Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 03:14 PM JST

PDB ID	:	6JI2
Title	:	Crystal structure of archaeal ribosomal protein aP1, aPelota, and GTP-bound aEF1A complex
Authors	:	Maruyama, K.; Imai, H.; Kawamura, M.; Ishino, S.; Ishino, Y.; Ito, K.; Uchiumi, T.
Deposited on	:	2019-02-20
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

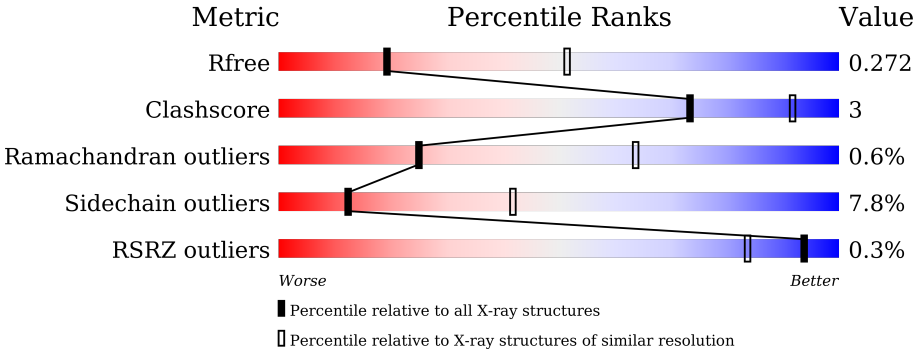
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	447	.% 85% 11% • •
1	E	447	85% 10% • •
2	B	376	81% 12% • 5%
2	F	376	.% 82% 10% • 5%
3	X	17	47% 6% 47%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12541 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 Elongation factor 1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	432	3391	2177	590	611	13	0	0	0
1	E	432	3391	2177	590	611	13	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9YAV0
A	-1	SER	-	expression tag	UNP Q9YAV0
A	0	HIS	-	expression tag	UNP Q9YAV0
A	438	LEU	-	expression tag	UNP Q9YAV0
A	439	ALA	-	expression tag	UNP Q9YAV0
A	440	ARG	-	expression tag	UNP Q9YAV0
A	441	GLY	-	expression tag	UNP Q9YAV0
A	442	SER	-	expression tag	UNP Q9YAV0
A	443	GLY	-	expression tag	UNP Q9YAV0
A	444	CYS	-	expression tag	UNP Q9YAV0
E	-2	GLY	-	expression tag	UNP Q9YAV0
E	-1	SER	-	expression tag	UNP Q9YAV0
E	0	HIS	-	expression tag	UNP Q9YAV0
E	438	LEU	-	expression tag	UNP Q9YAV0
E	439	ALA	-	expression tag	UNP Q9YAV0
E	440	ARG	-	expression tag	UNP Q9YAV0
E	441	GLY	-	expression tag	UNP Q9YAV0
E	442	SER	-	expression tag	UNP Q9YAV0
E	443	GLY	-	expression tag	UNP Q9YAV0
E	444	CYS	-	expression tag	UNP Q9YAV0

- Molecule 2 is a protein called Protein pelota homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	357	2765	1721	522	515	7	0	0	0
2	F	357	2765	1721	522	515	7	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q9YAZ5
B	-18	GLY	-	expression tag	UNP Q9YAZ5
B	-17	SER	-	expression tag	UNP Q9YAZ5
B	-16	SER	-	expression tag	UNP Q9YAZ5
B	-15	HIS	-	expression tag	UNP Q9YAZ5
B	-14	HIS	-	expression tag	UNP Q9YAZ5
B	-13	HIS	-	expression tag	UNP Q9YAZ5
B	-12	HIS	-	expression tag	UNP Q9YAZ5
B	-11	HIS	-	expression tag	UNP Q9YAZ5
B	-10	HIS	-	expression tag	UNP Q9YAZ5
B	-9	SER	-	expression tag	UNP Q9YAZ5
B	-8	SER	-	expression tag	UNP Q9YAZ5
B	-7	GLY	-	expression tag	UNP Q9YAZ5
B	-6	LEU	-	expression tag	UNP Q9YAZ5
B	-5	VAL	-	expression tag	UNP Q9YAZ5
B	-4	PRO	-	expression tag	UNP Q9YAZ5
B	-3	ARG	-	expression tag	UNP Q9YAZ5
B	-2	GLY	-	expression tag	UNP Q9YAZ5
B	-1	SER	-	expression tag	UNP Q9YAZ5
B	0	HIS	-	expression tag	UNP Q9YAZ5
F	-19	MET	-	initiating methionine	UNP Q9YAZ5
F	-18	GLY	-	expression tag	UNP Q9YAZ5
F	-17	SER	-	expression tag	UNP Q9YAZ5
F	-16	SER	-	expression tag	UNP Q9YAZ5
F	-15	HIS	-	expression tag	UNP Q9YAZ5
F	-14	HIS	-	expression tag	UNP Q9YAZ5
F	-13	HIS	-	expression tag	UNP Q9YAZ5
F	-12	HIS	-	expression tag	UNP Q9YAZ5
F	-11	HIS	-	expression tag	UNP Q9YAZ5
F	-10	HIS	-	expression tag	UNP Q9YAZ5
F	-9	SER	-	expression tag	UNP Q9YAZ5
F	-8	SER	-	expression tag	UNP Q9YAZ5
F	-7	GLY	-	expression tag	UNP Q9YAZ5
F	-6	LEU	-	expression tag	UNP Q9YAZ5
F	-5	VAL	-	expression tag	UNP Q9YAZ5

