



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:26 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

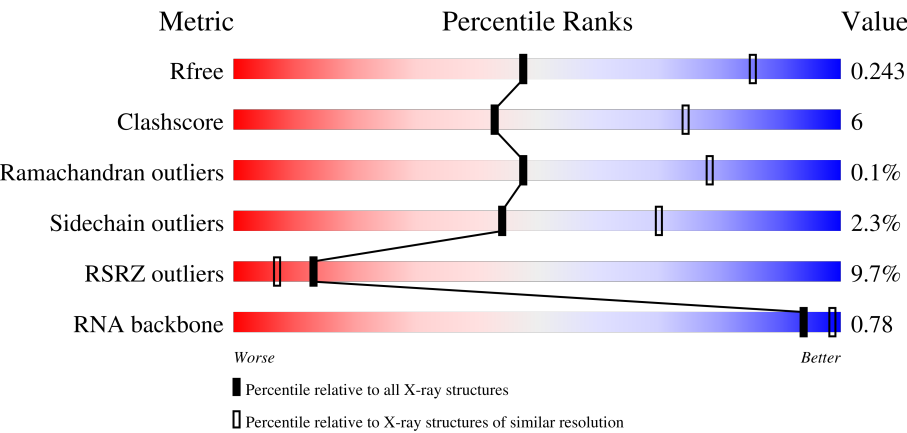
1 Overall quality at a glance i

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

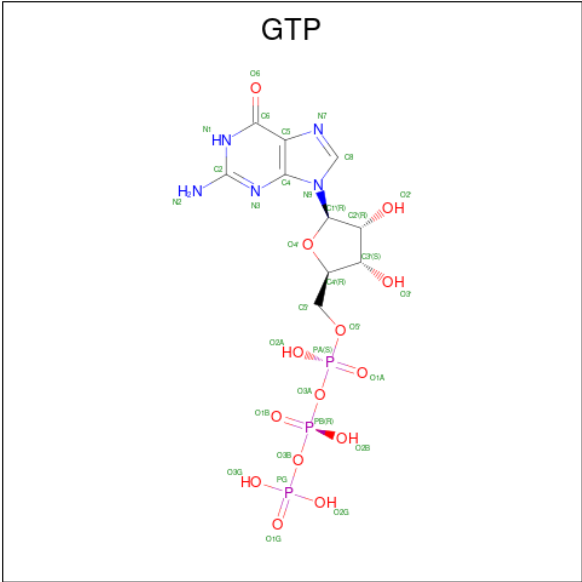
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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).

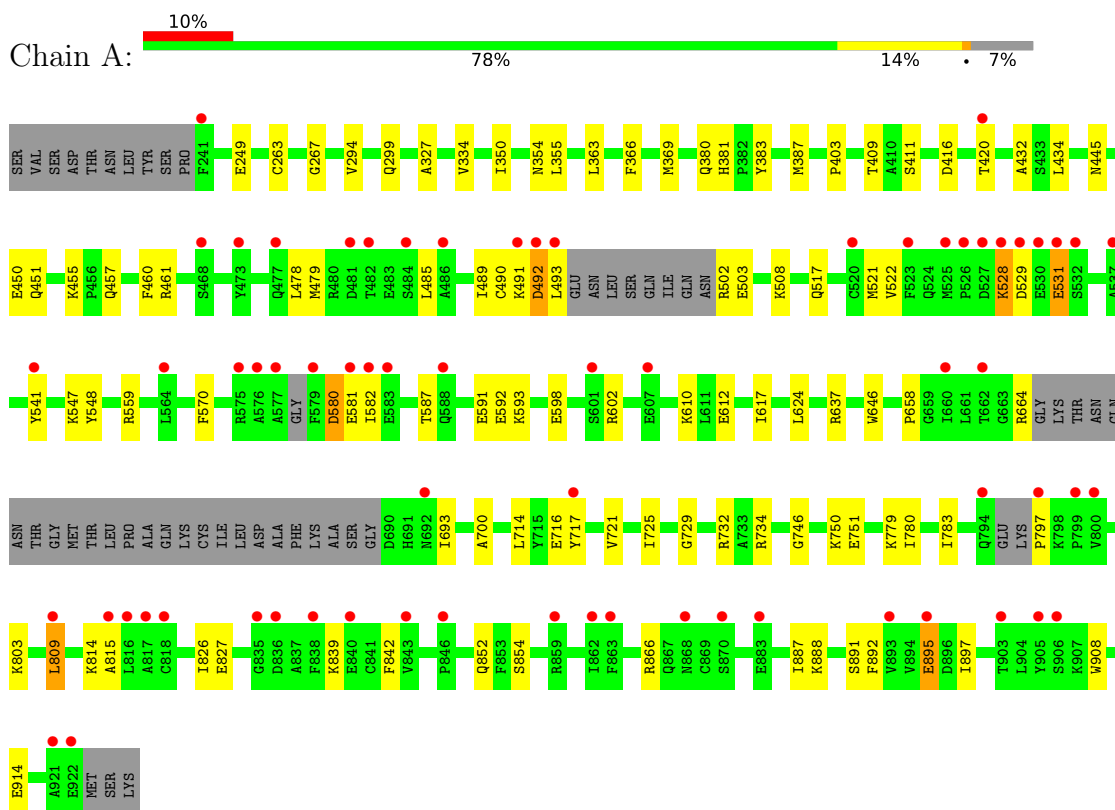


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	J	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	L	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

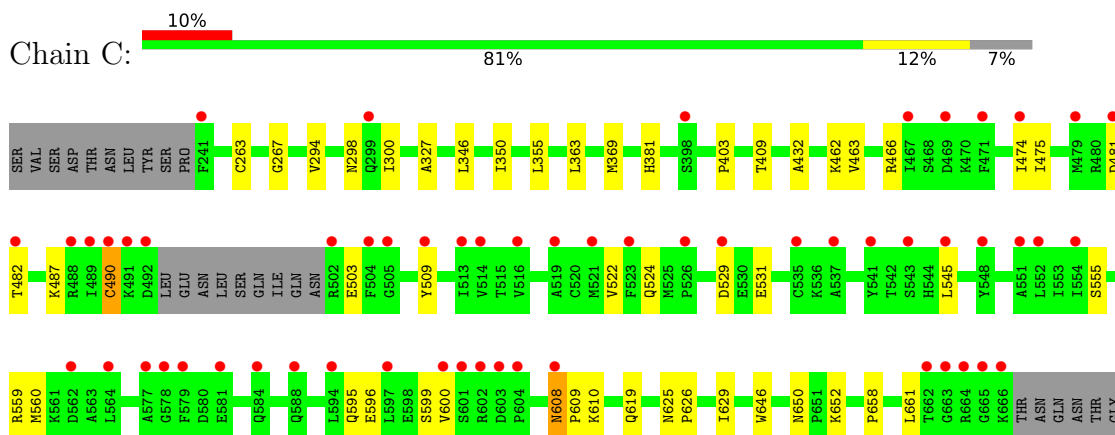
3 Residue-property plots [i](#)

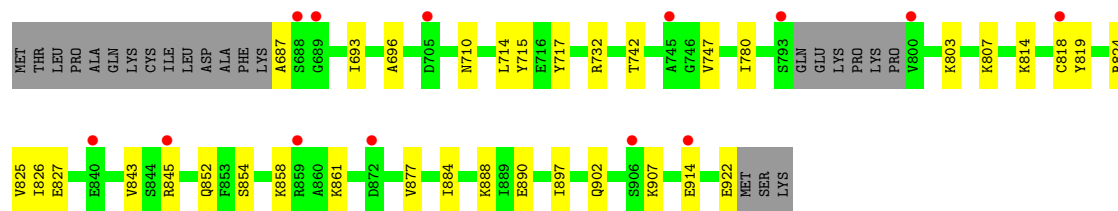
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

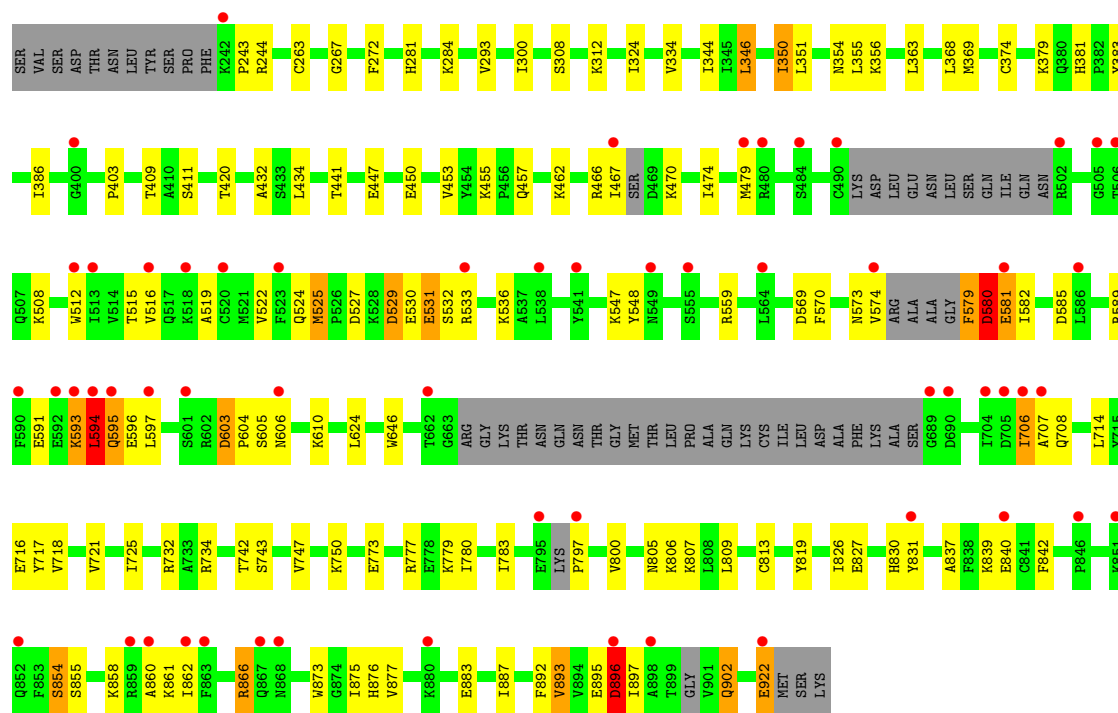
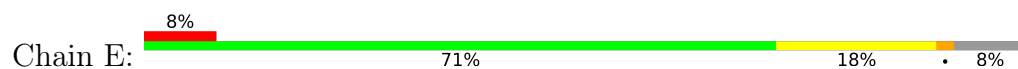


- Molecule 1: Probable ATP-dependent RNA helicase DDX58

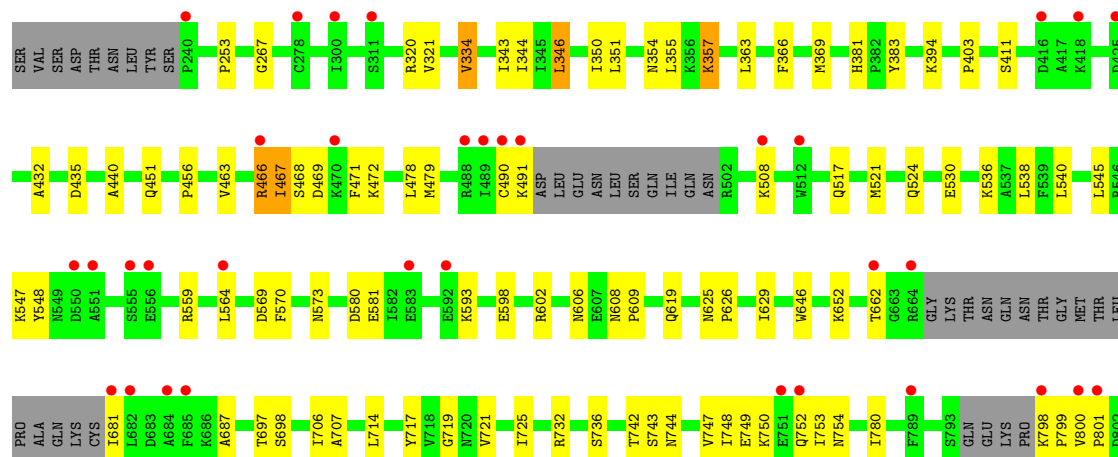
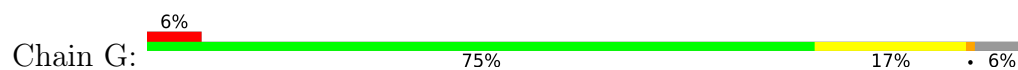


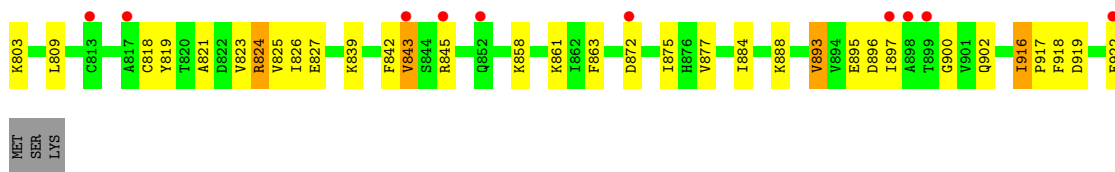


● Molecule 1: Probable ATP-dependent RNA helicase DDX58

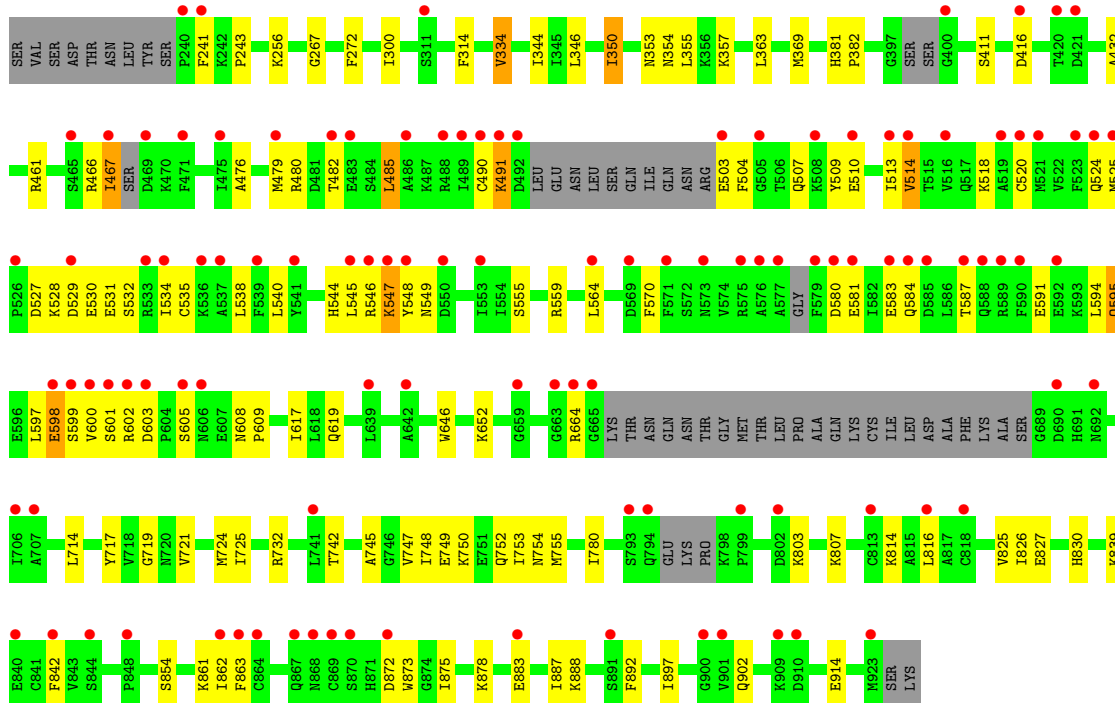
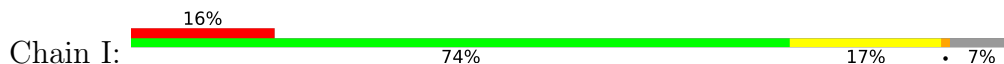


