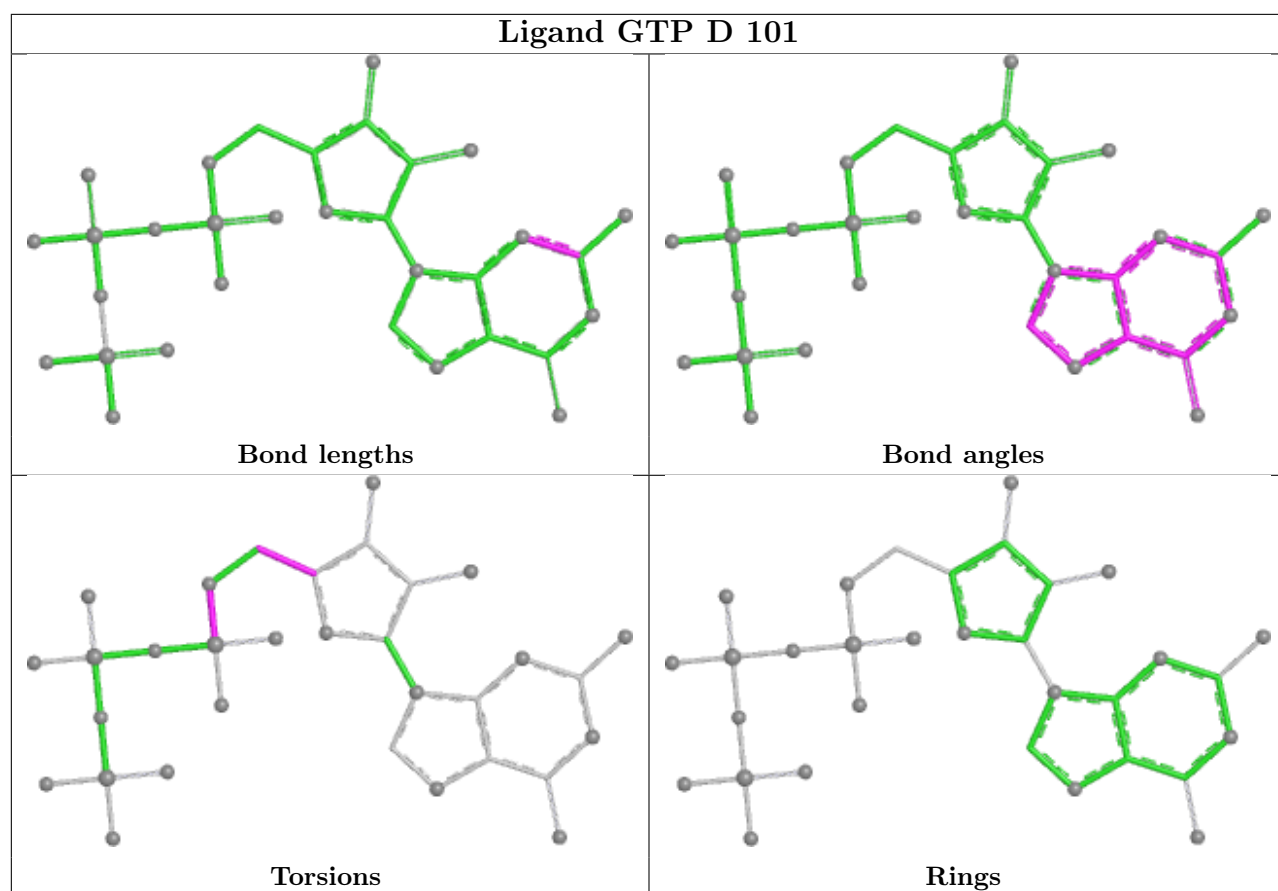
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand GTP H 101