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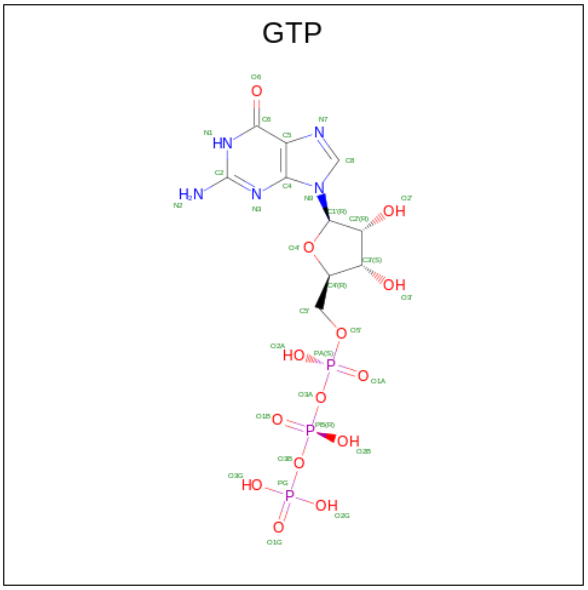
Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	PRO	-	expression tag	UNP Q9YAZ5
F	-3	ARG	-	expression tag	UNP Q9YAZ5
F	-2	GLY	-	expression tag	UNP Q9YAZ5
F	-1	SER	-	expression tag	UNP Q9YAZ5
F	0	HIS	-	expression tag	UNP Q9YAZ5

- Molecule 3 is a protein called Archaeal ribosomal stalk protein aP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	X	9	63	41	9	12	1	0	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	E	1	1	1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	A	1	1	1	0	0
			Total	Na		
6	E	1	1	1	0	0

- Molecule 7 is water.

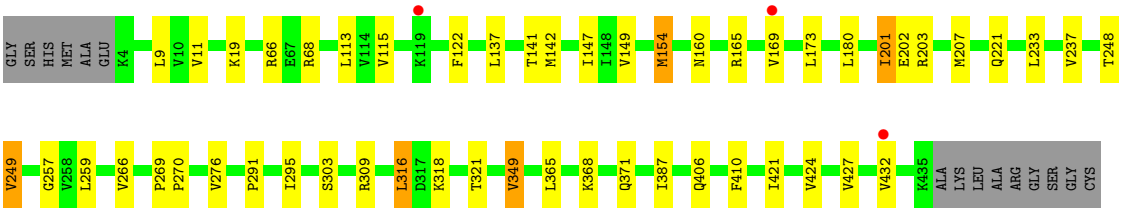
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	20	20	20	0	0
			Total	O		
7	B	31	31	31	0	0
			Total	O		
7	E	24	24	24	0	0
			Total	O		
7	F	22	22	22	0	0
			Total	O		
7	X	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

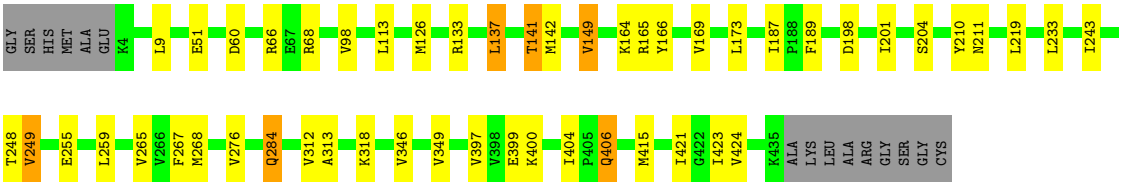
• Molecule 1: Elongation factor 1-alpha

Chain A:



