



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:07 AM GMT

PDB ID : 1VFN
Title : PURINE NUCLEOSIDE PHOSPHORYLASE
Authors : Koellner, G.; Bzowska, A.
Deposited on : 1996-10-08
Resolution : 2.15 Å(reported)

This is a full wwPDB validation 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>

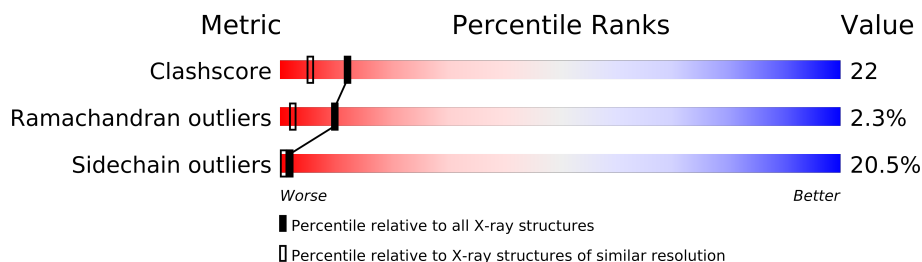
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.15 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	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)

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	281	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2243 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 PURINE-NUCLEOSIDE PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2102	1334	370	383	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	GLN	GLU	CONFLICT	UNP P55859

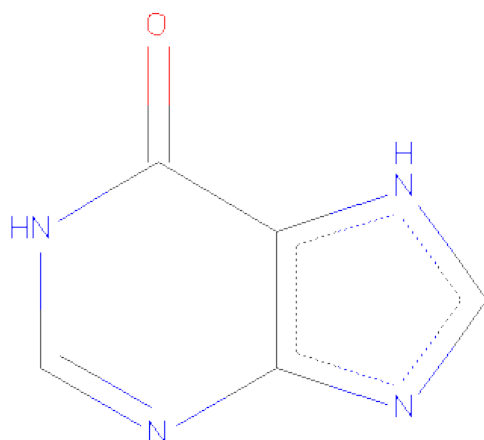
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is HYPOXANTHINE (three-letter code: HPA) (formula: C₅H₄N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	129	Total	O	0	0
			129	129		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	94.11Å 94.11Å 94.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15	Depositor
% Data completeness (in resolution range)	98.4 (20.00-2.15)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2243	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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: HPA, MG, ZN

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	1.21	13/2146 (0.6%)	1.61	43/2898 (1.5%)

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	A	1	0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLU	CD-OE2	8.12	1.34	1.25
1	A	262	GLU	CD-OE2	7.67	1.34	1.25
1	A	272	GLU	CD-OE2	7.50	1.33	1.25
1	A	259	GLU	CD-OE2	7.32	1.33	1.25
1	A	8	GLU	CD-OE2	6.66	1.32	1.25
1	A	153	GLU	CD-OE2	6.37	1.32	1.25
1	A	52	GLU	CD-OE2	6.30	1.32	1.25
1	A	258	GLU	CD-OE2	6.11	1.32	1.25
1	A	125	GLU	CD-OE2	6.03	1.32	1.25
1	A	152	GLU	CD-OE1	-5.98	1.19	1.25
1	A	89	GLU	CD-OE2	5.83	1.32	1.25
1	A	183	GLU	CD-OE2	5.17	1.31	1.25
1	A	109	GLU	CD-OE2	5.01	1.31	1.25

