



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:11 PM UTC

PDB ID : 1DAA / pdb\_00001daa  
Title : CRYSTALLOGRAPHIC STRUCTURE OF D-AMINO ACID AMINO-TRANSFERASE COMPLEXED WITH PYRIDOXAL-5'-PHOSPHATE  
Authors : Sugio, S.; Peisach, D.; Ringe, D.  
Deposited on : 1995-06-09  
Resolution : 1.94 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

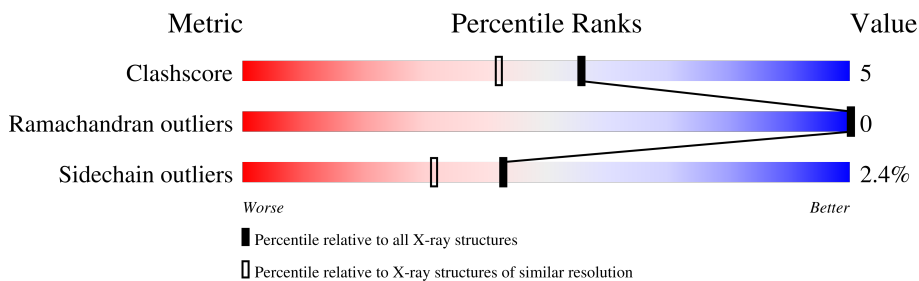
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	282	
1	B	282	

## 2 Entry composition [i](#)

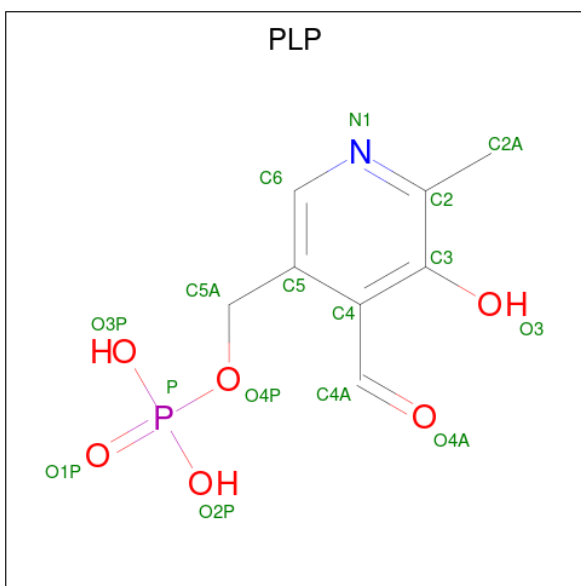
There are 3 unique types of molecules in this entry. The entry contains 4728 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-AMINO ACID AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	Total	C	N	O	S	31	0	0
			2232	1420	382	423	7			
1	B	277	Total	C	N	O	S	44	0	0
			2232	1420	382	423	7			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: 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	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is water.

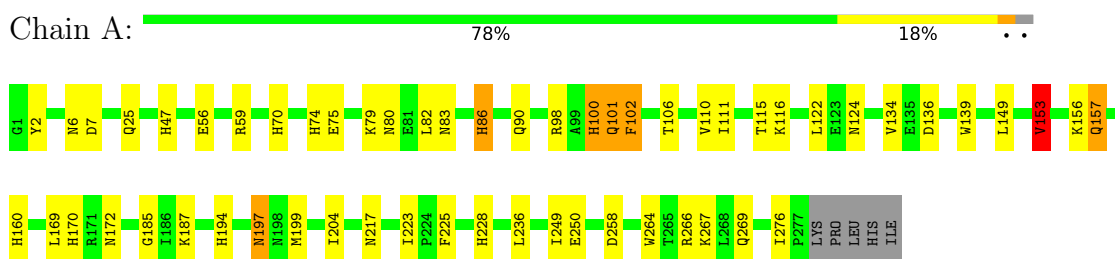
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	119	Total 119	O 119	0	0
3	B	113	Total 113	O 113	0	0

