Full wwPDB X-ray Structure Validation Report (i)

Apr 30, 2024 – 11:57 pm BST

PDB ID	:	5OVO
Title	:	Structure of DraG-GlnZ-delta42-54 complex from Azospirillum brasilense
Authors	:	Berthold, C.L.; Hogbom, M.
Deposited on	:	2017-08-29
Resolution	:	1.55 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:

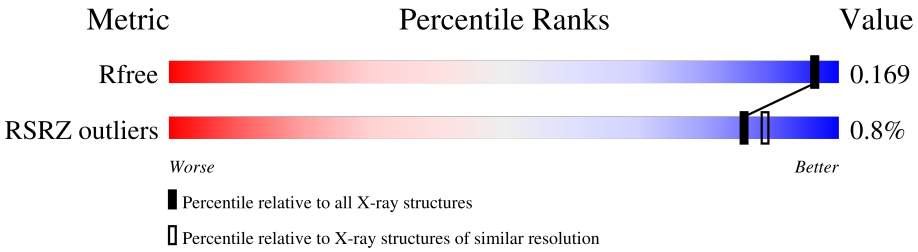
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.55 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	1483 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3637 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 ADP-ribosyl-(Dinitrogen reductase) hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	7	0
			2303	1443	417	430	13			

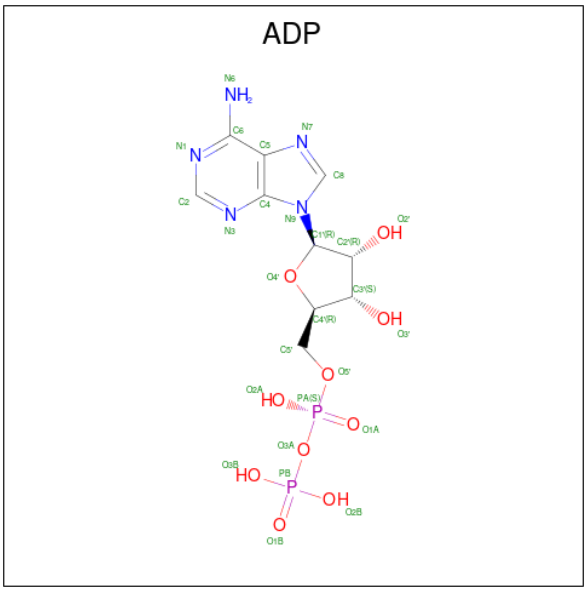
- Molecule 2 is a protein called Nitrogen regulatory protein P-II 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	2	0
			770	490	132	146	2			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	deletion	UNP P70731
B	?	-	THR	deletion	UNP P70731
B	?	-	GLU	deletion	UNP P70731
B	?	-	ILE	deletion	UNP P70731
B	?	-	TYR	deletion	UNP P70731
B	?	-	ARG	deletion	UNP P70731
B	?	-	GLY	deletion	UNP P70731
B	?	-	ALA	deletion	UNP P70731
B	?	-	GLU	deletion	UNP P70731
B	?	-	TYR	deletion	UNP P70731
B	?	-	SER	deletion	UNP P70731
B	?	-	VAL	deletion	UNP P70731
B	?	-	SER	deletion	UNP P70731

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mn 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	353	Total O 353 353	0	0
6	B	154	Total O 154 154	0	0

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

3 Data and refinement statistics (i)

Xtriage (Phenix) was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	116.74Å 116.74Å 105.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.60 – 1.55 45.60 – 1.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.60-1.55) 100.0 (45.60-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.144 , 0.165 0.149 , 0.169	Depositor DCC
R_{free} test set	3882 reflections (4.98%)	wwPDB-VP
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
Reported twinning fraction	0.588 for H, K, L 0.412 for K, H, -L	Depositor
Outliers	(Not available)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3637	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 5 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
3	ADP	B	201	-	24,29,29	0.97	2 (8%)	29,45,45	1.41	4 (13%)
3	ADP	A	301	4	24,29,29	1.34	3 (12%)	29,45,45	1.60	7 (24%)

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	ADP	B	201	-	-	0/12/32/32	0/3/3/3
3	ADP	A	301	4	-	2/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	ADP	C2'-C1'	-3.11	1.49	1.53
3	A	301	ADP	PA-O1A	-2.39	1.42	1.50
3	B	201	ADP	PA-O2A	-2.39	1.44	1.55
3	A	301	ADP	C2-N3	2.26	1.35	1.32
3	B	201	ADP	O4'-C1'	2.19	1.44	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	201	ADP	C5-C6-N6	3.11	125.08	120.35
3	A	301	ADP	C3'-C2'-C1'	3.04	105.55	100.98
3	B	201	ADP	N3-C2-N1	-2.83	124.25	128.68
3	A	301	ADP	O4'-C1'-C2'	-2.77	102.88	106.93
3	A	301	ADP	O2B-PB-O3A	-2.73	95.48	104.64
3	A	301	ADP	C4-C5-N7	-2.72	106.57	109.40
3	B	201	ADP	C4-C5-N7	-2.48	106.81	109.40
3	A	301	ADP	C5-C6-N6	2.42	124.02	120.35
3	A	301	ADP	C5-C6-N1	-2.35	115.01	120.35
3	B	201	ADP	O5'-PA-O1A	-2.29	100.11	109.07
3	A	301	ADP	O2'-C2'-C1'	-2.17	102.84	110.85

There are no chirality outliers.