● Molecule 1: Probable ATP-dependent RNA helicase DDX58

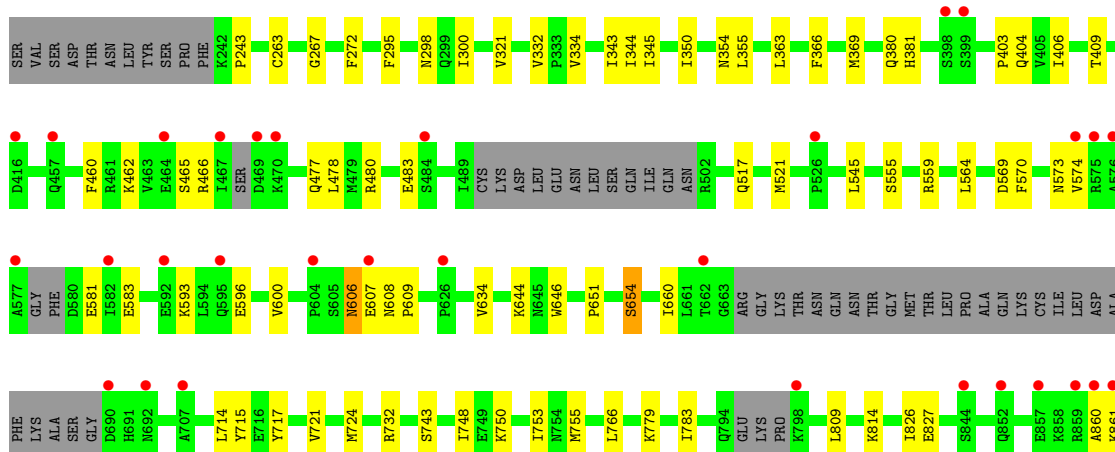
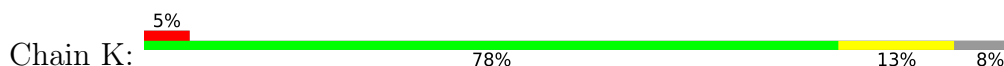




- Molecule 1: Probable ATP-dependent RNA helicase DDX58

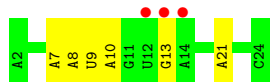
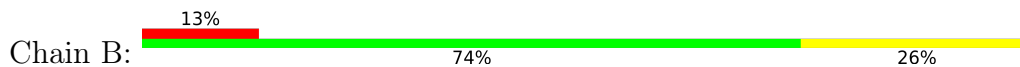


- Molecule 1: Probable ATP-dependent RNA helicase DDX58





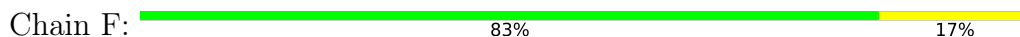
- Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*U
P*UP*AP*UP*AP*UP*UP*C)-3')



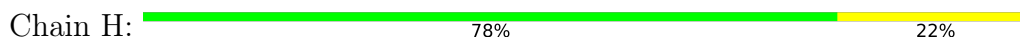
- Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*U
P*UP*AP*UP*AP*UP*UP*C)-3')



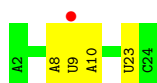
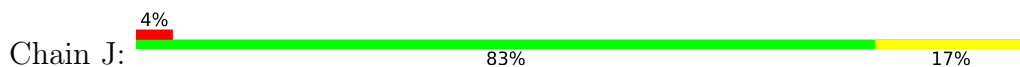
- Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*U
P*UP*AP*UP*AP*UP*UP*C)-3')



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





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

All (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
1	E	581	GLU	N-CA-C	6.98	125.66	110.80
1	A	797	PRO	N-CA-CB	6.74	110.42	103.00
1	E	797	PRO	N-CA-CB	6.72	110.40	103.00
1	I	598	GLU	CA-C-N	-6.65	111.57	122.54
1	I	598	GLU	C-N-CA	-6.65	111.57	122.54
1	A	492	ASP	CB-CA-C	-6.28	108.69	117.23
1	K	607	GLU	N-CA-C	6.23	119.29	110.50
1	E	603	ASP	CA-C-N	6.08	125.96	119.28
1	E	603	ASP	C-N-CA	6.08	125.96	119.28
1	C	608	ASN	CA-C-N	6.01	126.17	119.32
1	C	608	ASN	C-N-CA	6.01	126.17	119.32
1	K	867	GLN	CB-CA-C	-5.92	109.73	116.54
1	I	600	VAL	N-CA-C	-5.89	103.69	111.05
1	E	525	MET	CA-C-N	5.61	125.71	119.32
1	E	525	MET	C-N-CA	5.61	125.71	119.32
1	E	854	SER	CB-CA-C	-5.58	110.12	116.54
1	K	581	GLU	N-CA-C	5.52	116.70	108.31
1	I	854	SER	CB-CA-C	-5.42	110.30	116.54
1	A	854	SER	CB-CA-C	-5.38	110.35	116.54
1	C	884	ILE	N-CA-C	5.36	113.59	109.19
1	K	884	ILE	N-CA-C	5.34	113.57	109.19
1	E	379	LYS	CB-CA-C	-5.30	110.44	116.54
1	I	241	PHE	N-CA-C	-5.30	101.24	109.72
1	G	884	ILE	N-CA-C	5.28	113.52	109.19
1	I	491	LYS	CG-CD-CE	5.23	123.33	111.30
1	C	854	SER	CB-CA-C	-5.23	110.53	116.54
1	E	594	LEU	CA-C-N	5.21	127.21	120.44
1	E	594	LEU	C-N-CA	5.21	127.21	120.44
1	E	300	ILE	CB-CA-C	-5.13	108.91	114.35
1	K	880	LYS	CB-CA-C	-5.13	110.68	116.63
1	C	300	ILE	CB-CA-C	-5.05	109.00	114.35
1	I	314	PHE	N-CA-C	5.04	119.58	113.38
1	E	896	ASP	CA-C-N	5.04	127.09	120.60
1	E	896	ASP	C-N-CA	5.04	127.09	120.60
1	K	300	ILE	CB-CA-C	-5.04	109.01	114.35
1	I	300	ILE	CB-CA-C	-5.02	109.03	114.35

There are no chirality outliers.

All (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
1	G	466	ARG	Peptide
1	K	606	ASN	Peptide

