wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 03:11 AM EDT

PDB ID	:	1T91
Title	:	crystal structure of human small GTPase Rab7(GTP)
Authors	:	Song, H.; Hong, W.; Wu, M.; Wang, T.
Deposited on	:	2004-05-14
Resolution	:	1.90 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 (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:

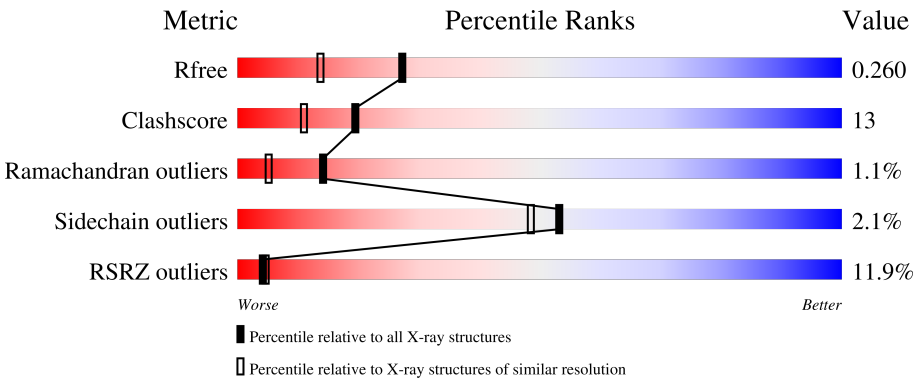
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	207	8% 65% 19% 15%
1	B	207	8% 65% 20% 15%
1	C	207	9% 66% 18% • 15%
1	D	207	16% 67% 17% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GTP	A	1401	-	-	X	-
3	GTP	B	1402	-	-	X	-
3	GTP	D	1404	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6251 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 Ras-related protein Rab-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	176	1404	896	236	266	6	0	0	0
1	B	176	1404	896	236	266	6	0	0	0
1	C	176	1404	896	236	266	6	0	0	0
1	D	176	1404	896	236	266	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

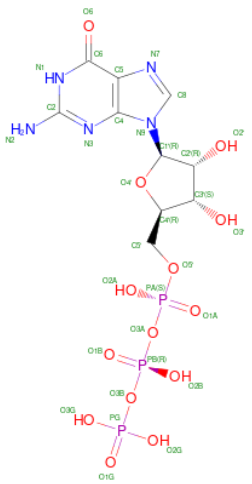
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	LEU	GLN	engineered mutation	UNP P51149
B	67	LEU	GLN	engineered mutation	UNP P51149
C	67	LEU	GLN	engineered mutation	UNP P51149
D	67	LEU	GLN	engineered mutation	UNP P51149

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP



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

- Molecule 4 is water.

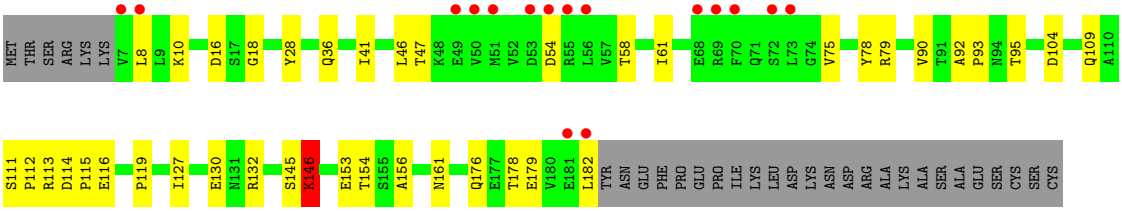
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	122	122	122	0	0
4	B	131	131	131	0	0
4	C	131	131	131	0	0
4	D	119	119	119	0	0

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.

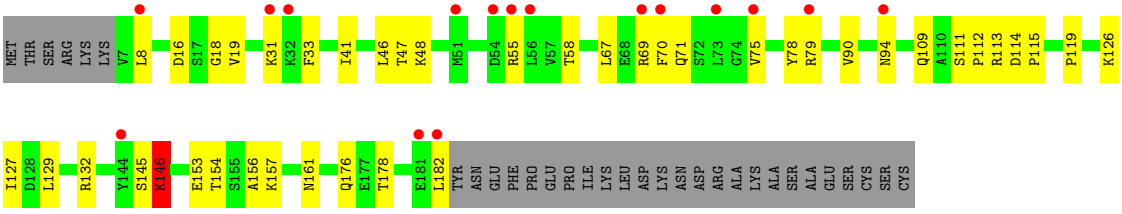
• Molecule 1: Ras-related protein Rab-7

Chain A:



