



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:50 am BST

PDB ID : 4JYB  
Title : MeaB, A Bacterial Homolog of MMAA, Bound to GMPPNP  
Authors : Koutmos, M.; Lofgren, M.; Padovani, D.; Banerjee, R.  
Deposited on : 2013-03-29  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray

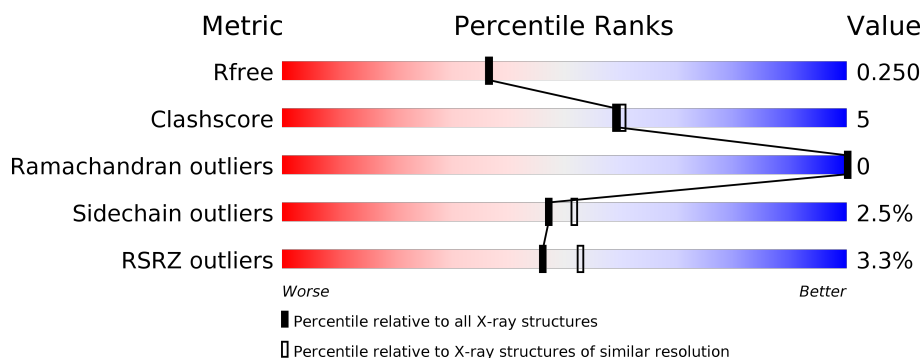
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10014 atoms, of which 4896 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 Methylmalonyl-CoA mutase accessory protein.













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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:HD3	1:B:42:ARG:HA	1.64	0.45
1:B:188:LYS:O	1:B:191:ILE:HG12	2.16	0.45
1:B:137:ARG:NH1	1:B:276:ASP:OD1	2.45	0.45
1:A:184:LEU:HD11	1:A:219:TYR:CZ	2.52	0.45
1:B:293:VAL:HG12	1:B:299:ARG:HG3	1.97	0.45
1:B:56:ILE:HG12	1:B:259[A]:ARG:HD2	1.98	0.45
1:A:34:ARG:NH2	3:A:622:HOH:O	2.50	0.44
1:A:20[B]:ARG:NH2	1:A:116:ARG:O	2.41	0.44
1:A:44:LEU:HD23	1:A:44:LEU:C	2.38	0.44
1:A:304:GLU:HG2	1:A:307[A]:ARG:HH21	1.82	0.44
1:A:133:ALA:O	1:A:168:LEU:HD21	2.19	0.43
1:A:192:PHE:HB3	1:B:193:GLU:CD	2.39	0.42
1:B:42:ARG:NH2	3:B:635:HOH:O	2.52	0.42
1:B:44:LEU:C	1:B:44:LEU:HD23	2.40	0.41
1:A:41:VAL:O	1:A:41:VAL:HG22	2.21	0.41
1:B:279:TRP:HA	1:B:279:TRP:CE3	2.57	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	324/337 (96%)	322 (99%)	2 (1%)	0	100	100
1	B	315/337 (94%)	306 (97%)	9 (3%)	0	100	100
All	All	639/674 (95%)	628 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	243/253 (96%)	234 (96%)	9 (4%)	34	35
1	B	239/253 (94%)	236 (99%)	3 (1%)	69	75
All	All	482/506 (95%)	470 (98%)	12 (2%)	47	52

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	68	LYS
1	A	97	ARG
1	A	107	THR
1	A	108	ARG
1	A	218	GLU
1	A	230	SER
1	A	232	THR
1	A	299	ARG
1	B	63	VAL
1	B	137	ARG
1	B	299	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GNP	B	401	-	28,34,34	2.74	9 (32%)	30,54,54	1.38	4 (13%)
2	GNP	A	401	-	28,34,34	2.89	8 (28%)	30,54,54	1.32	5 (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
2	GNP	B	401	-	-	3/17/38/38	0/3/3/3
2	GNP	A	401	-	-	3/17/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GNP	C4-N9	-11.66	1.32	1.47
2	B	401	GNP	C4-N9	-10.85	1.33	1.47
2	A	401	GNP	PG-N3B	5.61	1.78	1.63
2	B	401	GNP	PG-N3B	4.86	1.76	1.63
2	B	401	GNP	PB-N3B	4.29	1.74	1.63
2	A	401	GNP	PB-N3B	4.26	1.74	1.63
2	B	401	GNP	C8-N9	-3.07	1.35	1.45
2	A	401	GNP	C5-C6	-2.96	1.47	1.52
2	A	401	GNP	C8-N9	-2.78	1.36	1.45
2	B	401	GNP	PG-O1G	2.41	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GNP	C5-C6	-2.40	1.48	1.52
2	B	401	GNP	PG-O2G	2.39	1.63	1.56
2	B	401	GNP	C2-N1	-2.13	1.35	1.44
2	B	401	GNP	PG-O3G	2.10	1.62	1.56
2	A	401	GNP	C2-N1	-2.10	1.35	1.44
2	A	401	GNP	PG-O3G	2.05	1.62	1.56
2	A	401	GNP	PB-O3A	2.05	1.61	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GNP	O1G-PG-N3B	-2.95	107.42	111.77
2	A	401	GNP	O1G-PG-N3B	-2.94	107.44	111.77
2	A	401	GNP	O4'-C1'-N9	2.93	113.41	109.04
2	B	401	GNP	PA-O3A-PB	-2.89	122.45	132.62
2	A	401	GNP	C4-C5-N7	2.75	106.11	102.46
2	B	401	GNP	C4-C5-N7	2.72	106.06	102.46
2	A	401	GNP	O1B-PB-N3B	-2.64	107.88	111.77
2	B	401	GNP	O4'-C1'-N9	2.48	112.73	109.04
2	A	401	GNP	O2G-PG-O1G	-2.11	108.14	113.45