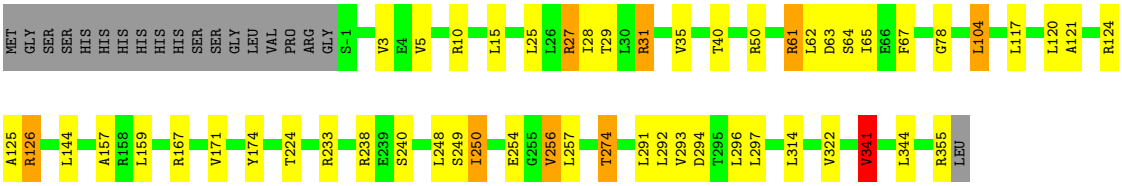
• Molecule 1: Elongation factor 1-alpha

Chain E:



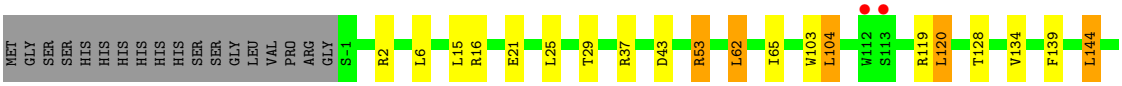
• Molecule 2: Protein pelota homolog

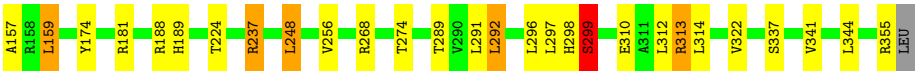
Chain B:



• Molecule 2: Protein pelota homolog

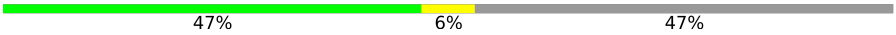
Chain F:





• Molecule 3: Archaeal ribosomal stalk protein aP1

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.45Å 73.41Å 108.14Å 98.64° 93.80° 100.44°	Depositor
Resolution (Å)	106.42 – 3.00 45.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (106.42-3.00) 98.6 (45.66-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.199 , 0.279 0.197 , 0.272	Depositor DCC
R_{free} test set	2154 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	76.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12541	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.38	0/3465	0.64	0/4686
1	E	0.38	0/3465	0.63	0/4686
2	B	0.41	0/2801	0.76	2/3783 (0.1%)
2	F	0.41	0/2801	0.74	1/3783 (0.0%)
3	X	0.60	0/64	0.77	0/81
All	All	0.40	0/12596	0.69	3/17019 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	104	LEU	CA-CB-CG	5.76	128.56	115.30
2	B	104	LEU	CA-CB-CG	5.32	127.53	115.30
2	B	341	VAL	CB-CA-C	-5.18	101.56	111.40

There are no chirality outliers.

There are no planarity outliers.

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	3391	0	3487	22	0
1	E	3391	0	3488	21	0
2	B	2765	0	2867	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2765	0	2867	21	0
3	X	63	0	56	0	0
4	A	32	0	12	0	0
4	E	32	0	12	0	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	20	0	0	0	0
7	B	31	0	0	0	0
7	E	24	0	0	0	0
7	F	22	0	0	0	0
7	X	1	0	0	0	0
All	All	12541	0	12789	82	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 3.

