



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 04:07 PM GMT

PDB ID : 2J9C  
Title : STRUCTURE OF GLNK1 WITH BOUND EFFECTORS INDICATES REGULATORY MECHANISM FOR AMMONIA UPTAKE  
Authors : Yildiz, O.; Kalthoff, C.; Raunser, S.; Kuehlbrandt, W.  
Deposited on : 2006-11-07  
Resolution : 1.30 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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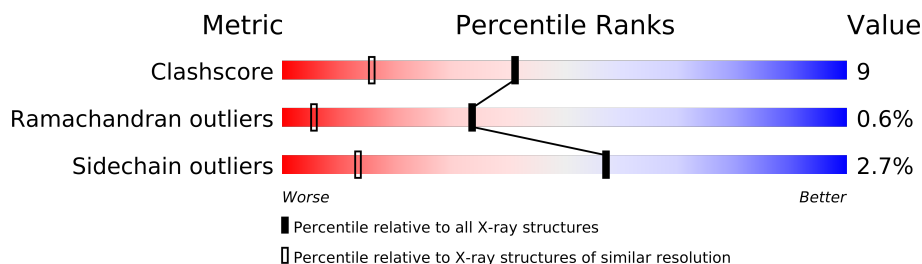
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.30 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))
Clashscore	79885	1140 (1.34-1.26)
Ramachandran outliers	78287	1093 (1.34-1.26)
Sidechain outliers	78261	1092 (1.34-1.26)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	119	
1	B	119	
1	C	119	

## 2 Entry composition i

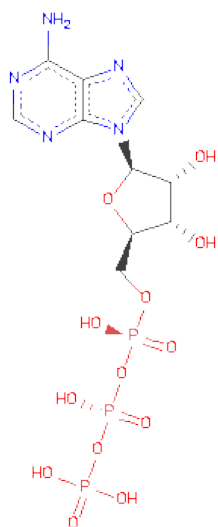
There are 7 unique types of molecules in this entry. The entry contains 3428 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	6	0
			946	602	165	175	4			
1	B	117	Total	C	N	O	S	0	4	0
			928	590	162	173	3			
1	C	117	Total	C	N	O	S	0	5	0
			939	595	164	177	3			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

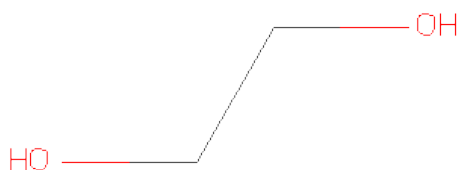
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

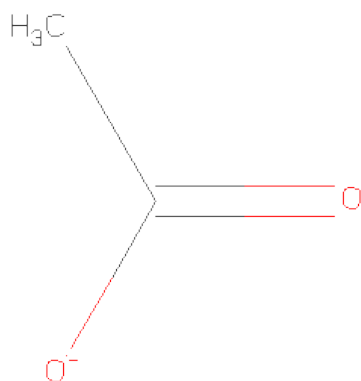
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	2	Total	Cl	0	0
			2	2		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	179	Total O 179 179	0	0
7	B	158	Total O 158 158	0	0
7	C	150	Total O 150 150	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain A: 



- Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain B: 



- Molecule 1: HYPOTHETICAL NITROGEN REGULATORY PII-LIKE PROTEIN MJ0059

Chain C: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.70Å 122.70Å 45.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.65 – 1.30	Depositor
% Data completeness (in resolution range)	100.0 (14.65-1.30)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.143 , 0.187	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACT, EDO, ATP, CL

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	1.03	3/969 (0.3%)	1.03	6/1298 (0.5%)
1	B	1.01	2/948 (0.2%)	1.04	6/1273 (0.5%)
1	C	1.11	2/962 (0.2%)	1.06	7/1290 (0.5%)
All	All	1.05	7/2879 (0.2%)	1.05	19/3861 (0.5%)