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	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:G:826:ILE:HG22	1:G:827:GLU:HG3	1.69	0.73
1:K:267:GLY:HA3	1:K:732:ARG:HD3	1.69	0.72
1:E:895:GLU:HG3	1:E:902:GLN:CG	2.19	0.72
1:C:803:LYS:NZ	1:C:914:GLU:OE1	2.18	0.72
1:E:806:LYS:HA	1:E:896:ASP:OD1	1.90	0.72
1:A:267:GLY:HA3	1:A:732:ARG:HD3	1.72	0.70
1:C:267:GLY:HA3	1:C:732:ARG:HD3	1.74	0.70
1:E:895:GLU:HG3	1:E:902:GLN:HG2	1.76	0.68
1:C:327:ALA:HA	1:C:852:GLN:HE22	1.58	0.68
1:G:478:LEU:HD11	1:G:593:LYS:HG3	1.76	0.67
1:A:432:ALA:HA	1:A:780:ILE:HG23	1.76	0.67
1:I:490:CYS:SG	1:I:491:LYS:N	2.63	0.66
1:G:843:VAL:HG22	1:G:863:PHE:HB2	1.77	0.66
1:I:564:LEU:HD21	1:I:598:GLU:HA	1.77	0.66
1:K:600:VAL:O	1:K:606:ASN:ND2	2.29	0.65
1:I:267:GLY:HA3	1:I:732:ARG:HD3	1.80	0.64
1:A:479:MET:HE2	1:A:548:TYR:HB3	1.79	0.64
1:E:559:ARG:HD3	1:E:646:TRP:HD1	1.62	0.64
1:C:462:LYS:NZ	1:C:463:VAL:O	2.26	0.64
1:E:594:LEU:HG	1:E:595:GLN:N	2.13	0.64
1:I:355:LEU:HD11	1:I:363:LEU:HD21	1.80	0.63
1:A:355:LEU:HD11	1:A:363:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:524:GLN:OE1	1:E:525:MET:N	2.28	0.63
1:E:861:LYS:HD2	1:E:875:ILE:HG22	1.81	0.62
1:C:596:GLU:O	1:C:600:VAL:HG23	1.98	0.62
1:I:888:LYS:HB3	5:J:101:GTP:H5'	1.81	0.61
1:I:466:ARG:NH2	1:I:555:SER:O	2.33	0.61
1:I:531:GLU:HA	1:I:534:ILE:HG12	1.80	0.61
1:G:559:ARG:HD3	1:G:646:TRP:HD1	1.66	0.61
1:G:821:ALA:O	1:G:824:ARG:NH2	2.34	0.60
1:I:580:ASP:OD1	1:I:581:GLU:N	2.34	0.60
2:J:9:U:H2'	2:J:10:A:C8	2.36	0.60
1:E:243:PRO:HB3	1:E:272:PHE:HE2	1.67	0.60
1:C:559:ARG:HD3	1:C:646:TRP:HD1	1.67	0.60
1:E:714:LEU:HB3	1:E:717:TYR:HB3	1.84	0.59
1:A:490:CYS:SG	1:A:491:LYS:N	2.75	0.59
1:A:451:GLN:NE2	1:E:447:GLU:OE1	2.35	0.59
1:A:637:ARG:HH12	1:A:664:ARG:HD2	1.68	0.59
1:A:826:ILE:HG22	1:A:827:GLU:HG3	1.84	0.59
1:G:466:ARG:NH2	1:G:606:ASN:O	2.36	0.58
1:G:748:ILE:O	1:G:752:GLN:HG2	2.03	0.58
1:A:327:ALA:HA	1:A:852:GLN:HE22	1.69	0.58
1:E:525:MET:HE1	1:E:531:GLU:H	1.69	0.58
1:I:587:THR:O	1:I:591:GLU:HG3	2.02	0.58
1:K:651:PRO:O	1:K:654:SER:OG	2.22	0.58
1:E:308:SER:OG	1:E:312:LYS:NZ	2.36	0.58
1:E:569:ASP:O	1:E:573:ASN:ND2	2.36	0.58
1:I:540:LEU:HD13	1:I:583:GLU:HG3	1.86	0.58
1:C:355:LEU:HD11	1:C:363:LEU:HD21	1.86	0.57
1:C:432:ALA:HA	1:C:780:ILE:HG23	1.86	0.57
1:G:471:PHE:HE1	1:G:564:LEU:HG	1.70	0.57
1:E:355:LEU:HD11	1:E:363:LEU:HD21	1.87	0.57
1:I:598:GLU:O	1:I:601:SER:HB2	2.05	0.57
1:C:595:GLN:O	1:C:599:SER:OG	2.22	0.56
1:G:824:ARG:HG2	1:G:918:PHE:HA	1.86	0.56
1:I:719:GLY:O	1:I:754:ASN:ND2	2.37	0.56
1:K:596:GLU:O	1:K:600:VAL:HG23	2.05	0.56
1:K:644:LYS:HD2	1:K:660:ILE:HD11	1.88	0.56
1:C:481:ASP:OD1	1:C:482:THR:N	2.38	0.56
1:E:381:HIS:HD1	1:E:383:TYR:H	1.52	0.56
1:I:714:LEU:HB3	1:I:717:TYR:HB3	1.86	0.56
1:E:525:MET:HE2	1:E:531:GLU:HB3	1.87	0.55
1:E:842:PHE:HB2	1:E:862:ILE:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:806:LYS:HA	1:E:896:ASP:CG	2.30	0.55
1:K:477:GLN:HA	1:K:480:ARG:CG	2.36	0.55
1:K:896:ASP:HB3	1:K:899:THR:HG22	1.88	0.55
1:A:559:ARG:HD3	1:A:646:TRP:HD1	1.70	0.55
1:E:267:GLY:HA3	1:E:732:ARG:HD3	1.88	0.55
1:I:664:ARG:NH2	2:J:23:U:OP2	2.40	0.55
1:A:420:THR:HG21	1:E:624:LEU:HD11	1.88	0.55
1:C:845:ARG:HH21	1:G:843:VAL:HG12	1.72	0.55
1:K:714:LEU:HB3	1:K:717:TYR:HB3	1.87	0.55
1:C:714:LEU:HB3	1:C:717:TYR:HB3	1.88	0.55
1:E:742:THR:HG21	1:E:747:VAL:HB	1.87	0.55
1:I:803:LYS:HG2	1:I:914:GLU:HB2	1.90	0.54
1:A:457:GLN:OE1	1:E:455:LYS:NZ	2.40	0.54
1:A:502:ARG:NE	1:A:503:GLU:OE2	2.36	0.54
1:I:830:HIS:HE1	5:J:101:GTP:HN22	1.56	0.54
1:K:809:LEU:HB2	1:K:893:VAL:HG13	1.89	0.54
1:A:528:LYS:O	1:A:531:GLU:HB2	2.07	0.54
1:G:355:LEU:HD11	1:G:363:LEU:HD21	1.89	0.54
1:A:714:LEU:HB3	1:A:717:TYR:HB3	1.90	0.54
1:E:369:MET:HE3	1:E:403:PRO:HG3	1.90	0.54
1:G:321:VAL:HG22	1:G:343:ILE:HB	1.90	0.54
1:K:355:LEU:HD11	1:K:363:LEU:HD21	1.90	0.54
1:C:845:ARG:NH2	1:G:843:VAL:HG12	2.23	0.53
1:G:823:VAL:O	1:G:916:ILE:HD11	2.08	0.53
1:I:559:ARG:HD3	1:I:646:TRP:HD1	1.73	0.53
1:G:432:ALA:HA	1:G:780:ILE:HG23	1.88	0.53
1:G:714:LEU:HB3	1:G:717:TYR:HB3	1.89	0.53
1:I:466:ARG:HG3	1:I:467:ILE:HG23	1.90	0.53
1:I:416:ASP:OD1	1:I:416:ASP:N	2.36	0.53
1:A:455:LYS:NZ	1:E:457:GLN:HE21	2.07	0.53
1:C:826:ILE:HG22	1:C:827:GLU:HG3	1.90	0.53
1:G:861:LYS:HD2	1:G:875:ILE:HG22	1.90	0.53
1:K:321:VAL:HG22	1:K:343:ILE:HB	1.91	0.52
1:E:895:GLU:HG3	1:E:902:GLN:HG3	1.91	0.52
1:G:896:ASP:O	1:G:900:GLY:N	2.38	0.52
1:K:569:ASP:O	1:K:573:ASN:ND2	2.30	0.52
1:G:451:GLN:N	1:G:451:GLN:OE1	2.42	0.52
1:I:461:ARG:HG3	1:I:617:ILE:HD11	1.91	0.52
1:K:861:LYS:HD2	1:K:875:ILE:HG22	1.91	0.52
1:G:895:GLU:HB2	1:G:902:GLN:HG2	1.92	0.52
1:K:919:ASP:HB3	1:K:922:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:837:ALA:O	1:E:840:GLU:HB2	2.10	0.52
1:E:862:ILE:HG22	1:E:873:TRP:HB2	1.92	0.52
1:G:369:MET:HE3	1:G:403:PRO:HG3	1.91	0.52
1:E:579:PHE:O	1:E:580:ASP:HB2	2.09	0.52
1:E:858:LYS:HA	1:E:877:VAL:HG12	1.91	0.52
1:G:888:LYS:HB3	5:H:101:GTP:H5'	1.90	0.52
1:E:293:VAL:HG22	1:E:368:LEU:HB3	1.92	0.52
1:I:353:ASN:O	1:I:357:LYS:HG2	2.09	0.51
1:I:411:SER:HB2	1:I:725:ILE:HD12	1.92	0.51
1:G:320:ARG:HD2	1:K:332:VAL:HG11	1.92	0.51
1:K:465:SER:HA	1:K:609:PRO:HG2	1.92	0.51
1:K:477:GLN:HA	1:K:480:ARG:HG2	1.90	0.51
1:K:350:ILE:O	1:K:354:ASN:ND2	2.40	0.51
1:C:298:ASN:HD21	1:C:381:HIS:CE1	2.28	0.51
1:I:528:LYS:O	1:I:531:GLU:N	2.44	0.51
1:G:469:ASP:HB3	1:G:472:LYS:HB3	1.93	0.51
1:A:746:GLY:O	1:A:750:LYS:HG2	2.11	0.51
1:C:807:LYS:HZ1	1:C:897:ILE:HG12	1.75	0.51
1:K:517:GLN:HG2	1:K:521:MET:HE3	1.93	0.51
1:E:525:MET:HE3	1:E:527:ASP:C	2.36	0.50
1:E:708:GLN:HE22	1:E:732:ARG:CZ	2.24	0.50
1:I:745:ALA:O	1:I:749:GLU:HG3	2.11	0.50
1:I:599:SER:HA	1:I:602:ARG:H	1.77	0.50
1:A:815:ALA:HB2	1:A:866:ARG:HD2	1.93	0.50
1:C:814:LYS:NZ	1:C:902:GLN:OE1	2.41	0.50
1:G:861:LYS:NZ	5:H:101:GTP:O1B	2.23	0.50
1:A:485:LEU:HB3	1:A:541:TYR:CZ	2.46	0.49
1:C:487:LYS:HA	1:C:490:CYS:SG	2.51	0.49
1:G:719:GLY:O	1:G:754:ASN:ND2	2.43	0.49
1:I:476:ALA:O	1:I:480:ARG:HG3	2.11	0.49
1:C:619:GLN:HE22	1:C:652:LYS:HE2	1.77	0.49
1:G:580:ASP:OD2	1:G:581:GLU:N	2.45	0.49
1:G:809:LEU:HB2	1:G:893:VAL:HG13	1.94	0.49
1:I:243:PRO:HB3	1:I:272:PHE:CE2	2.48	0.49
1:C:555:SER:OG	1:C:560:MET:HG2	2.12	0.49
1:K:559:ARG:HD3	1:K:646:TRP:HD1	1.77	0.49
1:G:824:ARG:HG3	1:G:916:ILE:HD13	1.94	0.49
1:A:508:LYS:HE2	2:B:9:U:H4'	1.94	0.49
1:C:369:MET:HE3	1:C:403:PRO:HG3	1.94	0.49
1:E:718:VAL:HG13	1:E:750:LYS:HG2	1.95	0.49
1:E:813:CYS:HB2	1:E:866:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:919:ASP:HB3	1:G:922:GLU:HG3	1.95	0.48
1:E:524:GLN:HG2	1:E:902:GLN:NE2	2.28	0.48
1:G:750:LYS:O	1:G:753:ILE:HG12	2.14	0.48
2:B:9:U:H2'	2:B:10:A:C8	2.47	0.48
1:G:629:ILE:HD11	1:G:687:ALA:HA	1.95	0.48
1:E:610:LYS:NZ	1:E:716:GLU:OE1	2.35	0.48
1:I:584:GLN:HA	1:I:587:THR:HG22	1.96	0.48
1:A:637:ARG:HH22	1:A:664:ARG:HG2	1.78	0.48
2:F:7:A:H2'	2:F:8:A:C8	2.49	0.48
1:K:243:PRO:HB3	1:K:272:PHE:CE2	2.49	0.48
1:A:461:ARG:HG3	1:A:617:ILE:HD11	1.95	0.48
1:K:814:LYS:NZ	1:K:902:GLN:OE1	2.36	0.48
1:A:888:LYS:HE3	1:A:891:SER:HB2	1.96	0.47
1:E:519:ALA:HA	1:E:522:VAL:HG22	1.95	0.47
1:G:363:LEU:HD13	1:G:369:MET:HE1	1.96	0.47
1:A:581:GLU:HB3	1:A:582:ILE:H	1.25	0.47
1:A:610:LYS:NZ	1:A:716:GLU:OE1	2.41	0.47
1:G:744:ASN:HB3	1:G:747:VAL:HG23	1.96	0.47
1:K:899:THR:HG23	1:K:901:VAL:H	1.78	0.47
1:G:742:THR:HG21	1:G:747:VAL:HB	1.96	0.47
1:A:450:GLU:OE2	1:E:734:ARG:NH1	2.44	0.47
1:C:503:GLU:O	1:C:509:TYR:HB2	2.15	0.47
1:E:809:LEU:HB2	1:E:893:VAL:HG13	1.97	0.47
1:G:818:CYS:SG	1:G:819:TYR:N	2.88	0.47
1:G:839:LYS:HA	1:G:842:PHE:CE2	2.50	0.47
1:I:344:ILE:HG22	1:I:346:LEU:HD13	1.96	0.47
1:I:479:MET:HE2	1:I:548:TYR:HB3	1.96	0.47
1:I:529:ASP:N	1:I:529:ASP:OD1	2.44	0.47
1:I:830:HIS:CE1	5:J:101:GTP:HN22	2.32	0.47
1:A:460:PHE:HE1	1:A:751:GLU:HG2	1.79	0.47
1:E:411:SER:HB2	1:E:725:ILE:HD12	1.97	0.47
1:E:826:ILE:HG22	1:E:827:GLU:HG3	1.95	0.47
1:E:854:SER:OG	1:E:855:SER:N	2.47	0.47
1:E:860:ALA:HB3	1:E:876:HIS:HB3	1.95	0.47
1:K:462:LYS:NZ	1:K:743:SER:O	2.47	0.47
1:I:520:CYS:SG	1:I:538:LEU:HD23	2.55	0.47
1:K:460:PHE:HB3	1:K:748:ILE:HD12	1.96	0.47
1:E:356:LYS:HD2	1:E:356:LYS:O	2.14	0.47
1:I:750:LYS:HE3	2:J:8:A:H5''	1.96	0.47
1:I:861:LYS:HD2	1:I:875:ILE:HG22	1.96	0.47
1:E:603:ASP:OD2	1:E:605:SER:OG	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:724:MET:HE1	1:I:755:MET:HG3	1.97	0.46
1:I:839:LYS:HA	1:I:842:PHE:CE2	2.51	0.46
1:K:860:ALA:HB3	1:K:876:HIS:HB3	1.97	0.46
1:G:467:ILE:HG22	1:G:468:SER:N	2.30	0.46
1:I:748:ILE:O	1:I:752:GLN:HG2	2.16	0.46
1:K:478:LEU:HD11	1:K:593:LYS:HE2	1.97	0.46
1:C:742:THR:HG21	1:C:747:VAL:HB	1.97	0.46
1:C:858:LYS:HA	1:C:877:VAL:HG12	1.98	0.46
1:G:706:ILE:HG12	1:G:707:ALA:H	1.79	0.46
1:A:598:GLU:OE1	1:A:602:ARG:NH2	2.48	0.46
1:C:861:LYS:NZ	5:D:101:GTP:O1B	2.38	0.46
1:I:749:GLU:O	1:I:753:ILE:HG23	2.16	0.46
1:K:480:ARG:HA	1:K:483:GLU:HB2	1.98	0.46
1:A:411:SER:HB2	1:A:725:ILE:HD12	1.98	0.46
1:C:524:GLN:HA	1:C:531:GLU:OE2	2.15	0.46
1:G:747:VAL:HA	1:G:750:LYS:HG2	1.97	0.46
1:I:503:GLU:CG	1:I:504:PHE:N	2.79	0.46
1:G:479:MET:HE2	1:G:548:TYR:HB3	1.97	0.46
1:I:514:VAL:O	1:I:518:LYS:HG3	2.16	0.46
1:C:650:ASN:OD1	1:C:652:LYS:HG3	2.16	0.46
1:G:463:VAL:O	1:G:743:SER:HA	2.15	0.46
1:G:749:GLU:O	1:G:753:ILE:HG23	2.16	0.46
1:E:529:ASP:O	1:E:532:SER:HB3	2.16	0.46
1:E:922:GLU:H	1:E:922:GLU:HG2	1.53	0.46
1:E:479:MET:HE2	1:E:548:TYR:HB3	1.98	0.45
2:F:18:U:H2'	2:F:19:A:C8	2.51	0.45
1:I:594:LEU:O	1:I:597:LEU:HB2	2.17	0.45
1:G:536:LYS:NZ	1:G:580:ASP:OD1	2.48	0.45
1:I:598:GLU:HG2	1:I:599:SER:N	2.31	0.45
1:K:298:ASN:HD21	1:K:381:HIS:CE1	2.35	0.45
1:A:502:ARG:HG2	1:A:503:GLU:HG3	1.97	0.45
1:E:243:PRO:HB3	1:E:272:PHE:CE2	2.50	0.45
1:E:603:ASP:HA	1:E:604:PRO:HD3	1.84	0.45
1:I:807:LYS:HD2	1:I:816:LEU:HD13	1.99	0.45
1:K:363:LEU:HD13	1:K:369:MET:HE1	1.99	0.45
1:A:637:ARG:NH2	2:B:21:A:OP2	2.41	0.45
1:C:824:ARG:NH2	1:C:922:GLU:OE1	2.39	0.45
1:I:527:ASP:OD1	1:I:530:GLU:HB3	2.17	0.45
1:C:466:ARG:HB2	1:C:608:ASN:OD1	2.17	0.45
1:C:714:LEU:HD13	1:C:717:TYR:CD2	2.51	0.45
1:E:525:MET:SD	1:E:530:GLU:HB3	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:594:LEU:HG	1:E:595:GLN:H	1.81	0.45
1:E:708:GLN:HE22	1:E:732:ARG:NH1	2.14	0.45
1:I:363:LEU:HD13	1:I:369:MET:HE1	1.98	0.45
1:I:432:ALA:HA	1:I:780:ILE:HG23	1.98	0.45
1:K:724:MET:HE1	1:K:755:MET:HG3	1.98	0.45
1:A:779:LYS:O	1:A:783:ILE:HG13	2.16	0.45
1:A:350:ILE:O	1:A:354:ASN:ND2	2.43	0.45
1:I:510:GLU:HA	1:I:513:ILE:HG22	1.99	0.45
1:K:263:CYS:HA	1:K:409:THR:O	2.17	0.45
1:E:805:ASN:HD21	1:E:819:TYR:HD2	1.65	0.44
1:I:534:ILE:HG13	1:I:535:CYS:N	2.32	0.44
1:I:826:ILE:HG22	1:I:827:GLU:HG3	1.98	0.44
1:K:295:PHE:HB3	1:K:345:ILE:HG13	2.00	0.44
1:K:779:LYS:O	1:K:783:ILE:HG13	2.18	0.44
1:E:462:LYS:NZ	1:E:743:SER:O	2.51	0.44
1:A:734:ARG:NH1	1:E:450:GLU:OE2	2.31	0.44
1:C:888:LYS:HB3	5:D:101:GTP:H5'	1.99	0.44
1:E:470:LYS:O	1:E:474:ILE:HG13	2.18	0.44
1:E:585:ASP:O	1:E:589:ARG:HG3	2.16	0.44
1:G:569:ASP:OD1	1:G:573:ASN:ND2	2.51	0.44
1:G:863:PHE:HD2	1:G:872:ASP:HA	1.83	0.44
1:C:363:LEU:HD13	1:C:369:MET:HE1	1.99	0.44
1:E:432:ALA:HA	1:E:780:ILE:HG23	2.00	0.44
1:A:517:GLN:HG2	1:A:521:MET:HE3	1.99	0.44
1:I:503:GLU:HG3	1:I:504:PHE:CD1	2.52	0.44
1:I:814:LYS:NZ	1:I:902:GLN:OE1	2.37	0.44
1:E:263:CYS:HA	1:E:409:THR:O	2.17	0.44
1:G:366:PHE:O	1:G:403:PRO:HB3	2.18	0.44
1:K:750:LYS:HA	1:K:753:ILE:HG12	1.99	0.44
2:L:11:G:N2	2:L:14:A:OP2	2.44	0.44
1:A:299:GLN:NE2	1:A:700:ALA:HB3	2.33	0.43
1:G:411:SER:HB2	1:G:725:ILE:HD12	1.99	0.43
1:A:547:LYS:HG3	1:A:570:PHE:CE1	2.54	0.43
1:A:839:LYS:HA	1:A:842:PHE:CE2	2.53	0.43
1:E:895:GLU:O	1:E:896:ASP:CG	2.61	0.43
1:E:512:TRP:O	1:E:516:VAL:HG23	2.19	0.43
1:E:839:LYS:HA	1:E:842:PHE:CE2	2.53	0.43
1:G:524:GLN:NE2	1:G:895:GLU:OE2	2.52	0.43
2:L:9:U:H2'	2:L:10:A:C8	2.53	0.43
1:A:263:CYS:HA	1:A:409:THR:O	2.18	0.43
1:A:366:PHE:O	1:A:403:PRO:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:357:LYS:HB3	1:G:357:LYS:HE2	1.83	0.43
1:I:528:LYS:HA	1:I:531:GLU:HB3	2.00	0.43
1:E:524:GLN:NE2	1:E:531:GLU:OE1	2.51	0.43
1:I:595:GLN:HA	1:I:598:GLU:OE1	2.19	0.43
1:I:887:ILE:HB	1:I:892:PHE:HE2	1.83	0.43
1:E:524:GLN:HG2	1:E:902:GLN:HE22	1.83	0.43
2:F:18:U:H2'	2:F:19:A:H8	1.83	0.43
1:G:467:ILE:HG22	1:G:468:SER:H	1.83	0.43
1:G:839:LYS:HA	1:G:842:PHE:HE2	1.84	0.43
1:I:742:THR:HG21	1:I:747:VAL:HB	2.01	0.43
1:E:858:LYS:HG2	1:E:875:ILE:HD12	2.00	0.43
1:G:253:PRO:HG2	1:G:440:ALA:HB2	2.00	0.43
1:A:416:ASP:OD1	1:A:416:ASP:N	2.41	0.43
1:A:492:ASP:HB3	1:A:493:LEU:H	1.42	0.43
1:C:466:ARG:NH2	1:C:555:SER:O	2.52	0.43
1:G:608:ASN:HA	1:G:609:PRO:HD2	1.88	0.43
1:I:524:GLN:O	1:I:525:MET:HG3	2.19	0.43
1:E:779:LYS:O	1:E:783:ILE:HG13	2.19	0.42
1:G:598:GLU:O	1:G:602:ARG:HG3	2.19	0.42
1:I:466:ARG:HG2	1:I:467:ILE:HG12	2.01	0.42
1:K:369:MET:HE3	1:K:403:PRO:HG3	2.00	0.42
1:G:490:CYS:SG	1:G:491:LYS:N	2.92	0.42
1:G:619:GLN:NE2	1:G:652:LYS:HB3	2.34	0.42
1:G:800:VAL:HA	1:G:801:PRO:HD3	1.91	0.42
1:I:608:ASN:HA	1:I:609:PRO:HD2	1.90	0.42
1:K:404:GLN:HE21	1:K:406:ILE:HD11	1.84	0.42
1:A:363:LEU:HD13	1:A:369:MET:HE1	2.01	0.42
1:I:878:LYS:HD3	1:I:883:GLU:HG2	2.02	0.42
1:K:564:LEU:HD23	1:K:564:LEU:HA	1.87	0.42
1:G:344:ILE:HG22	1:G:346:LEU:HD13	2.02	0.42
1:G:564:LEU:HD23	1:G:564:LEU:HA	1.85	0.42
1:I:540:LEU:O	1:I:544:HIS:ND1	2.47	0.42
1:K:298:ASN:HD21	1:K:381:HIS:HE2	1.67	0.42
1:K:634:VAL:HG12	1:K:715:TYR:HB3	2.00	0.42
1:K:826:ILE:HG22	1:K:827:GLU:HG3	2.01	0.42
1:G:698:SER:HG	2:H:20:U:HO2'	1.61	0.42
1:E:591:GLU:HA	1:E:594:LEU:HB2	2.02	0.42
1:G:858:LYS:HA	1:G:877:VAL:HG12	2.01	0.42
2:B:7:A:H2'	2:B:8:A:C8	2.54	0.42
1:E:453:VAL:HG22	1:E:732:ARG:HD2	2.01	0.42
1:E:533:ARG:HA	1:E:536:LYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:773:GLU:OE2	1:E:777:ARG:NH2	2.44	0.42
1:I:714:LEU:HD13	1:I:717:TYR:CD2	2.55	0.42
1:K:887:ILE:HB	1:K:892:PHE:HE2	1.84	0.42
1:A:521:MET:O	1:A:814:LYS:NZ	2.32	0.42
1:G:350:ILE:O	1:G:354:ASN:ND2	2.43	0.42
1:I:619:GLN:NE2	1:I:652:LYS:HB3	2.35	0.42
1:A:249:GLU:OE1	1:A:445:ASN:ND2	2.33	0.42
1:A:587:THR:O	1:A:591:GLU:HG3	2.19	0.42
1:A:729:GLY:O	1:A:732:ARG:HG3	2.20	0.42
1:G:381:HIS:HD1	1:G:383:TYR:H	1.67	0.42
2:L:13:G:H2'	2:L:14:A:C8	2.55	0.42
2:D:13:G:H2'	2:D:14:A:C8	2.55	0.42
1:E:363:LEU:HD13	1:E:369:MET:HE1	2.02	0.42
1:E:714:LEU:HD13	1:E:717:TYR:CD2	2.55	0.42
2:H:11:G:N2	2:H:14:A:OP2	2.40	0.42
1:E:344:ILE:HG22	1:E:346:LEU:HD13	2.02	0.41
1:G:517:GLN:HG2	1:G:521:MET:HE3	2.02	0.41
1:G:662:THR:HG22	1:G:697:THR:HG23	2.02	0.41
1:I:863:PHE:HD2	1:I:872:ASP:HA	1.84	0.41
1:E:830:HIS:C	1:E:831:TYR:HD1	2.29	0.41
1:G:916:ILE:HA	1:G:917:PRO:HD3	1.96	0.41
1:C:629:ILE:H	1:C:710:ASN:HD21	1.67	0.41
1:E:466:ARG:NH2	1:E:606:ASN:O	2.39	0.41
1:G:394:LYS:NZ	1:G:435:ASP:OD1	2.52	0.41
1:G:625:ASN:HA	1:G:626:PRO:HD2	1.90	0.41
1:I:334:VAL:HG11	1:I:354:ASN:OD1	2.20	0.41
1:I:503:GLU:O	1:I:509:TYR:HB2	2.20	0.41
1:K:480:ARG:HG2	1:K:480:ARG:H	1.65	0.41
1:A:624:LEU:HD11	1:E:420:THR:HG21	2.01	0.41
1:C:608:ASN:HA	1:C:609:PRO:HD2	1.76	0.41
1:C:625:ASN:HA	1:C:626:PRO:HD2	1.96	0.41
1:C:658:PRO:HA	1:C:693:ILE:HG23	2.01	0.41
1:E:346:LEU:HD23	1:E:351:LEU:HB2	2.03	0.41
1:E:807:LYS:HE3	1:E:819:TYR:CE2	2.54	0.41
1:G:798:LYS:HA	1:G:799:PRO:HD3	1.94	0.41
1:C:629:ILE:HD11	1:C:687:ALA:HA	2.01	0.41
1:G:897:ILE:HG12	1:G:897:ILE:O	2.21	0.41
1:I:546:ARG:O	1:I:549:ASN:HB3	2.20	0.41
1:C:610:LYS:HE2	1:C:715:TYR:HE1	1.85	0.41
1:E:334:VAL:HG21	1:E:354:ASN:ND2	2.35	0.41
1:E:547:LYS:HG3	1:E:570:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:456:PRO:HB3	1:G:736:SER:HB2	2.03	0.41
1:I:528:LYS:O	1:I:532:SER:N	2.46	0.41
2:L:18:U:H2'	2:L:19:A:C8	2.56	0.41
1:A:387:MET:HE2	1:A:434:LEU:HA	2.02	0.41
1:E:324:ILE:HG22	1:E:350:ILE:HG12	2.03	0.41
2:L:18:U:H2'	2:L:19:A:H8	1.86	0.41
1:A:658:PRO:HA	1:A:693:ILE:HG23	2.02	0.41
1:A:888:LYS:HA	1:A:908:TRP:HE1	1.86	0.41
1:C:661:LEU:HB3	1:C:696:ALA:HB2	2.02	0.41
1:C:818:CYS:SG	1:C:819:TYR:N	2.94	0.41
1:E:508:LYS:HE2	1:E:508:LYS:HB3	1.71	0.41
1:E:706:ILE:HD12	1:E:707:ALA:O	2.20	0.41
1:G:547:LYS:HG3	1:G:570:PHE:CE1	2.56	0.41
1:I:381:HIS:CG	1:I:382:PRO:HD2	2.56	0.41
1:I:482:THR:HA	1:I:485:LEU:HD22	2.03	0.41
1:I:507:GLN:HE22	2:J:9:U:H1'	1.85	0.41
1:I:862:ILE:HG22	1:I:873:TRP:HB2	2.03	0.41
1:A:299:GLN:HE21	1:A:700:ALA:HB3	1.86	0.41
1:A:369:MET:HE3	1:A:403:PRO:HG3	2.03	0.41
1:G:825:VAL:HG12	1:G:916:ILE:O	2.20	0.41
1:I:545:LEU:HD12	1:I:545:LEU:HA	1.86	0.41
1:K:714:LEU:HD13	1:K:717:TYR:CD2	2.56	0.41
1:A:803:LYS:HD2	1:A:914:GLU:HG3	2.03	0.40
1:A:809:LEU:HD11	1:A:895:GLU:HG3	2.03	0.40
1:A:887:ILE:HB	1:A:892:PHE:HE2	1.86	0.40
1:C:843:VAL:HG12	1:G:845:ARG:HE	1.86	0.40
1:E:374:CYS:HB2	1:E:434:LEU:HD11	2.02	0.40
1:G:334:VAL:HG11	1:G:354:ASN:OD1	2.22	0.40
1:I:547:LYS:NZ	1:I:570:PHE:CE1	2.87	0.40
1:I:861:LYS:HB3	1:I:861:LYS:HE3	1.87	0.40
1:C:263:CYS:HA	1:C:409:THR:O	2.21	0.40
1:E:281:HIS:O	1:E:284:LYS:HG2	2.20	0.40
1:G:545:LEU:HD12	1:G:545:LEU:HA	1.85	0.40
2:H:9:U:H2'	2:H:10:A:C8	2.56	0.40
1:I:350:ILE:O	1:I:354:ASN:ND2	2.54	0.40
1:K:334:VAL:HG11	1:K:354:ASN:OD1	2.21	0.40
1:K:366:PHE:O	1:K:403:PRO:HB3	2.21	0.40
1:A:363:LEU:HD22	1:A:369:MET:HE1	2.03	0.40
1:G:346:LEU:HD23	1:G:351:LEU:HB2	2.03	0.40
1:K:363:LEU:HD22	1:K:369:MET:HE1	2.04	0.40
1:K:570:PHE:O	1:K:574:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:CYS:HB3	1:E:441:THR:HG22	2.03	0.40
1:E:593:LYS:O	1:E:594:LEU:C	2.65	0.40
1:I:603:ASP:OD1	1:I:605:SER:N	2.49	0.40
1:K:888:LYS:HB3	5:L:101:GTP:H5'	2.04	0.40
1:A:381:HIS:HD1	1:A:383:TYR:H	1.68	0.40
1:A:888:LYS:HB3	5:B:101:GTP:H5'	2.04	0.40
1:E:351:LEU:HD23	1:E:386:ILE:HD13	2.03	0.40
1:E:887:ILE:HB	1:E:892:PHE:HE2	1.87	0.40
1:K:608:ASN:HA	1:K:609:PRO:HD2	1.90	0.40
1:K:888:LYS:HA	1:K:908:TRP:HE1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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Mol	Chain	Res	Type
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

