



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:27 PM GMT

PDB ID : 1PYX  
Title : GSK-3 Beta complexed with AMP-PNP  
Authors : Bertrand, J.A.; Thieffine, S.; Vulpetti, A.; Cristiani, C.; Valsasina, B.; Knapp, S.; Kalisz, H.M.; Flocco, M.  
Deposited on : 2003-07-09  
Resolution : 2.40 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>

---

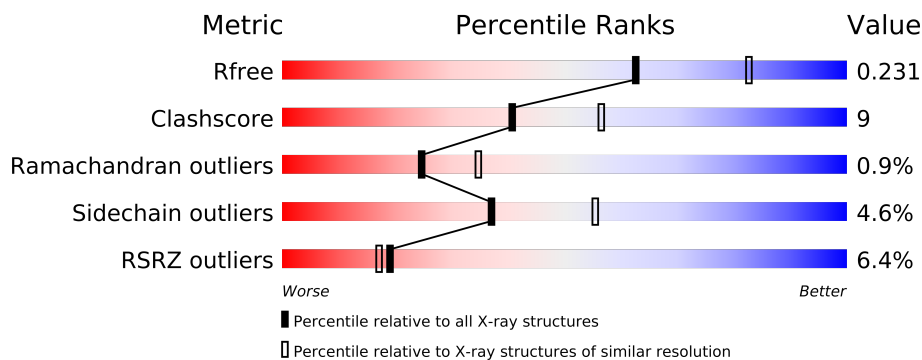
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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.

Mol	Chain	Length	Quality of chain
1	A	422	
1	B	422	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5682 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 Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2743	1767	472	493	11			
1	B	338	Total	C	N	O	S	0	0	0
			2706	1744	465	486	11			

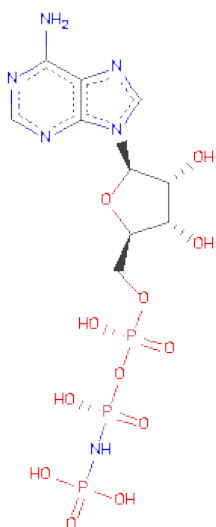
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP P49841
A	0	PRO	-	CLONING ARTIFACT	UNP P49841
B	-1	GLY	-	CLONING ARTIFACT	UNP P49841
B	0	PRO	-	CLONING ARTIFACT	UNP P49841

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	85	Total O 85 85	0	0
4	B	82	Total O 82 82	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.69Å 85.21Å 178.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.40 19.92 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.92-2.40) 98.7 (19.92-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.38Å)	Xtriage
Refinement program	CNX 2002 (ACCELRYN)	Depositor
R, $R_{free}$	0.206 , 0.233 0.203 , 0.231	Depositor DCC
$R_{free}$ test set	2468 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 43.3	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 49993 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP

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	0.52	0/2811	0.70	1/3823 (0.0%)
1	B	0.49	0/2773	0.68	0/3770
All	All	0.50	0/5584	0.69	1/7593 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ASN	N-CA-C	5.35	125.45	111.00

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	2743	0	2777	59	0
1	B	2706	0	2740	47	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	13	1	0
3	B	31	0	13	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	85	0	0	0	0
4	B	82	0	0	0	0
All	All	5682	0	5543	103	0

