



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:50 am 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

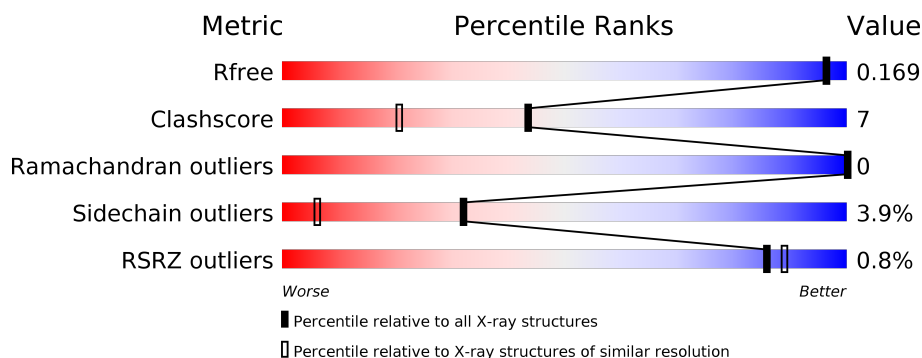
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	297	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>80%</span> <span>15%</span> <span>...</span> </div> </div>
2	B	99	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>87%</span> <span>11%</span> <span>..</span> </div> </div>

## 2 Entry composition

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<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

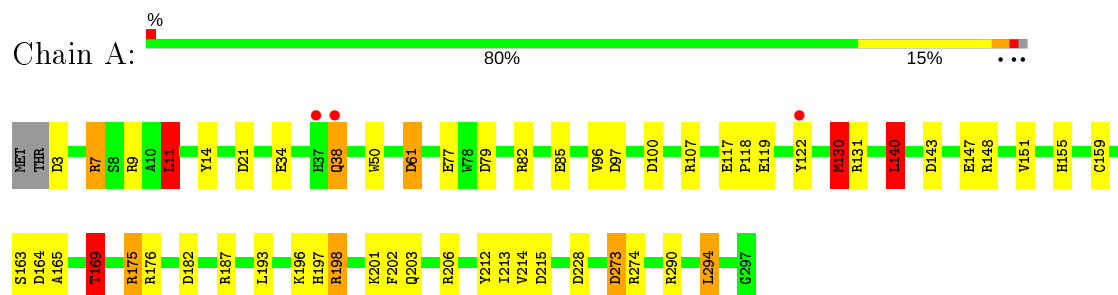
- Molecule 6 is water.

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

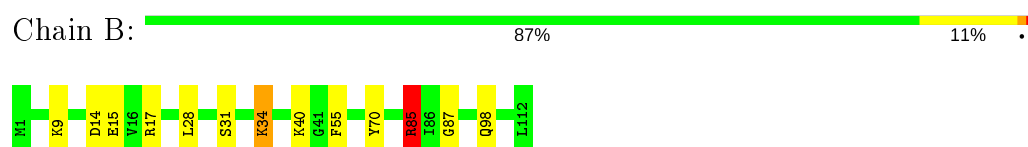
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: ADP-ribosyl-(Dinitrogen reductase) hydrolase



- Molecule 2: Nitrogen regulatory protein P-II 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 1.55Å)	Xtriage
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
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.588 for H, K, L 0.412 for K, H, -L	Depositor
Outliers	0 of 77906 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3637	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, MN, ADP

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	1.25	6/2371 (0.3%)	1.47	40/3214 (1.2%)
2	B	1.29	0/782	1.29	5/1048 (0.5%)
All	All	1.26	6/3153 (0.2%)	1.43	45/4262 (1.1%)

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	A	1	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	GLU	CD-OE2	7.90	1.34	1.25
1	A	82	ARG	CD-NE	-6.05	1.36	1.46
1	A	147	GLU	CD-OE1	6.04	1.32	1.25
1	A	119	GLU	CD-OE1	5.54	1.31	1.25
1	A	130	MET	CA-CB	-5.10	1.42	1.53
1	A	50	TRP	CG-CD1	-5.06	1.29	1.36

