



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2016 – 12:00 PM EDT

PDB ID : 5IKP  
Title : Crystal structure of human brain glycogen phosphorylase bound to AMP  
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Deposited on : 2016-03-03  
Resolution : 3.40 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](mailto: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.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

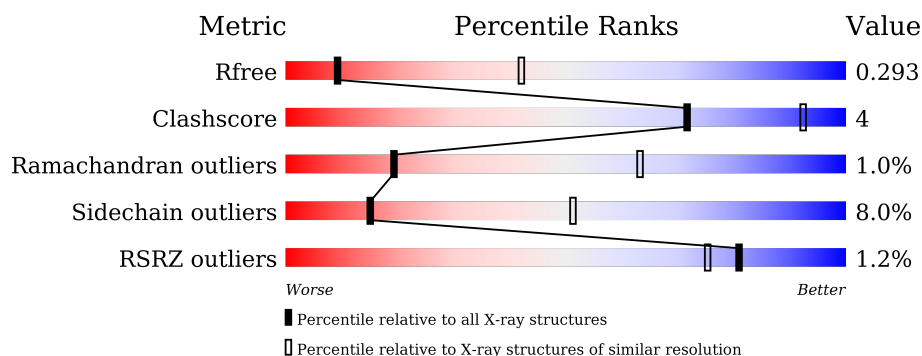
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	846	<div> <div></div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6558 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.

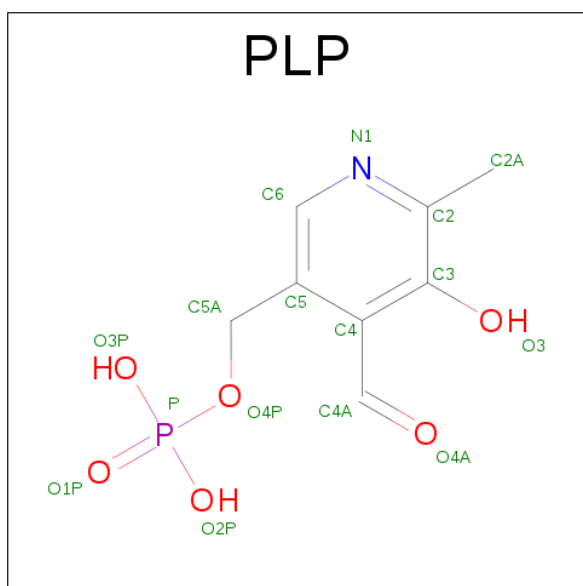
- Molecule 1 is a protein called Glycogen phosphorylase, brain form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	806	6520	4169	1126	1194	31	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

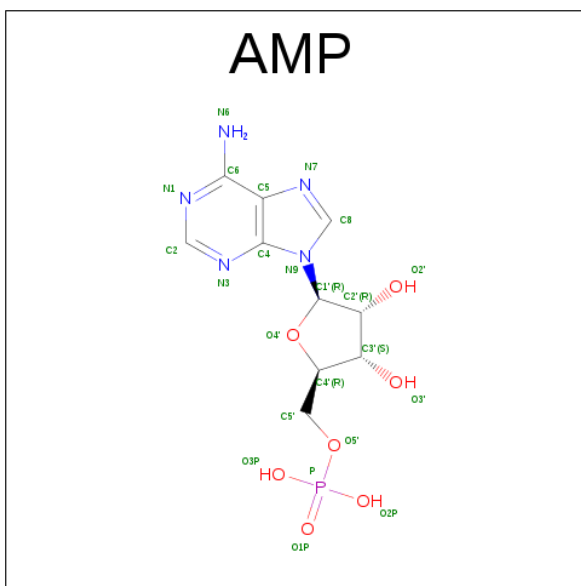
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P11216
A	-2	SER	-	expression tag	UNP P11216
A	-1	HIS	-	expression tag	UNP P11216

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.04Å 172.04Å 123.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.56 – 3.40 47.56 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.56-3.40) 99.8 (47.56-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.202 , 0.295 0.203 , 0.293	Depositor DCC
$R_{free}$ test set	768 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	112.6	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 90.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6558	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: AMP, 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	0.51	0/6669	0.67	0/9028

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	6520	0	6468	56	0
2	A	15	0	6	0	0
3	A	23	0	12	0	0
All	All	6558	0	6486	56	0

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 4.