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	GNP	PG-N3B-PB-O1B
2	B	401	GNP	PA-O3A-PB-O1B
2	B	401	GNP	C2'-C1'-N9-C4
2	A	401	GNP	PG-N3B-PB-O1B
2	A	401	GNP	PA-O3A-PB-O1B
2	A	401	GNP	C2'-C1'-N9-C4

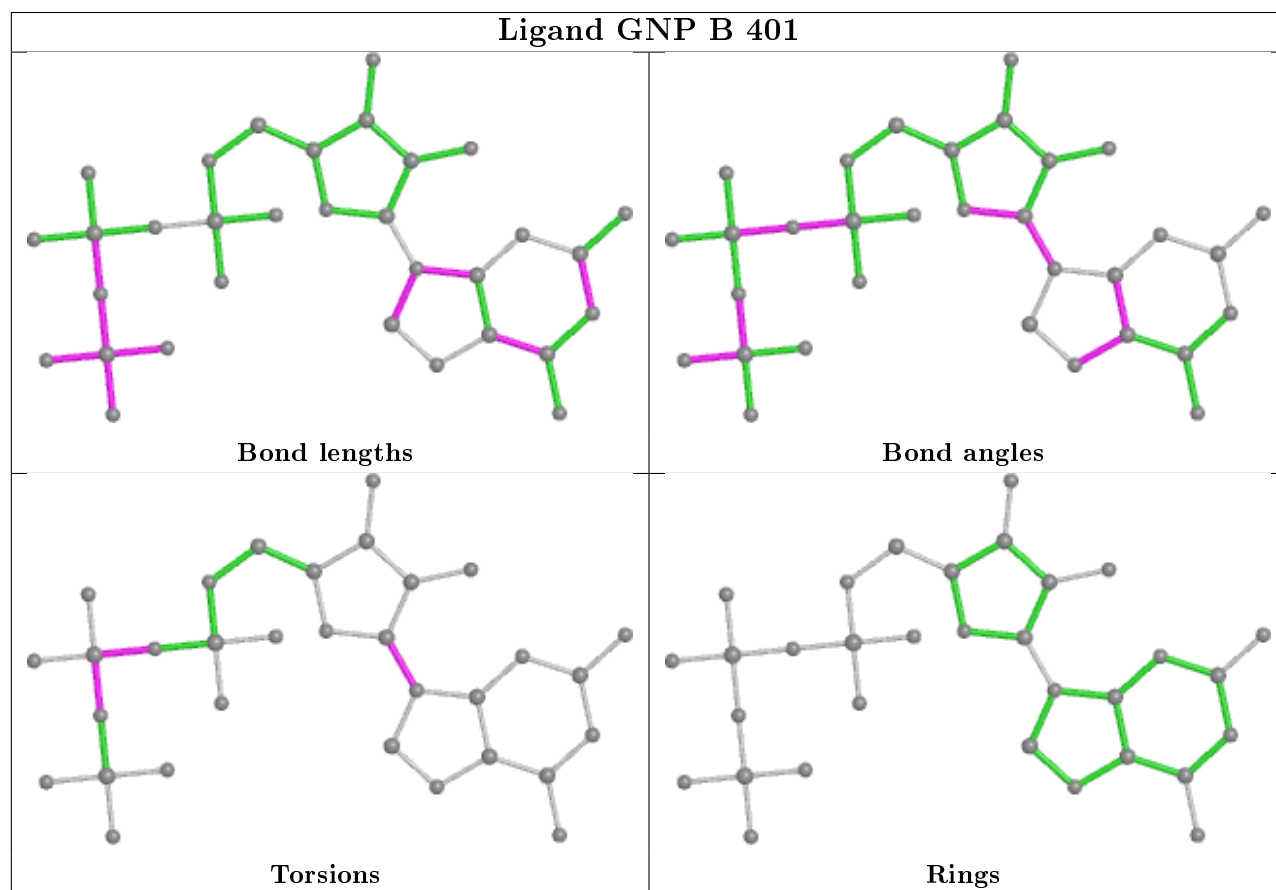
There are no ring outliers.