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	294	VAL
1	A	334	VAL
1	A	380	GLN
1	A	489	ILE
1	A	522	VAL
1	A	528	LYS
1	A	529	ASP
1	A	531	GLU
1	A	580	ASP
1	A	592	GLU
1	A	612	GLU
1	A	721	VAL
1	A	809	LEU
1	A	895	GLU
1	A	897	ILE
1	C	294	VAL

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Mol	Chain	Res	Type
1	C	346	LEU
1	C	350	ILE
1	C	474	ILE
1	C	475	ILE
1	C	490	CYS
1	C	522	VAL
1	C	529	ASP
1	C	545	LEU
1	C	825	VAL
1	C	890	GLU
1	C	907	LYS
1	E	244	ARG
1	E	346	LEU
1	E	350	ILE
1	E	467	ILE
1	E	515	THR
1	E	529	ASP
1	E	531	GLU
1	E	574	VAL
1	E	582	ILE
1	E	706	ILE
1	E	721	VAL
1	E	800	VAL
1	E	866	ARG
1	E	883	GLU
1	E	893	VAL
1	E	897	ILE
1	E	902	GLN
1	E	922	GLU
1	G	334	VAL
1	G	346	LEU
1	G	357	LYS
1	G	508	LYS
1	G	530	GLU
1	G	538	LEU
1	G	540	LEU
1	G	681	ILE
1	G	721	VAL
1	G	803	LYS
1	G	824	ARG
1	G	843	VAL
1	G	893	VAL