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:220:ARG:CD	1:A:221:TYR:H	1.65	1.09
1:B:220:ARG:CD	1:B:221:TYR:H	1.66	1.08
1:B:220:ARG:HD3	1:B:221:TYR:H	1.19	1.07
1:A:220:ARG:HD3	1:A:221:TYR:H	1.20	1.05
1:A:370:ASN:HD22	1:A:372:PRO:HD2	1.41	0.83
1:B:106:HIS:HD2	1:B:108:ASN:H	1.24	0.82
1:A:106:HIS:CD2	1:A:108:ASN:H	1.98	0.81
1:A:106:HIS:HD2	1:A:108:ASN:H	1.24	0.81
1:B:106:HIS:CD2	1:B:108:ASN:H	1.99	0.80
1:B:220:ARG:CD	1:B:221:TYR:N	2.47	0.77
1:B:370:ASN:HD22	1:B:372:PRO:HD2	1.51	0.76
1:A:370:ASN:ND2	1:A:372:PRO:HD2	2.01	0.75
1:A:220:ARG:CD	1:A:221:TYR:N	2.46	0.75
1:A:285:ASN:HB3	1:A:286:PRO:CD	2.16	0.75
1:A:220:ARG:HH11	1:A:220:ARG:HG2	1.56	0.71
1:B:220:ARG:HD2	1:B:221:TYR:H	1.56	0.70
1:A:220:ARG:HD2	1:A:221:TYR:H	1.54	0.68
1:B:220:ARG:HH11	1:B:220:ARG:HG2	1.58	0.68
1:A:220:ARG:HD3	1:A:221:TYR:CG	2.33	0.64
1:A:60:LYS:HE2	1:A:72:GLN:NE2	2.13	0.64
1:A:91:LYS:HE2	1:A:126:VAL:HG23	1.79	0.62
1:B:307:PRO:O	1:B:308:ARG:HB2	2.00	0.61
1:B:291:PHE:CE2	1:B:293:PHE:HB2	2.35	0.61
1:B:279:GLU:O	1:B:283:GLU:HG2	2.00	0.60
1:A:153:LEU:HD23	1:A:153:LEU:H	1.65	0.60
1:A:370:ASN:C	1:A:370:ASN:HD22	2.04	0.59
1:B:220:ARG:HD2	1:B:221:TYR:N	2.14	0.59
1:A:220:ARG:HD2	1:A:221:TYR:N	2.13	0.59
1:B:220:ARG:HD3	1:B:221:TYR:CG	2.38	0.59
1:B:307:PRO:O	1:B:308:ARG:CB	2.50	0.58
1:A:349:LYS:HE2	1:A:355:ASP:OD1	2.04	0.58
1:A:220:ARG:HD3	1:A:221:TYR:N	2.05	0.58
1:B:91:LYS:O	1:B:91:LYS:HD3	2.03	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:296:ILE:HD11	1:B:67:PHE:CE1	2.40	0.57
1:A:98:LEU:O	1:A:102:ARG:HG3	2.05	0.57
1:B:212:PRO:HB3	1:B:232:THR:HG23	1.88	0.56
1:A:285:ASN:CB	1:A:286:PRO:CD	2.82	0.56
1:B:370:ASN:ND2	1:B:372:PRO:HD2	2.18	0.56
1:A:285:ASN:HB3	1:A:286:PRO:HD3	1.86	0.56
1:B:98:LEU:O	1:B:102:ARG:HG3	2.06	0.55
1:B:316:LEU:HD22	1:B:320:LEU:HD22	1.89	0.55
1:B:220:ARG:HD3	1:B:221:TYR:N	2.04	0.54
1:A:144:ARG:HD2	1:A:148:ARG:NH2	2.23	0.54
1:B:212:PRO:HB3	1:B:232:THR:CG2	2.39	0.53
1:A:91:LYS:HE2	1:A:126:VAL:CG2	2.39	0.53
1:B:62:ILE:HG21	1:B:72:GLN:HB2	1.90	0.52
1:A:316:LEU:HD22	1:A:320:LEU:HD22	1.91	0.51
1:A:106:HIS:HD2	1:A:108:ASN:N	2.01	0.51
1:B:106:HIS:HD2	1:B:108:ASN:N	2.00	0.51
1:B:137:GLU:HG3	1:B:191:PRO:HG3	1.94	0.50
1:B:276:PRO:HB2	1:B:281:ILE:HG13	1.93	0.50