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ARG	NE-CZ-NH1	17.38	128.99	120.30
1	A	24	ARG	NE-CZ-NH2	-13.81	113.39	120.30
1	A	158	ARG	NE-CZ-NH2	-12.71	113.94	120.30
1	A	84	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	A	84	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	A	171	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	229	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	A	158	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	A	171	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	A	24	ARG	CD-NE-CZ	8.54	135.55	123.60
1	A	248	ASP	CB-CG-OD1	8.20	125.68	118.30
1	A	134	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	243	ASN	CA-C-N	7.41	133.49	117.20
1	A	243	ASN	C-N-CA	7.20	139.69	121.70
1	A	134	ASP	CB-CG-OD1	7.12	124.70	118.30
1	A	207	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	176	SER	N-CA-CB	6.86	120.79	110.50
1	A	248	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	A	164	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	260	VAL	N-CA-C	-6.59	93.21	111.00
1	A	78	CYS	CA-CB-SG	-6.30	102.66	114.00
1	A	245	VAL	N-CA-C	6.24	127.86	111.00
1	A	78	CYS	CB-CA-C	-6.21	97.98	110.40
1	A	168	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	243	ASN	O-C-N	-6.06	113.00	122.70
1	A	210	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	73	LEU	C-N-CA	-5.87	107.03	121.70
1	A	243	ASN	CB-CA-C	5.74	121.89	110.40
1	A	84	ARG	CD-NE-CZ	5.58	131.41	123.60
1	A	76	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	243	ASN	N-CA-C	5.50	125.85	111.00
1	A	47	THR	N-CA-CB	-5.42	99.99	110.30
1	A	39	VAL	N-CA-C	-5.39	96.44	111.00
1	A	49	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	239	SER	CB-CA-C	-5.29	100.04	110.10
1	A	131	LEU	CB-CA-C	-5.28	100.17	110.20
1	A	49	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	175	HIS	N-CA-C	-5.24	96.85	111.00
1	A	207	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	164	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	169	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	247	MET	CB-CA-C	-5.15	100.10	110.40
1	A	215	ASP	CB-CG-OD1	5.01	122.81	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	243	ASN	CA

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	2102	0	2061	90	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	10	0	4	0	0
5	A	129	0	0	11	0
All	All	2243	0	2065	90	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 22.