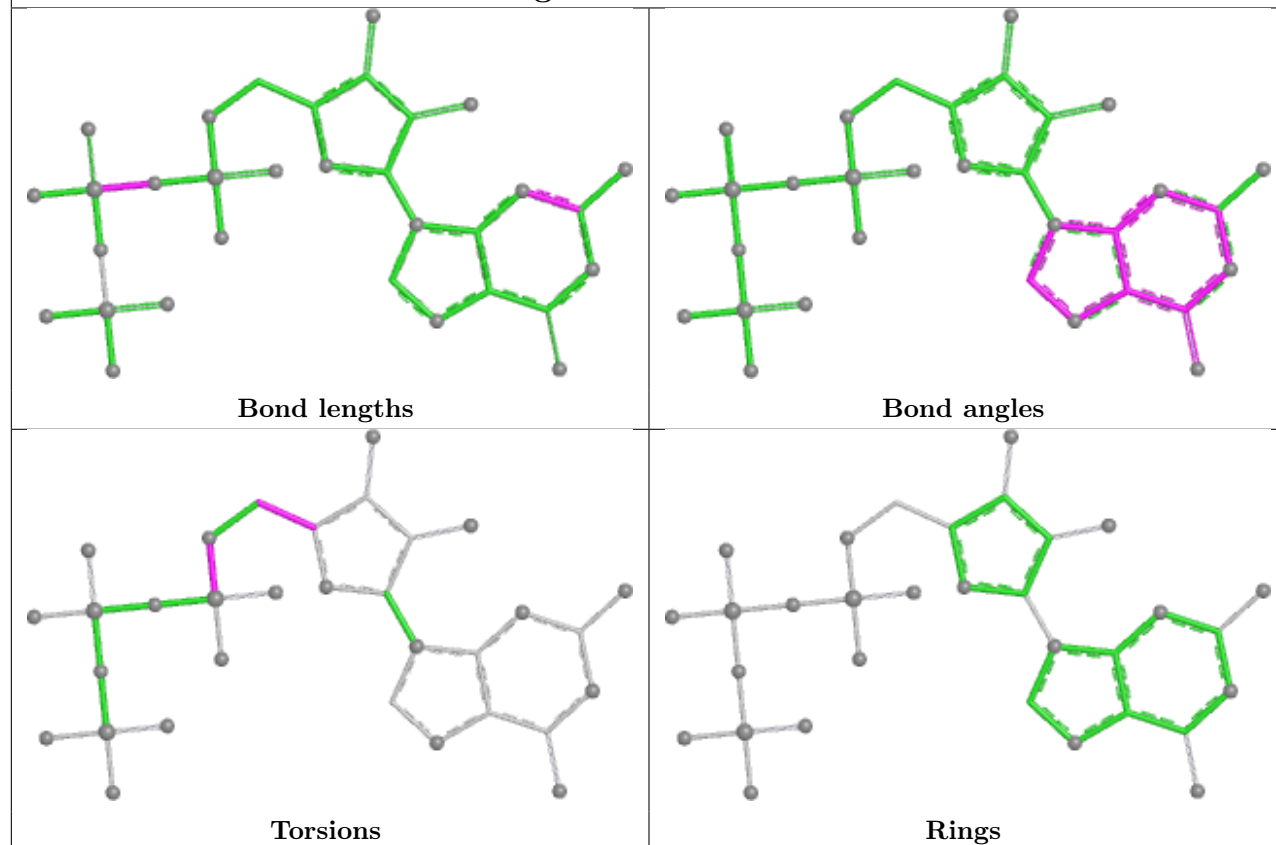


Ligand GTP L 101

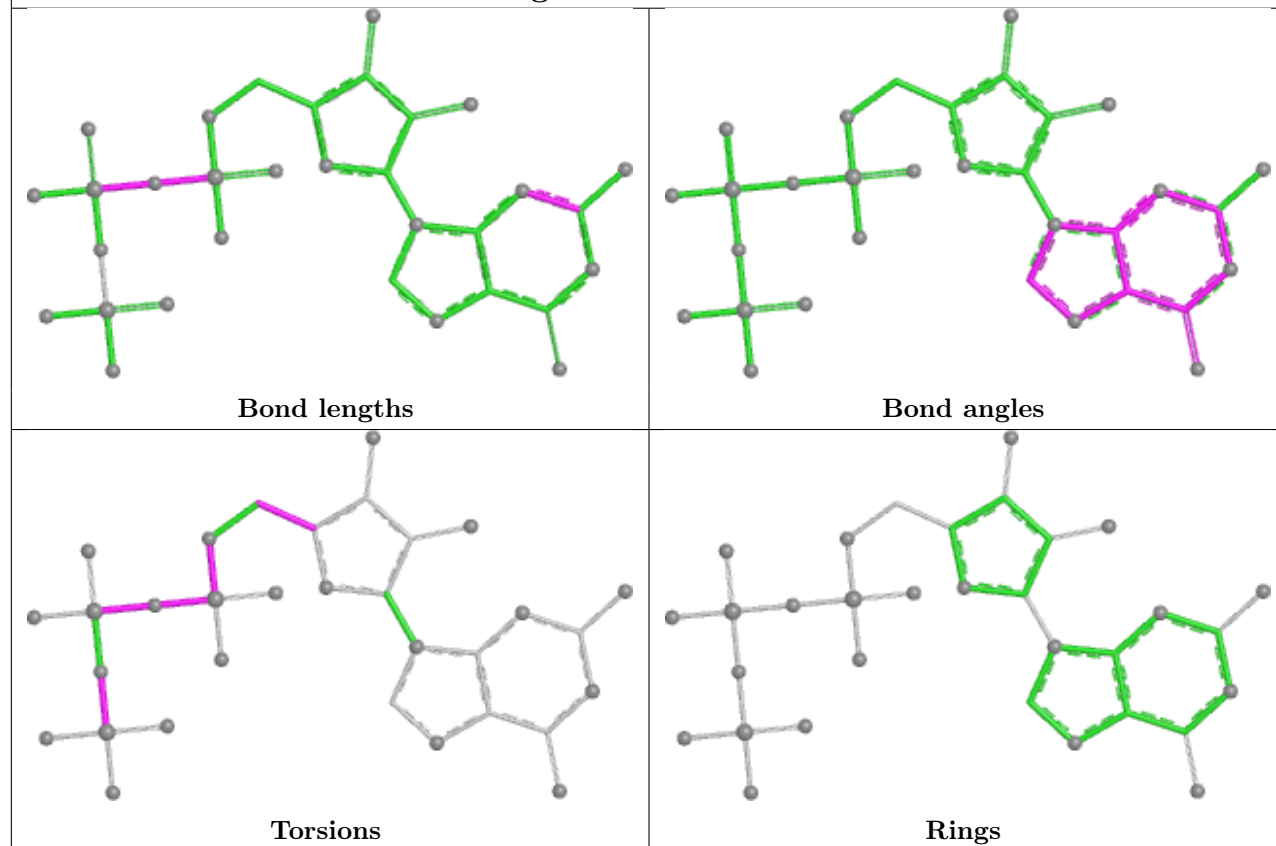




Ligand GTP J 101



Ligand GTP B 101



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	646/695 (92%)	0.55	67 (10%) 11 6	23, 53, 121, 244	0
1	C	647/695 (93%)	0.64	70 (10%) 11 6	25, 56, 126, 229	0
1	E	638/695 (91%)	0.67	57 (8%) 15 8	33, 59, 133, 252	0
1	G	653/695 (93%)	0.69	44 (6%) 24 13	34, 61, 108, 186	0
1	I	644/695 (92%)	0.96	111 (17%) 4 2	34, 63, 151, 267	0
1	K	637/695 (91%)	0.49	37 (5%) 29 16	30, 58, 115, 220	0
2	B	23/23 (100%)	0.25	3 (13%) 7 4	32, 47, 158, 204	0
2	D	23/23 (100%)	0.16	0 100 100	32, 48, 135, 159	0
2	F	23/23 (100%)	-0.13	0 100 100	40, 47, 117, 132	0
2	H	23/23 (100%)	0.52	0 100 100	36, 58, 138, 154	0
2	J	23/23 (100%)	0.39	1 (4%) 40 22	35, 55, 133, 159	0
2	L	23/23 (100%)	-0.17	0 100 100	37, 49, 133, 169	0
All	All	4003/4308 (92%)	0.65	390 (9%) 13 7	23, 59, 130, 267	0