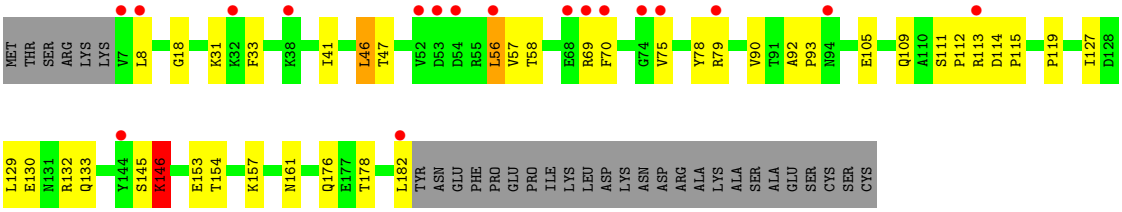
• Molecule 1: Ras-related protein Rab-7

Chain B:



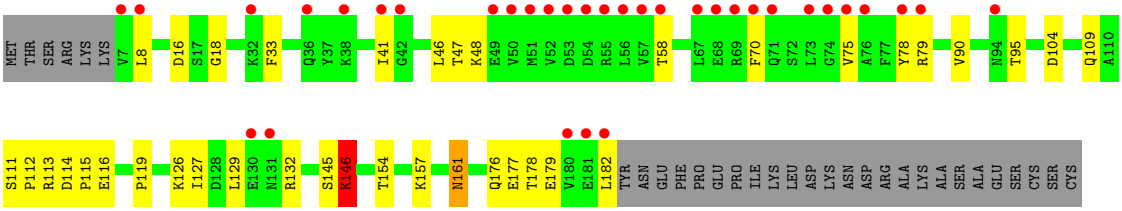
• Molecule 1: Ras-related protein Rab-7

Chain C:



• Molecule 1: Ras-related protein Rab-7

Chain D:


MET
THR
SER
ARG
LYS
LYS
V7
L8
D16
S17
G18
K32
F33
Q36
Y37
K38
I41
G42
L46
T47
K48
E49
V50
M51
V52
D53
D54
R55
L56
V57
T58
L67
E68
R69
F70
Q71
S72
L73
G74
V75
A76
F77
Y78
R79
V90
N94
T95
D104
Q109
A110
S111
P112
R113
D114
P115
E116
P119
K126
I127
D128
L129
E130
M131
R132
S145
K146
T154
K157
N161
Q176
E177
T178
E179
V180
E181
L182
TYR
ASN
GLU
PHE
PRO
GLU
PRO
ILE
LYS
LEU
ASP
LYS
ASN
ASP
ARG
ALA
LYS
ALA
SER
ALA
GLU
SER
CYS
SER
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.70Å 56.78Å 74.51Å 71.51° 71.72° 77.75°	Depositor
Resolution (Å)	20.00 – 1.90 33.05 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-1.90) 93.7 (33.05-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.243 , 0.247 0.252 , 0.260	Depositor DCC
R_{free} test set	1883 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 28.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.467 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6251	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2581e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MG, GTP

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	0.35	0/1430	0.64	2/1937 (0.1%)
1	B	0.35	0/1430	0.64	2/1937 (0.1%)
1	C	0.35	0/1430	0.64	2/1937 (0.1%)
1	D	0.35	0/1430	0.64	2/1937 (0.1%)
All	All	0.35	0/5720	0.64	8/7748 (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	B	0	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	113	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	C	113	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	113	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	113	ARG	NE-CZ-NH1	-6.65	116.98	120.30
1	A	113	ARG	NE-CZ-NH1	6.57	123.58	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	55	ARG	Sidechain

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	1404	0	1395	30	0
1	B	1404	0	1395	32	0
1	C	1404	0	1395	30	0
1	D	1404	0	1395	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	32	0	11	9	0
3	B	32	0	11	11	0
3	C	32	0	11	8	0
3	D	32	0	11	11	0
4	A	122	0	0	8	0
4	B	131	0	0	7	0
4	C	131	0	0	6	0
4	D	119	0	0	4	0
All	All	6251	0	5624	145	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 145 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)
3:B:1402:GTP:C1'	3:B:1402:GTP:N9	1.68	1.57
3:C:1403:GTP:C1'	3:C:1403:GTP:N9	1.68	1.56
3:A:1401:GTP:C1'	3:A:1401:GTP:N9	1.68	1.55
3:D:1404:GTP:C1'	3:D:1404:GTP:N9	1.68	1.51
3:A:1401:GTP:N9	3:A:1401:GTP:C2'	2.40	0.85