All (56) 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:149:THR:HG22	1:A:233:TYR:H	1.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASN:HA	1:A:277:ARG:HB2	1.61	0.81
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.81	0.61
1:A:95:LEU:HD23	1:A:123:GLU:HG3	1.87	0.56
1:A:196:TYR:HD2	1:A:242:ARG:HH22	1.53	0.56
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.89	0.55
1:A:26:GLU:HA	1:A:29:LYS:HD2	1.88	0.55
1:A:702:GLU:HG3	1:A:807:CYS:HB3	1.89	0.53
1:A:828:GLU:HB3	1:A:831:ASP:HB2	1.91	0.52
1:A:233:TYR:HB2	1:A:489:ARG:HD3	1.91	0.52
1:A:162:GLU:HA	1:A:183:LEU:HD12	1.91	0.52
1:A:482:LYS:HE3	1:A:823:GLU:HB2	1.91	0.52
1:A:308:ILE:HD13	1:A:352:ILE:HG21	1.92	0.51
1:A:583:VAL:HG11	1:A:642:VAL:HG22	1.92	0.50
1:A:374:TYR:HB3	1:A:452:VAL:HG22	1.94	0.50
1:A:281:PRO:HG2	1:A:291:LEU:HD23	1.94	0.49
1:A:459:HIS:HA	1:A:462:ILE:HD12	1.95	0.48
1:A:70:THR:HA	1:A:834:ILE:HG12	1.96	0.48
1:A:69:ARG:HE	1:A:837:PRO:HB3	1.79	0.47
1:A:81:ARG:HB3	1:A:155:TYR:HE1	1.79	0.47
1:A:490:ARG:HG3	1:A:494:LEU:HD12	1.96	0.47
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.95	0.47
1:A:578:LEU:HB3	1:A:666:ILE:HD12	1.97	0.47
1:A:567:VAL:HG12	1:A:606:GLY:HA3	1.97	0.47
1:A:503:ILE:HG23	1:A:507:ILE:HD12	1.97	0.46
1:A:95:LEU:O	1:A:99:MET:HG2	2.16	0.46
1:A:578:LEU:HG	1:A:780:TYR:CD2	2.51	0.45
1:A:662:LEU:HD21	1:A:689:ILE:CD1	2.46	0.45
1:A:364:ALA:HA	1:A:367:ILE:HD12	1.99	0.45
1:A:144:LEU:HA	1:A:147:MET:HE2	1.97	0.45
1:A:610:ALA:HB3	1:A:613:TYR:HB2	1.98	0.45
1:A:492:LEU:HD13	1:A:683:LEU:HG	1.99	0.45
1:A:799:LYS:O	1:A:802:ILE:HG22	2.17	0.45
1:A:446:VAL:HG22	1:A:452:VAL:HG21	1.99	0.44
1:A:69:ARG:HA	1:A:72:GLN:HG2	1.99	0.44
1:A:455:VAL:O	1:A:483:THR:HA	2.17	0.43
1:A:772:LYS:HB3	1:A:775:ALA:HB3	1.99	0.43
1:A:381:PRO:HG3	1:A:467:VAL:HA	1.99	0.43
1:A:380:LEU:HA	1:A:381:PRO:HD3	1.95	0.43
1:A:530:PHE:CE2	1:A:802:ILE:HD11	2.53	0.43
1:A:231:PRO:HA	1:A:238:VAL:HG22	2.02	0.42
1:A:731:TYR:CE2	1:A:775:ALA:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:ILE:HA	1:A:835:PRO:HD3	1.93	0.42
1:A:579:ASN:O	1:A:583:VAL:HG23	2.19	0.42
1:A:507:ILE:HD11	1:A:521:LEU:HB3	2.02	0.41
1:A:662:LEU:HD21	1:A:689:ILE:HD12	2.02	0.41
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.92	0.41
1:A:101:ASN:HD22	1:A:231:PRO:HG2	1.86	0.41
1:A:89:PHE:O	1:A:131:LEU:HB2	2.21	0.40
1:A:138:ARG:HA	1:A:138:ARG:HD2	1.91	0.40
1:A:272:ALA:HA	1:A:275:ILE:HD12	2.03	0.40
1:A:738:LEU:HB2	1:A:777:TYR:CE2	2.56	0.40
1:A:369:LYS:O	1:A:450:HIS:HB3	2.22	0.40
1:A:449:SER:O	1:A:478:LYS:HD2	2.20	0.40
1:A:562:MET:HB3	1:A:601:ARG:HG2	2.04	0.40
1:A:82:ILE:HA	1:A:334:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	798/846 (94%)	721 (90%)	69 (9%)	8 (1%)	<span>19</span> <span>63</span>