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	C	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	107	GLU	CB-CG	-7.32	1.38	1.52
1	B	5	GLU	CD-OE1	-6.06	1.19	1.25
1	C	39	GLN	CG-CD	5.83	1.64	1.51
1	A	3	LYS	CD-CE	-5.65	1.37	1.51
1	A	31	SER	CA-CB	5.45	1.61	1.52
1	A	3	LYS	CE-NZ	5.43	1.62	1.49
1	B	31	SER	CA-CB	5.13	1.60	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	ASP	CB-CG-OD2	8.07	125.56	118.30
1	C	45	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	49	ARG	NE-CZ-NH1	-6.67	116.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	C	49	ARG	N-CA-C	6.63	128.90	111.00
1	B	101	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	C	98	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	63	LEU	CB-CG-CD1	-6.08	100.66	111.00
1	B	5	GLU	OE1-CD-OE2	-5.96	116.14	123.30
1	C	54	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	1[A]	MET	CG-SD-CE	-5.70	91.08	100.20
1	A	1[B]	MET	CG-SD-CE	-5.70	91.08	100.20
1	C	45	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	B	22	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	49	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	C	101	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	101	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	C	54	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	82	ARG	NE-CZ-NH2	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	49	ARG	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	946	0	0	7	0
1	B	928	0	0	7	0
1	C	939	0	0	12	1
2	A	31	0	0	0	0
2	B	31	0	0	1	0
2	C	31	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	2	0
4	C	1	0	0	2	0
5	A	4	0	0	0	0
5	B	8	0	0	0	0
5	C	4	0	0	2	0
6	A	8	0	0	2	0
6	C	4	0	0	1	0
7	A	179	0	0	6	0
7	B	158	0	0	5	0
7	C	150	0	0	5	0
All	All	3428	0	0	27	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (27) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105:LYS:NZ	7:A:2167:HOH:O	1.87	1.06
1:C:98:ARG:NH2	4:C:1118:CL:CL	2.33	0.97
1:B:39:GLN:NE2	7:B:2064:HOH:O	2.08	0.85
1:A:105:LYS:NZ	7:A:2166:HOH:O	2.11	0.84
1:C:107:GLU:OE1	7:C:2138:HOH:O	1.93	0.84
1:A:62[B]:GLU:OE2	7:A:2119:HOH:O	1.98	0.81
1:C:98:ARG:CD	4:C:1118:CL:CL	2.66	0.81
1:C:71[A]:ASP:OD1	7:C:2095:HOH:O	1.98	0.81
1:B:28:MET:CE	1:B:61[A]:ILE:CG2	2.58	0.80
1:C:5[B]:GLU:OE2	7:C:2006:HOH:O	2.03	0.77
1:C:98:ARG:NE	7:C:2138:HOH:O	2.16	0.77
1:A:115:HIS:CD2	7:A:2169:HOH:O	2.45	0.69
1:B:46:TYR:OH	7:B:2076:HOH:O	2.14	0.63
1:C:32:GLU:OE1	5:C:1119:EDO:O1	2.19	0.60
1:B:14:GLU:OE2	7:B:2029:HOH:O	2.17	0.60
1:C:113:LEU:CD1	7:C:2141:HOH:O	2.52	0.57
1:A:115:HIS:ND1	7:A:2174:HOH:O	2.33	0.56
1:C:34:LYS:NZ	6:C:1120:ACT:O	2.38	0.55
1:B:41:GLY:N	7:B:2067:HOH:O	2.46	0.48
1:B:90:LYS:NZ	4:B:1118:CL:CL	2.84	0.47
6:A:1121:ACT:CH3	1:C:32:GLU:O	2.63	0.47
1:C:109:LYS:CB	1:C:109:LYS:NZ	2.80	0.45
1:B:98:ARG:NH1	7:B:2134:HOH:O	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:HIS:CE1	7:A:2174:HOH:O	2.70	0.44
1:C:33:VAL:O	5:C:1119:EDO:C1	2.66	0.43
1:A:31:SER:OG	6:A:1122:ACT:CH3	2.68	0.41
2:B:1116:ATP:N6	4:B:1118:CL:CL	2.91	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:45:ARG:NH2	1:C:72[A]:ASN:OD1[4_664]	2.11	0.09

## 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	121/119 (102%)	119 (98%)	2 (2%)	0	100	100
1	B	119/119 (100%)	117 (98%)	2 (2%)	0	100	100
1	C	120/119 (101%)	117 (98%)	1 (1%)	2 (2%)	14	0
All	All	360/357 (101%)	353 (98%)	5 (1%)	2 (1%)	33	5