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	174/207 (84%)	169 (97%)	3 (2%)	2 (1%)	14	5
1	B	174/207 (84%)	169 (97%)	3 (2%)	2 (1%)	14	5
1	C	174/207 (84%)	168 (97%)	4 (2%)	2 (1%)	14	5
1	D	174/207 (84%)	169 (97%)	3 (2%)	2 (1%)	14	5
All	All	696/828 (84%)	675 (97%)	13 (2%)	8 (1%)	14	5

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	ARG
1	C	79	ARG
1	A	79	ARG
1	A	146	LYS
1	D	146	LYS

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	153/181 (84%)	150 (98%)	3 (2%)	55	51
1	B	153/181 (84%)	150 (98%)	3 (2%)	55	51
1	C	153/181 (84%)	149 (97%)	4 (3%)	46	39
1	D	153/181 (84%)	150 (98%)	3 (2%)	55	51
All	All	612/724 (84%)	599 (98%)	13 (2%)	53	48

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	56	LEU
1	C	146	LYS
1	D	161	ASN
1	D	46	LEU
1	D	146	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	94	ASN
1	C	133	GLN
1	D	161	ASN
1	D	35	ASN
1	D	36	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	GTP	B	1402	2	26,34,34	3.78	9 (34%)	32,54,54	2.03	5 (15%)
3	GTP	D	1404	2	26,34,34	3.77	10 (38%)	32,54,54	2.03	5 (15%)
3	GTP	C	1403	2	26,34,34	3.78	10 (38%)	32,54,54	2.03	5 (15%)
3	GTP	A	1401	2	26,34,34	3.78	9 (34%)	32,54,54	2.03	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	B	1402	2	-	2/18/38/38	0/3/3/3
3	GTP	D	1404	2	-	2/18/38/38	0/3/3/3
3	GTP	C	1403	2	-	2/18/38/38	0/3/3/3
3	GTP	A	1401	2	-	2/18/38/38	0/3/3/3

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1403	GTP	C2'-C1'	-14.35	1.32	1.53
3	A	1401	GTP	C2'-C1'	-14.34	1.32	1.53
3	B	1402	GTP	C2'-C1'	-14.33	1.32	1.53
3	D	1404	GTP	C2'-C1'	-14.32	1.32	1.53
3	A	1401	GTP	C3'-C4'	-8.99	1.30	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1403	GTP	O4'-C4'-C3'	7.91	120.76	105.11
3	A	1401	GTP	O4'-C4'-C3'	7.90	120.75	105.11
3	D	1404	GTP	O4'-C4'-C3'	7.89	120.73	105.11
3	B	1402	GTP	O4'-C4'-C3'	7.89	120.73	105.11
3	C	1403	GTP	PB-O3B-PG	-4.39	117.77	132.83

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1401	GTP	PA-O3A-PB-O1B
3	B	1402	GTP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	C	1403	GTP	PA-O3A-PB-O1B
3	D	1404	GTP	PA-O3A-PB-O1B
3	A	1401	GTP	PA-O3A-PB-O2B

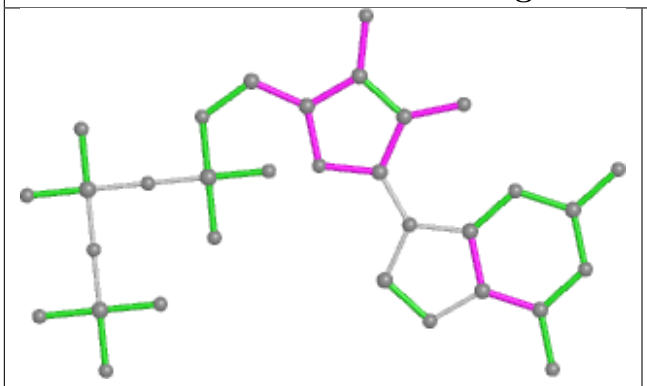
There are no ring outliers.