1:A:137:GLU:HG3	1:A:191:PRO:HG3	1.93	0.50
1:A:294:PRO:HG2	1:B:67:PHE:CE2	2.47	0.49
1:B:369:SER:O	1:B:370:ASN:HB2	2.12	0.49
1:B:220:ARG:O	1:B:223:ARG:HG3	2.14	0.48
1:A:276:PRO:HG3	1:A:323:TYR:CZ	2.48	0.48
1:A:220:ARG:O	1:A:223:ARG:HG3	2.13	0.48
1:A:296:ILE:HD11	1:B:67:PHE:CZ	2.50	0.47
1:A:38:THR:O	1:A:55:SER:HA	2.15	0.47
1:B:370:ASN:C	1:B:370:ASN:HD22	2.18	0.46
1:A:285:ASN:HB3	1:A:286:PRO:HD2	1.96	0.46
1:A:279:GLU:HG3	1:A:282:ARG:HH12	1.79	0.46
1:A:153:LEU:HD23	1:A:153:LEU:N	2.31	0.46
1:A:305:PHE:CD2	1:A:314:ILE:HG12	2.51	0.46
1:A:220:ARG:HD3	1:A:221:TYR:CD2	2.50	0.46
1:A:153:LEU:H	1:A:153:LEU:CD2	2.26	0.46
1:A:193:THR:O	1:A:357:PRO:HG3	2.15	0.46
1:B:344:ARG:HG2	1:B:379:PRO:HG3	1.96	0.45
1:B:106:HIS:HE1	1:B:366:GLU:OE1	1.98	0.45
1:B:88:LEU:HD11	1:B:125:GLU:OE1	2.16	0.45
1:A:112:LEU:HA	1:A:132:LEU:HD23	1.97	0.45
1:A:46:GLN:HE21	1:A:46:GLN:HB3	1.55	0.45
1:A:135:VAL:HA	1:A:136:PRO:HD3	1.75	0.45
1:A:225:PRO:HB2	1:A:284:MET:SD	2.57	0.45
1:A:371:PRO:HB2	1:A:372:PRO:HD3	1.98	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:196:LEU:HD23	1:A:196:LEU:C	2.37	0.44
1:B:316:LEU:HD22	1:B:320:LEU:CD2	2.47	0.44
1:A:92:ARG:O	1:A:93:PHE:CD1	2.71	0.44
1:B:220:ARG:HH11	1:B:220:ARG:CG	2.29	0.43
1:B:64:ASN:HB3	1:B:65:GLY:H	1.54	0.43
1:A:94:LYS:HD2	1:A:99:GLN:NE2	2.34	0.42
1:A:195:VAL:HG22	1:A:357:PRO:HB3	2.01	0.42
1:A:250:LEU:HA	1:A:250:LEU:HD12	1.87	0.42
1:B:115:PHE:HA	1:B:129:ASN:O	2.19	0.42
1:A:316:LEU:HD22	1:A:320:LEU:CD2	2.49	0.42
1:A:65:GLY:HA3	3:A:1001:ANP:O1B	2.20	0.42
1:B:211:GLU:HA	1:B:212:PRO:HD3	1.92	0.42
1:B:80:GLU:CD	1:B:113:ARG:HH22	2.23	0.42
1:B:135:VAL:HA	1:B:136:PRO:HD3	1.76	0.42
1:B:220:ARG:HD3	1:B:221:TYR:CD2	2.55	0.41
1:A:379:PRO:HA	1:A:380:PRO:HD3	1.93	0.41
1:A:52:GLN:NE2	1:A:114:TYR:HE2	2.17	0.41
1:A:267:VAL:HG12	1:A:271:LYS:HE3	2.02	0.41
1:B:196:LEU:HD23	1:B:196:LEU:C	2.41	0.41
1:A:91:LYS:HE2	1:A:126:VAL:CB	2.51	0.41
1:A:301:TRP:O	1:A:304:VAL:HB	2.21	0.41
1:B:93:PHE:CD1	1:B:93:PHE:N	2.89	0.41
1:B:60:LYS:O	1:B:62:ILE:HG23	2.20	0.41
1:A:266:LEU:HA	1:A:266:LEU:HD12	1.84	0.41
1:A:370:ASN:C	1:A:370:ASN:ND2	2.73	0.40
1:B:267:VAL:HG12	1:B:271:LYS:HE3	2.03	0.40
1:B:193:THR:O	1:B:194:ALA:HB3	2.21	0.40
1:A:293:PHE:HA	1:A:294:PRO:HD3	1.94	0.40

