



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 11:23 PM GMT

PDB ID : 2OID
Title : Crystal structure of IRAK4 kinase domain complexed with AMPPNP
Authors : Kuglstatter, A.; Villasenor, A.G.; Browner, M.F.
Deposited on : 2007-01-10
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

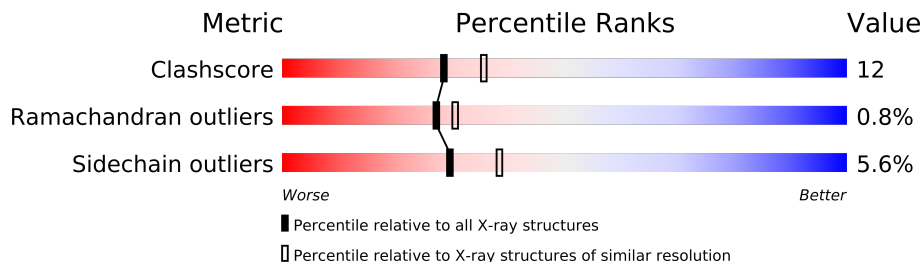
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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 ≥ 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	301	
1	B	301	
1	C	301	
1	D	301	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8921 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.

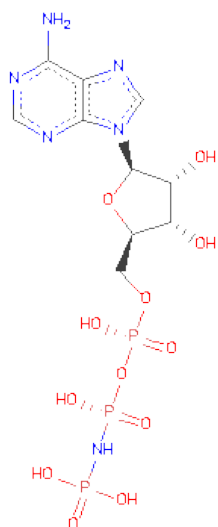
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	P	S	0	0	0
			2105	1321	356	412	3	13			
1	B	274	Total	C	N	O	P	S	0	0	0
			2171	1364	368	424	2	13			
1	C	259	Total	C	N	O	P	S	0	0	0
			2052	1286	344	405	3	14			
1	D	277	Total	C	N	O	P	S	0	0	0
			2190	1370	369	434	3	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	342	TPO	THR	MODIFIED RESIDUE	UNP Q9NWZ3
A	345	TPO	THR	MODIFIED RESIDUE	UNP Q9NWZ3
A	346	SEP	SER	MODIFIED RESIDUE	UNP Q9NWZ3
B	342	TPO	THR	MODIFIED RESIDUE	UNP Q9NWZ3
B	345	TPO	THR	MODIFIED RESIDUE	UNP Q9NWZ3
B	346	SEP	SER	MODIFIED RESIDUE	UNP Q9NWZ3
C	342	TPO	THR	MODIFIED RESIDUE	UNP Q9NWZ3
C	345	TPO	THR	MODIFIED RESIDUE	UNP Q9NWZ3
C	346	SEP	SER	MODIFIED RESIDUE	UNP Q9NWZ3
D	342	TPO	THR	MODIFIED RESIDUE	UNP Q9NWZ3
D	345	TPO	THR	MODIFIED RESIDUE	UNP Q9NWZ3
D	346	SEP	SER	MODIFIED RESIDUE	UNP Q9NWZ3

- Molecule 2 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	89	Total	O	0	0
			89	89		
3	B	83	Total	O	0	0
			83	83		
3	C	56	Total	O	0	0
			56	56		
3	D	51	Total	O	0	0
			51	51		

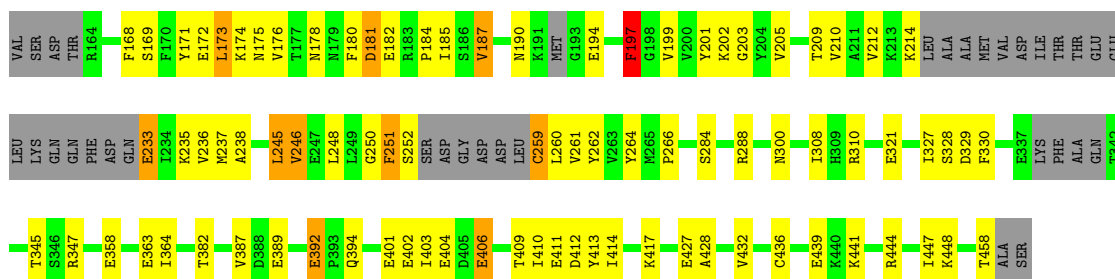
3 Residue-property plots

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.