4 monomers are involved in 39 short contacts:

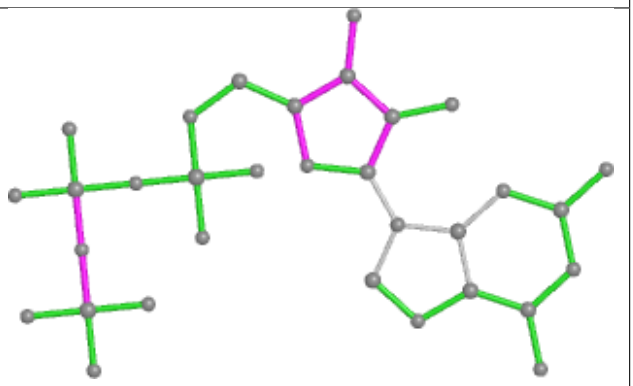
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1402	GTP	11	0
3	D	1404	GTP	11	0
3	C	1403	GTP	8	0
3	A	1401	GTP	9	0

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

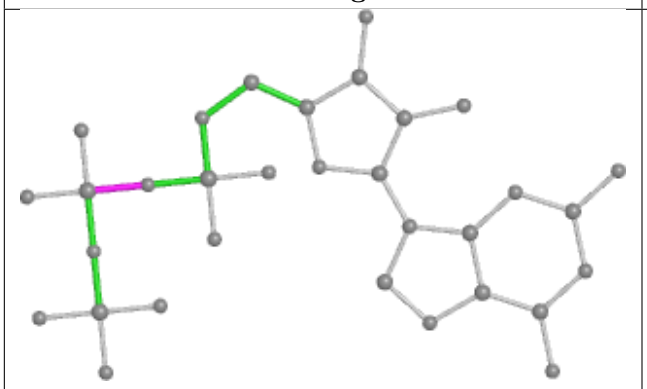
Ligand GTP B 1402



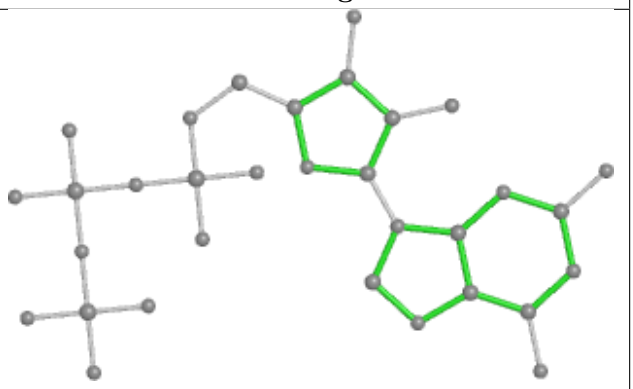
Bond lengths



Bond angles