All (82) 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:198:ASP:OD2	1:E:204:SER:OG	1.68	1.09
1:A:169:VAL:O	1:A:173:LEU:HD13	1.82	0.80
2:F:43:ASP:OD1	2:F:53:ARG:HD3	1.84	0.77
2:F:134:VAL:HG13	2:F:139:PHE:HD1	1.54	0.73
1:E:259:LEU:HD11	1:E:276:VAL:HG21	1.75	0.69
2:F:134:VAL:CG1	2:F:139:PHE:HD1	2.09	0.65
2:F:134:VAL:CG1	2:F:139:PHE:CD1	2.80	0.64
1:E:421:ILE:HD12	1:E:421:ILE:C	2.17	0.64
2:B:3:VAL:HG11	2:B:121:ALA:HB2	1.80	0.63
2:F:21:GLU:O	2:F:25:LEU:HD23	1.99	0.63
2:B:157:ALA:HB2	2:B:174:TYR:CE1	2.35	0.62
1:A:141:THR:HG21	1:A:421:ILE:HG21	1.81	0.62
2:B:27:ARG:NH1	2:B:294:ASP:OD2	2.33	0.60
1:E:421:ILE:HD12	1:E:421:ILE:O	2.01	0.60
2:F:292:LEU:CB	2:F:341:VAL:HG12	2.32	0.60
2:B:159:LEU:HD21	2:B:171:VAL:HG12	1.83	0.59
2:F:134:VAL:HG13	2:F:139:PHE:CD1	2.36	0.59
1:A:122:PHE:CE1	1:A:173:LEU:HD11	2.38	0.58
2:B:3:VAL:CG1	2:B:121:ALA:HB2	2.36	0.55
2:F:292:LEU:HB3	2:F:341:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:423:ILE:HG13	1:E:423:ILE:O	2.07	0.55
1:A:137:LEU:O	1:A:141:THR:HG23	2.06	0.55
2:F:144:LEU:HD12	2:F:248:LEU:HD23	1.88	0.54
1:A:259:LEU:HD11	1:A:276:VAL:HG21	1.90	0.54
2:F:310:GLU:OE1	2:F:313:ARG:NH2	2.40	0.54
1:A:349:VAL:HG13	1:A:410:PHE:HB3	1.91	0.53
2:B:157:ALA:HB2	2:B:174:TYR:CZ	2.44	0.53
2:B:27:ARG:HG3	2:B:67:PHE:HB3	1.91	0.53
1:A:248:THR:HG21	1:A:303:SER:HA	1.90	0.53
1:E:169:VAL:O	1:E:173:LEU:HD13	2.08	0.53
2:F:298:HIS:O	2:F:299:SER:O	2.27	0.52
2:F:157:ALA:HB1	2:F:159:LEU:HD13	1.91	0.52
1:A:249:VAL:HG22	1:A:249:VAL:O	2.09	0.52
1:E:400:LYS:HA	1:E:424:VAL:HG22	1.91	0.52
1:A:173:LEU:N	1:A:173:LEU:CD1	2.73	0.51
2:F:296:LEU:CD1	2:F:341:VAL:HG13	2.41	0.50
1:E:284:GLN:HE21	1:E:284:GLN:HA	1.75	0.50
1:E:415:MET:SD	2:F:237:ARG:NH1	2.85	0.49
2:B:35:VAL:HG22	2:B:61:ARG:HA	1.95	0.49
2:B:249:SER:O	2:B:250:ILE:C	2.51	0.49
1:A:365:LEU:HD11	1:A:387:ILE:HD11	1.94	0.48
1:A:11:VAL:HG12	1:A:19:LYS:HG2	1.94	0.48
2:B:296:LEU:CD1	2:B:341:VAL:HG22	2.45	0.47
2:F:16:ARG:HD2	2:F:103:TRP:CE2	2.50	0.46
2:F:25:LEU:HD12	2:F:119:ARG:O	2.16	0.46
1:E:399:GLU:HG2	1:E:404:ILE:HD12	1.98	0.46
2:F:128:THR:HG21	2:F:189:HIS:HB3	1.97	0.46
1:A:122:PHE:HE1	1:A:173:LEU:HD11	1.79	0.45
1:A:349:VAL:CG1	1:A:410:PHE:HB3	2.46	0.45
2:F:29:THR:HG21	2:F:120:LEU:HD13	1.98	0.45
2:B:5:VAL:HG11	2:B:10:ARG:NH2	2.31	0.45
1:E:9:LEU:HD11	1:E:219:LEU:HD22	1.98	0.45
1:A:266:VAL:HB	1:A:316:LEU:HD22	1.98	0.44
1:E:421:ILE:C	1:E:421:ILE:CD1	2.85	0.44
2:F:298:HIS:O	2:F:299:SER:C	2.55	0.44
2:F:157:ALA:HB2	2:F:174:TYR:CE1	2.53	0.43
2:B:28:ILE:O	2:B:31:ARG:NH1	2.50	0.43
2:B:124:ARG:O	2:B:126:ARG:N	2.52	0.43
2:B:248:LEU:O	2:B:249:SER:C	2.57	0.43
2:B:25:LEU:HD13	2:B:28:ILE:HD11	2.00	0.43
1:A:321:THR:HG21	1:A:427:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ASP:HB2	2:B:78:GLY:HA2	2.01	0.42
1:E:126:MET:O	1:E:133:ARG:NH1	2.52	0.42
1:A:154:MET:HG2	1:A:207:MET:SD	2.59	0.42
1:A:173:LEU:N	1:A:173:LEU:HD12	2.35	0.42
1:E:60:ASP:O	1:E:66:ARG:NH2	2.53	0.42
1:A:237:VAL:HG23	1:A:309:ARG:HA	2.01	0.41
1:E:137:LEU:O	1:E:141:THR:HG23	2.21	0.41
1:E:149:VAL:HG11	1:E:189:PHE:CE2	2.55	0.41
1:A:365:LEU:HD11	1:A:387:ILE:CD1	2.49	0.41
2:B:256:VAL:HG22	2:B:257:LEU:N	2.35	0.41
1:E:255:GLU:HB3	1:E:406:GLN:HG3	2.03	0.41
2:B:29:THR:HG21	2:B:120:LEU:HD13	2.01	0.41
2:B:167:ARG:O	2:B:171:VAL:HG13	2.20	0.41
1:A:201:ILE:HG12	1:A:202:GLU:HG3	2.03	0.41
1:E:312:VAL:HG21	1:E:397:VAL:HG11	2.03	0.41
1:E:267:PHE:CE2	1:E:313:ALA:HB2	2.56	0.41
2:F:62:LEU:HD23	2:F:65:ILE:HD11	2.03	0.41
1:A:269:PRO:N	1:A:270:PRO:CD	2.84	0.40
1:E:243:ILE:HD12	1:E:249:VAL:HG11	2.04	0.40
1:A:257:GLY:O	1:A:291:PRO:HD3	2.22	0.40
1:E:166:TYR:HA	1:E:169:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	430/447 (96%)	401 (93%)	28 (6%)	1 (0%)	47 82
1	E	430/447 (96%)	413 (96%)	14 (3%)	3 (1%)	22 60
2	B	355/376 (94%)	341 (96%)	11 (3%)	3 (1%)	19 57
2	F	355/376 (94%)	340 (96%)	13 (4%)	2 (1%)	25 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	X	7/17 (41%)	2 (29%)	4 (57%)	1 (14%)	0	1
All	All	1577/1663 (95%)	1497 (95%)	70 (4%)	10 (1%)	25	64