The worst 5 of 390 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	471	PHE	6.0
1	K	577	ALA	5.3
1	C	579	PHE	5.3
1	A	662	THR	5.2
1	G	685	PHE	5.2

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

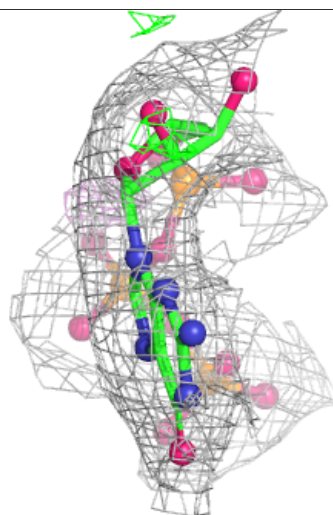
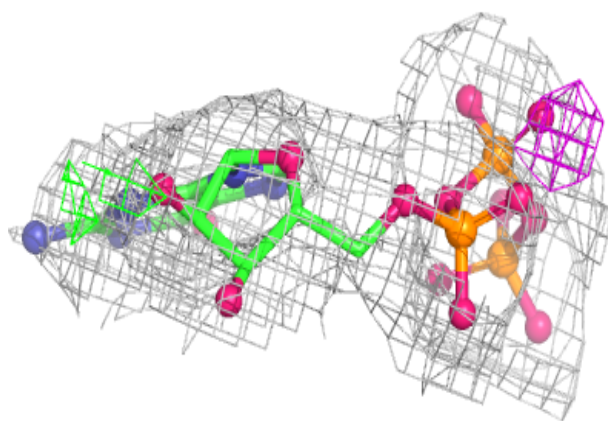
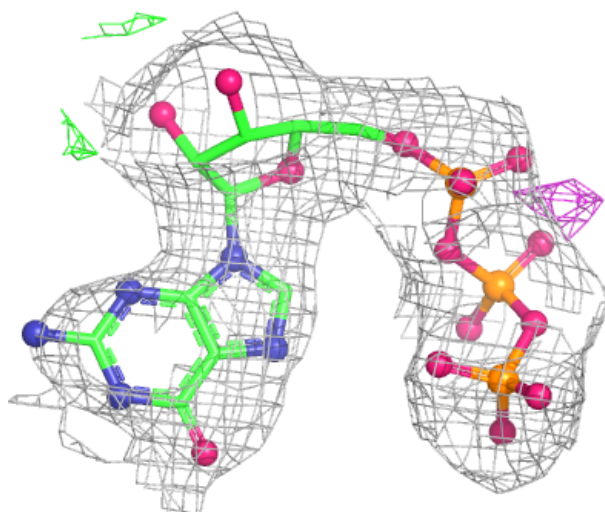
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	G	1002	1/1	0.88	0.10	24,24,24,24	0
5	GTP	F	101	32/32	0.90	0.11	36,60,84,88	0
4	MG	A	1003	1/1	0.91	0.13	56,56,56,56	0
5	GTP	B	101	32/32	0.92	0.10	33,47,88,95	0
5	GTP	H	101	32/32	0.93	0.09	22,44,88,90	0
5	GTP	L	101	32/32	0.93	0.09	27,56,96,105	0
4	MG	K	1002	1/1	0.94	0.06	39,39,39,39	0
5	GTP	D	101	32/32	0.95	0.09	4,45,89,97	0
5	GTP	J	101	32/32	0.95	0.09	11,44,98,125	0
3	ZN	I	1001	1/1	0.95	0.08	74,74,74,74	0
3	ZN	E	1001	1/1	0.96	0.07	82,82,82,82	0
4	MG	I	1002	1/1	0.96	0.06	13,13,13,13	0
4	MG	A	1004	1/1	0.96	0.11	50,50,50,50	0
4	MG	E	1002	1/1	0.97	0.06	46,46,46,46	0
4	MG	G	1003	1/1	0.97	0.13	25,25,25,25	0
3	ZN	A	1001	1/1	0.98	0.03	75,75,75,75	0
4	MG	A	1002	1/1	0.98	0.04	28,28,28,28	0
3	ZN	G	1001	1/1	0.98	0.04	77,77,77,77	0
3	ZN	C	1001	1/1	0.99	0.04	74,74,74,74	0
3	ZN	K	1001	1/1	0.99	0.04	75,75,75,75	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.