### 3 Residue-property plots [i](#)

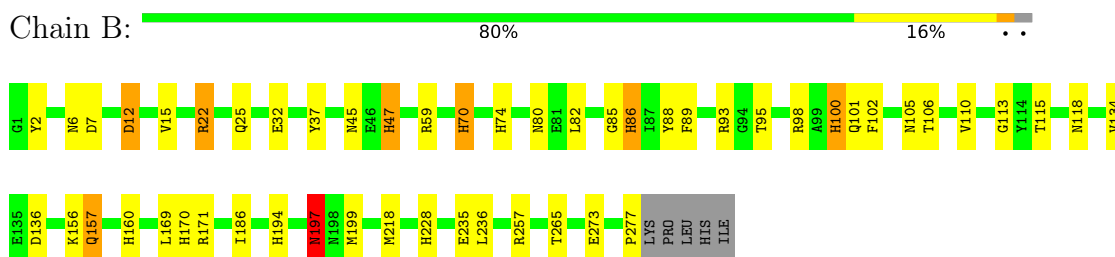
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: D-AMINO ACID AMINOTRANSFERASE



- Molecule 1: D-AMINO ACID AMINOTRANSFERASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.50Å 76.20Å 73.30Å 90.00° 103.90° 90.00°	Depositor
Resolution (Å)	10.00 – 1.94	Depositor
% Data completeness (in resolution range)	88.0 (10.00-1.94)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	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: 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	0.95	10/2277 (0.4%)	1.53	25/3081 (0.8%)
1	B	0.93	10/2277 (0.4%)	1.51	24/3081 (0.8%)
All	All	0.94	20/4554 (0.4%)	1.52	49/6162 (0.8%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	VAL	CA-CB	6.96	1.63	1.54
1	B	170	HIS	CD2-NE2	-6.94	1.30	1.37
1	B	86	HIS	CD2-NE2	-6.72	1.30	1.37
1	B	47	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	86	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	47	HIS	CD2-NE2	-6.46	1.30	1.37
1	B	100	HIS	CD2-NE2	-6.37	1.30	1.37
1	B	74	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	170	HIS	CD2-NE2	-6.22	1.31	1.37
1	B	228	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	74	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	228	HIS	CD2-NE2	-6.00	1.31	1.37
1	B	160	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	70	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	100	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	194	HIS	CD2-NE2	-5.54	1.31	1.37
1	B	70	HIS	CD2-NE2	-5.49	1.31	1.37
1	B	194	HIS	CD2-NE2	-5.47	1.31	1.37
1	B	47	HIS	CG-ND1	-5.33	1.32	1.38
1	A	160	HIS	CD2-NE2	-5.18	1.32	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	GLN	OE1-CD-NE2	-8.40	114.20	122.60
1	A	187	LYS	CA-CB-CG	-7.50	99.09	114.10
1	B	7	ASP	CA-CB-CG	7.41	120.01	112.60
1	B	22	ARG	NE-CZ-NH2	-7.25	112.68	119.20
1	A	59	ARG	N-CA-C	7.11	121.21	111.54
1	A	217	ASN	CA-CB-CG	-7.00	105.59	112.60
1	B	106	THR	CA-C-O	6.95	128.45	120.60
1	B	59	ARG	N-CA-C	6.81	120.93	111.74
1	A	106	THR	CA-C-O	6.76	127.50	120.40
1	B	197	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	B	70	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	A	258	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	122	LEU	N-CA-C	6.32	118.17	111.28
1	B	170	HIS	CB-CG-CD2	-6.20	123.15	131.20
1	B	70	HIS	CB-CG-ND1	6.18	131.97	122.70
1	B	12	ASP	CA-CB-CG	6.08	118.69	112.60
1	A	124	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	B	218	MET	CA-C-N	6.03	125.79	119.76
1	B	218	MET	C-N-CA	6.03	125.79	119.76
1	A	7	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	102	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	276	ILE	N-CA-CB	-5.97	102.85	111.21
1	A	217	ASN	N-CA-C	5.89	119.78	112.24
1	B	86	HIS	CB-CG-CD2	-5.89	123.55	131.20
1	A	100	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	B	157	GLN	OE1-CD-NE2	-5.81	116.79	122.60
1	A	157	GLN	CG-CD-NE2	5.81	125.11	116.40
1	A	90	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	B	105	ASN	N-CA-C	-5.52	100.30	109.46
1	A	228	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	A	197	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	B	273	GLU	CB-CA-C	-5.50	100.46	110.63
1	A	172	ASN	CA-CB-CG	5.49	118.09	112.60
1	B	100	HIS	CB-CG-CD2	-5.48	124.08	131.20
1	A	225	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	86	HIS	CB-CG-CD2	-5.39	124.20	131.20
1	A	160	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	B	85	GLY	O-C-N	-5.33	119.38	123.80
1	B	265	THR	N-CA-C	-5.31	105.57	111.36
1	B	228	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	A	83	ASN	CA-CB-CG	-5.29	107.31	112.60
1	A	204	ILE	CA-CB-CG1	-5.29	101.41	110.40
1	B	89	PHE	CA-CB-CG	5.27	119.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	A	74	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	B	118	ASN	CA-C-N	5.20	125.48	119.92
1	B	118	ASN	C-N-CA	5.20	125.48	119.92
1	B	47	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	A	139	TRP	CA-CB-CG	5.03	123.15	113.60