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	125	ALA
1	E	51	GLU
1	E	210	TYR
1	E	211	ASN
2	F	299	SER
1	A	432	VAL
2	B	274	THR
2	B	250	ILE
2	F	274	THR
3	X	104	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/378 (98%)	344 (93%)	25 (7%)	16	48
1	E	369/378 (98%)	348 (94%)	21 (6%)	20	56
2	B	295/311 (95%)	266 (90%)	29 (10%)	8	30
2	F	295/311 (95%)	266 (90%)	29 (10%)	8	30
3	X	6/14 (43%)	6 (100%)	0	100	100
All	All	1334/1392 (96%)	1230 (92%)	104 (8%)	12	42

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	66	ARG

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Mol	Chain	Res	Type
1	A	68	ARG
1	A	113	LEU
1	A	115	VAL
1	A	142	MET
1	A	147	ILE
1	A	149	VAL
1	A	154	MET
1	A	160	ASN
1	A	165	ARG
1	A	180	LEU
1	A	201	ILE
1	A	203	ARG
1	A	221	GLN
1	A	233	LEU
1	A	249	VAL
1	A	295	ILE
1	A	316	LEU
1	A	318	LYS
1	A	349	VAL
1	A	368	LYS
1	A	371	GLN
1	A	406	GLN
1	A	424	VAL
2	B	15	LEU
2	B	27	ARG
2	B	31	ARG
2	B	40	THR
2	B	50	ARG
2	B	61	ARG
2	B	62	LEU
2	B	64	SER
2	B	65	ILE
2	B	104	LEU
2	B	117	LEU
2	B	126	ARG
2	B	144	LEU
2	B	224	THR
2	B	233	ARG
2	B	238	ARG
2	B	240	SER
2	B	254	GLU
2	B	256	VAL

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Mol	Chain	Res	Type
2	B	274	THR
2	B	291	LEU
2	B	292	LEU
2	B	293	VAL
2	B	297	LEU
2	B	314	LEU
2	B	322	VAL
2	B	341	VAL
2	B	344	LEU
2	B	355	ARG
1	E	68	ARG
1	E	98	VAL
1	E	113	LEU
1	E	137	LEU
1	E	141	THR
1	E	142	MET
1	E	149	VAL
1	E	164	LYS
1	E	165	ARG
1	E	187	ILE
1	E	201	ILE
1	E	233	LEU
1	E	248	THR
1	E	249	VAL
1	E	265	VAL
1	E	268	MET
1	E	284	GLN
1	E	318	LYS
1	E	346	VAL
1	E	349	VAL
1	E	406	GLN
2	F	2	ARG
2	F	6	LEU
2	F	15	LEU
2	F	37	ARG
2	F	53	ARG
2	F	62	LEU
2	F	104	LEU
2	F	120	LEU
2	F	144	LEU
2	F	159	LEU
2	F	181	ARG