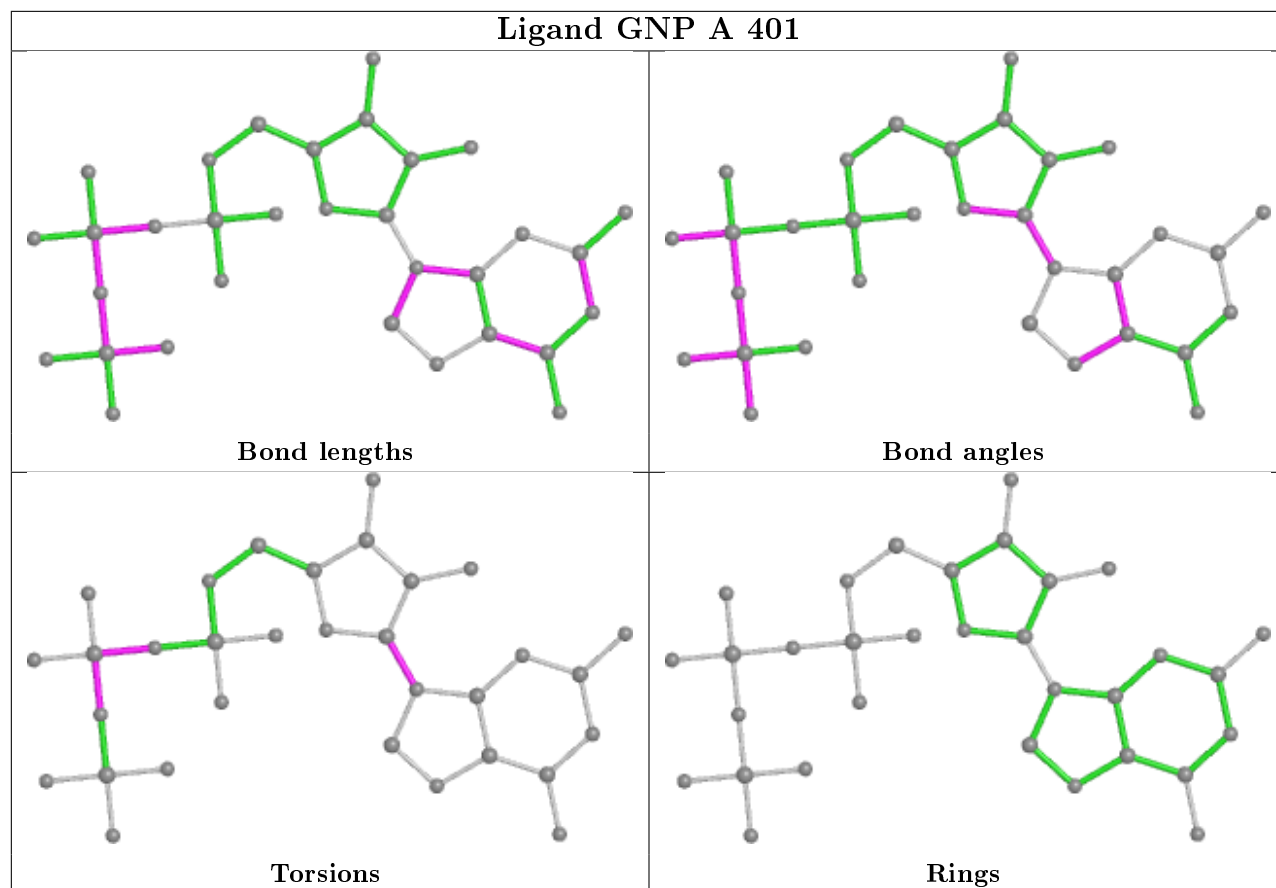
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	GNP	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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	323/337 (95%)	0.11	8 (2%) 57 62	25, 39, 65, 88	0
1	B	315/337 (93%)	0.06	13 (4%) 37 43	24, 40, 64, 94	2 (0%)
All	All	638/674 (94%)	0.08	21 (3%) 46 53	24, 40, 65, 94	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	206	GLY	4.6
1	A	229	PRO	4.4
1	A	329	LEU	3.8
1	B	205	ASP	3.6
1	B	158	VAL	3.3
1	B	179	GLY	3.1
1	B	8	MET	3.1
1	A	231	ALA	2.8
1	A	207	ASP	2.8
1	A	230	SER	2.8
1	B	65	GLY	2.7
1	A	107	THR	2.7
1	B	192	PHE	2.7
1	B	243	LEU	2.4
1	B	178	PRO	2.4
1	B	210	ARG	2.2
1	B	64	PRO	2.2
1	B	327	ILE	2.1
1	B	177	LEU	2.1
1	A	105	ASP	2.0
1	A	228	PRO	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

