WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB Geometry-Only Validation Summary Report (i)

Oct 2, 2023 – 05:56 PM EDT

PDB ID	:	4RSG
Title	:	Neutron crystal structure of Ras bound to the GTP analogue GppNHp
Authors	:	Knihtila, R.R.; Holzapfel, G.; Weiss, K.L.; Meilleur, F.; Mattos, C.
Deposited on	:	2014-11-07
Resolution	:	1.91 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
NEUTRON DIFFRACTION

The reported resolution of this entry is 1.91 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 2639 atoms, of which 1015 are hydrogens and 309 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 GTPase HRas.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S			
1	A	162	2433	759	218	1008	208	234	6	0	82	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).
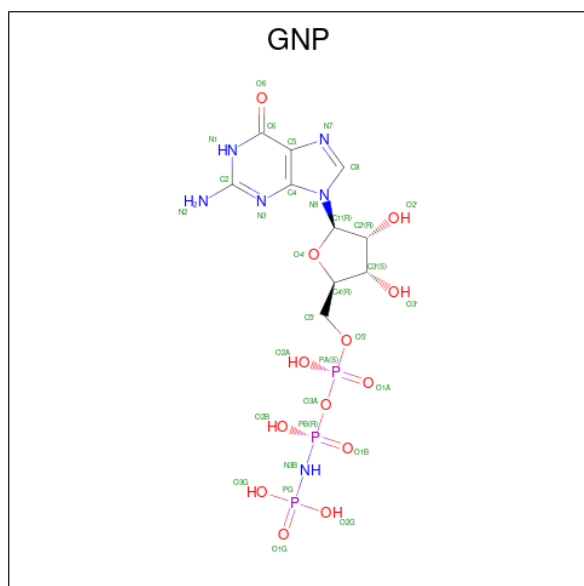
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	D	H	N	O	P		
2	A	1	46	10	7	7	6	13	3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	75	Total 159	D 84	O 75	0	0

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.

3 Model quality ⓘ

3.1 Standard geometry ⓘ

MolProbity failed to run properly - this section is therefore empty.

3.2 Too-close contacts ⓘ

MolProbity failed to run properly - this section is therefore empty.

3.3 Torsion angles ⓘ

3.3.1 Protein backbone ⓘ

MolProbity failed to run properly - this section is therefore empty.

3.3.2 Protein sidechains ⓘ

MolProbity failed to run properly - this section is therefore empty.

3.3.3 RNA ⓘ

MolProbity failed to run properly - this section is therefore empty.

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

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

3.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

3.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#|Z| > 2$
2	GNP	A	201	3	29,34,34	2.82	11 (37%)	33,54,54	2.86	16 (48%)

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	A	201	3	-	6/14/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	GNP	PG-O1G	7.99	1.58	1.46
2	A	201	GNP	PG-O2G	-6.17	1.40	1.56
2	A	201	GNP	PB-N3B	4.50	1.75	1.63
2	A	201	GNP	O4'-C1'	-4.40	1.34	1.41
2	A	201	GNP	PG-N3B	4.22	1.74	1.63

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	GNP	C4-C5-C6	-7.45	113.68	120.80
2	A	201	GNP	O1G-PG-N3B	-6.09	102.80	111.77
2	A	201	GNP	O2B-PB-O1B	5.55	121.55	109.92
2	A	201	GNP	O2'-C2'-C3'	4.36	125.92	111.82
2	A	201	GNP	O2B-PB-O3A	3.77	117.23	104.64

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	GNP	PB-N3B-PG-O1G
2	A	201	GNP	PG-N3B-PB-O1B
2	A	201	GNP	PG-N3B-PB-O3A
2	A	201	GNP	PA-O3A-PB-O2B
2	A	201	GNP	C5'-O5'-PA-O3A

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 GNP A 201

Bond lengths

Bond angles

Torsions

Rings
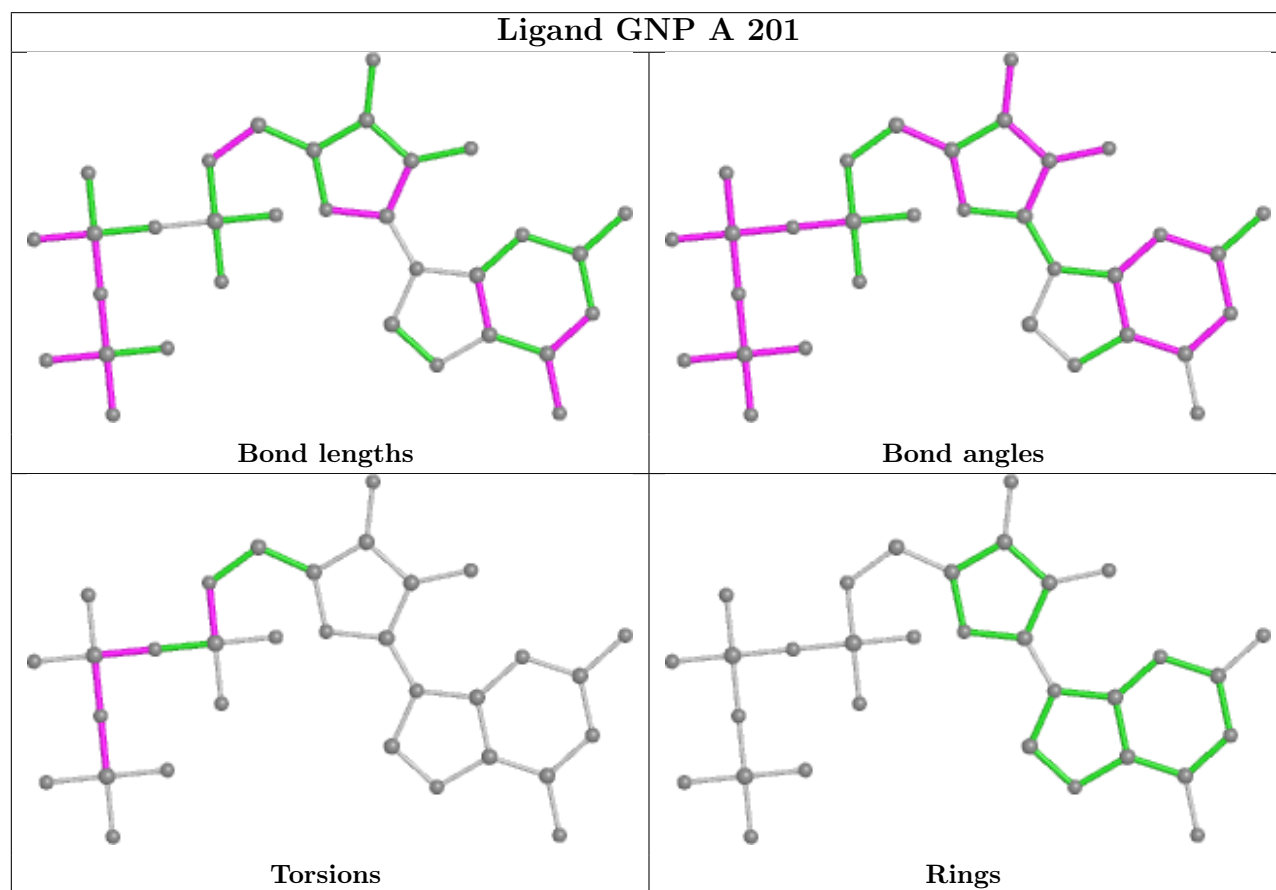
3.7 Other polymers ⓘ

There are no such residues in this entry.

3.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.