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	337/422 (80%)	322 (96%)	11 (3%)	4 (1%)	19 26

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	332/422 (79%)	315 (95%)	15 (4%)	2 (1%)	33	47
All	All	669/844 (79%)	637 (95%)	26 (4%)	6 (1%)	25	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ASN
1	A	220	ARG
1	B	220	ARG
1	B	308	ARG
1	A	77	ASP
1	A	218	CYS

### 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	305/365 (84%)	292 (96%)	13 (4%)	40	59
1	B	301/365 (82%)	286 (95%)	15 (5%)	34	51
All	All	606/730 (83%)	578 (95%)	28 (5%)	37	55

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	77	ASP
1	A	169	LEU
1	A	220	ARG
1	A	227	LEU
1	A	232	THR
1	A	250	LEU
1	A	266	LEU
1	A	286	PRO
1	A	295	GLN
1	A	316	LEU
1	A	320	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	370	ASN
1	B	49	ASP
1	B	67	PHE
1	B	91	LYS
1	B	151	GLN
1	B	169	LEU
1	B	220	ARG
1	B	227	LEU
1	B	232	THR
1	B	250	LEU
1	B	266	LEU
1	B	279	GLU
1	B	316	LEU
1	B	320	LEU
1	B	370	ASN
1	B	383	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	72	GLN
1	A	99	GLN
1	A	106	HIS
1	A	108	ASN
1	A	365	GLN
1	A	370	ASN
1	B	72	GLN
1	B	106	HIS
1	B	108	ASN
1	B	365	GLN
1	B	370	ASN

### 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 6 ligands modelled in this entry, 4 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	ANP	A	1001	2	33,33,33	2.70	7 (21%)	51,52,52	2.16	12 (23%)
3	ANP	B	2001	2	33,33,33	3.08	6 (18%)	51,52,52	2.13	15 (29%)

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	ANP	A	1001	2	-	0/18/38/38	0/1/3/3
3	ANP	B	2001	2	-	0/18/38/38	0/1/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	ANP	PG-O1G	10.16	1.58	1.46
3	B	2001	ANP	PG-N3B	-8.97	1.56	1.64
3	A	1001	ANP	PG-O1G	8.91	1.57	1.46
3	A	1001	ANP	PG-N3B	-7.40	1.57	1.64
3	B	2001	ANP	PB-N3B	-6.28	1.58	1.64
3	B	2001	ANP	PB-O1B	6.04	1.53	1.46
3	A	1001	ANP	PB-O1B	5.78	1.53	1.46
3	A	1001	ANP	PB-N3B	-5.77	1.59	1.64
3	B	2001	ANP	C4-N3	3.99	1.41	1.35
3	B	2001	ANP	C5-C4	3.80	1.49	1.40
3	A	1001	ANP	C4-N3	3.36	1.40	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	ANP	C5-C4	3.13	1.47	1.40
3	A	1001	ANP	PA-O3A	2.30	1.64	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	ANP	O4'-C1'-N9	6.62	114.59	108.44
3	A	1001	ANP	N3-C2-N1	-6.17	123.55	128.71
3	B	2001	ANP	N3-C2-N1	-5.84	123.83	128.71
3	B	2001	ANP	O4'-C1'-N9	5.70	113.74	108.44
3	B	2001	ANP	C8-N9-C4	5.61	111.18	106.90
3	A	1001	ANP	C8-N9-C4	5.33	110.96	106.90
3	A	1001	ANP	PA-O3A-PB	-4.18	117.54	131.81
3	A	1001	ANP	N3-C4-N9	4.02	132.69	125.43
3	B	2001	ANP	N3-C4-N9	3.97	132.61	125.43
3	B	2001	ANP	O3G-PG-O1G	-3.87	103.65	113.60
3	A	1001	ANP	O3G-PG-O1G	-3.80	103.83	113.60
3	B	2001	ANP	PB-N3B-PG	3.73	136.35	130.07
3	A	1001	ANP	PB-N3B-PG	3.62	136.16	130.07
3	B	2001	ANP	PA-O3A-PB	-3.47	119.95	131.81
3	B	2001	ANP	C5-C4-N9	-3.12	102.66	107.16
3	A	1001	ANP	C5-C4-N9	-2.83	103.08	107.16
3	B	2001	ANP	C2-N1-C6	2.68	123.62	118.77
3	A	1001	ANP	O2A-PA-O1A	-2.59	97.73	112.21
3	B	2001	ANP	O2A-PA-O1A	-2.54	98.03	112.21
3	B	2001	ANP	O1G-PG-N3B	-2.45	108.13	111.83
3	B	2001	ANP	C6-C5-C4	-2.27	113.08	117.25
3	A	1001	ANP	C2-N1-C6	2.25	122.83	118.77
3	A	1001	ANP	C6-C5-C4	-2.23	113.15	117.25
3	B	2001	ANP	O3G-PG-N3B	2.18	112.53	106.61
3	B	2001	ANP	O2B-PB-O3A	2.16	115.39	105.14
3	A	1001	ANP	O2A-PA-O3A	2.13	115.25	105.14
3	B	2001	ANP	O2A-PA-O3A	2.05	114.87	105.14

