



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:47 am GMT

PDB ID : 2QN7
Title : Glycogen Phosphorylase b in complex with N-4-hydroxybenzoyl-N'-4-beta-D-glucopyranosyl urea
Authors : Chrysina, E.D.; Tiraidis, K.; Alexacou, K.-M.; Zographos, S.E.; Leonidas, D.D.; Oikonomakos, N.G.
Deposited on : 2007-07-18
Resolution : 1.83 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

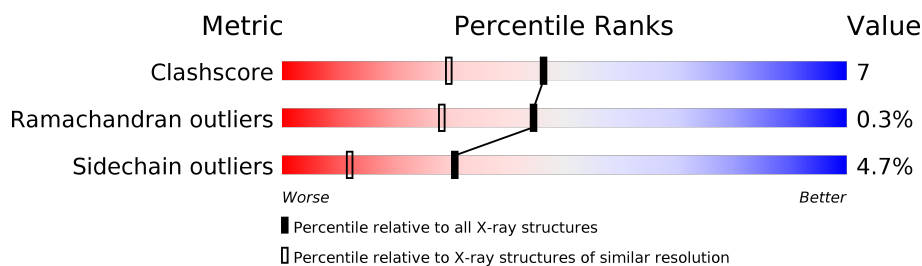
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	112137	3197 (1.86-1.82)
Ramachandran outliers	110173	3164 (1.86-1.82)
Sidechain outliers	110143	3165 (1.86-1.82)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6955 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.

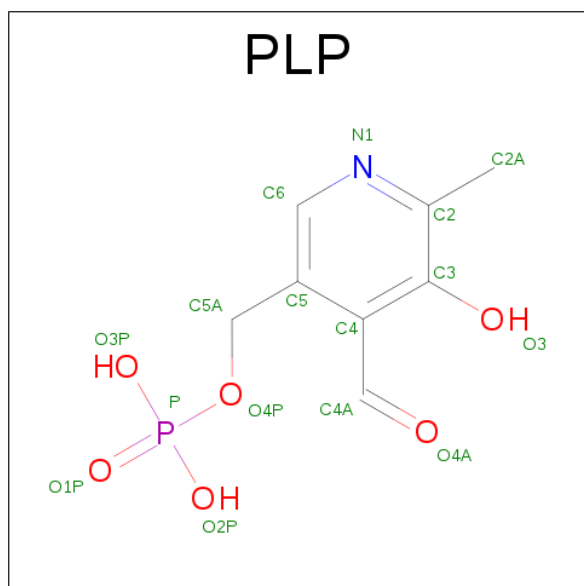
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	805	6546	4173	1153	1191	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

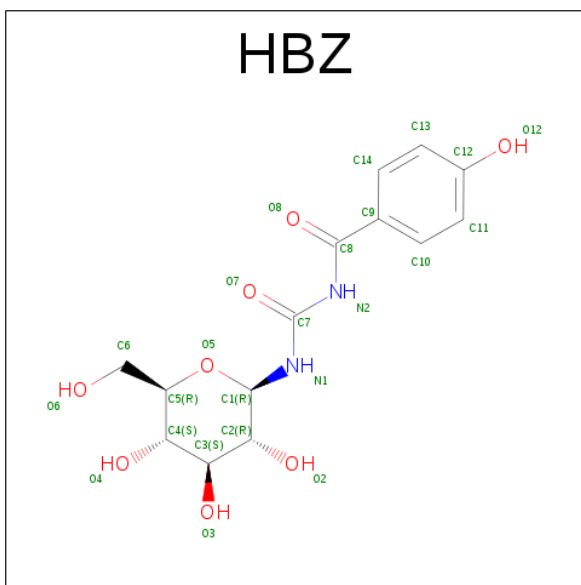
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	SEE REMARK 999	UNP P00489

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



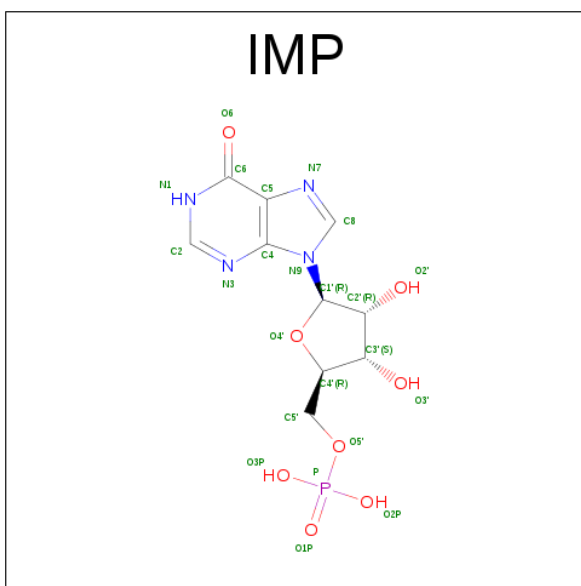
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	15	8	1	5	1	0	0