All (2) torsion outliers are listed below:

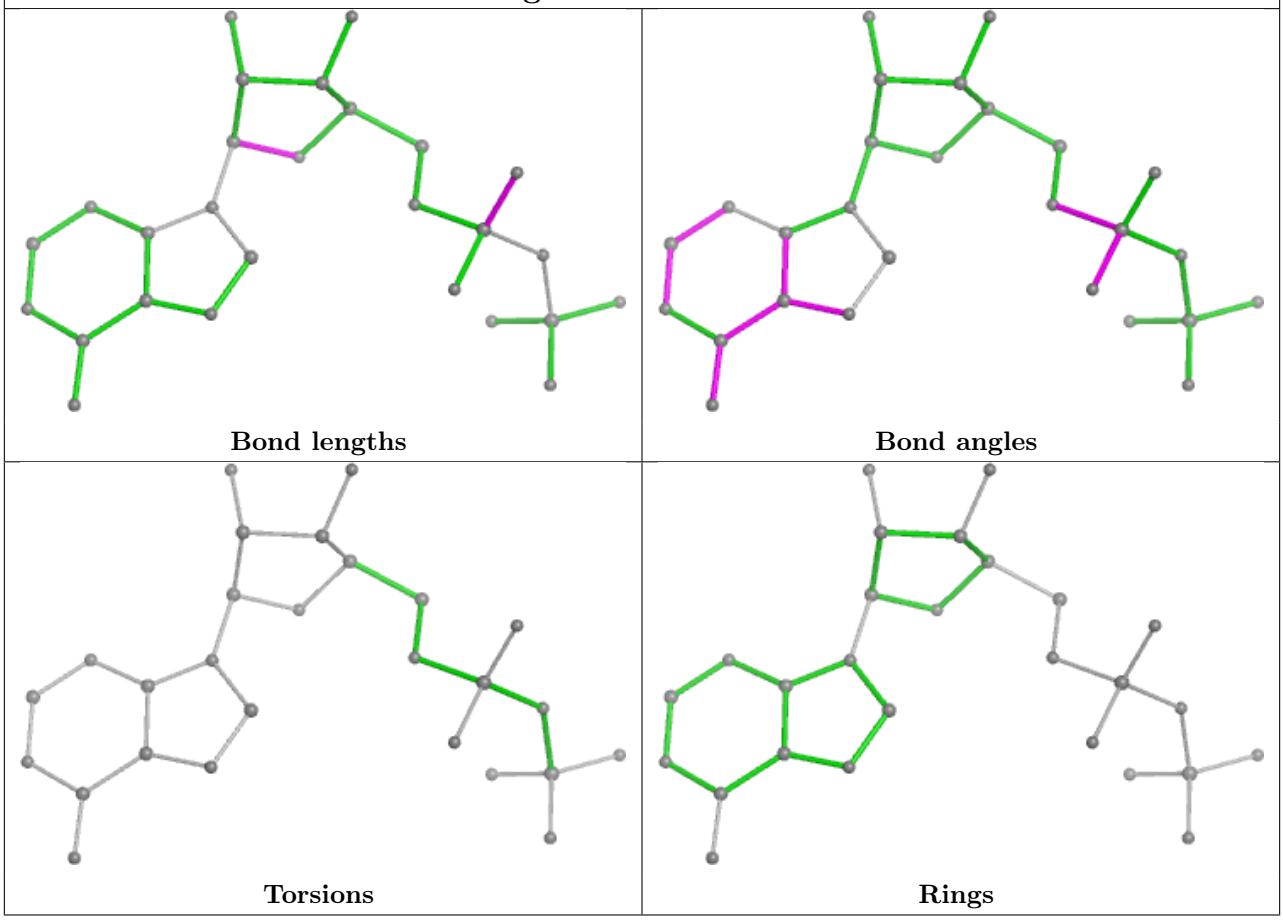
Mol	Chain	Res	Type	Atoms
3	A	301	ADP	PB-O3A-PA-O1A
3	A	301	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