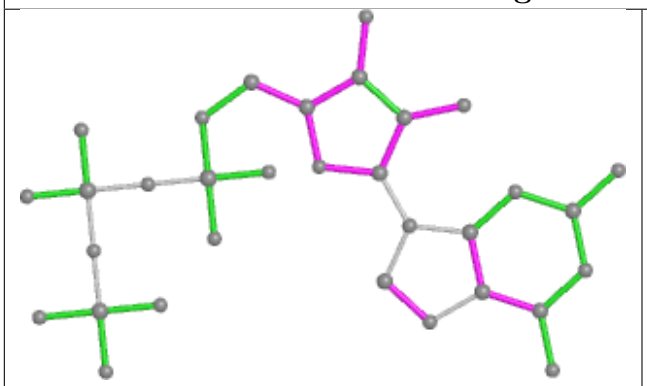


Torsions

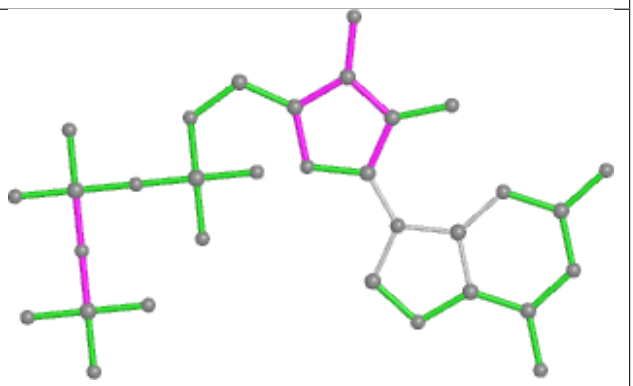


Rings

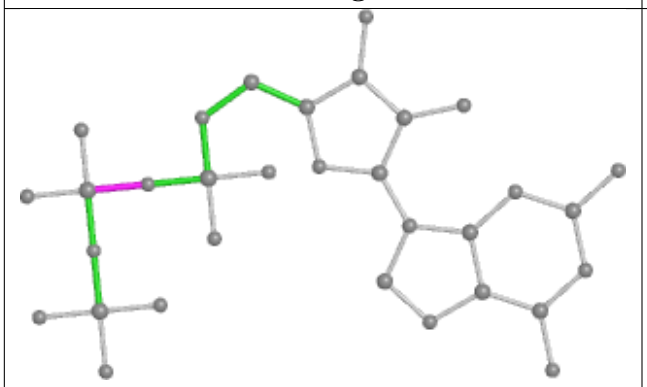
Ligand GTP D 1404



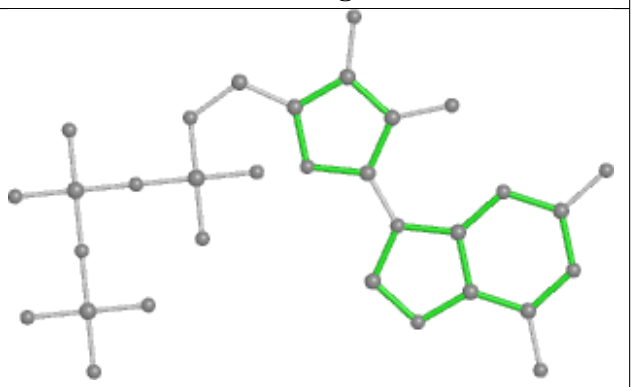
Bond lengths



Bond angles

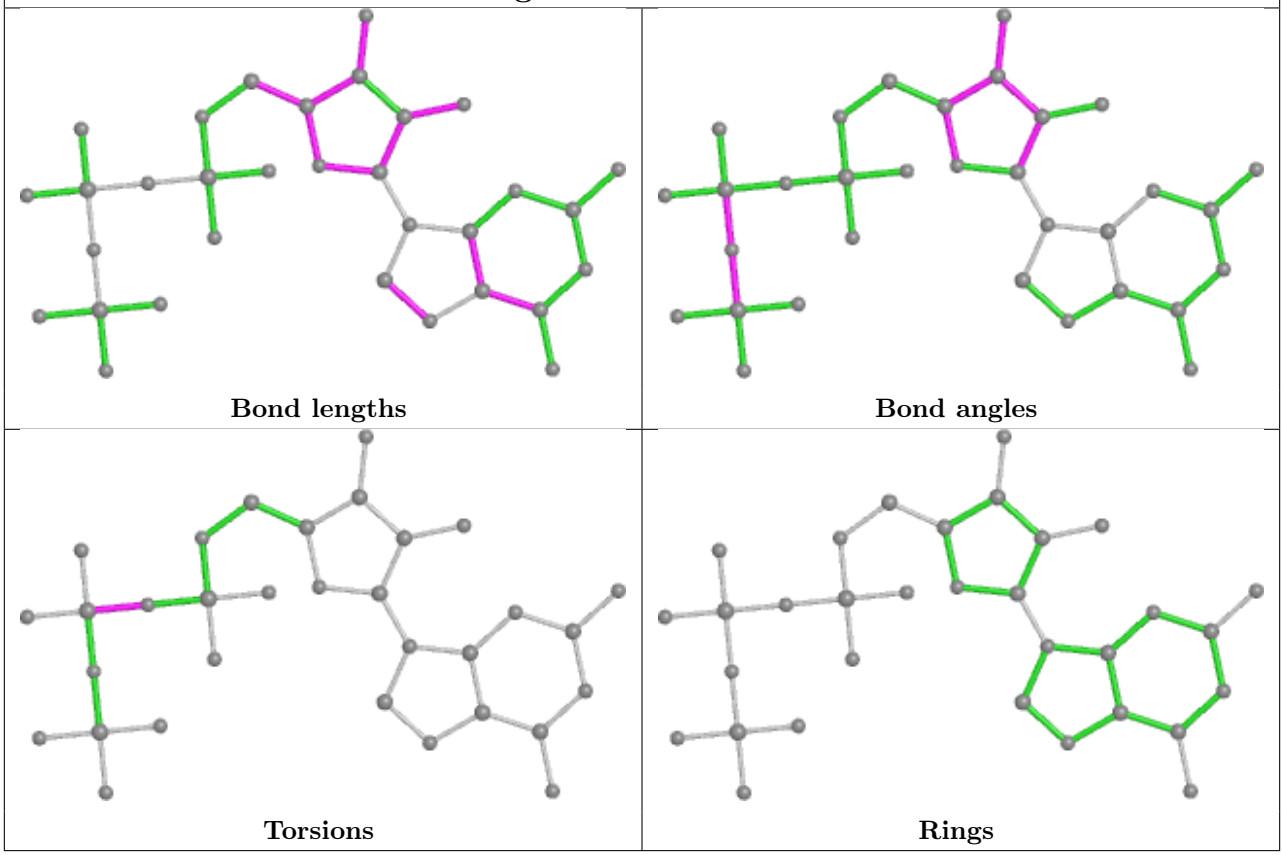


Torsions

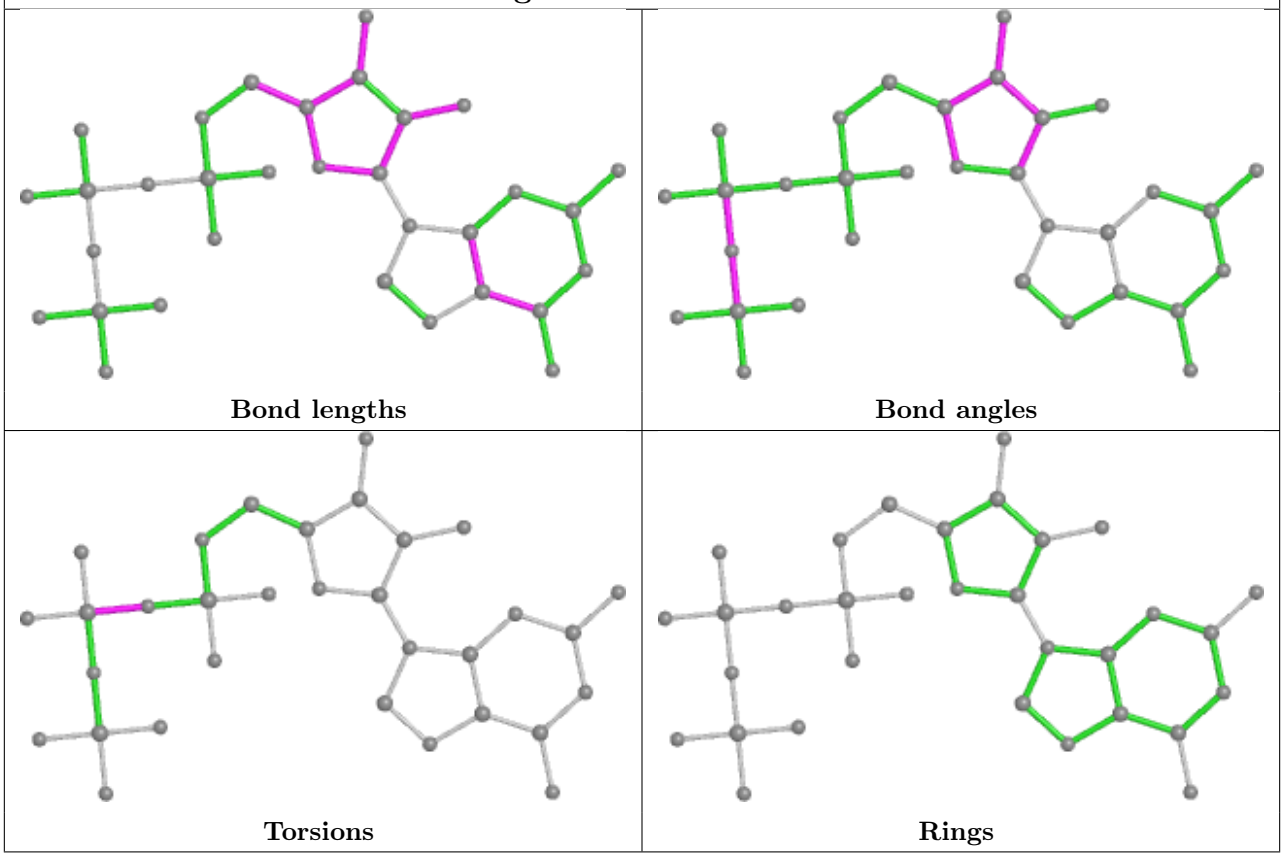


Rings

Ligand GTP C 1403



Ligand GTP A 1401



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	176/207 (85%)	0.38	16 (9%)	9	10	6, 12, 20, 23	0
1	B	176/207 (85%)	0.85	16 (9%)	9	10	18, 26, 36, 41	0
1	C	176/207 (85%)	0.85	18 (10%)	6	8	17, 26, 36, 41	0
1	D	176/207 (85%)	1.02	34 (19%)	1	1	16, 26, 37, 40	0
All	All	704/828 (85%)	0.77	84 (11%)	4	5	6, 24, 36, 41	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	70	PHE	8.8
1	D	69	ARG	7.2
1	D	73	LEU	7.2
1	A	70	PHE	6.4
1	A	69	ARG	5.9