- Molecule 3 is N-[[[(4-HYDROXYPHENYL)CARBONYL]CARBAMOYL]-BETA-D-GLUCOPYRANOSYLAMINE (three-letter code: HBZ) (formula: C₁₄H₁₈N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	14	2	8		

- Molecule 4 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	347	Total 347	O 347	0	0



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.34Å 128.34Å 116.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.83	Depositor
% Data completeness (in resolution range)	91.1 (30.00-1.83)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6955	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: IMP, HBZ, PLP

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	0.31	0/6692	0.60	0/9056

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6546	0	6492	95	0
2	A	15	0	7	0	0
3	A	24	0	18	0	0
4	A	23	0	11	0	0
5	A	347	0	0	10	1
All	All	6955	0	6528	95	1

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 (95) 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:42:ASP:HB2	1:A:45:VAL:HG22	1.32	1.05
1:A:282:ASN:HB3	5:A:1291:HOH:O	1.81	0.79
1:A:455:VAL:H	1:A:459:HIS:HD2	1.33	0.76
1:A:678:ASN:HD22	1:A:679:MET:H	1.35	0.74
1:A:719:ASP:O	1:A:723:GLN:HG2	1.88	0.73
1:A:834:LEU:HG	1:A:835:PRO:HD2	1.74	0.69
1:A:739:ARG:O	1:A:743:GLU:HG3	1.95	0.67
1:A:550:GLU:O	1:A:554:LYS:HD3	1.95	0.66
1:A:69:ARG:CZ	1:A:836:ALA:HB2	2.26	0.65
1:A:516:ASP:O	1:A:519:ARG:HG3	1.97	0.64
1:A:42:ASP:HB2	1:A:45:VAL:CG2	2.19	0.62
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.82	0.62
1:A:235:ASN:H	1:A:235:ASN:HD22	1.48	0.61
1:A:65:GLY:O	1:A:69:ARG:HG2	2.00	0.61
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.83	0.61
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.84	0.61
1:A:642:VAL:C	1:A:643:ILE:HD12	2.22	0.59
1:A:551:ARG:NH1	1:A:552:GLU:OE2	2.37	0.58
1:A:550:GLU:HG2	1:A:555:VAL:O	2.05	0.57
1:A:474:LEU:HD13	1:A:475:GLU:HG3	1.87	0.57
1:A:207:GLU:OE1	1:A:214:LYS:NZ	2.36	0.56
1:A:510:GLU:HB2	5:A:1174:HOH:O	2.06	0.56
1:A:678:ASN:HD22	1:A:679:MET:N	2.03	0.55
1:A:214:LYS:HZ3	1:A:214:LYS:HB3	1.72	0.55
1:A:557:ILE:O	1:A:559:PRO:HD3	2.06	0.55
1:A:250:ASN:HA	1:A:269:ARG:HH21	1.73	0.54
1:A:34:HIS:HE1	1:A:61:ASP:OD1	1.91	0.54
1:A:501:GLU:O	1:A:505:GLU:HG3	2.07	0.54
1:A:423:ASP:O	1:A:426:ARG:HG2	2.10	0.52
1:A:519:ARG:HD2	5:A:1335:HOH:O	2.10	0.51
1:A:285:PHE:CD1	1:A:382:GLU:HB2	2.46	0.51
1:A:15:VAL:HG13	1:A:501:GLU:OE1	2.11	0.51
1:A:678:ASN:ND2	1:A:679:MET:H	2.06	0.51
1:A:18:LEU:HD22	1:A:18:LEU:N	2.25	0.51
1:A:16:ARG:HB2	1:A:106:ASN:ND2	2.26	0.51
1:A:21:VAL:HG23	1:A:22:GLU:N	2.25	0.50
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.93	0.50
1:A:380:ILE:CG2	1:A:382:GLU:CD	2.80	0.50
