



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:30 AM GMT

PDB ID : 1B4D  
Title : AMIDOCARBAMATE INHIBITOR OF GLYCOGEN PHOSPHORYLASE  
Authors : Tsitsanou, K.E.; Oikonomakos, N.G.; Zographos, S.E.; Skamnaki, V.T.; Gregoriou, M.; Watson, K.A.; Johnson, L.N.; Fleet, G.W.J.  
Deposited on : 1998-12-18  
Resolution : 2.00 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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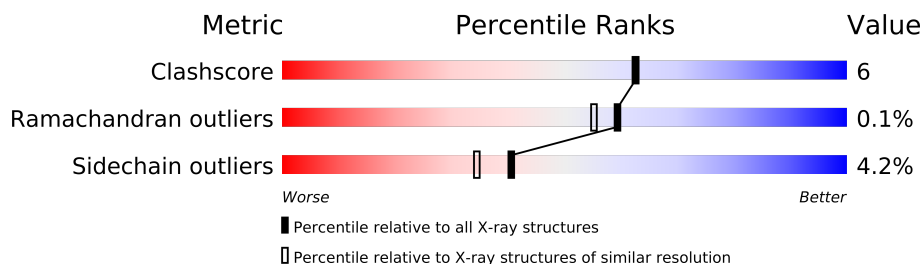
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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	842	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7419 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.

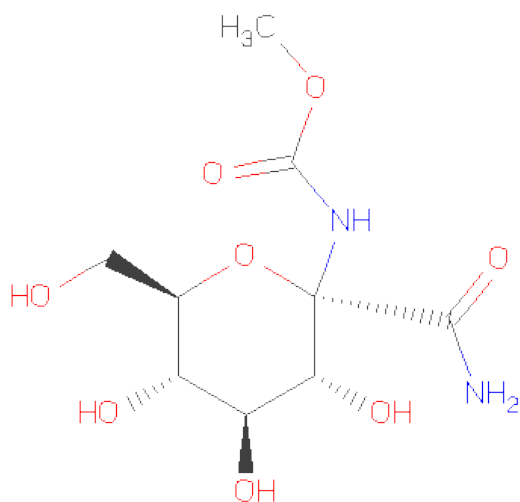
- Molecule 1 is a protein called PROTEIN (GLYCOGEN PHOSPHORYLASE B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	804	6542	4172	1153	1188	29	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

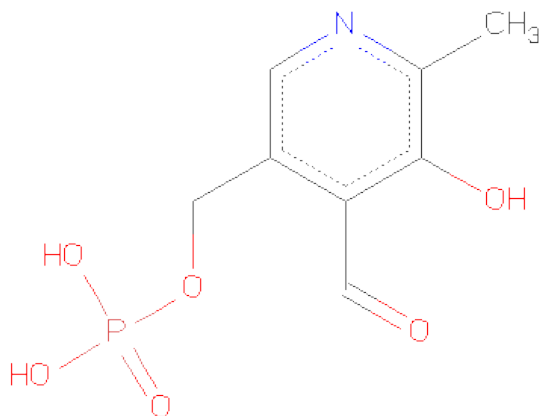
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	SEE REMARK 999	UNP P00489
A	609	ALA	PRO	SEE REMARK 999	UNP P00489

- Molecule 2 is 2-DEOXY-2-METHOXYCARBAMIDO-BETA-D-GLUCO-2-HEPTULOPYRANOSONAMIDE (three-letter code: CRA) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>2</sub>O<sub>8</sub>).



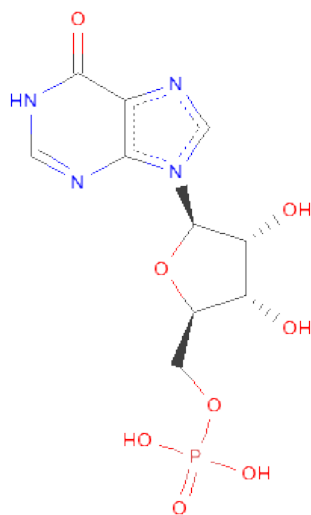
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	19	9	2	8	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