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)

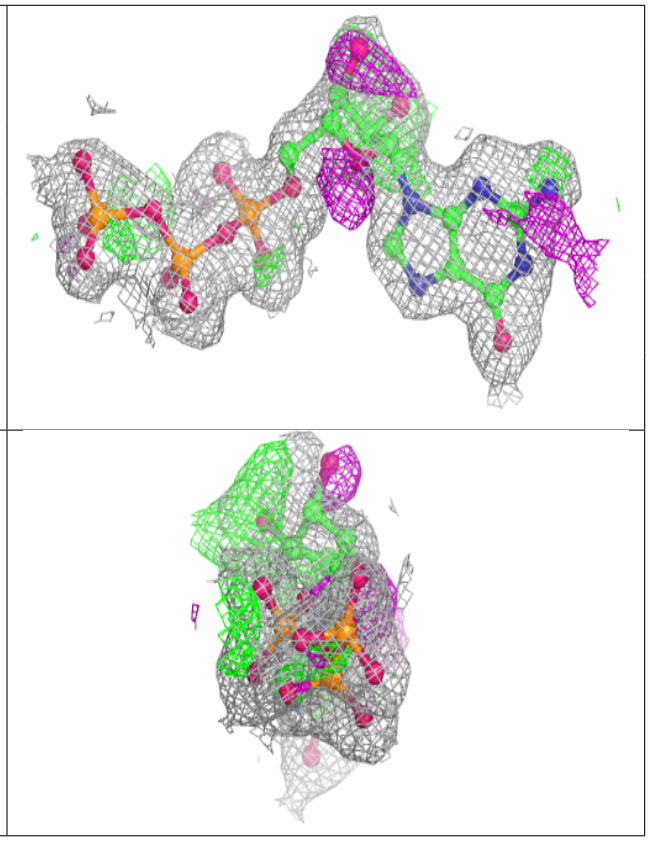
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	1302	1/1	0.85	0.14	27,27,27,27	0
2	MG	A	1301	1/1	0.87	0.15	25,25,25,25	0
2	MG	D	1304	1/1	0.88	0.15	25,25,25,25	0
2	MG	C	1303	1/1	0.89	0.14	27,27,27,27	0
3	GTP	A	1401	32/32	0.89	0.17	18,25,33,41	0
3	GTP	B	1402	32/32	0.89	0.18	18,29,38,45	0
3	GTP	C	1403	32/32	0.89	0.17	18,27,36,43	0
3	GTP	D	1404	32/32	0.89	0.20	19,25,33,44	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.

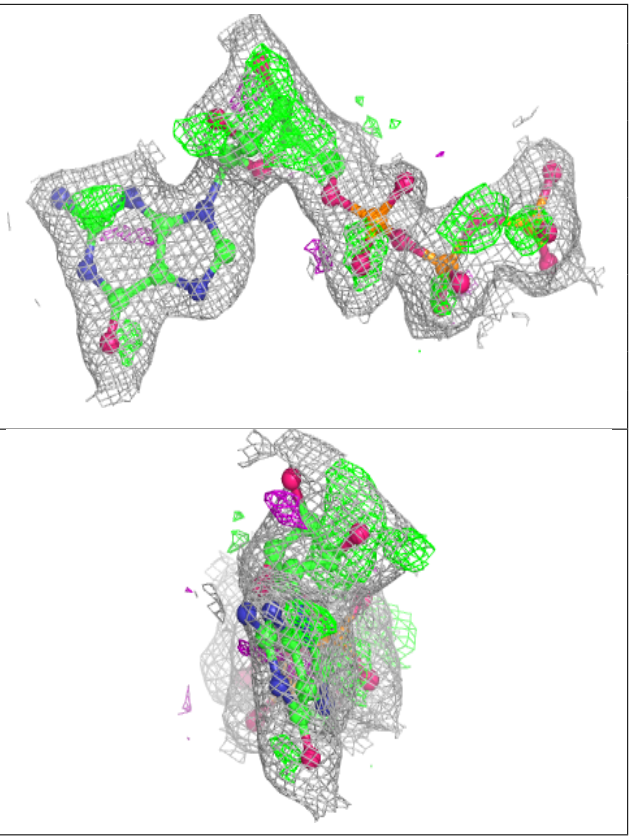
Electron density around GTP A 1401:

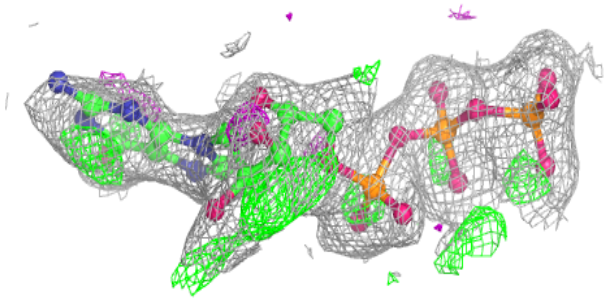
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GTP B 1402:

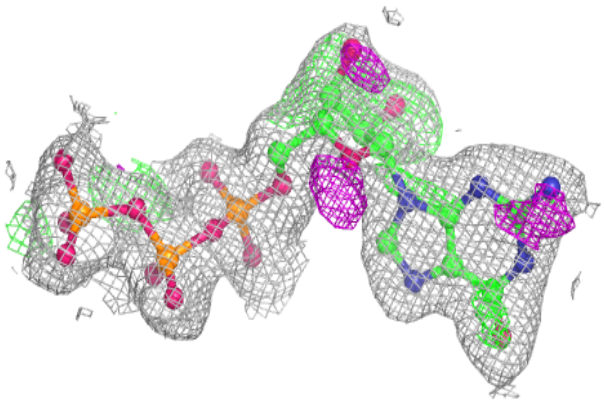
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

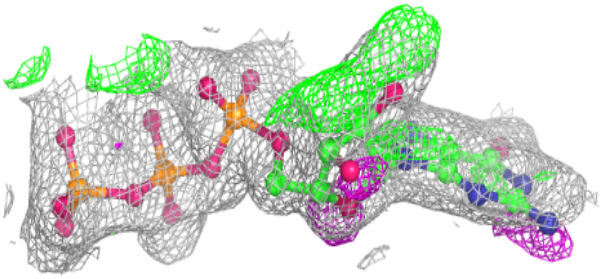


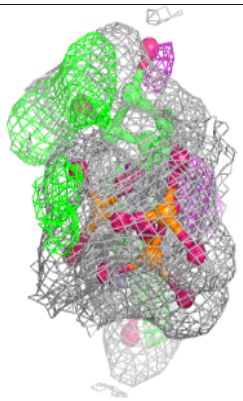


Electron density around GTP C 1403:

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

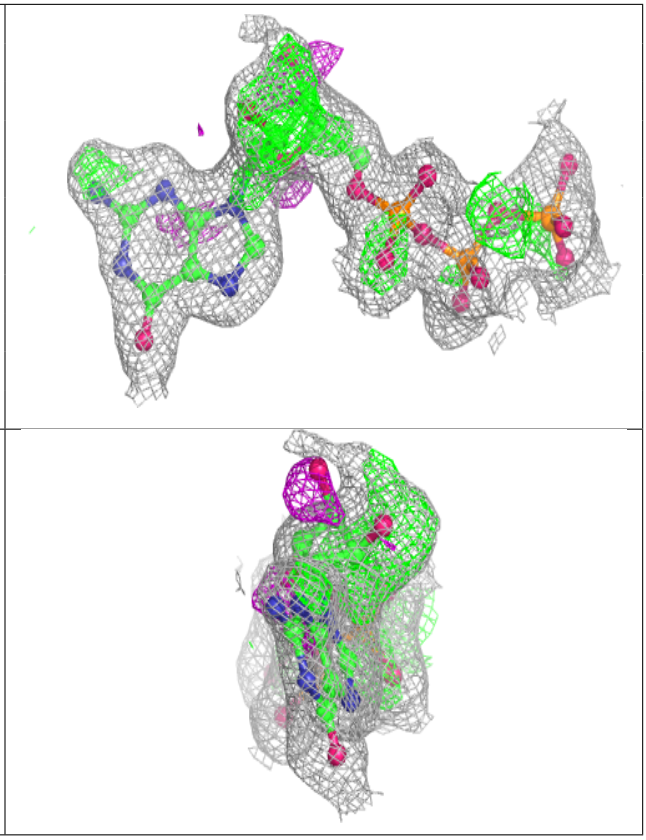






Electron density around GTP D 1404:

$2mF_o$-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.