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Mol	Chain	Res	Type
2	F	188	ARG
2	F	224	THR
2	F	237	ARG
2	F	248	LEU
2	F	256	VAL
2	F	268	ARG
2	F	289	THR
2	F	291	LEU
2	F	292	LEU
2	F	297	LEU
2	F	299	SER
2	F	312	LEU
2	F	313	ARG
2	F	314	LEU
2	F	322	VAL
2	F	337	SER
2	F	344	LEU
2	F	355	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	183	GLN
1	A	376	ASN
1	A	378	GLN
1	E	284	GLN
2	F	68	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	GTP	A	501	5,6	26,34,34	0.91	0	32,54,54	1.43	5 (15%)
4	GTP	E	501	5,6	26,34,34	0.95	1 (3%)	32,54,54	1.28	4 (12%)

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
4	GTP	A	501	5,6	-	0/18/38/38	0/3/3/3
4	GTP	E	501	5,6	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	501	GTP	C6-N1	-2.29	1.34	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	GTP	PB-O3B-PG	-3.98	119.16	132.83
4	E	501	GTP	PB-O3B-PG	-3.48	120.88	132.83
4	A	501	GTP	PA-O3A-PB	-3.05	122.34	132.83
4	A	501	GTP	C8-N7-C5	2.51	107.77	102.99
4	E	501	GTP	C8-N7-C5	2.46	107.67	102.99
4	E	501	GTP	PA-O3A-PB	-2.39	124.62	132.83
4	E	501	GTP	C5-C6-N1	2.25	117.93	113.95
4	A	501	GTP	C5-C6-N1	2.24	117.91	113.95
4	A	501	GTP	O3G-PG-O2G	2.11	115.69	107.64

There are no chirality outliers.

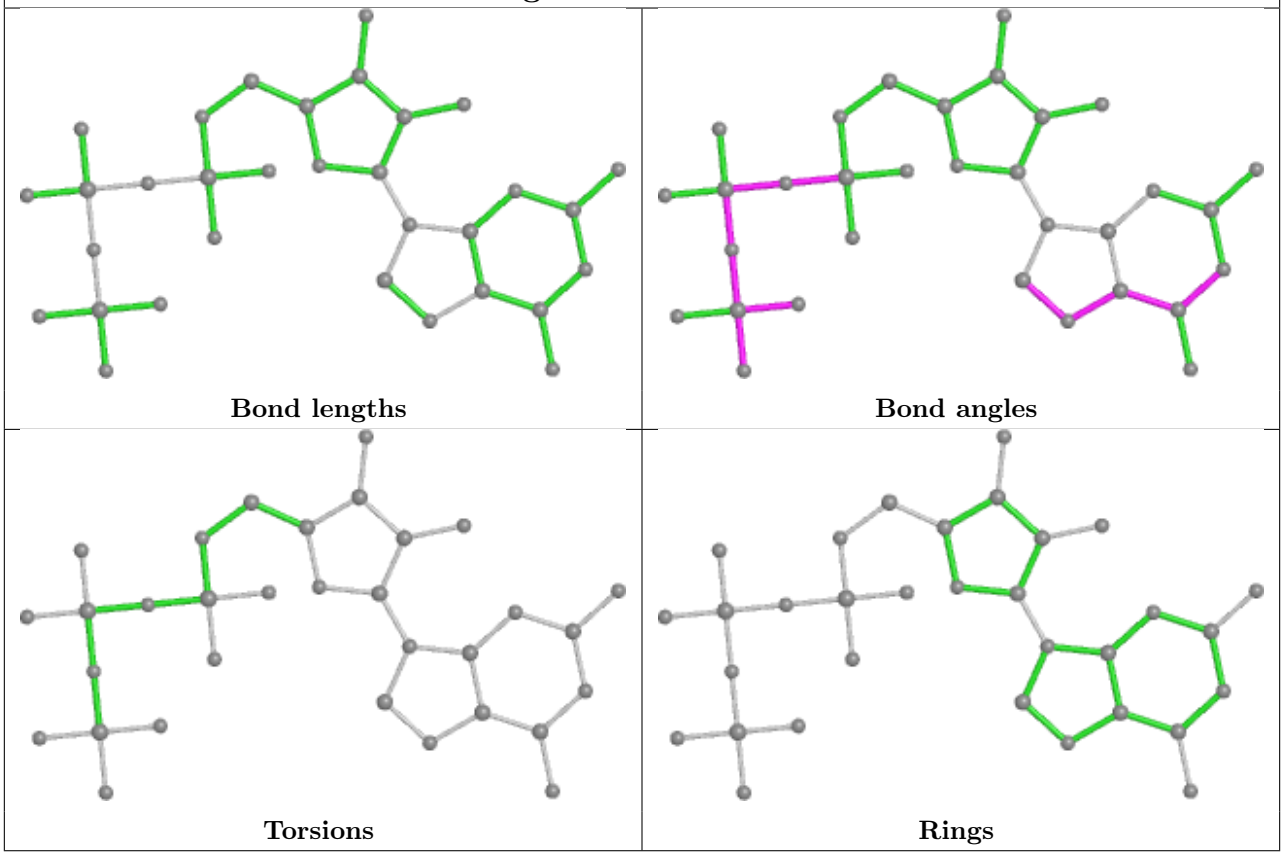
There are no torsion outliers.