1:A:380:ILE:HG22	1:A:382:GLU:CD	2.32	0.50
1:A:678:ASN:HD22	1:A:678:ASN:N	2.11	0.49
1:A:831:ARG:HE	1:A:831:ARG:HA	1.77	0.48
1:A:636:VAL:O	1:A:639:ARG:HD3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LYS:O	1:A:473:GLU:HG3	2.13	0.48
1:A:568:LYS:HG3	1:A:574:LYS:HD3	1.96	0.48
1:A:831:ARG:O	1:A:833:ARG:NH1	2.46	0.48
1:A:119:MET:O	1:A:123:GLU:HG3	2.14	0.47
1:A:450:HIS:HD2	5:A:1171:HOH:O	1.97	0.47
1:A:363:LYS:HD3	1:A:363:LYS:C	2.34	0.47
1:A:534:VAL:O	1:A:537:VAL:HG22	2.15	0.47
1:A:617:LYS:HD3	5:A:1201:HOH:O	2.15	0.47
1:A:551:ARG:HH11	1:A:551:ARG:HB3	1.80	0.46
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.98	0.46
1:A:360:ASP:OD1	1:A:363:LYS:HB2	2.16	0.46
1:A:380:ILE:HG22	1:A:382:GLU:OE1	2.16	0.46
1:A:434:GLY:O	1:A:435:ALA:C	2.53	0.46
1:A:81:ARG:CG	1:A:155:TYR:HE2	2.29	0.46
1:A:261:GLY:HA3	5:A:1337:HOH:O	2.15	0.46
1:A:363:LYS:HD3	1:A:363:LYS:O	2.15	0.46
1:A:450:HIS:HE1	5:A:1116:HOH:O	1.98	0.46
1:A:214:LYS:NZ	1:A:214:LYS:CB	2.80	0.45
1:A:81:ARG:HG2	1:A:155:TYR:HE2	1.81	0.45
1:A:193:ARG:NH1	5:A:1253:HOH:O	2.50	0.45
1:A:510:GLU:HB3	1:A:517:GLN:HE22	1.82	0.44
1:A:209:THR:O	1:A:211:GLN:N	2.51	0.44
1:A:499:LEU:HD12	1:A:502:ILE:HD11	1.99	0.44
1:A:398:ARG:NH1	1:A:402:ILE:HG13	2.33	0.44
1:A:504:ALA:HA	1:A:508:GLY:O	2.18	0.44
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.53	0.44
1:A:280:TYR:OH	1:A:291:LEU:HB3	2.18	0.44
1:A:510:GLU:HB3	1:A:517:GLN:NE2	2.33	0.44
1:A:285:PHE:HD1	1:A:382:GLU:HB2	1.82	0.43
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.19	0.43
1:A:781:VAL:O	1:A:785:GLU:HG3	2.18	0.43
1:A:20:GLY:O	1:A:24:VAL:HG23	2.19	0.43
1:A:426:ARG:HG3	1:A:427:ARG:N	2.33	0.43
1:A:235:ASN:HA	1:A:833:ARG:HG3	2.01	0.43
1:A:81:ARG:HG2	1:A:155:TYR:CE2	2.53	0.42
1:A:33:ARG:NH2	5:A:1261:HOH:O	2.50	0.42
1:A:706:GLU:H	1:A:706:GLU:CD	2.23	0.42
1:A:341:HIS:HB2	1:A:342:PRO:HD3	2.02	0.42
1:A:165:ILE:HG12	5:A:1276:HOH:O	2.18	0.42
1:A:36:HIS:O	1:A:40:VAL:HA	2.19	0.42
1:A:834:LEU:HA	1:A:835:PRO:HD3	1.90	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:VAL:HG13	1:A:400:LEU:HD11	2.02	0.41
1:A:751:SER:N	1:A:752:PRO:HD3	2.34	0.41
1:A:410:PHE:O	1:A:413:ARG:HB2	2.20	0.41
1:A:834:LEU:HG	1:A:835:PRO:CD	2.49	0.41
1:A:463:LEU:HA	1:A:467:ILE:HG22	2.03	0.41
1:A:80:LYS:HE2	1:A:334:ALA:HB2	2.03	0.41
1:A:397:PRO:O	1:A:401:GLN:HG3	2.20	0.40
1:A:457:ARG:HH12	1:A:701:GLU:CD	2.25	0.40
1:A:87:LEU:HD21	1:A:296:GLU:HG2	2.04	0.40
1:A:678:ASN:N	1:A:678:ASN:ND2	2.67	0.40
1:A:282:ASN:OD1	1:A:284:ASN:OD1	2.40	0.40
1:A:689:ILE:O	1:A:689:ILE:HG23	2.20	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	Interatomic distance (Å)	Clash overlap (Å)
5:A:1262:HOH:O	5:A:1262:HOH:O[7_556]	2.19	0.01