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ARG	NE-CZ-NH1	23.80	132.20	120.30
1	A	82	ARG	NE-CZ-NH2	-22.78	108.91	120.30
1	A	130	MET	CG-SD-CE	-11.70	81.47	100.20
2	B	17	ARG	NE-CZ-NH1	10.63	125.62	120.30
1	A	187	ARG	NE-CZ-NH1	9.03	124.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	A	97	ASP	CB-CG-OD2	8.74	126.17	118.30
1	A	140	LEU	CB-CG-CD1	8.67	125.74	111.00
1	A	164	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	A	182	ASP	CB-CG-OD1	8.06	125.56	118.30
1	A	82	ARG	CD-NE-CZ	8.00	134.80	123.60
1	A	143	ASP	CB-CG-OD1	7.81	125.33	118.30
1	A	176	ARG	NE-CZ-NH2	7.75	124.18	120.30
1	A	215	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	169	THR	CA-CB-CG2	7.08	122.31	112.40
1	A	148	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	A	164	ASP	CB-CG-OD1	6.83	124.45	118.30
2	B	17	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	100	ASP	CB-CG-OD1	6.63	124.26	118.30
1	A	107	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	21	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	A	131	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	202	PHE	CB-CG-CD2	-6.22	116.45	120.80
1	A	273[A]	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	273[B]	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	290	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	82	ARG	CG-CD-NE	-6.06	99.07	111.80
1	A	100	ASP	CB-CG-OD2	-6.04	112.86	118.30
2	B	15	GLU	OE1-CD-OE2	6.03	130.53	123.30
1	A	11	LEU	CA-CB-CG	5.91	128.89	115.30
1	A	9	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	202	PHE	CB-CG-CD1	5.75	124.82	120.80
1	A	11	LEU	CB-CG-CD1	5.59	120.50	111.00
2	B	85	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	79	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	206	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	97	ASP	OD1-CG-OD2	-5.45	112.95	123.30
2	B	70	TYR	CD1-CE1-CZ	-5.26	115.07	119.80
1	A	61	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	273[A]	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	273[B]	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	228	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	7	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	198	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	175	ARG	NE-CZ-NH2	5.12	122.86	120.30

All (1) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	A	169	THR	CB

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	2303	0	2270	33	0
2	B	770	0	821	9	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	353	0	0	11	0
6	B	154	0	0	6	0
All	All	3637	0	3115	42	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 7.

All (42) 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:A:85:GLU:HG2	6:A:758:HOH:O	1.40	1.22
1:A:213:ILE:HG12	6:A:682:HOH:O	1.56	1.05
1:A:34:GLU:O	1:A:38[A]:GLN:HG2	1.62	1.00
1:A:273[A]:ASP:OD2	6:A:501:HOH:O	1.80	0.98
1:A:163:SER:HA	6:A:682:HOH:O	1.63	0.96
1:A:96:VAL:HG23	6:A:547:HOH:O	1.77	0.85
1:A:198:ARG:HH11	1:A:198:ARG:HG3	1.44	0.83
1:A:96:VAL:CG2	6:A:547:HOH:O	2.29	0.80
2:B:34[A]:LYS:NZ	6:B:301:HOH:O	2.15	0.80
2:B:55:PHE:HE2	6:B:415:HOH:O	1.67	0.76
1:A:117:GLU:HB2	1:A:118:PRO:CD	2.17	0.73
1:A:130:MET:HE2	6:A:704:HOH:O	1.91	0.71
1:A:130:MET:CE	6:A:704:HOH:O	2.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASP:OD1	6:A:503:HOH:O	2.10	0.69
1:A:122[A]:TYR:CE1	6:A:781:HOH:O	2.48	0.67
1:A:151:VAL:HG13	1:A:155:HIS:CE1	2.30	0.66
2:B:34[A]:LYS:HB3	2:B:55:PHE:CE1	2.32	0.64
1:A:169:THR:HG21	1:A:193:LEU:HB2	1.79	0.64
2:B:55:PHE:CE2	6:B:415:HOH:O	2.47	0.62
1:A:165:ALA:O	1:A:169:THR:HG23	2.01	0.60
1:A:198:ARG:HH11	1:A:198:ARG:CG	2.15	0.59
2:B:14:ASP:OD1	6:B:302:HOH:O	2.17	0.58
1:A:122[A]:TYR:CD1	6:A:781:HOH:O	2.57	0.57
1:A:117:GLU:HB2	1:A:118:PRO:HD3	1.87	0.56
2:B:28:LEU:HD12	2:B:28:LEU:C	2.29	0.53
1:A:117:GLU:CB	1:A:118:PRO:CD	2.88	0.52
1:A:201:LYS:HE2	1:A:203:GLN:O	2.12	0.50
1:A:117:GLU:HB2	1:A:118:PRO:HD2	1.92	0.49
1:A:61:ASP:HA	1:A:130:MET:SD	2.54	0.48
2:B:85:ARG:HD2	6:B:388:HOH:O	2.14	0.47
1:A:117:GLU:O	1:A:159[A]:CYS:SG	2.74	0.46
1:A:140:LEU:HD13	1:A:175:ARG:HG2	1.97	0.46
1:A:151:VAL:CG1	1:A:155:HIS:CE1	3.00	0.45
1:A:7:ARG:O	1:A:11:LEU:HB2	2.19	0.43
2:B:9:LYS:HE3	2:B:87:GLY:C	2.39	0.43
1:A:274[B]:ARG:HD2	1:A:274[B]:ARG:HA	1.75	0.43
1:A:151:VAL:HG13	1:A:155:HIS:NE2	2.33	0.42
1:A:130:MET:SD	1:A:130:MET:C	2.97	0.42
2:B:98:GLN:NE2	6:B:312:HOH:O	2.52	0.42
1:A:196:LYS:HG2	1:A:197:HIS:CD2	2.55	0.41
1:A:294:LEU:HD23	1:A:294:LEU:N	2.35	0.41
1:A:212:TYR:CE2	1:A:214:VAL:HB	2.56	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	300/297 (101%)	292 (97%)	8 (3%)	0	100	100
2	B	99/99 (100%)	99 (100%)	0	0	100	100
All	All	399/396 (101%)	391 (98%)	8 (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	235/230 (102%)	225 (96%)	10 (4%)	29	5
2	B	83/81 (102%)	78 (94%)	5 (6%)	19	2
All	All	318/311 (102%)	303 (95%)	15 (5%)	32	4