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	736	PRO
1	A	772	LYS
1	A	78	ASP
1	A	166	PHE
1	A	380	LEU
1	A	492	LEU
1	A	509	GLU

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Mol	Chain	Res	Type
1	A	794	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	703/737 (95%)	647 (92%)	56 (8%)	15 51

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	33	ARG
1	A	34	HIS
1	A	35	LEU
1	A	39	LEU
1	A	69	ARG
1	A	90	TYR
1	A	96	GLN
1	A	105	GLN
1	A	136	LEU
1	A	169	LYS
1	A	216	LEU
1	A	217	ASP
1	A	224	MET
1	A	228	THR
1	A	234	LYS
1	A	245	SER
1	A	261	ASP
1	A	264	GLU
1	A	274	ASN
1	A	277	ARG
1	A	299	VAL
1	A	316	PHE
1	A	327	GLU
1	A	328	THR

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Mol	Chain	Res	Type
1	A	340	THR
1	A	363	LYS
1	A	380	LEU
1	A	392	PHE
1	A	458	ILE
1	A	474	LEU
1	A	489	ARG
1	A	505	GLU
1	A	538	LYS
1	A	549	LEU
1	A	560	SER
1	A	568	LYS
1	A	586	LEU
1	A	591	LYS
1	A	613	TYR
1	A	652	LEU
1	A	667	SER
1	A	678	ASN
1	A	729	ARG
1	A	730	GLU
1	A	735	LEU
1	A	746	SER
1	A	754	GLU
1	A	759	LYS
1	A	790	LEU
1	A	800	LYS
1	A	813	SER
1	A	816	THR
1	A	830	SER
1	A	838	ASN
1	A	839	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	459	HIS
1	A	763	ASN
1	A	767	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

2 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	PLP	A	901	1	15,15,16	3.39	3 (20%)	21,22,23	1.42	5 (23%)
3	AMP	A	902	-	22,25,25	1.14	1 (4%)	22,38,38	1.97	3 (13%)

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	PLP	A	901	1	-	0/6/6/8	0/1/1/1
3	AMP	A	902	-	-	0/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	PLP	C3-C4	2.76	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	AMP	C5-C4	3.54	1.48	1.40
2	A	901	PLP	C5-C4	7.57	1.49	1.40
2	A	901	PLP	C3-C2	10.02	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	AMP	N3-C2-N1	-7.25	123.17	128.87
2	A	901	PLP	P-O4P-C5A	-2.29	115.49	120.79
2	A	901	PLP	C3-C4-C5	-2.09	116.23	118.68
3	A	902	AMP	O3P-P-O2P	2.07	115.05	107.44
2	A	901	PLP	C6-C5-C4	2.10	119.91	118.12
2	A	901	PLP	O3P-P-O2P	2.15	115.33	107.44
2	A	901	PLP	O3-C3-C2	2.16	120.70	117.53
3	A	902	AMP	C4'-O4'-C1'	2.31	112.09	109.64

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	806/846 (95%)	0.06	10 (1%) 81 75	78, 117, 154, 190	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	ALA	2.8
1	A	734	HIS	2.6
1	A	584	VAL	2.5
1	A	256	ASP	2.4
1	A	831	ASP	2.2
1	A	569	ARG	2.2
1	A	750	PHE	2.1
1	A	753	LYS	2.1
1	A	839	ILE	2.1
1	A	526	SER	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AMP	A	902	23/23	0.89	0.20	0.35	123,130,136,145	0
2	PLP	A	901	15/16	0.93	0.30	0.02	101,111,127,139	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.