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Mol	Chain	Res	Type
1	G	916	ILE
1	I	256	LYS
1	I	334	VAL
1	I	350	ILE
1	I	467	ILE
1	I	485	LEU
1	I	514	VAL
1	I	547	LYS
1	I	721	VAL
1	I	825	VAL
1	I	897	ILE
1	K	344	ILE
1	K	380	GLN
1	K	545	LEU
1	K	583	GLU
1	K	654	SER
1	K	721	VAL
1	K	766	LEU
1	K	893	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	ASN
1	A	299	GLN
1	A	517	GLN
1	A	549	ASN
1	A	852	GLN
1	A	871	HIS
1	C	298	ASN
1	C	353	ASN
1	C	389	ASN
1	C	419	ASN
1	C	549	ASN
1	C	619	GLN
1	C	625	ASN
1	C	710	ASN
1	C	744	ASN
1	C	852	GLN
1	C	876	HIS
1	E	298	ASN
1	E	306	GLN

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Mol	Chain	Res	Type
1	E	389	ASN
1	E	457	GLN
1	E	549	ASN
1	E	692	ASN
1	E	708	GLN
1	E	902	GLN
1	G	298	ASN
1	G	331	ASN
1	G	389	ASN
1	G	511	GLN
1	G	549	ASN
1	G	557	HIS
1	G	805	ASN
1	G	902	GLN
1	I	289	GLN
1	I	306	GLN
1	I	349	GLN
1	I	507	GLN
1	I	619	GLN
1	I	805	ASN
1	I	876	HIS
1	K	298	ASN
1	K	389	ASN
1	K	549	ASN
1	K	557	HIS
1	K	619	GLN
1	K	708	GLN
1	K	876	HIS

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
5	B	101	GTP	C2-N3	2.27	1.38	1.33
5	L	101	GTP	C2-N3	2.26	1.38	1.33
5	B	101	GTP	PB-O3A	2.24	1.61	1.59
5	B	101	GTP	PA-O3A	2.16	1.61	1.59

All (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
5	H	101	GTP	C5-C4-N3	-5.44	119.73	128.39
5	B	101	GTP	C2-N3-C4	4.85	120.65	112.30
5	F	101	GTP	C2-N3-C4	4.84	120.63	112.30
5	D	101	GTP	C2-N3-C4	4.83	120.61	112.30
5	J	101	GTP	C2-N3-C4	4.82	120.60	112.30
5	H	101	GTP	C2-N3-C4	4.76	120.49	112.30
5	L	101	GTP	C2-N3-C4	4.75	120.48	112.30
5	F	101	GTP	N9-C4-N3	3.89	133.74	125.95
5	B	101	GTP	N9-C4-N3	3.78	133.52	125.95
5	J	101	GTP	N9-C4-N3	3.78	133.50	125.95
5	D	101	GTP	N9-C4-N3	3.78	133.50	125.95
5	H	101	GTP	N9-C4-N3	3.72	133.40	125.95
5	L	101	GTP	N9-C4-N3	3.63	133.22	125.95
5	F	101	GTP	C2-N1-C6	-3.04	119.60	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	101	GTP	C2-N1-C6	-3.01	119.64	125.11
5	H	101	GTP	C2-N1-C6	-3.01	119.66	125.11
5	L	101	GTP	C2-N1-C6	-3.00	119.67	125.11
5	B	101	GTP	C2-N1-C6	-3.00	119.67	125.11
5	D	101	GTP	C2-N1-C6	-2.97	119.72	125.11
5	J	101	GTP	C5-C6-N1	2.56	119.78	113.25
5	B	101	GTP	C5-C6-N1	2.54	119.72	113.25
5	D	101	GTP	C5-C6-N1	2.53	119.70	113.25
5	H	101	GTP	C5-C6-N1	2.51	119.65	113.25
5	L	101	GTP	C5-C6-N1	2.51	119.65	113.25
5	F	101	GTP	C5-C6-N1	2.51	119.65	113.25
5	J	101	GTP	O6-C6-C5	-2.51	119.90	126.53
5	F	101	GTP	C8-N7-C5	2.50	108.72	104.26
5	H	101	GTP	O6-C6-C5	-2.50	119.93	126.53
5	B	101	GTP	O6-C6-C5	-2.49	119.95	126.53
5	L	101	GTP	C8-N7-C5	2.48	108.67	104.26
5	D	101	GTP	O6-C6-C5	-2.48	119.99	126.53
5	F	101	GTP	O6-C6-C5	-2.47	120.02	126.53
5	H	101	GTP	C8-N7-C5	2.47	108.65	104.26
5	H	101	GTP	N9-C8-N7	-2.46	108.84	113.40
5	L	101	GTP	N9-C8-N7	-2.45	108.85	113.40
5	B	101	GTP	C8-N7-C5	2.44	108.60	104.26
5	D	101	GTP	C8-N7-C5	2.44	108.60	104.26
5	J	101	GTP	N9-C8-N7	-2.44	108.88	113.40
5	J	101	GTP	C8-N7-C5	2.43	108.60	104.26
5	F	101	GTP	N9-C8-N7	-2.43	108.90	113.40
5	B	101	GTP	N9-C8-N7	-2.42	108.91	113.40
5	L	101	GTP	O6-C6-C5	-2.38	120.24	126.53
5	D	101	GTP	N9-C8-N7	-2.38	108.98	113.40

There are no chirality outliers.

All (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
5	F	101	GTP	C5'-O5'-PA-O1A
5	H	101	GTP	C5'-O5'-PA-O3A
5	H	101	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	H	101	GTP	C5'-O5'-PA-O2A
5	J	101	GTP	C5'-O5'-PA-O3A
5	J	101	GTP	C5'-O5'-PA-O1A
5	J	101	GTP	C5'-O5'-PA-O2A
5	L	101	GTP	C5'-O5'-PA-O3A
5	L	101	GTP	C5'-O5'-PA-O1A
5	L	101	GTP	C5'-O5'-PA-O2A
5	B	101	GTP	O4'-C4'-C5'-O5'
5	B	101	GTP	C3'-C4'-C5'-O5'
5	D	101	GTP	C3'-C4'-C5'-O5'
5	H	101	GTP	O4'-C4'-C5'-O5'
5	H	101	GTP	C3'-C4'-C5'-O5'
5	L	101	GTP	O4'-C4'-C5'-O5'
5	L	101	GTP	C3'-C4'-C5'-O5'
5	D	101	GTP	O4'-C4'-C5'-O5'
5	J	101	GTP	O4'-C4'-C5'-O5'
5	J	101	GTP	C3'-C4'-C5'-O5'
5	F	101	GTP	C3'-C4'-C5'-O5'
5	B	101	GTP	PA-O3A-PB-O1B
5	B	101	GTP	PB-O3A-PA-O2A
5	F	101	GTP	O4'-C4'-C5'-O5'
5	B	101	GTP	C5'-O5'-PA-O2A
5	F	101	GTP	C5'-O5'-PA-O3A
5	F	101	GTP	C5'-O5'-PA-O2A
5	F	101	GTP	PB-O3A-PA-O2A
5	L	101	GTP	PB-O3A-PA-O1A
5	B	101	GTP	PB-O3B-PG-O1G
5	B	101	GTP	PA-O3A-PB-O2B
5	F	101	GTP	PA-O3A-PB-O1B
5	B	101	GTP	PB-O3B-PG-O2G
5	B	101	GTP	PB-O3B-PG-O3G
5	F	101	GTP	PB-O3A-PA-O1A
5	L	101	GTP	PB-O3A-PA-O2A

There are no ring outliers.

5 monomers are involved in 9 short contacts:

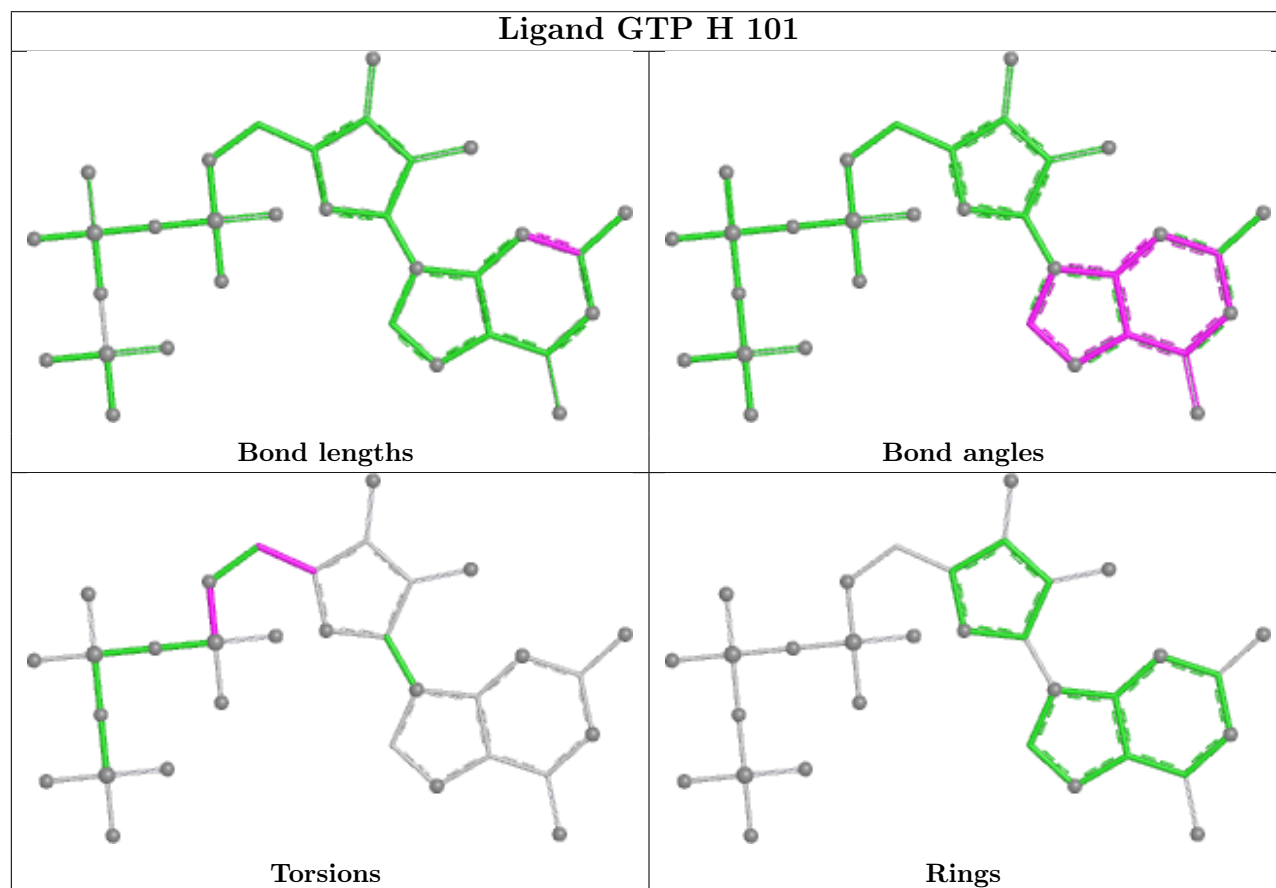
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	101	GTP	2	0
5	L	101	GTP	1	0
5	D	101	GTP	2	0
5	J	101	GTP	3	0

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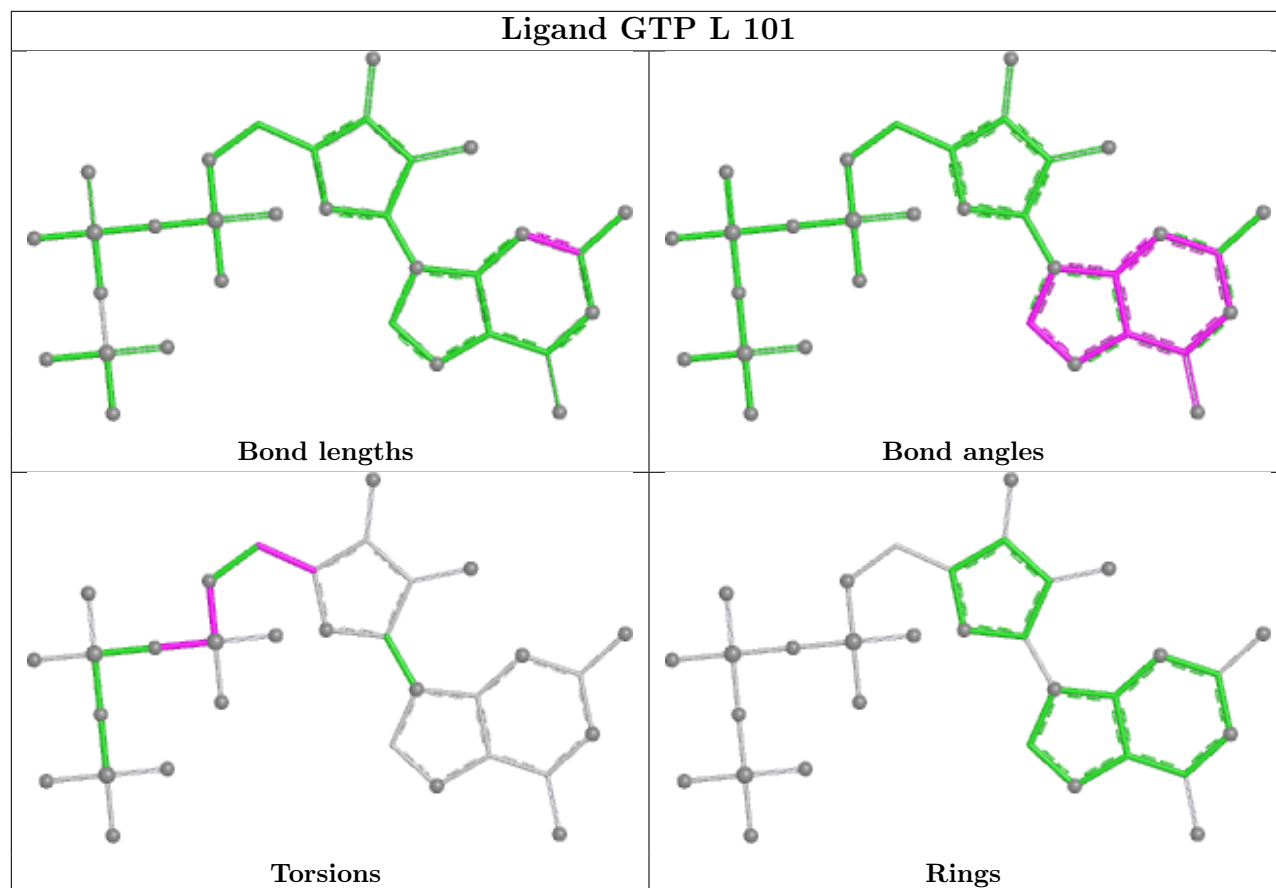
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	101	GTP	1	0