All (90) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35:LEU:HD23	1:A:114:THR:HG23	1.33	1.08
1:A:145:ASN:HD22	1:A:147:LEU:H	1.02	0.98
1:A:38:LEU:H	1:A:38:LEU:HD12	1.34	0.92
1:A:261:LEU:HD11	1:A:265:LYS:NZ	1.85	0.91
1:A:88:TYR:CE2	1:A:219:MET:HE3	2.12	0.85
1:A:35:LEU:HD23	1:A:114:THR:CG2	2.06	0.84
1:A:145:ASN:ND2	1:A:147:LEU:H	1.77	0.82
1:A:261:LEU:HD11	1:A:265:LYS:HZ2	1.44	0.81
1:A:125:GLU:HG3	5:A:309:HOH:O	1.82	0.78
1:A:267:ALA:HB1	1:A:271:LEU:HD12	1.66	0.77
1:A:152:GLU:OE2	1:A:154:ARG:HB2	1.86	0.76
1:A:244:LYS:C	1:A:244:LYS:HE2	2.06	0.76
1:A:267:ALA:HB1	1:A:271:LEU:CD1	2.16	0.75
1:A:244:LYS:HB3	1:A:244:LYS:NZ	1.91	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:206:CYS:SG	1:A:244:LYS:HE3	2.31	0.71
1:A:176:SER:N	5:A:427:HOH:O	2.24	0.70
1:A:185:ARG:HG3	1:A:186:GLU:N	2.08	0.68
1:A:35:LEU:C	5:A:333:HOH:O	2.31	0.68
1:A:207:ARG:O	1:A:211:ASN:ND2	2.30	0.65
1:A:261:LEU:HD11	1:A:265:LYS:HZ3	1.63	0.64
1:A:38:LEU:N	1:A:38:LEU:HD12	2.09	0.64
1:A:264:GLY:O	1:A:266:GLN:N	2.31	0.63
1:A:269:GLN:O	1:A:273:GLN:HG2	1.99	0.62
1:A:33:SER:HB2	5:A:324:HOH:O	1.99	0.62
1:A:32:GLY:O	1:A:35:LEU:HD22	1.99	0.62
1:A:262:GLU:HA	1:A:265:LYS:HB2	1.81	0.61
1:A:238:PHE:HE1	1:A:271:LEU:HD21	1.66	0.60
1:A:84:ARG:NH2	1:A:114:THR:O	2.30	0.59
1:A:39:VAL:HG12	1:A:40:ASN:N	2.17	0.59
1:A:258:GLU:O	1:A:259:GLU:HG3	2.03	0.59
1:A:282:ILE:N	1:A:282:ILE:HD12	2.19	0.56
1:A:76:ARG:NH2	1:A:282:ILE:HB	2.20	0.56
1:A:145:ASN:HD22	1:A:147:LEU:N	1.87	0.56
1:A:32:GLY:O	1:A:35:LEU:HB2	2.06	0.56
1:A:240:LEU:HG	1:A:271:LEU:HD11	1.88	0.56
1:A:178:TRP:CZ2	1:A:183:GLU:HG3	2.42	0.55
1:A:88:TYR:HE2	1:A:219:MET:HE3	1.66	0.55
1:A:172:GLN:O	1:A:175:HIS:O	2.25	0.55
1:A:38:LEU:HD13	1:A:80:MET:HE1	1.88	0.54
1:A:282:ILE:HG22	1:A:282:ILE:O	2.07	0.54
1:A:40:ASN:C	1:A:41:LYS:HG3	2.27	0.54
1:A:21:THR:O	1:A:24:ARG:NH2	2.42	0.53
1:A:73:LEU:HB3	1:A:279:MET:HG3	1.91	0.52
1:A:76:ARG:CG	1:A:76:ARG:HH11	2.22	0.52
1:A:210:ARG:O	1:A:210:ARG:HD2	2.10	0.52
1:A:7:TYR:HE2	1:A:11:GLN:OE1	1.93	0.52
1:A:238:PHE:HE1	1:A:271:LEU:CD2	2.22	0.52
1:A:244:LYS:HA	5:A:423:HOH:O	2.09	0.52
1:A:271:LEU:O	1:A:275:VAL:HG23	2.11	0.50
1:A:76:ARG:HH21	1:A:282:ILE:HB	1.76	0.50
1:A:265:LYS:O	1:A:266:GLN:HB3	2.11	0.50
1:A:32:GLY:HA3	1:A:84:ARG:HH21	1.78	0.49
1:A:40:ASN:C	1:A:42:LEU:H	2.15	0.49
1:A:138:LEU:HB2	1:A:194:MET:O	2.12	0.49
1:A:170:MET:HE1	1:A:236:PHE:HB3	1.95	0.48
1:A:94:TRP:CZ3	1:A:95:LYS:HG3	2.49	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:221:THR:HA	1:A:224:GLU:OE1	2.14	0.48
1:A:282:ILE:N	1:A:282:ILE:CD1	2.77	0.47
1:A:67:ARG:HD3	1:A:82:GLN:HG2	1.96	0.47
1:A:238:PHE:CE1	1:A:271:LEU:CD2	2.98	0.47
1:A:4:GLY:HA3	5:A:377:HOH:O	2.13	0.47
1:A:243:ASN:HB2	5:A:423:HOH:O	2.14	0.46
1:A:208:LEU:C	1:A:208:LEU:HD23	2.36	0.46
1:A:40:ASN:O	1:A:41:LYS:HG3	2.17	0.45
1:A:10:TYR:HB3	1:A:105:LEU:HD23	1.97	0.45
1:A:145:ASN:HB2	5:A:370:HOH:O	2.17	0.44
1:A:80:MET:HE3	1:A:80:MET:HB3	1.70	0.44
1:A:270:LYS:HA	1:A:273:GLN:HE21	1.83	0.44
1:A:170:MET:SD	1:A:234:ARG:HD2	2.58	0.44
1:A:211:ASN:ND2	5:A:338:HOH:O	2.50	0.43
1:A:274:PHE:O	1:A:278:LEU:HB2	2.17	0.43
1:A:136:ILE:HG22	1:A:138:LEU:HD13	2.00	0.43
1:A:246:ILE:HD12	1:A:246:ILE:C	2.39	0.42
1:A:76:ARG:CG	1:A:76:ARG:NH1	2.82	0.42
1:A:244:LYS:HE2	1:A:245:VAL:N	2.35	0.42
1:A:45:ALA:HA	1:A:70:PHE:O	2.19	0.42
1:A:154:ARG:HE	1:A:154:ARG:HB2	1.74	0.42
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.90	0.42
1:A:148:ARG:NH1	5:A:420:HOH:O	2.39	0.41
1:A:35:LEU:N	1:A:35:LEU:CD1	2.82	0.41
1:A:259:GLU:HA	1:A:262:GLU:HG2	2.00	0.41
1:A:73:LEU:HA	1:A:73:LEU:HD23	1.63	0.41
1:A:133:ARG:NE	5:A:413:HOH:O	2.53	0.41
1:A:54:PRO:O	1:A:55:ASN:HB2	2.20	0.41
1:A:242:THR:O	1:A:243:ASN:HB3	2.19	0.41
1:A:114:THR:HG23	1:A:115:ASN:N	2.34	0.41
1:A:245:VAL:HG21	1:A:253:GLY:O	2.20	0.41
1:A:170:MET:CE	1:A:236:PHE:CB	2.98	0.41
1:A:266:GLN:O	1:A:269:GLN:HG2	2.20	0.41
1:A:267:ALA:O	1:A:268:ALA:C	2.60	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	264/281 (94%)	244 (92%)	14 (5%)	6 (2%)	10 2