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 ⓘ

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	343/422 (81%)	0.08	24 (6%) 16 14	25, 40, 74, 91	0
1	B	338/422 (80%)	-0.02	20 (5%) 22 20	24, 38, 69, 95	0
All	All	681/844 (80%)	0.03	44 (6%) 19 17	24, 39, 72, 95	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	386	ALA	6.6
1	B	35	SER	6.5
1	A	35	SER	6.3
1	A	93	PHE	6.2
1	A	119	SER	4.3
1	A	92	ARG	4.2
1	B	92	ARG	4.1
1	A	278	ARG	3.8
1	B	282	ARG	3.8
1	A	282	ARG	3.5
1	A	77	ASP	3.3
1	B	148	ARG	3.3
1	B	119	SER	3.2
1	A	148	ARG	3.1
1	A	90	ASP	3.1
1	A	285	ASN	3.1
1	B	65	GLY	3.0
1	A	295	GLN	3.0
1	B	308	ARG	2.9
1	B	278	ARG	2.9
1	B	279	GLU	2.9
1	B	125	GLU	2.8
1	A	385	GLN	2.8
1	B	36	LYS	2.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	307	PRO	2.7
1	A	125	GLU	2.7
1	B	91	LYS	2.7
1	B	93	PHE	2.6
1	A	91	LYS	2.6
1	A	308	ARG	2.6
1	A	36	LYS	2.5
1	A	126	VAL	2.5
1	A	47	GLY	2.4
1	B	130	LEU	2.4
1	B	64	ASN	2.4
1	A	297	LYS	2.4
1	B	295	GLN	2.3
1	A	130	LEU	2.3
1	A	210	GLY	2.3
1	B	94	LYS	2.3
1	B	209	ARG	2.3
1	A	303	LYS	2.2
1	A	209	ARG	2.0
1	B	77	ASP	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ANP	A	1001	31/31	0.10	-0.76	27,34,42,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ANP	B	2001	31/31	0.11	-0.84	34,40,51,52	0
2	MG	B	2003	1/1	0.06	-1.21	46,46,46,46	0
2	MG	A	1003	1/1	0.07	-1.38	35,35,35,35	0
2	MG	B	2002	1/1	0.04	-2.46	59,59,59,59	0
2	MG	A	1002	1/1	0.05	-2.76	44,44,44,44	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.