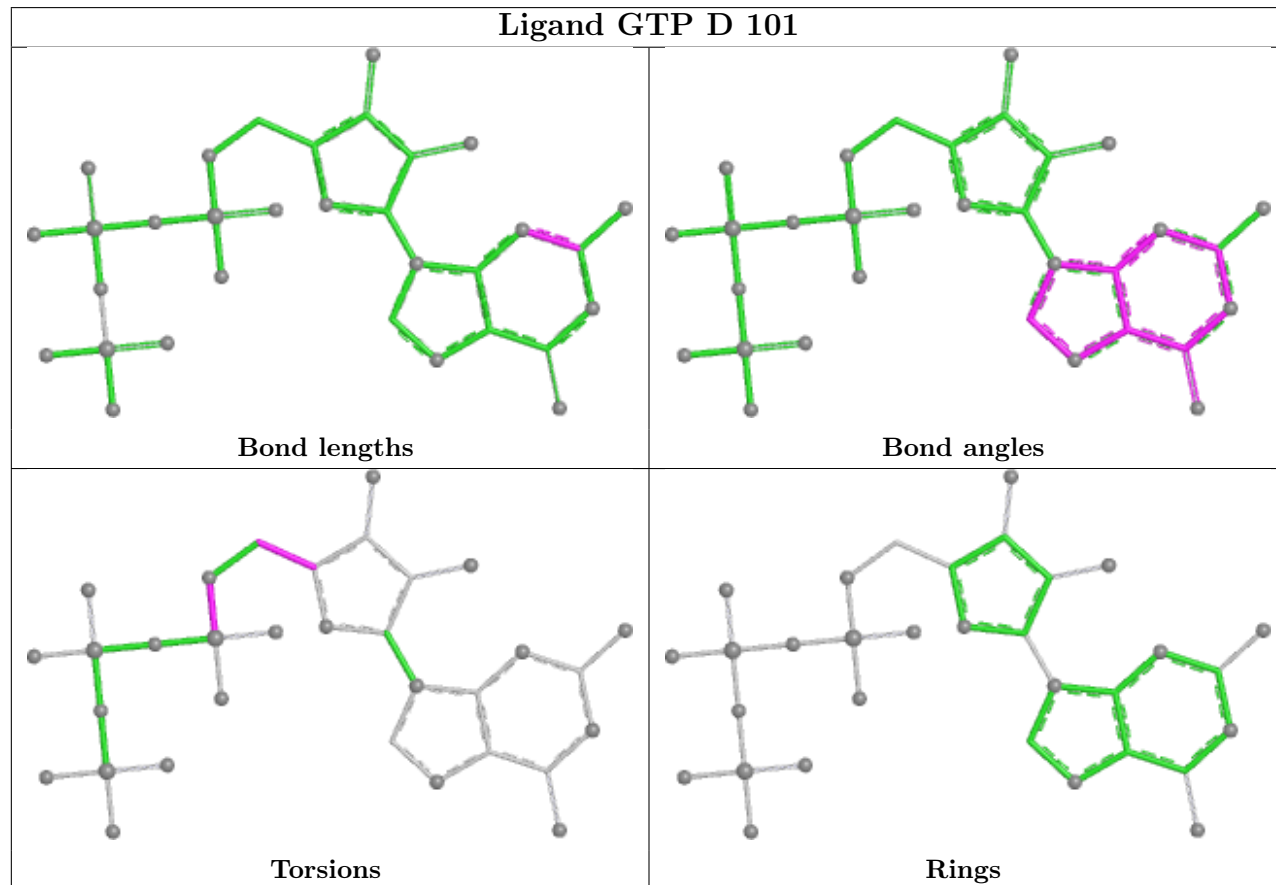
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