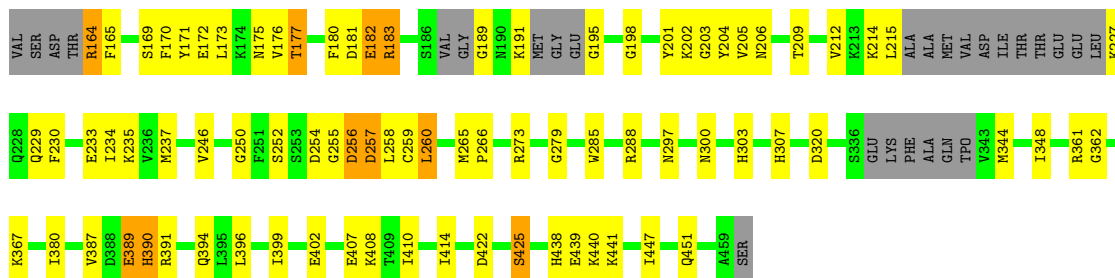
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A:



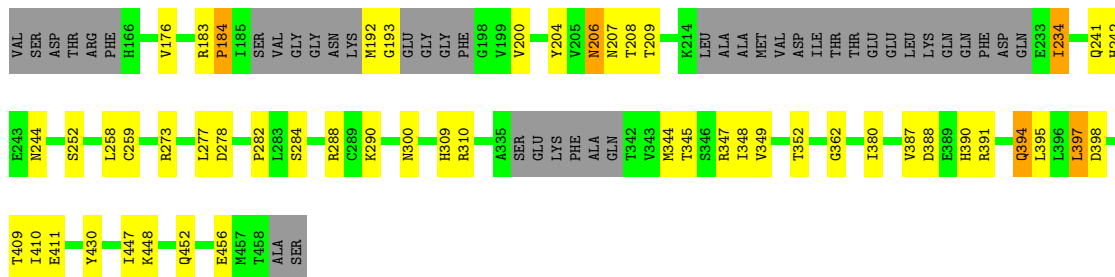
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain B:



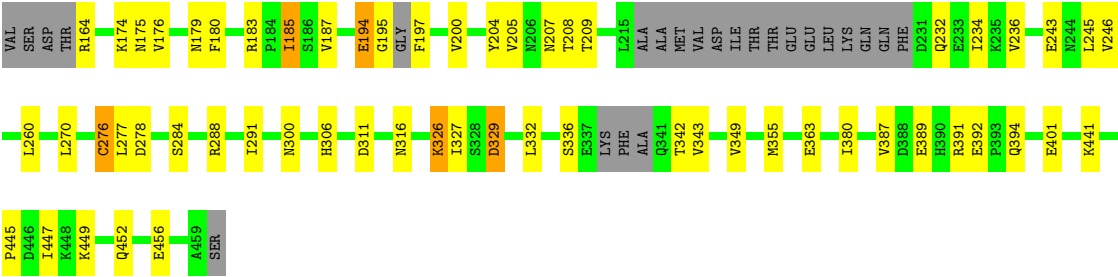
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain C:



- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.12Å 138.97Å 89.20Å 90.00° 126.43° 90.00°	Depositor
Resolution (Å)	49.94 – 2.30	Depositor
% Data completeness (in resolution range)	99.3 (49.94-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.241 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8921	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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: TPO, ANP, SEP

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	0.62	0/2106	0.66	0/2833
1	B	0.61	0/2184	0.66	0/2938
1	C	0.53	0/2051	0.62	1/2762 (0.0%)
1	D	0.54	1/2191 (0.0%)	0.60	0/2948
All	All	0.58	1/8532 (0.0%)	0.64	1/11481 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	276	CYS	CB-SG	-5.02	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	397	LEU	CA-CB-CG	6.21	129.59	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2105	0	2077	73	2
1	B	2171	0	2138	73	3
1	C	2052	0	2024	36	0
1	D	2190	0	2148	34	1
2	A	31	0	13	1	0
2	B	31	0	13	0	0
2	C	31	0	13	4	0
2	D	31	0	13	3	0
3	A	89	0	0	7	0
3	B	83	0	0	2	1
3	C	56	0	0	1	0
3	D	51	0	0	2	0
All	All	8921	0	8439	213	4

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 12.

The worst 5 of 213 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:170:PHE:HA	1:B:173:LEU:HD12	1.34	1.09
1:B:233:GLU:O	1:B:237:MET:HG2	1.59	1.02
1:B:265:MET:HE1	1:B:320:ASP:HB3	1.41	1.02
1:D:195:GLY:HA3	2:D:4:ANP:O2G	1.70	0.92
1:B:265:MET:CE	1:B:320:ASP:HB3	2.03	0.87

All (4) 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)
3:B:2108:HOH:O	3:B:2108:HOH:O[2_555]	1.85	0.35
1:A:175:ASN:ND2	1:B:176:VAL:CG1[2_555]	1.89	0.31
1:A:176:VAL:CG1	1:B:175:ASN:ND2[2_555]	2.15	0.05
1:B:361:ARG:NH1	1:D:355:MET:O[4_546]	2.17	0.03

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	254/301 (84%)	242 (95%)	9 (4%)	3 (1%)	19	19
1	B	262/301 (87%)	245 (94%)	15 (6%)	2 (1%)	27	30
1	C	247/301 (82%)	228 (92%)	17 (7%)	2 (1%)	27	30
1	D	266/301 (88%)	255 (96%)	10 (4%)	1 (0%)	43	52
All	All	1029/1204 (86%)	970 (94%)	51 (5%)	8 (1%)	27	30

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	A	197	PHE
1	B	257	ASP
1	C	207	ASN
1	B	390	HIS