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	50	GLU
1	C	49	ARG

### 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	106/102 (104%)	101 (95%)	5 (5%)	36 3
1	B	104/102 (102%)	101 (97%)	3 (3%)	55 12
1	C	105/102 (103%)	103 (98%)	2 (2%)	69 26
All	All	315/306 (103%)	305 (97%)	10 (3%)	57 9

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	MET
1	A	1[B]	MET
1	A	18	LYS
1	A	109[A]	LYS
1	A	109[B]	LYS
1	B	45	ARG
1	B	49	ARG
1	B	109	LYS
1	C	49	ARG
1	C	115	HIS

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 chains 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 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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	ATP	A	1116	3	33,33,33	1.37	4 (12%)	52,52,52	1.56	6 (11%)
5	EDO	A	1120	-	3,3,3	0.73	0	2,2,2	0.14	0
6	ACT	A	1121	-	1,3,3	0.23	0	0,3,3	0.00	-
6	ACT	A	1122	-	1,3,3	1.36	0	0,3,3	0.00	-
2	ATP	B	1116	3	33,33,33	0.93	1 (3%)	52,52,52	1.55	7 (13%)
5	EDO	B	1119	-	3,3,3	0.44	0	2,2,2	0.72	0
5	EDO	B	1120	-	3,3,3	0.51	0	2,2,2	0.77	0
2	ATP	C	1116	3	33,33,33	1.39	5 (15%)	52,52,52	1.15	3 (5%)
5	EDO	C	1119	-	3,3,3	0.41	0	2,2,2	0.76	0
6	ACT	C	1120	-	1,3,3	1.41	0	0,3,3	0.00	-

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	ATP	A	1116	3	-	0/22/38/38	0/1/3/3
5	EDO	A	1120	-	-	0/1/1/1	0/0/0/0
6	ACT	A	1121	-	-	0/0/0/0	0/0/0/0
6	ACT	A	1122	-	-	0/0/0/0	0/0/0/0
2	ATP	B	1116	3	-	0/22/38/38	0/1/3/3
5	EDO	B	1119	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1120	-	-	0/1/1/1	0/0/0/0
2	ATP	C	1116	3	-	0/22/38/38	0/1/3/3
5	EDO	C	1119	-	-	0/1/1/1	0/0/0/0
6	ACT	C	1120	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1116	ATP	PG-O3B	4.28	1.67	1.60
2	C	1116	ATP	C4-N9	-3.89	1.32	1.37
2	C	1116	ATP	PG-O3B	3.87	1.66	1.60
2	A	1116	ATP	C2'-C1'	-3.09	1.49	1.53
2	B	1116	ATP	C4-N9	-2.88	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1116	ATP	C4-N9	-2.55	1.34	1.37
2	A	1116	ATP	O4'-C1'	2.51	1.45	1.41
2	C	1116	ATP	C2'-C1'	-2.34	1.50	1.53
2	C	1116	ATP	C8-N9	2.13	1.39	1.36
2	C	1116	ATP	PA-O3A	2.12	1.63	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1116	ATP	N3-C2-N1	-5.25	124.32	128.71
2	A	1116	ATP	O4'-C1'-N9	-4.25	104.49	108.44
2	A	1116	ATP	N3-C2-N1	-4.17	125.22	128.71
2	A	1116	ATP	N3-C4-N9	3.68	132.09	125.43
2	B	1116	ATP	C4'-O4'-C1'	-3.63	105.81	109.75
2	A	1116	ATP	C4'-O4'-C1'	-3.63	105.81	109.75
2	B	1116	ATP	C2-N1-C6	3.61	125.28	118.77
2	A	1116	ATP	O3G-PG-O1G	3.53	121.99	110.44
2	B	1116	ATP	N6-C6-N1	3.15	125.55	119.36
2	C	1116	ATP	C8-N9-C4	3.05	109.23	106.90
2	B	1116	ATP	C4-C5-N7	-2.99	106.96	109.52
2	B	1116	ATP	N3-C4-N9	2.98	130.82	125.43
2	A	1116	ATP	O4'-C1'-C2'	2.79	111.05	106.77
2	B	1116	ATP	C8-N9-C4	2.67	108.94	106.90
2	C	1116	ATP	N3-C2-N1	-2.66	126.48	128.71
2	C	1116	ATP	N3-C4-N9	2.57	130.06	125.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.