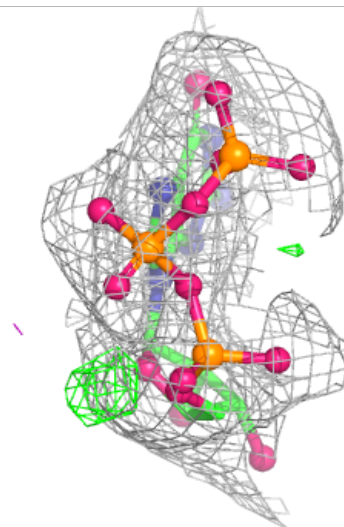
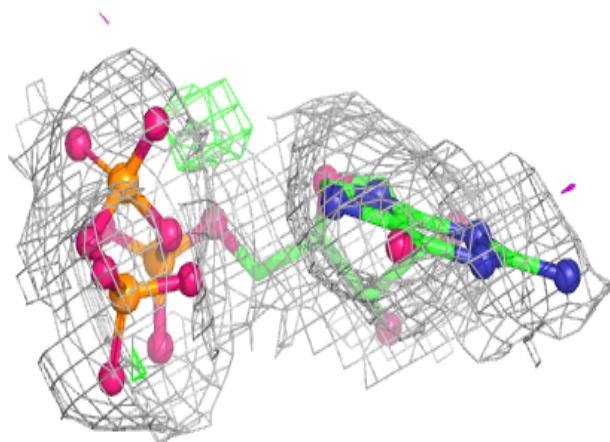
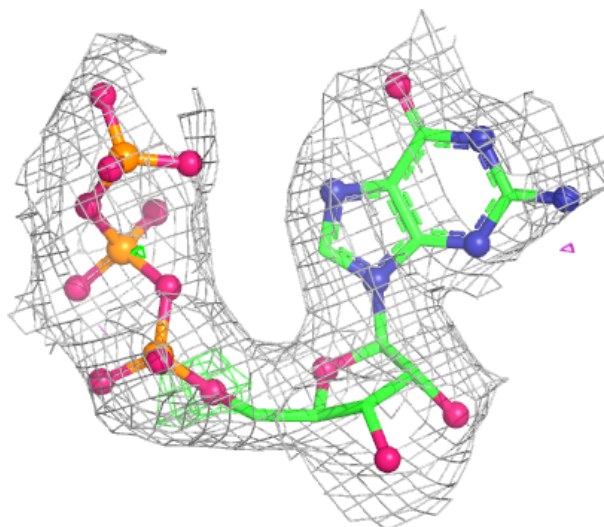
Electron density around GTP F 101:

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



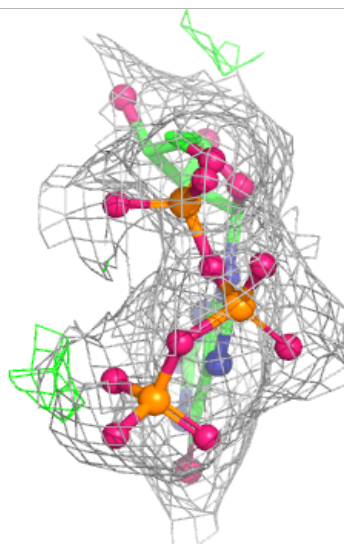
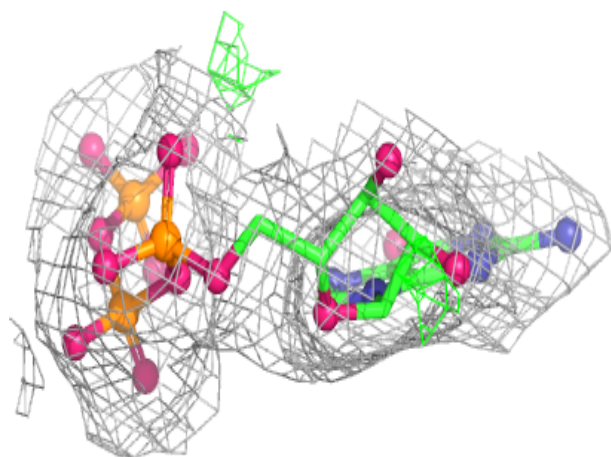
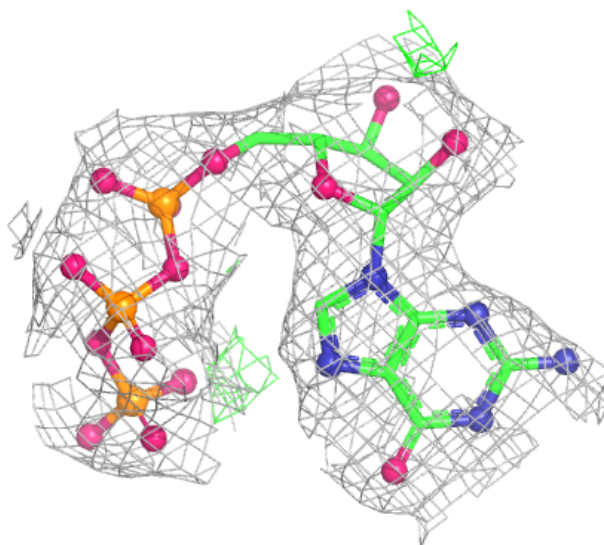
Electron density around GTP B 101:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



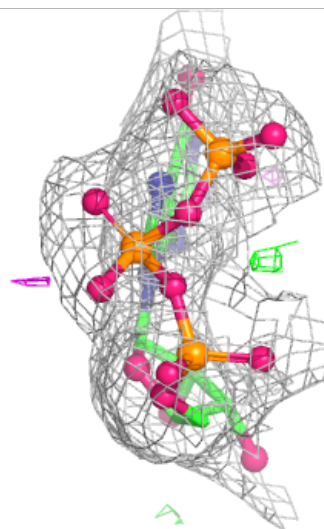
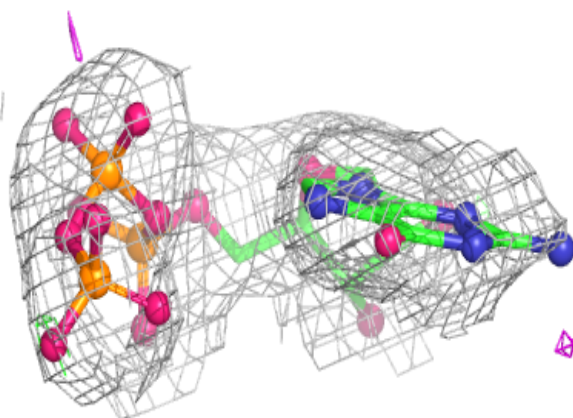
Electron density around GTP H 101:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