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	14	TYR
1	A	38[A]	GLN
1	A	38[B]	GLN
1	A	77[A]	GLU
1	A	77[B]	GLU
1	A	130	MET
1	A	140	LEU
1	A	169	THR
1	A	294	LEU
2	B	31	SER
2	B	34[A]	LYS
2	B	34[B]	LYS
2	B	40	LYS
2	B	85	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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(°)	Ideal(°)
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.

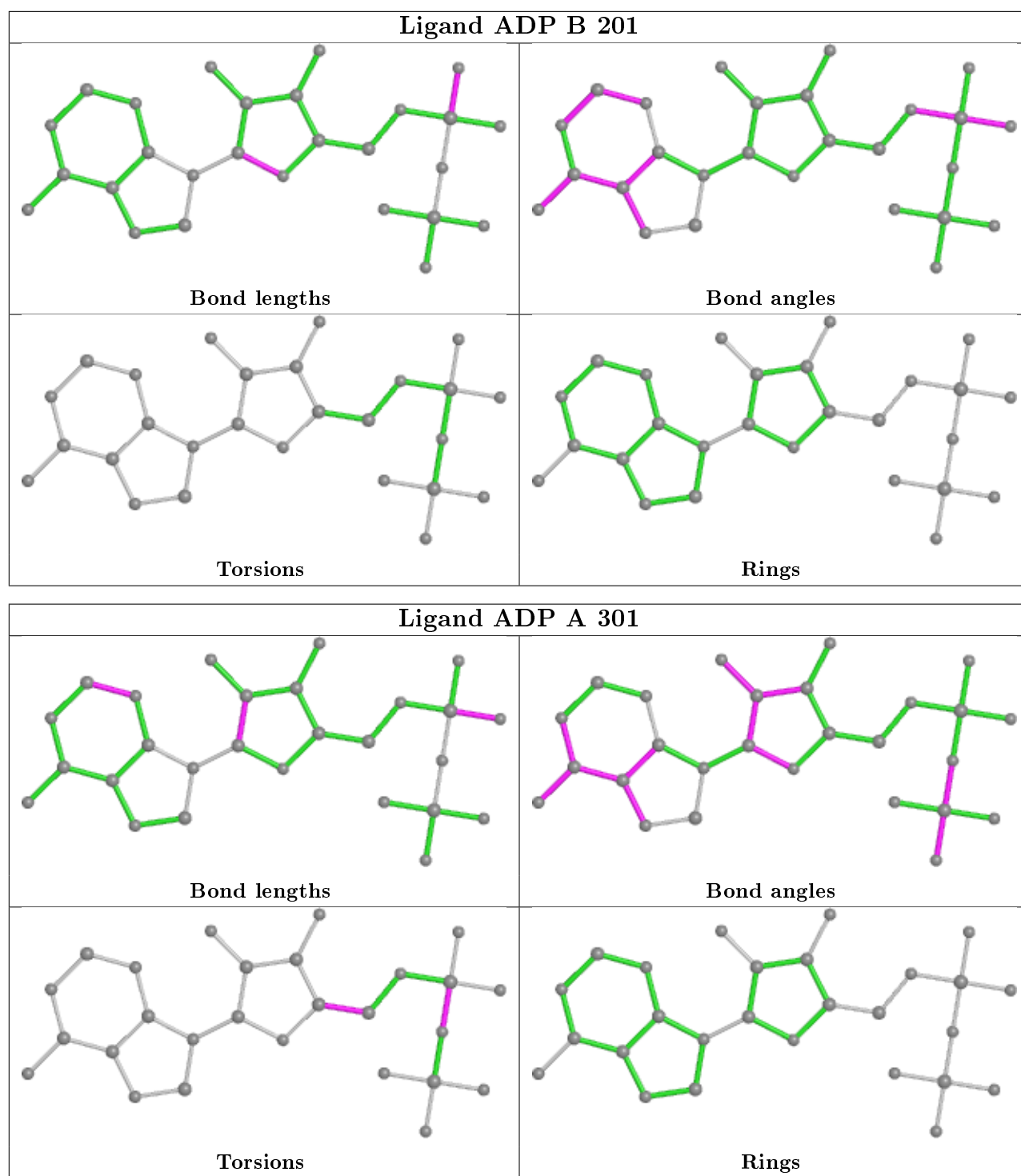
All (2) torsion outliers are listed below:

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 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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	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

### 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(Å <sup>2</sup> )	Q<0.9
3	ADP	B	201	27/27	0.98	0.07	11,12,14,21	0
3	ADP	A	301	27/27	0.98	0.05	12,16,18,19	0

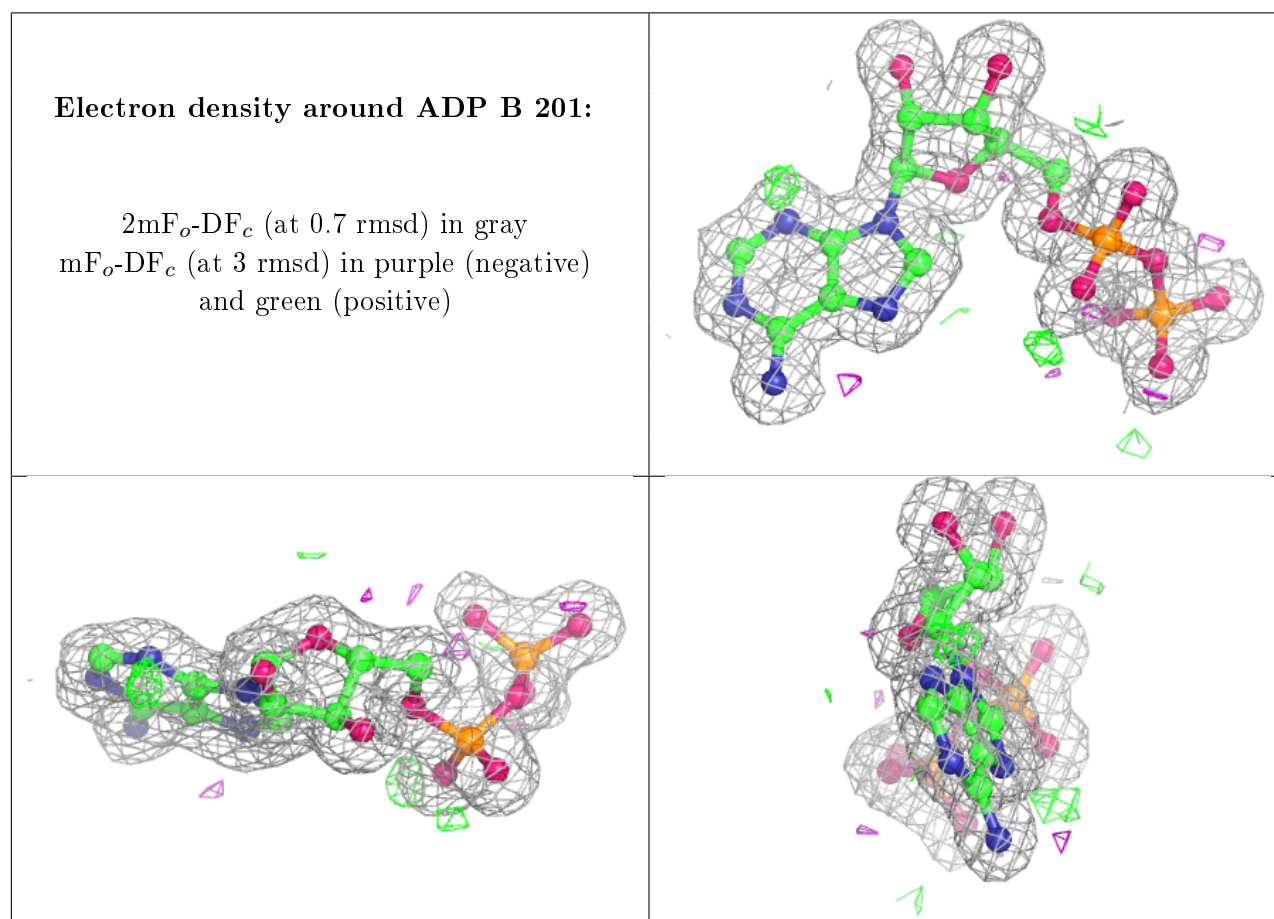