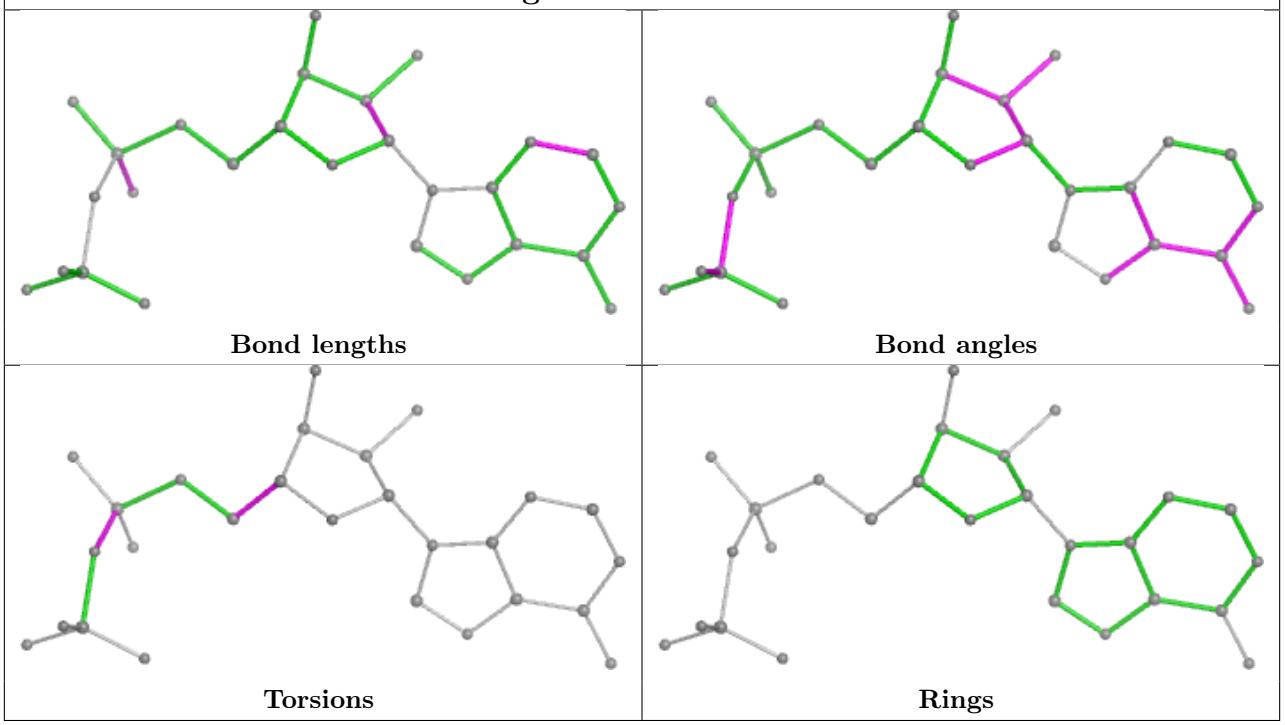
No monomer is involved in short contacts.

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 ADP B 201



Ligand ADP A 301



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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^{th} 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	295/297 (99%)	-0.47	3 (1%) 82 86	9, 12, 21, 27	0
2	B	99/99 (100%)	-0.39	0 100 100	10, 13, 19, 24	0
All	All	394/396 (99%)	-0.45	3 (0%) 86 89	9, 13, 20, 27	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	HIS	2.8
1	A	38[A]	GLN	2.3
1	A	122[A]	TYR	2.3

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

There are no monosaccharides in this entry.

5.4 Ligands

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^{th} 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
3	ADP	A	301	27/27	0.98	0.05	12,16,18,19	0
3	ADP	B	201	27/27	0.98	0.07	11,12,14,21	0

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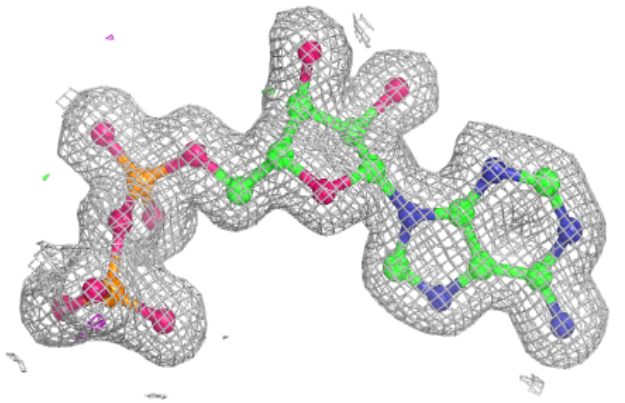
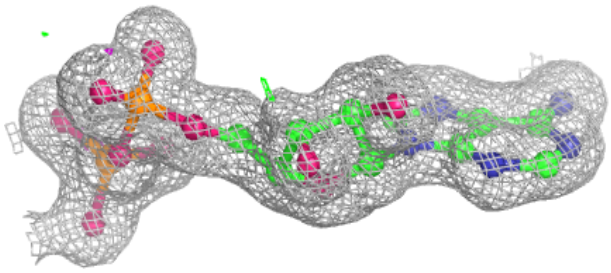
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	302	1/1	0.99	0.03	19,19,19,19	0
4	MG	A	303	1/1	0.99	0.03	21,21,21,21	0
5	MN	B	202	1/1	1.00	0.03	24,24,24,24	0