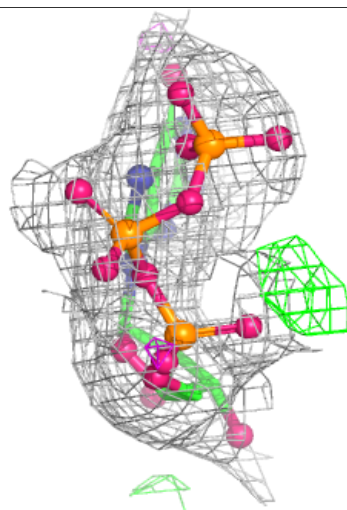
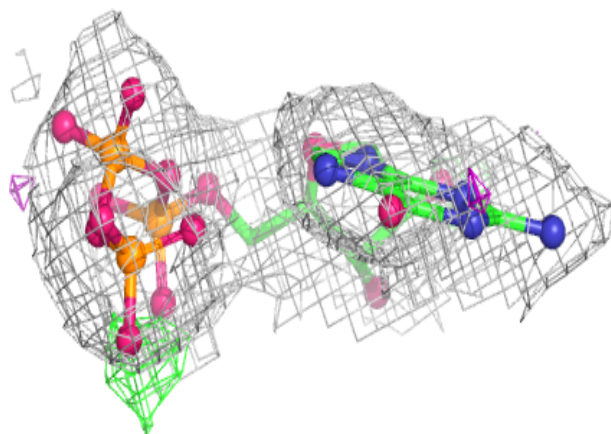
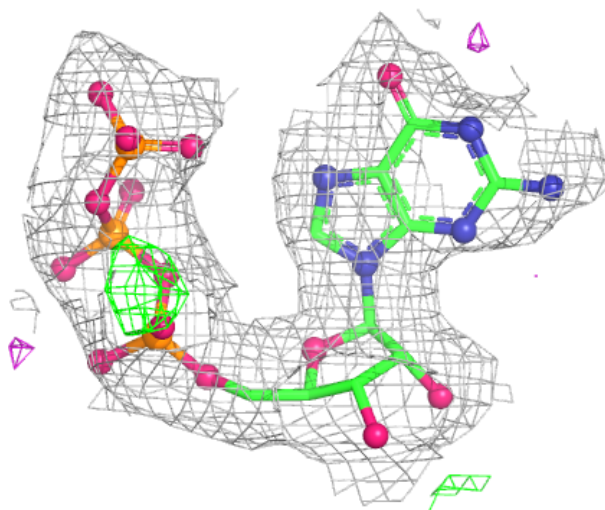
Electron density around GTP L 101:

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and green (positive)



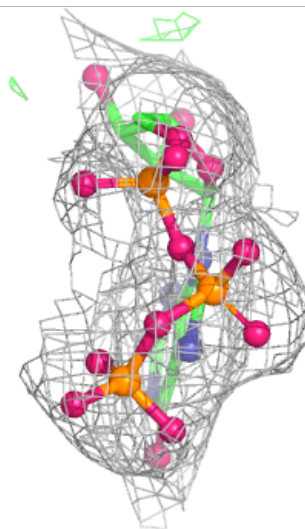
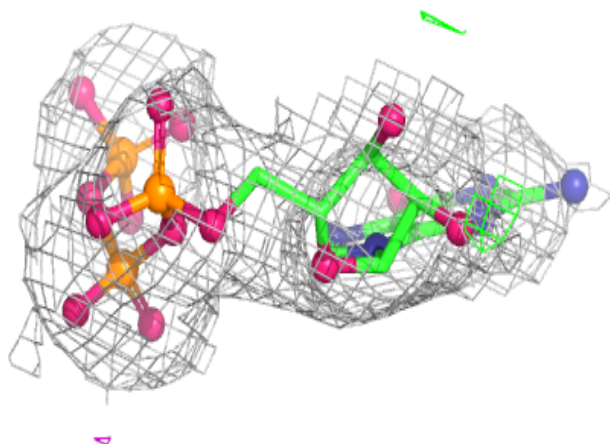
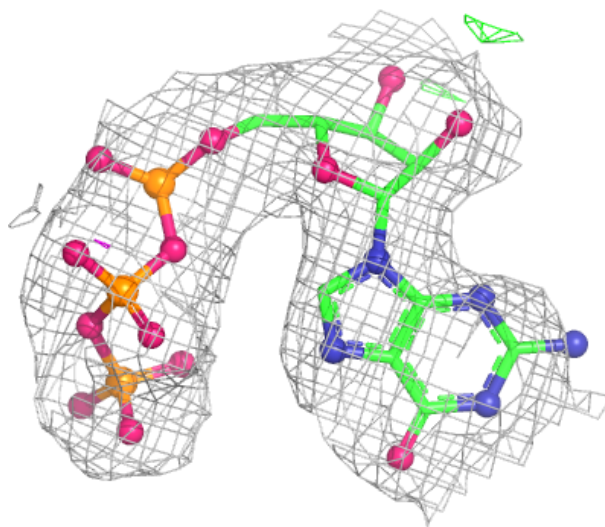
Electron density around GTP D 101:

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and green (positive)



Electron density around GTP J 101:

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.