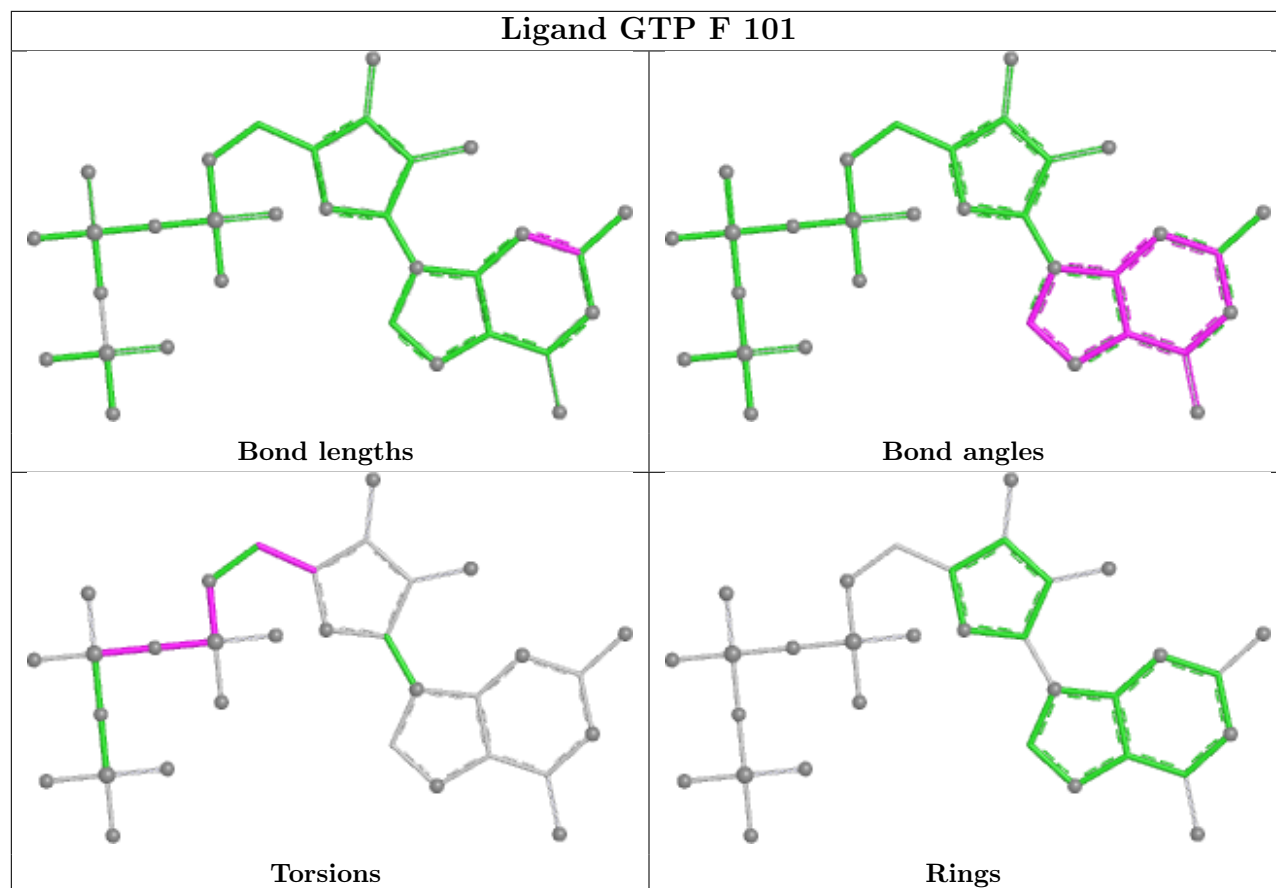
Ligand GTP L 101



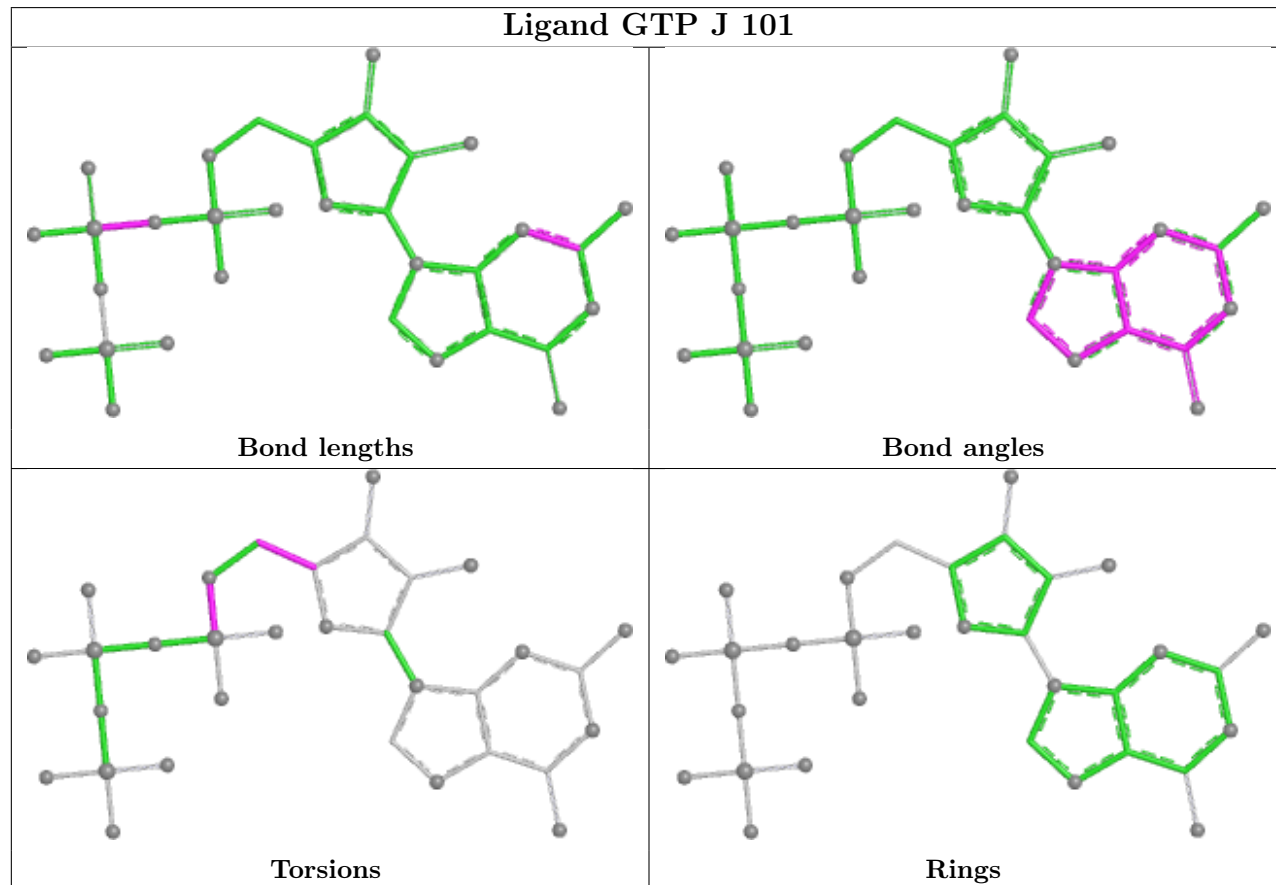
Ligand GTP D 101

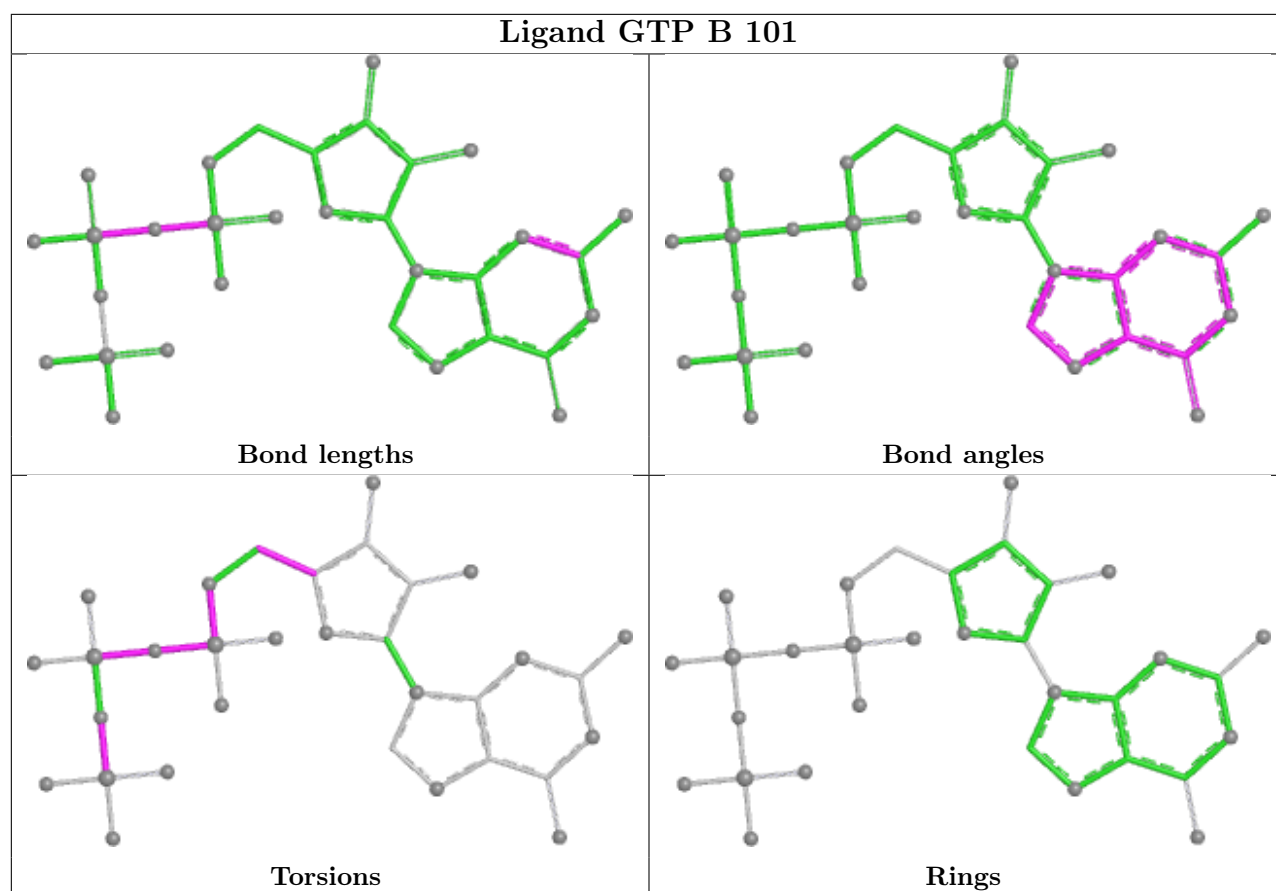


Ligand GTP F 101



Ligand GTP J 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

All (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
1	I	794	GLN	5.2
1	C	241	PHE	5.0
1	I	583	GLU	4.8
1	E	707	ALA	4.7
1	I	601	SER	4.7
1	G	491	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	I	868	ASN	4.7
1	A	241	PHE	4.6
1	A	816	LEU	4.5
1	E	896	ASP	4.5
1	G	681	ILE	4.2
1	E	490	CYS	4.2
1	I	867	GLN	4.2
1	C	481	ASP	4.1
1	G	551	ALA	4.1
1	I	870	SER	4.1
1	A	493	LEU	4.1
1	E	594	LEU	4.1
1	K	595	GLN	4.0
1	C	504	PHE	4.0
1	C	664	ARG	3.9
1	E	502	ARG	3.9
1	E	574	VAL	3.9
1	C	479	MET	3.9
1	I	486	ALA	3.8
1	K	867	GLN	3.8
1	A	530	GLU	3.8
1	A	577	ALA	3.7
1	K	862	ILE	3.7
1	E	592	GLU	3.7
1	G	592	GLU	3.7
1	A	921	ALA	3.7
1	E	868	ASN	3.7
1	I	606	ASN	3.6
1	G	488	ARG	3.6
1	I	240	PRO	3.6
1	E	467	ILE	3.6
1	C	482	THR	3.6
1	I	523	PHE	3.5
1	I	863	PHE	3.5
1	A	843	VAL	3.5
1	G	897	ILE	3.5
1	I	475	ILE	3.5
1	C	548	TYR	3.5
1	A	525	MET	3.5
1	E	593	LYS	3.4
1	C	608	ASN	3.4
1	A	840	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	467	ILE	3.4
1	A	846	PRO	3.4
1	E	922	GLU	3.4
1	I	514	VAL	3.4
1	I	536	LYS	3.4
1	E	523	PHE	3.4
1	A	537	ALA	3.4
1	G	489	ILE	3.4
1	A	526	PRO	3.4
1	A	523	PHE	3.3
1	A	482	THR	3.3
1	E	581	GLU	3.3
1	A	532	SER	3.3
1	I	869	CYS	3.3
1	I	581	GLU	3.3
1	A	468	SER	3.3
1	K	467	ILE	3.3
1	K	844	SER	3.3
1	G	490	CYS	3.3
1	C	666	LYS	3.3
1	C	541	TYR	3.3
1	C	793	SER	3.3
1	G	682	LEU	3.3
1	G	800	VAL	3.2
1	I	576	ALA	3.2
1	C	502	ARG	3.2
1	A	529	ASP	3.2
1	E	706	ILE	3.2
1	I	534	ILE	3.2
1	I	400	GLY	3.2
1	C	906	SER	3.2
1	I	923	MET	3.2
1	E	533	ARG	3.2
1	A	870	SER	3.2
1	C	545	LEU	3.1
1	A	717	TYR	3.1
1	I	489	ILE	3.1
1	K	457	GLN	3.1
1	C	469	ASP	3.1
1	E	564	LEU	3.1
1	C	872	ASP	3.1
1	C	564	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	883	GLU	3.1
1	A	859	ARG	3.1
1	A	800	VAL	3.1
1	G	751	GLU	3.1
1	I	526	PRO	3.1
1	I	573	ASN	3.0
1	I	584	GLN	3.0
1	E	505	GLY	3.0
1	I	589	ARG	3.0
1	A	906	SER	3.0
1	E	852	GLN	3.0
1	C	552	LEU	3.0
1	A	486	ALA	3.0
1	C	509	TYR	3.0
1	K	861	LYS	3.0
1	E	595	GLN	3.0
1	G	278	CYS	3.0
1	G	843	VAL	3.0
1	A	581	GLU	3.0
1	E	518	LYS	2.9
1	C	523	PHE	2.9
1	I	588	GLN	2.9
1	A	818	CYS	2.9
1	I	545	LEU	2.9
1	I	664	ARG	2.9
1	C	601	SER	2.9
1	I	579	PHE	2.9
1	I	529	ASP	2.9
1	G	555	SER	2.9
1	I	571	PHE	2.9
1	I	793	SER	2.9
1	K	852	GLN	2.9
1	K	526	PRO	2.9
1	A	922	GLU	2.9
1	I	602	ARG	2.9
1	E	797	PRO	2.8
1	C	602	ARG	2.8
1	C	537	ALA	2.8
1	E	898	ALA	2.8
1	I	799	PRO	2.8
1	C	705	ASP	2.8
1	I	510	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	520	CYS	2.8
1	I	521	MET	2.8
1	E	846	PRO	2.8
1	I	491	LYS	2.8
1	C	490	CYS	2.8
1	E	520	CYS	2.8
1	K	857	GLU	2.8
1	I	471	PHE	2.8
1	I	539	PHE	2.8
1	C	514	VAL	2.8
1	E	555	SER	2.8
1	E	513	ILE	2.8
1	E	862	ILE	2.8
1	I	575	ARG	2.7
1	I	577	ALA	2.7
1	A	799	PRO	2.7
1	C	604	PRO	2.7
1	C	665	GLY	2.7
1	E	400	GLY	2.7
1	E	597	LEU	2.7
1	I	467	ILE	2.7
1	K	582	ILE	2.7
1	K	484	SER	2.7
1	A	528	LYS	2.7
1	E	851	LYS	2.7
1	G	416	ASP	2.7
1	K	921	ALA	2.7
1	A	893	VAL	2.7
1	C	584	GLN	2.7
1	E	689	GLY	2.7
1	I	483	GLU	2.7
1	I	490	CYS	2.7
1	C	492	ASP	2.7
1	I	550	ASP	2.7
1	A	838	PHE	2.6
1	I	587	THR	2.6
1	G	512	TRP	2.6
1	I	580	ASP	2.6
1	I	603	ASP	2.6
1	I	241	PHE	2.6
1	I	900	GLY	2.6
1	A	527	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	588	GLN	2.6
1	I	840	GLU	2.6
1	K	607	GLU	2.6
1	I	537	ALA	2.6
1	I	553	ILE	2.6
1	I	469	ASP	2.6
1	A	868	ASN	2.6
1	I	488	ARG	2.6
1	C	818	CYS	2.6
1	G	845	ARG	2.6
1	A	862	ILE	2.5
1	I	492	ASP	2.5
1	I	872	ASP	2.5
1	C	505	GLY	2.5
1	G	311	SER	2.5
1	I	642	ALA	2.5
1	K	464	GLU	2.5
1	K	690	ASP	2.5
1	K	707	ALA	2.5
1	C	662	THR	2.5
1	E	512	TRP	2.5
1	K	662	THR	2.5
1	A	835	GLY	2.5
1	I	813	CYS	2.5
1	C	398	SER	2.5
1	I	901	VAL	2.5
1	K	574	VAL	2.5
1	A	481	ASP	2.5
1	I	690	ASP	2.5
1	I	910	ASP	2.5
1	A	863	PHE	2.5
1	C	859	ARG	2.5
1	C	800	VAL	2.5
1	A	582	ILE	2.5
1	C	840	GLU	2.5
1	E	690	ASP	2.5
1	I	590	PHE	2.5
1	K	416	ASP	2.5
1	I	547	LYS	2.5
1	I	816	LEU	2.5
1	G	564	LEU	2.4
1	E	516	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	659	GLY	2.4
1	I	525	MET	2.4
1	E	601	SER	2.4
1	I	533	ARG	2.4
1	A	903	THR	2.4
1	I	802	ASP	2.4
1	G	240	PRO	2.4
1	A	809	LEU	2.4
1	E	586	LEU	2.4
1	I	818	CYS	2.4
1	A	692	ASN	2.4
1	K	576	ALA	2.4
1	K	860	ALA	2.4
1	G	470	LYS	2.4
1	I	842	PHE	2.4
1	C	581	GLU	2.4
1	C	543	SER	2.4
1	K	399	SER	2.4
1	I	600	VAL	2.4
1	C	562	ASP	2.4
1	G	898	ALA	2.4
1	I	548	TYR	2.4
1	I	508	LYS	2.4
1	G	466	ARG	2.4
1	K	859	ARG	2.4
1	A	531	GLU	2.4
1	E	840	GLU	2.4
1	G	922	GLU	2.4
1	I	505	GLY	2.3
1	C	577	ALA	2.3
1	E	831	TYR	2.3
1	A	420	THR	2.3
1	I	663	GLY	2.3
1	K	798	LYS	2.3
1	A	815	ALA	2.3
1	I	848	PRO	2.3
1	C	663	GLY	2.3
1	A	576	ALA	2.3
1	E	506	THR	2.3
2	B	14	A	2.3
1	A	836	ASP	2.3
1	K	469	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	477	GLN	2.3
1	K	592	GLU	2.3
1	C	554	ILE	2.3
1	C	578	GLY	2.3
1	I	862	ILE	2.3
1	I	479	MET	2.3
1	K	863	PHE	2.3
1	C	603	ASP	2.3
1	E	705	ASP	2.3
1	I	416	ASP	2.3
1	I	524	GLN	2.3
1	C	491	LYS	2.3
1	I	598	GLU	2.3
1	C	521	MET	2.3
1	I	639	LEU	2.3
1	E	541	TYR	2.3
1	E	880	LYS	2.3
1	C	745	ALA	2.2
1	G	813	CYS	2.2
1	I	421	ASP	2.2
1	I	883	GLU	2.2
1	C	489	ILE	2.2
1	A	794	GLN	2.2
1	K	922	GLU	2.2
1	A	492	ASP	2.2
1	G	550	ASP	2.2
1	C	526	PRO	2.2
1	G	801	PRO	2.2
1	A	491	LYS	2.2
1	K	470	LYS	2.2
1	A	601	SER	2.2
1	I	599	SER	2.2
1	K	398	SER	2.2
1	A	607	GLU	2.2
1	I	503	GLU	2.2
1	I	692	ASN	2.2
1	K	692	ASN	2.2
2	B	13	G	2.2
1	I	707	ALA	2.2
1	A	575	ARG	2.2
1	C	488	ARG	2.2
1	G	789	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	482	THR	2.2
1	C	299	GLN	2.2
1	C	513	ILE	2.2
1	G	583	GLU	2.2
1	C	845	ARG	2.2
1	E	662	THR	2.1
1	I	564	LEU	2.1
1	E	479	MET	2.1
1	C	914	GLU	2.1
1	E	860	ALA	2.1
1	G	684	ALA	2.1
1	I	465	SER	2.1
1	I	605	SER	2.1
1	K	575	ARG	2.1
1	E	606	ASN	2.1
1	K	626	PRO	2.1
1	C	529	ASP	2.1
2	B	12	U	2.1
1	C	519	ALA	2.1
1	C	551	ALA	2.1
1	E	859	ARG	2.1
1	G	664	ARG	2.1
1	A	484	SER	2.1
1	A	895	GLU	2.1
1	I	844	SER	2.1
1	E	549	ASN	2.1
1	I	516	VAL	2.1
1	I	420	THR	2.1
1	A	541	TYR	2.1
1	I	541	TYR	2.1
1	I	546	ARG	2.1
1	G	752	GLN	2.1
1	G	852	GLN	2.1
1	A	583	GLU	2.1
1	C	689	GLY	2.1
1	A	579	PHE	2.1
1	E	484	SER	2.1
1	K	882	PHE	2.1
1	G	508	LYS	2.1
1	I	585	ASP	2.1
1	I	909	LYS	2.1
1	E	704	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	706	ILE	2.1
1	E	867	GLN	2.1
2	J	9	U	2.1
1	A	797	PRO	2.1
1	C	688	SER	2.1
1	I	891	SER	2.1
1	C	600	VAL	2.1
1	C	474	ILE	2.1
1	C	594	LEU	2.1
1	E	480	ARG	2.1
1	I	741	LEU	2.1
1	G	425	ASP	2.1
1	G	662	THR	2.1
1	G	899	THR	2.1
1	I	864	CYS	2.1
1	G	817	ALA	2.1
1	I	519	ALA	2.1
1	A	588	GLN	2.1
1	I	665	GLY	2.1
1	E	590	PHE	2.1
1	I	592	GLU	2.1
1	K	604	PRO	2.1
1	C	516	VAL	2.0
1	I	513	ILE	2.0
1	A	520	CYS	2.0
1	A	817	ALA	2.0
1	C	535	CYS	2.0
1	E	863	PHE	2.0
1	E	242	LYS	2.0
1	E	795	GLU	2.0
1	G	418	LYS	2.0
1	A	564	LEU	2.0
1	A	660	ILE	2.0
1	G	300	ILE	2.0
1	I	311	SER	2.0
1	A	473	TYR	2.0
1	A	905	TYR	2.0
1	G	872	ASP	2.0
1	I	569	ASP	2.0
1	G	798	LYS	2.0
1	G	556	GLU	2.0
1	C	597	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	538	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

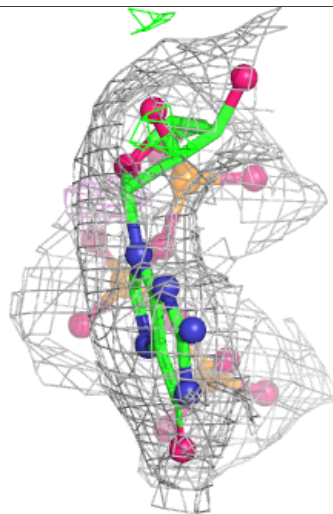
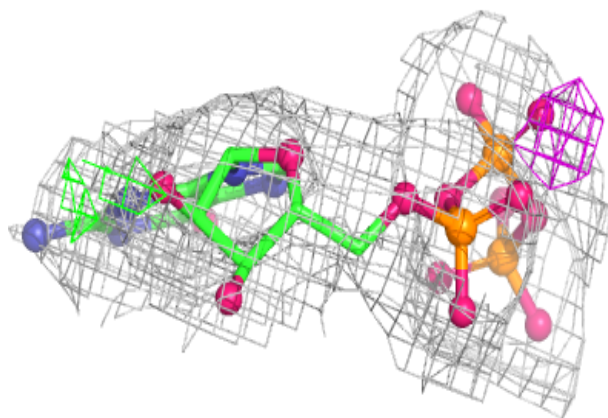
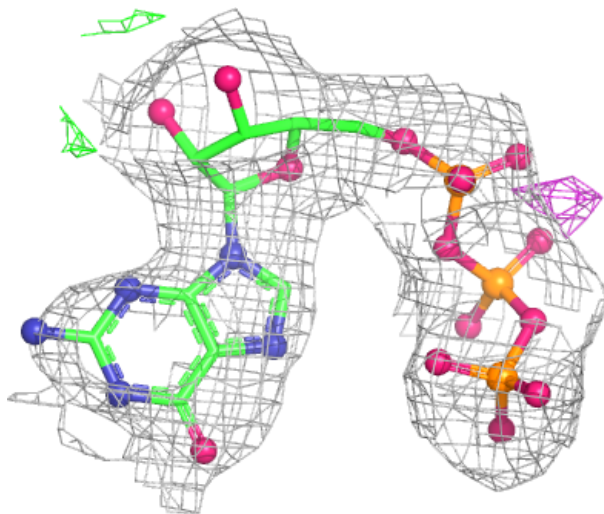
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	G	1002	1/1	0.88	0.10	24,24,24,24	0
5	GTP	F	101	32/32	0.90	0.11	36,60,84,88	0
4	MG	A	1003	1/1	0.91	0.13	56,56,56,56	0
5	GTP	B	101	32/32	0.92	0.10	33,47,88,95	0
5	GTP	H	101	32/32	0.93	0.09	22,44,88,90	0
5	GTP	L	101	32/32	0.93	0.09	27,56,96,105	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.