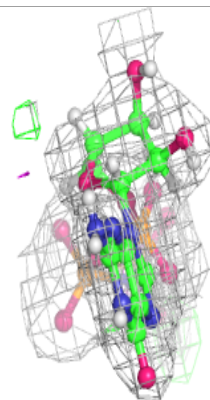
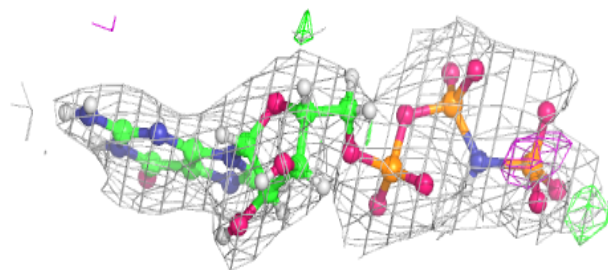
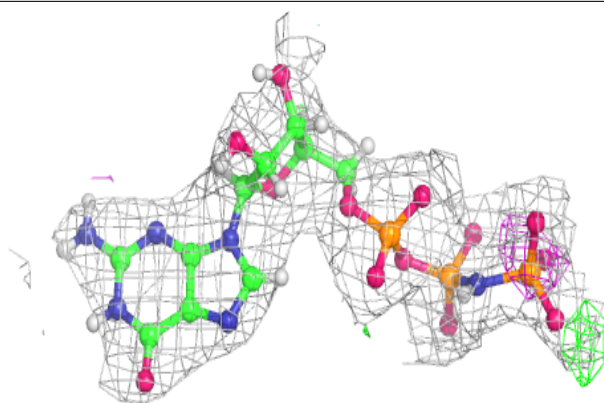
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GNP	B	401	32/32	0.90	0.17	55,63,77,90	0
2	GNP	A	401	32/32	0.95	0.11	38,43,58,63	0

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.

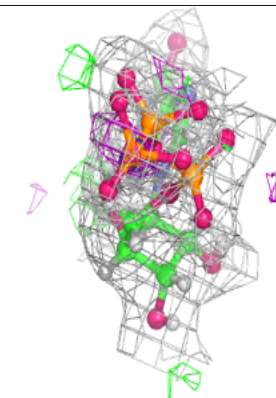
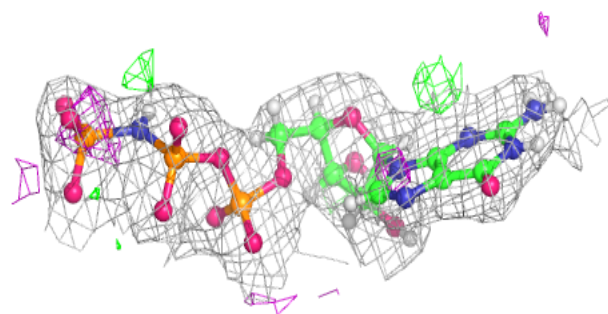
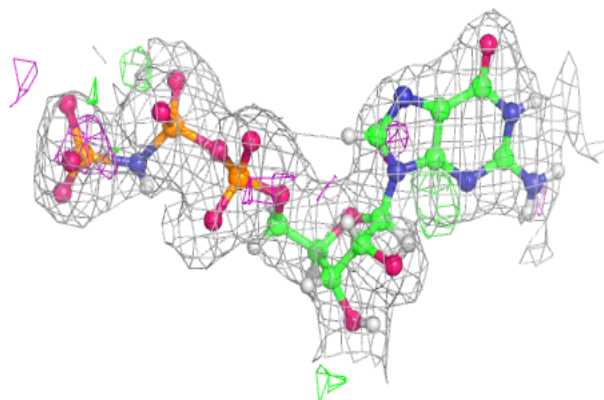


**Electron density around GNP B 401:**

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

**Electron density around GNP A 401:**

$2mF_o-DF_c$  (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.