There are no ring outliers.

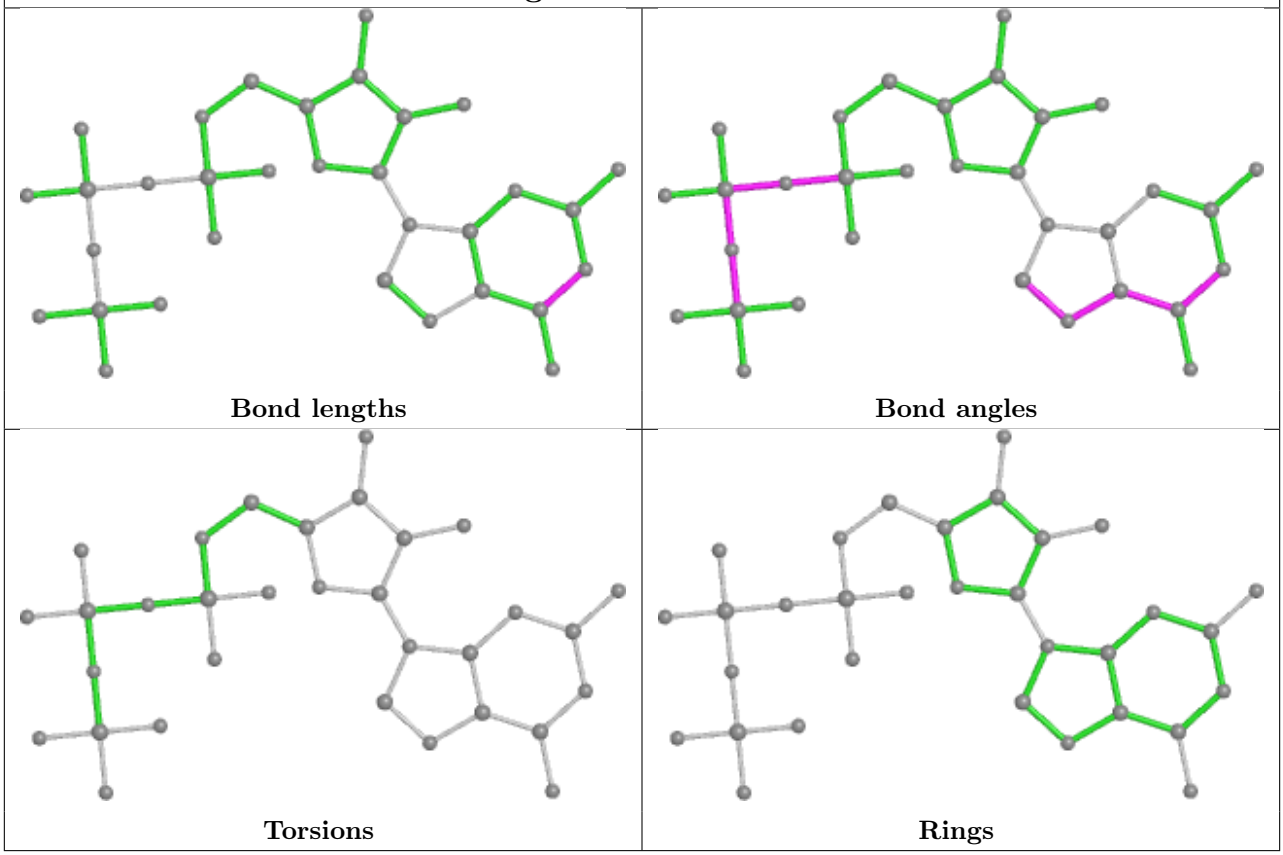
No monomer is involved in short contacts.