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

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	820	Total 820	O 820	0	0

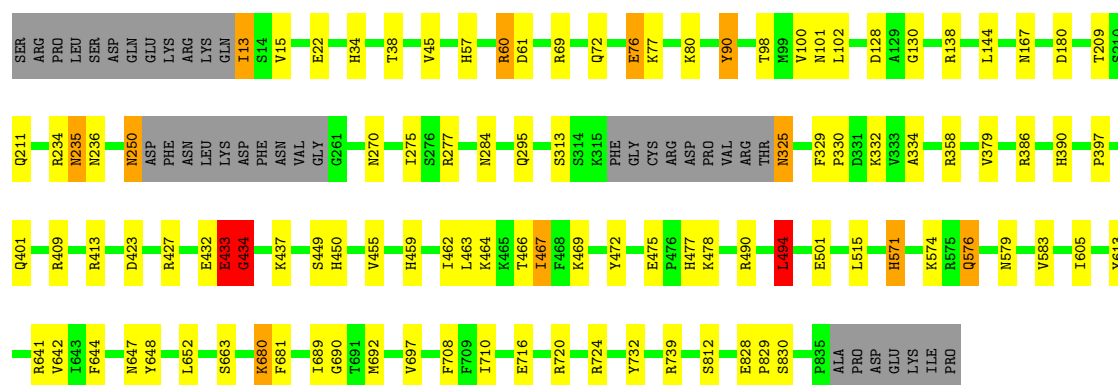
### 3 Residue-property plots

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: PROTEIN (GLYCOGEN PHOSPHORYLASE B)

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.68Å 126.68Å 115.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.4 (20.00-2.00)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.182 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7419	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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: IMP, CRA, 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	0.65	1/6688 (0.0%)	0.67	5/9049 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LYS	N-CA	42.66	2.31	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LYS	N-CA-CB	-11.92	89.15	110.60
1	A	680	LYS	CD-CE-NZ	-9.27	90.38	111.70
1	A	433	GLU	N-CA-C	7.31	130.74	111.00
1	A	494	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	434	GLY	N-CA-C	5.02	125.65	113.10

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	6542	0	6498	72	0
2	A	19	0	16	0	0
3	A	15	0	7	0	0
4	A	23	0	11	0	0
5	A	820	0	0	16	0
All	All	7419	0	6532	72	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 6.