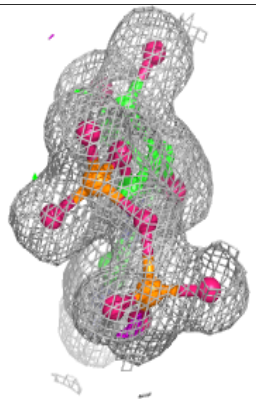
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 301:

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

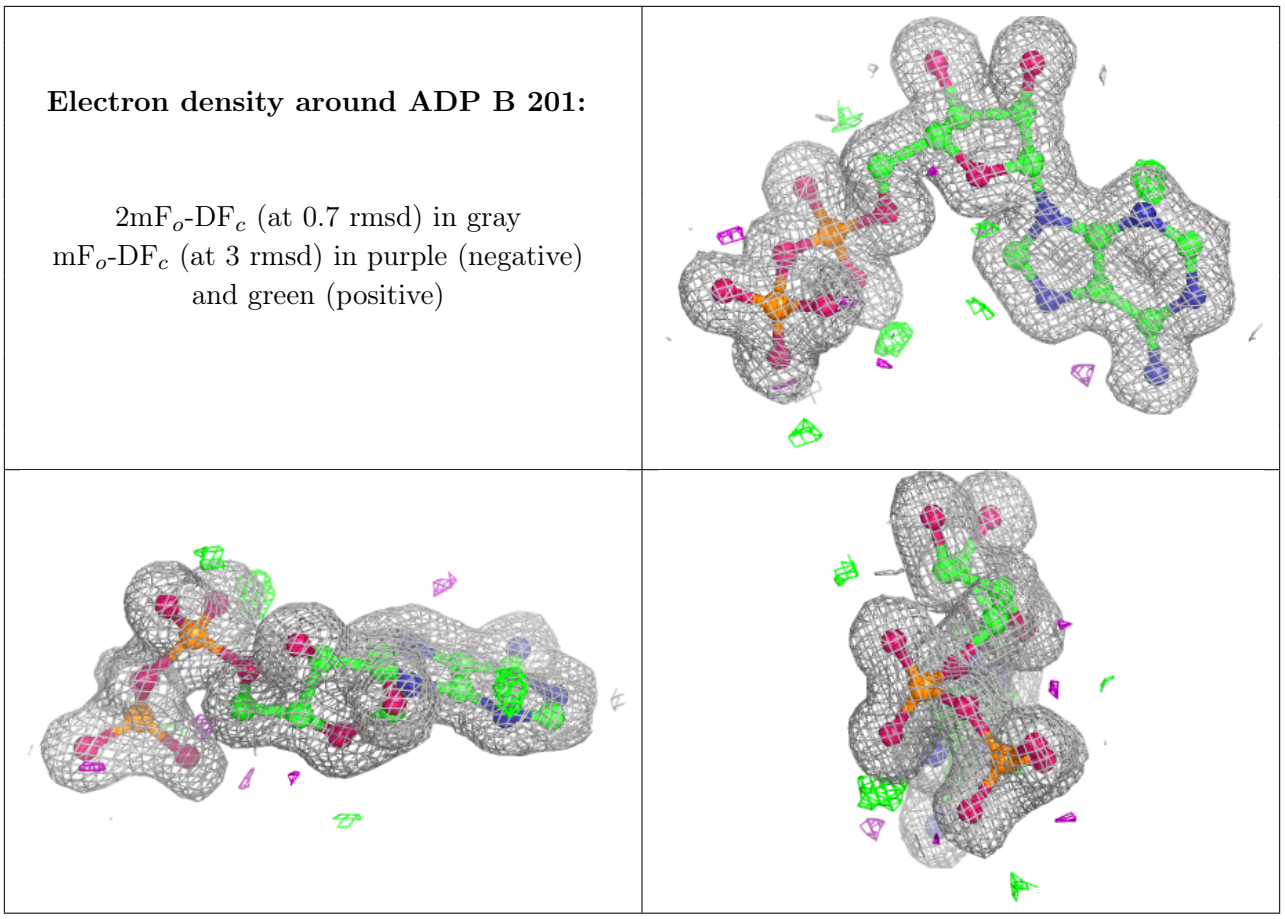






Electron density around ADP B 201:

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



5.5 Other polymers

There are no such residues in this entry.