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

Ligand GTP A 501



Ligand GTP E 501



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	432/447 (96%)	-0.19	3 (0%) 87 69	56, 79, 114, 139	0
1	E	432/447 (96%)	-0.30	0 100 100	56, 78, 112, 127	0
2	B	357/376 (94%)	-0.30	0 100 100	53, 75, 100, 123	0
2	F	357/376 (94%)	-0.33	2 (0%) 89 72	60, 80, 113, 127	0
3	X	9/17 (52%)	0.18	0 100 100	95, 101, 106, 108	0
All	All	1587/1663 (95%)	-0.27	5 (0%) 94 84	53, 78, 111, 139	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	112	TRP	3.2
1	A	119	LYS	2.9
1	A	432	VAL	2.6
1	A	169	VAL	2.0
2	F	113	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

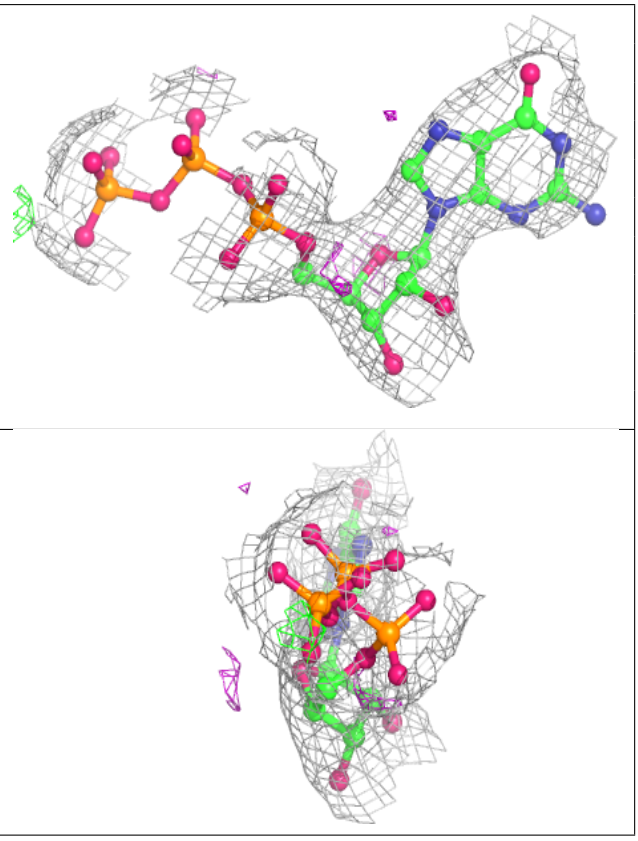
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	E	503	1/1	0.94	0.11	71,71,71,71	0
4	GTP	E	501	32/32	0.96	0.18	65,82,98,101	0
6	NA	A	503	1/1	0.97	0.14	60,60,60,60	0
4	GTP	A	501	32/32	0.97	0.16	65,73,84,85	0
5	MG	E	502	1/1	0.98	0.11	52,52,52,52	0
5	MG	A	502	1/1	1.00	0.16	64,64,64,64	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.

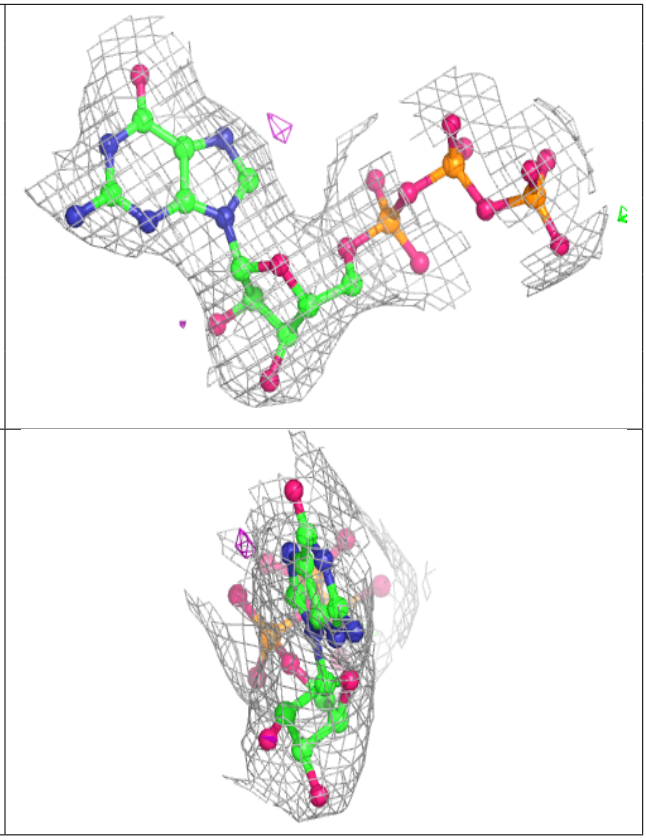
Electron density around GTP E 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GTP A 501:

$2mF_o$-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.