All (72) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:490:ARG:HA	1:A:494:LEU:HG	1.42	0.99
1:A:100:VAL:HG21	1:A:494:LEU:HD22	1.47	0.97
1:A:680:LYS:N	1:A:680:LYS:CA	2.31	0.93
1:A:463:LEU:HD23	1:A:467:ILE:HD13	1.53	0.89
1:A:270:ASN:HB2	5:A:1817:HOH:O	1.82	0.79
1:A:102:LEU:HG	5:A:1801:HOH:O	1.86	0.75
1:A:235:ASN:H	1:A:235:ASN:HD22	1.38	0.72
1:A:379:VAL:HG22	5:A:1651:HOH:O	1.89	0.71
1:A:455:VAL:H	1:A:459:HIS:HD2	1.39	0.70
1:A:98:THR:O	5:A:1801:HOH:O	2.10	0.69
1:A:250:ASN:HA	5:A:1567:HOH:O	1.92	0.69
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.77	0.65
1:A:463:LEU:HA	1:A:467:ILE:HD12	1.80	0.63
1:A:716:GLU:HG3	1:A:720:ARG:HH21	1.64	0.63
1:A:60:ARG:HD3	5:A:1740:HOH:O	1.97	0.62
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.83	0.61
1:A:325:ASN:N	1:A:325:ASN:OD1	2.34	0.61
1:A:100:VAL:HG21	1:A:494:LEU:CD2	2.25	0.60
1:A:235:ASN:HD22	1:A:235:ASN:N	1.98	0.58
1:A:90:TYR:CE1	1:A:130:GLY:HA2	2.40	0.57
1:A:211:GLN:O	1:A:358:ARG:NH1	2.38	0.57
1:A:386:ARG:HD2	1:A:432:GLU:OE1	2.04	0.57
1:A:716:GLU:HG3	1:A:720:ARG:NH2	2.20	0.56
1:A:235:ASN:H	1:A:235:ASN:ND2	2.02	0.56
1:A:462:ILE:HG22	1:A:467:ILE:HD11	1.89	0.55
1:A:80:LYS:HE2	1:A:334:ALA:HB2	1.87	0.55
1:A:450:HIS:HD2	5:A:1075:HOH:O	1.89	0.54
1:A:732:TYR:O	1:A:739:ARG:HD3	2.08	0.54
1:A:692:MET:CE	1:A:697:VAL:HG13	2.38	0.54
1:A:167:ASN:ND2	1:A:647:ASN:HD21	2.07	0.53
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:515:LEU:HD22	1:A:812:SER:HB2	1.90	0.52
1:A:475:GLU:OE1	1:A:478:LYS:HE3	2.10	0.51
1:A:101:ASN:HB2	5:A:1801:HOH:O	2.10	0.51
1:A:449:SER:O	1:A:478:LYS:HE2	2.11	0.51
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.93	0.50
1:A:277:ARG:HD2	5:A:1495:HOH:O	2.12	0.49
1:A:692:MET:HE1	1:A:697:VAL:HG13	1.95	0.49
1:A:692:MET:HE3	1:A:697:VAL:HG22	1.94	0.49
1:A:690:GLY:O	1:A:710:ILE:HA	2.13	0.49
1:A:680:LYS:N	1:A:680:LYS:CB	2.75	0.48
1:A:477:HIS:HB2	5:A:1770:HOH:O	2.13	0.48
1:A:464:LYS:HD2	1:A:472:TYR:CE1	2.49	0.47
1:A:397:PRO:O	1:A:401:GLN:HG3	2.14	0.47
1:A:455:VAL:H	1:A:459:HIS:CD2	2.26	0.47
1:A:515:LEU:CD2	1:A:812:SER:HB2	2.44	0.47
1:A:409:ARG:O	1:A:413:ARG:HG3	2.15	0.46
1:A:72:GLN:NE2	1:A:76:GLU:OE2	2.49	0.45
1:A:13:ILE:CG2	1:A:15:VAL:HG22	2.46	0.45
1:A:571:HIS:HB2	1:A:574:LYS:HD2	1.98	0.45
1:A:466:THR:OG1	1:A:467:ILE:N	2.47	0.45
1:A:689:ILE:O	1:A:689:ILE:HG23	2.15	0.45
1:A:433:GLU:O	1:A:434:GLY:O	2.35	0.44
1:A:167:ASN:HD22	1:A:647:ASN:HD21	1.65	0.44
1:A:275:ILE:O	1:A:295:GLN:HG2	2.17	0.43
1:A:423:ASP:O	1:A:427:ARG:HG3	2.17	0.43
1:A:663:SER:HB2	1:A:681:PHE:CG	2.53	0.43
1:A:455:VAL:N	1:A:459:HIS:HD2	2.13	0.43
1:A:209:THR:HG23	5:A:1694:HOH:O	2.19	0.42
1:A:463:LEU:HA	1:A:467:ILE:CD1	2.47	0.42
1:A:390:HIS:HD2	5:A:1606:HOH:O	2.02	0.42
1:A:235:ASN:N	1:A:235:ASN:ND2	2.62	0.42
1:A:332:LYS:HG3	5:A:1543:HOH:O	2.19	0.42
1:A:605:ILE:O	1:A:644:PHE:HA	2.19	0.42
1:A:69:ARG:HD2	5:A:1014:HOH:O	2.20	0.42
1:A:13:ILE:HG23	1:A:501:GLU:OE1	2.20	0.42
1:A:45:VAL:HG21	5:A:1775:HOH:O	2.19	0.41
1:A:57:HIS:HE1	5:A:1239:HOH:O	2.02	0.41
1:A:235:ASN:O	1:A:236:ASN:HB2	2.21	0.41
1:A:583:VAL:HG11	1:A:642:VAL:HG21	2.03	0.41
1:A:571:HIS:H	1:A:576:GLN:HE22	1.69	0.40
1:A:828:GLU:HA	1:A:829:PRO:HD2	1.97	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	798/842 (95%)	769 (96%)	28 (4%)	1 (0%)	59	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLY