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	SER
1	A	265	LYS
1	A	266	GLN
1	A	33	SER
1	A	36	GLY
1	A	268	ALA

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	220/233 (94%)	175 (80%)	45 (20%)	2 0

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	27	VAL
1	A	33	SER
1	A	35	LEU
1	A	38	LEU
1	A	39	VAL
1	A	42	LEU
1	A	43	THR

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Mol	Chain	Res	Type
1	A	56	PHE
1	A	67	ARG
1	A	72	ILE
1	A	73	LEU
1	A	74	ASN
1	A	76	ARG
1	A	82	GLN
1	A	84	ARG
1	A	87	MET
1	A	96	VAL
1	A	104	ARG
1	A	105	LEU
1	A	114	THR
1	A	120	LEU
1	A	125	GLU
1	A	131	LEU
1	A	138	LEU
1	A	145	ASN
1	A	154	ARG
1	A	158	ARG
1	A	168	ARG
1	A	176	SER
1	A	179	LYS
1	A	185	ARG
1	A	186	GLU
1	A	187	LEU
1	A	195	LEU
1	A	212	LEU
1	A	240	LEU
1	A	244	LYS
1	A	251	SER
1	A	254	LYS
1	A	265	LYS
1	A	266	GLN
1	A	269	GLN
1	A	271	LEU
1	A	277	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN

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Mol	Chain	Res	Type
1	A	55	ASN
1	A	74	ASN
1	A	86	HIS
1	A	145	ASN
1	A	199	ASN
1	A	211	ASN
1	A	269	GLN

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
4	HPA	A	300	-	11,11,11	1.69	5 (45%)	9,15,15	2.86	2 (22%)

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
4	HPA	A	300	-	-	0/0/0/0	0/0/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	300	HPA	C8-N9	2.69	1.40	1.34
4	A	300	HPA	C6-N1	2.38	1.41	1.37
4	A	300	HPA	C8-N7	-2.37	1.30	1.34
4	A	300	HPA	C2-N3	2.03	1.35	1.31
4	A	300	HPA	C4-N9	2.01	1.38	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	300	HPA	C8-N7-C5	-7.05	103.51	108.52
4	A	300	HPA	C4-C5-N7	4.00	110.36	106.02

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.