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	229/259 (88%)	216 (94%)	13 (6%)	29	37
1	B	238/259 (92%)	225 (94%)	13 (6%)	30	39
1	C	225/259 (87%)	213 (95%)	12 (5%)	32	41
1	D	239/259 (92%)	225 (94%)	14 (6%)	28	35
All	All	931/1036 (90%)	879 (94%)	52 (6%)	30	38

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	344	MET
1	C	241	GLN
1	D	329	ASP
1	B	389	GLU
1	C	206	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	206	ASN
1	B	394	GLN
1	D	166	HIS
1	B	166	HIS
1	D	175	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

11 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	342	1	10,10,11	6.12	1 (10%)	12,14,16	1.20	2 (16%)
1	TPO	A	345	1	10,10,11	5.83	1 (10%)	12,14,16	1.39	1 (8%)
1	SEP	A	346	1	9,9,10	6.02	3 (33%)	10,12,14	1.56	2 (20%)
1	TPO	B	345	1	10,10,11	5.66	1 (10%)	12,14,16	1.54	2 (16%)
1	SEP	B	346	1	9,9,10	6.17	3 (33%)	10,12,14	1.41	1 (10%)
1	TPO	C	342	1	10,10,11	6.16	1 (10%)	12,14,16	1.30	2 (16%)
1	TPO	C	345	1	10,10,11	5.81	1 (10%)	12,14,16	1.62	1 (8%)
1	SEP	C	346	1	9,9,10	6.05	3 (33%)	10,12,14	1.33	2 (20%)
1	TPO	D	342	1	10,10,11	5.90	1 (10%)	12,14,16	1.28	1 (8%)
1	TPO	D	345	1	10,10,11	5.62	1 (10%)	12,14,16	1.33	1 (8%)
1	SEP	D	346	1	9,9,10	6.13	3 (33%)	10,12,14	1.34	2 (20%)

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
1	TPO	A	342	1	-	0/9/11/13	0/0/0/0
1	TPO	A	345	1	-	1/9/11/13	0/0/0/0
1	SEP	A	346	1	-	0/6/8/10	0/0/0/0
1	TPO	B	345	1	-	1/9/11/13	0/0/0/0
1	SEP	B	346	1	-	0/6/8/10	0/0/0/0
1	TPO	C	342	1	-	0/9/11/13	0/0/0/0
1	TPO	C	345	1	-	1/9/11/13	0/0/0/0
1	SEP	C	346	1	-	0/6/8/10	0/0/0/0
1	TPO	D	342	1	-	0/9/11/13	0/0/0/0
1	TPO	D	345	1	-	1/9/11/13	0/0/0/0
1	SEP	D	346	1	-	0/6/8/10	0/0/0/0

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	TPO	O-C	19.34	1.24	1.11
1	A	342	TPO	O-C	19.19	1.24	1.11
1	D	342	TPO	O-C	18.52	1.24	1.11
1	A	345	TPO	O-C	18.26	1.24	1.11
1	C	345	TPO	O-C	18.23	1.24	1.11

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	345	TPO	CB-CA-N	4.69	116.16	109.60
1	A	346	SEP	C-CA-N	-3.66	110.17	113.83
1	B	346	SEP	C-CA-N	-3.58	110.26	113.83
1	A	345	TPO	CB-CA-N	3.43	114.39	109.60
1	B	345	TPO	CB-CA-N	3.27	114.17	109.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	OG1-CB-CA-N
1	B	345	TPO	OG1-CB-CA-N
1	C	345	TPO	OG1-CB-CA-N
1	D	345	TPO	OG1-CB-CA-N

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	ANP	A	1	-	33,33,33	3.58	6 (18%)	51,52,52	2.35	12 (23%)
2	ANP	B	2	-	33,33,33	3.60	7 (21%)	51,52,52	2.19	13 (25%)
2	ANP	C	3	-	33,33,33	3.56	7 (21%)	51,52,52	2.18	12 (23%)
2	ANP	D	4	-	33,33,33	3.68	7 (21%)	51,52,52	1.87	8 (15%)

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	ANP	A	1	-	-	0/18/38/38	0/1/3/3
2	ANP	B	2	-	-	0/18/38/38	0/1/3/3
2	ANP	C	3	-	-	0/18/38/38	0/1/3/3
2	ANP	D	4	-	-	0/18/38/38	0/1/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	ANP	PB-N3B	13.88	1.76	1.64
2	A	1	ANP	PG-N3B	13.64	1.76	1.64
2	B	2	ANP	PG-N3B	13.23	1.75	1.64
2	C	3	ANP	PG-N3B	13.13	1.75	1.64
2	D	4	ANP	PG-N3B	13.09	1.75	1.64

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ANP	PB-N3B-PG	-8.70	115.43	130.07
2	A	1	ANP	N3-C2-N1	-7.61	122.35	128.71
2	B	2	ANP	N3-C2-N1	-7.44	122.49	128.71
2	C	3	ANP	N3-C2-N1	-7.36	122.56	128.71
2	C	3	ANP	PB-N3B-PG	-7.09	118.15	130.07

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.