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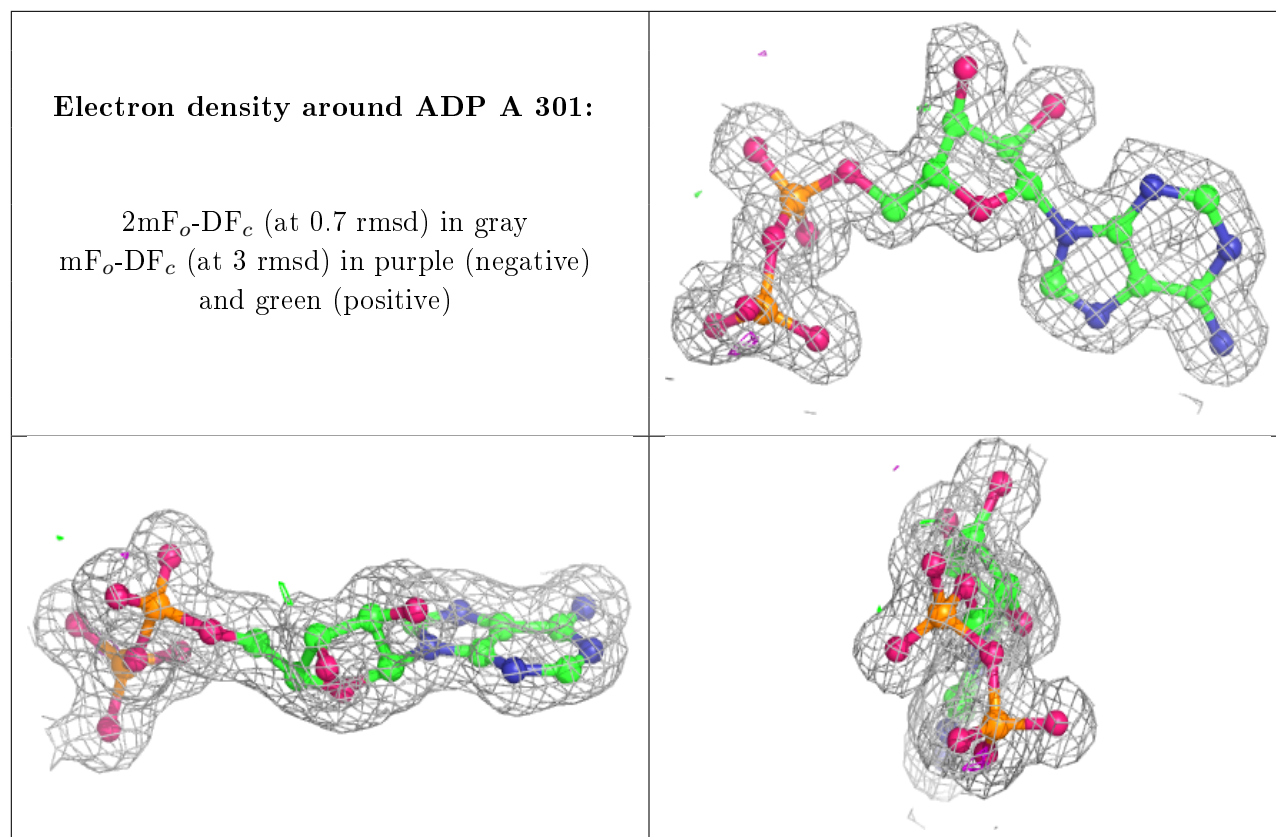


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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	303	1/1	0.99	0.03	21,21,21,21	0
4	MG	A	302	1/1	0.99	0.03	19,19,19,19	0
5	MN	B	202	1/1	1.00	0.03	24,24,24,24	0

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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.