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	799/842 (95%)	768 (96%)	29 (4%)	2 (0%)	44 28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	SER
1	A	835	PRO

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	696/731 (95%)	663 (95%)	33 (5%)	30	12

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	39	LEU
1	A	90	TYR
1	A	104	LEU
1	A	115	LEU
1	A	205	ARG
1	A	211	GLN
1	A	214	LYS
1	A	235	ASN
1	A	243	LEU
1	A	306	ASP
1	A	325	ASN
1	A	363	LYS
1	A	400	LEU
1	A	433	GLU
1	A	474	LEU
1	A	489	ARG
1	A	510	GLU
1	A	549	LEU
1	A	568	LYS
1	A	579	ASN
1	A	596	LYS
1	A	613	TYR
1	A	645	LEU
1	A	678	ASN
1	A	706	GLU
1	A	708	PHE
1	A	714	ARG
1	A	720	ARG
1	A	721	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	790	LEU
1	A	831	ARG
1	A	833	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	211	GLN
1	A	235	ASN
1	A	325	ASN
1	A	390	HIS
1	A	412	ASN
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	560	ASN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	A	767	HIS
1	A	832	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
4	IMP	A	930	-	21,25,25	2.20	9 (42%)	22,38,38	2.50	7 (31%)
3	HBZ	A	998	-	25,25,25	2.72	11 (44%)	34,35,35	0.95	1 (2%)
2	PLP	A	999	1	15,15,16	1.51	2 (13%)	20,22,23	1.05	0

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	IMP	A	930	-	-	0/6/26/26	0/3/3/3
3	HBZ	A	998	-	-	0/14/34/34	0/2/2/2
2	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	PLP	C3-C2	-3.03	1.38	1.40
4	A	930	IMP	C5-C4	-2.28	1.35	1.40
4	A	930	IMP	C2'-C1'	-2.21	1.50	1.53
4	A	930	IMP	C2-N3	-2.20	1.28	1.32
3	A	998	HBZ	C7-N2	-2.13	1.34	1.39
3	A	998	HBZ	O4-C4	2.06	1.47	1.43
4	A	930	IMP	O4'-C1'	2.27	1.44	1.41
4	A	930	IMP	C6-C5	2.69	1.46	1.41
3	A	998	HBZ	C3-C2	2.70	1.59	1.52
4	A	930	IMP	C5'-C4'	2.97	1.61	1.51
2	A	999	PLP	C4A-C4	3.08	1.57	1.51
3	A	998	HBZ	C13-C12	3.08	1.44	1.38
3	A	998	HBZ	C11-C12	3.34	1.45	1.38
4	A	930	IMP	C6-N1	3.68	1.39	1.33
3	A	998	HBZ	C10-C9	3.75	1.45	1.39
3	A	998	HBZ	C14-C13	3.97	1.45	1.38
4	A	930	IMP	C2-N1	4.07	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	998	HBZ	C14-C9	4.49	1.46	1.39
3	A	998	HBZ	C11-C10	4.53	1.46	1.38
4	A	930	IMP	C8-N7	4.88	1.43	1.34
3	A	998	HBZ	C2-C1	5.45	1.58	1.52
3	A	998	HBZ	O5-C1	5.98	1.52	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	930	IMP	N3-C2-N1	-7.15	122.63	128.86
4	A	930	IMP	O4'-C4'-C5'	-2.70	100.28	109.40
3	A	998	HBZ	O5-C1-C2	-2.64	107.14	109.84
4	A	930	IMP	O2'-C2'-C1'	-2.31	104.38	111.61
4	A	930	IMP	O4'-C4'-C3'	-2.30	100.59	105.17
4	A	930	IMP	C4-C5-N7	2.65	111.97	109.41
4	A	930	IMP	C4'-O4'-C1'	3.20	113.17	109.77
4	A	930	IMP	C2-N1-C6	6.09	126.08	115.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.