### 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%)	667 (96%)	29 (4%)	40	34

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	22	GLU
1	A	60	ARG
1	A	76	GLU
1	A	77	LYS
1	A	90	TYR
1	A	128	ASP
1	A	138	ARG
1	A	144	LEU
1	A	180	ASP
1	A	234	ARG
1	A	235	ASN
1	A	250	ASN

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Mol	Chain	Res	Type
1	A	284	ASN
1	A	313	SER
1	A	325	ASN
1	A	433	GLU
1	A	437	LYS
1	A	467	ILE
1	A	469	LYS
1	A	494	LEU
1	A	571	HIS
1	A	576	GLN
1	A	579	ASN
1	A	613	TYR
1	A	641	ARG
1	A	708	PHE
1	A	724	ARG
1	A	830	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	57	HIS
1	A	97	ASN
1	A	106	ASN
1	A	167	ASN
1	A	235	ASN
1	A	284	ASN
1	A	325	ASN
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	614	HIS
1	A	767	HIS
1	A	768	HIS

### 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 ⓘ

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	-	25,25,25	1.70	7 (28%)	35,38,38	11.08	8 (22%)
2	CRA	A	998	-	19,19,19	1.80	4 (21%)	28,28,28	1.61	5 (17%)
3	PLP	A	999	1	14,15,16	2.35	4 (28%)	20,22,23	1.83	6 (30%)

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	-	-	0/10/26/26	0/1/3/3
2	CRA	A	998	-	-	2/15/38/38	0/1/1/1
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C3-C2	-5.96	1.36	1.40
2	A	998	CRA	O8-C7	4.50	1.40	1.34
4	A	930	IMP	C8-N7	4.45	1.43	1.34
2	A	998	CRA	C1-C2	4.31	1.60	1.53
3	A	999	PLP	C5A-C5	4.27	1.62	1.51
3	A	999	PLP	O3-C3	3.03	1.44	1.37
4	A	930	IMP	C6-C5	2.88	1.45	1.41
3	A	999	PLP	P-O3P	-2.67	1.45	1.54
4	A	930	IMP	C5'-C4'	2.60	1.60	1.51
2	A	998	CRA	O5-C1	2.43	1.47	1.43
4	A	930	IMP	O4'-C1'	2.30	1.44	1.41
4	A	930	IMP	C2-N1	2.29	1.41	1.35
4	A	930	IMP	P-O3P	-2.21	1.46	1.54
4	A	930	IMP	C6-N1	2.16	1.40	1.37
2	A	998	CRA	C3-C4	2.05	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	930	IMP	C6-C5-N7	-64.94	125.39	134.14
2	A	998	CRA	O8-C7-N2	5.43	114.51	109.44
4	A	930	IMP	C8-N9-C4	3.81	109.81	106.90
3	A	999	PLP	O3P-P-O1P	3.68	122.47	110.44
3	A	999	PLP	C2A-C2-C3	3.42	125.18	121.02
4	A	930	IMP	C4-C5-N7	3.03	112.12	109.52
3	A	999	PLP	O4P-C5A-C5	-2.77	103.63	109.26
3	A	999	PLP	O2P-P-O4P	-2.65	99.34	106.65
4	A	930	IMP	O4'-C4'-C3'	-2.52	100.06	105.17
2	A	998	CRA	O2-C2-C1	2.48	113.12	108.16
2	A	998	CRA	O5-C1-C2	2.45	111.59	107.77
4	A	930	IMP	C5-C6-N1	-2.34	107.70	113.81
3	A	999	PLP	C6-N1-C2	2.34	124.29	119.28
4	A	930	IMP	C4'-O4'-C1'	2.23	112.17	109.75
4	A	930	IMP	O4'-C4'-C5'	-2.22	101.44	109.36
2	A	998	CRA	O5-C1-N2	-2.05	103.99	110.11
2	A	998	CRA	O8-C7-O7	-2.04	122.03	124.64
3	A	999	PLP	O3-C3-C2	2.02	121.20	117.61
4	A	930	IMP	O4'-C1'-C2'	-2.02	103.68	106.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	998	CRA	O5-C1-C9-N1
2	A	998	CRA	C2-C1-C9-N1

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.