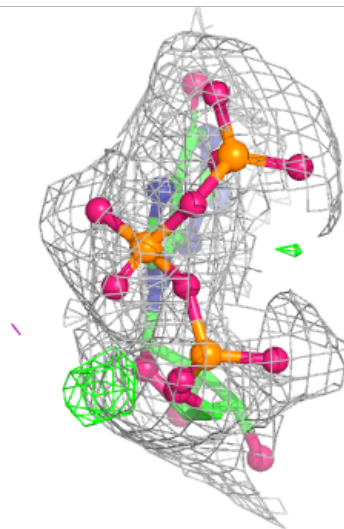
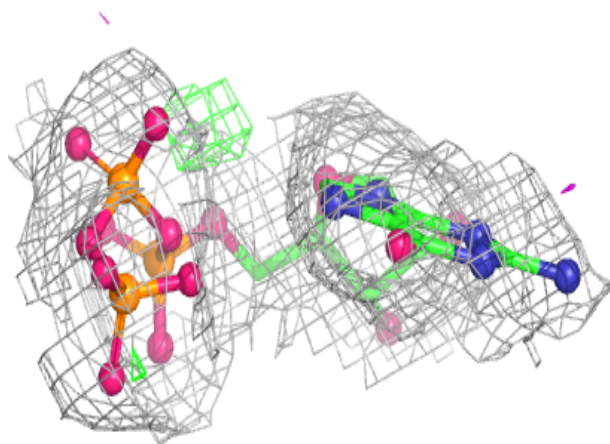
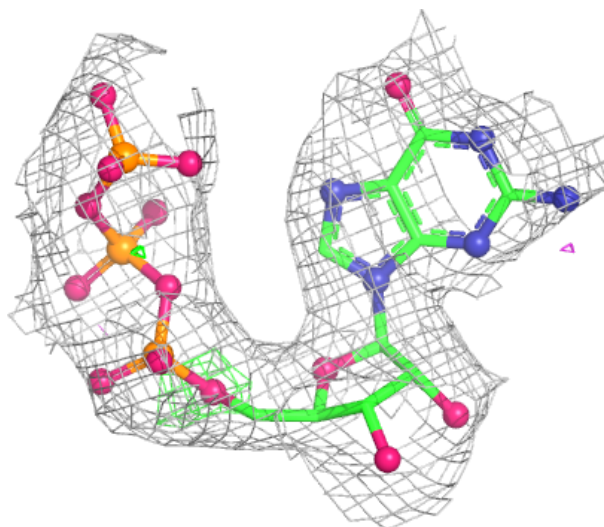
Electron density around GTP F 101:

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



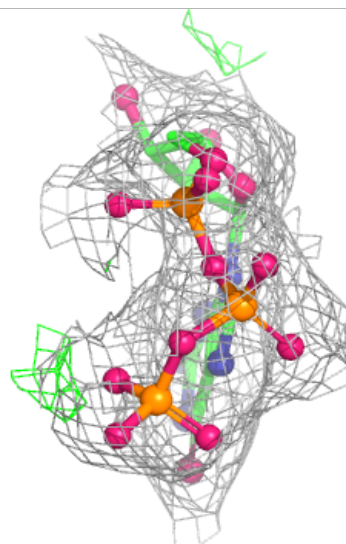
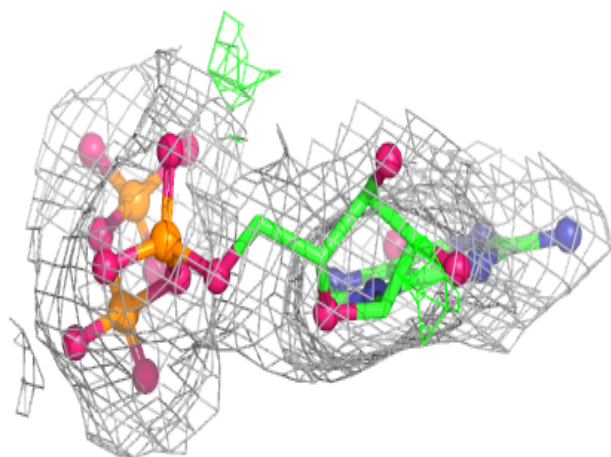
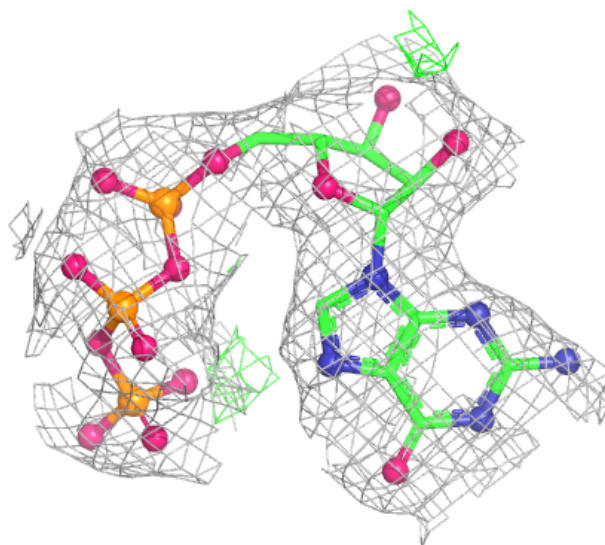
Electron density around GTP B 101:

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



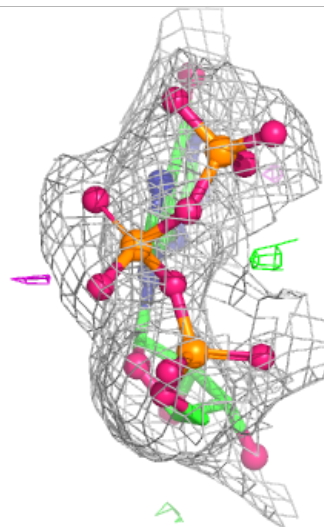
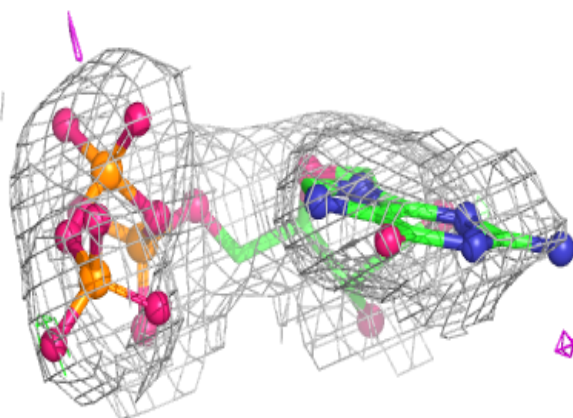
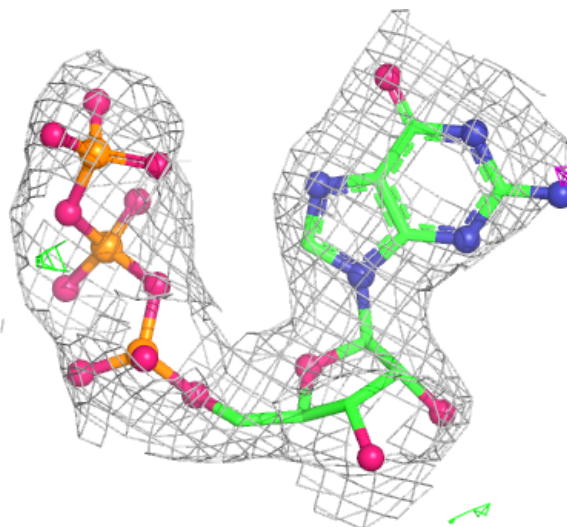
Electron density around GTP H 101:

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



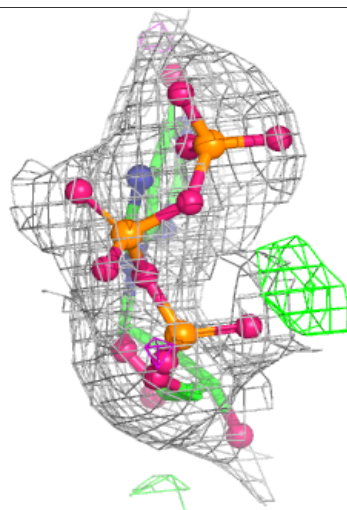
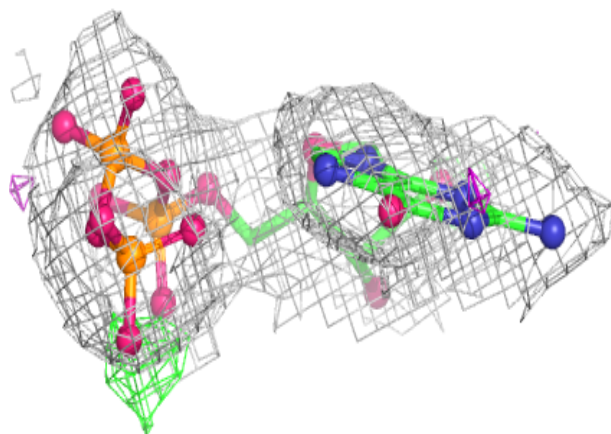
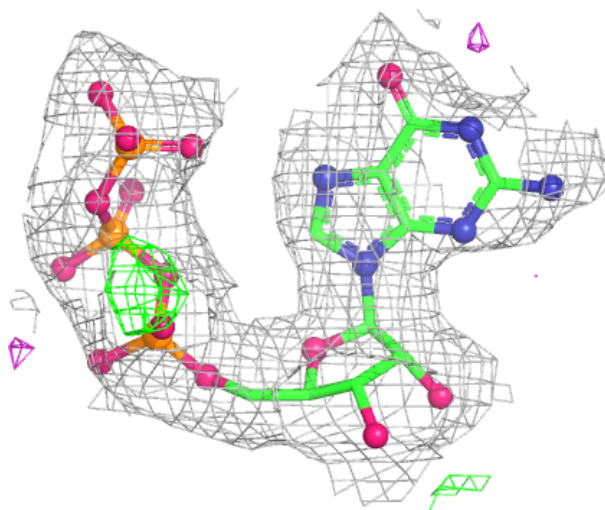
Electron density around GTP L 101:

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



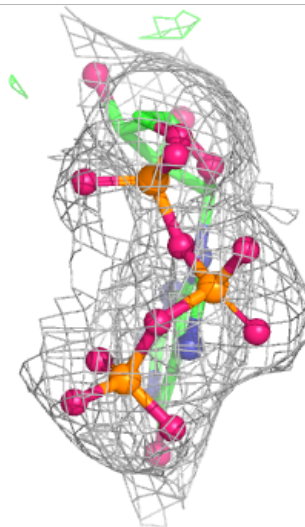
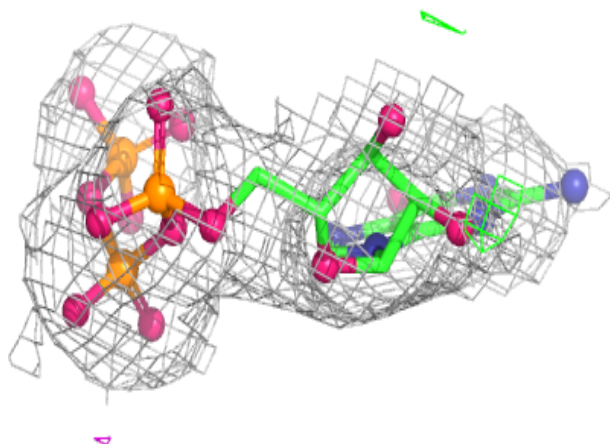
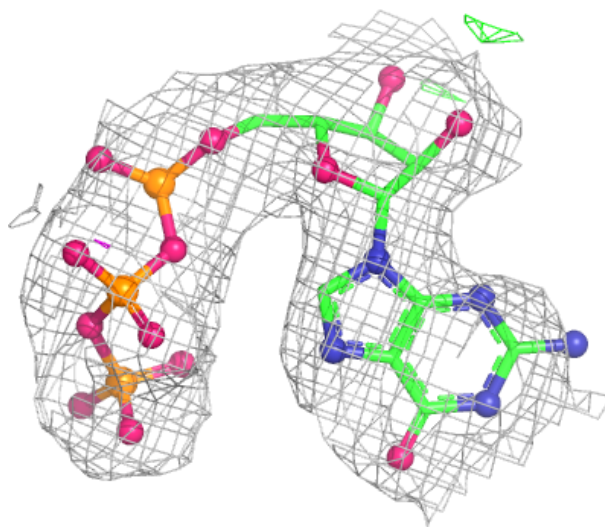
Electron density around GTP D 101:

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



Electron density around GTP 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 [i](#)

There are no such residues in this entry.