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	2232	0	2239	21	0
1	B	2232	0	2239	27	0
2	A	16	0	8	0	0
2	B	16	0	8	0	0
3	A	119	0	0	2	0
3	B	113	0	0	3	0
All	All	4728	0	4494	41	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 5.

All (41) 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:100:HIS:HB2	1:B:156:LYS:HD2	1.69	0.75
1:B:2:TYR:H	1:B:80:ASN:HD21	1.36	0.74
1:A:266:ARG:HH11	1:A:269:GLN:HE22	1.42	0.66
1:B:6:ASN:HD21	1:B:110:VAL:HA	1.62	0.64
1:A:2:TYR:H	1:A:80:ASN:HD21	1.47	0.62
1:B:25:GLN:HE22	1:B:98:ARG:HB2	1.71	0.55
1:A:6:ASN:HD21	1:A:110:VAL:HA	1.74	0.52
1:A:86:HIS:HD2	3:A:652:HOH:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:TYR:HB2	1:B:277:PRO:HG2	1.91	0.52
1:A:157:GLN:NE2	1:B:102:PHE:H	2.07	0.51
1:B:47:HIS:HE1	3:B:715:HOH:O	1.93	0.50
1:A:101:GLN:HB3	1:B:156:LYS:HD3	1.92	0.49
1:B:82:LEU:HD22	1:B:115:THR:HB	1.95	0.49
1:B:134:VAL:O	1:B:169:LEU:HA	2.11	0.49
1:A:157:GLN:NE2	1:B:101:GLN:HB2	2.29	0.48
1:B:136:ASP:HB3	1:B:171:ARG:HG2	1.95	0.48
1:A:149:LEU:O	1:A:153:VAL:HG13	2.14	0.47
1:A:185:GLY:HA2	1:A:236:LEU:HD23	1.95	0.47
1:A:264:TRP:HA	1:A:267:LYS:HG2	1.95	0.47
1:A:102:PHE:H	1:B:157:GLN:NE2	2.13	0.47
3:A:732:HOH:O	1:B:86:HIS:HE1	1.98	0.47
1:A:134:VAL:O	1:A:169:LEU:HA	2.15	0.47
1:B:45:ASN:HD21	1:B:70:HIS:HD2	1.61	0.46
1:B:197:ASN:ND2	1:B:199:MET:H	2.13	0.46
1:A:136:ASP:HB2	1:A:169:LEU:HB3	1.98	0.46
1:A:75:GLU:O	1:A:79:LYS:HG2	2.17	0.45
1:B:12:ASP:O	1:B:15:VAL:HG12	2.17	0.45
1:A:6:ASN:HA	1:A:111:ILE:HB	1.99	0.44
1:B:45:ASN:HD21	1:B:70:HIS:CD2	2.37	0.43
1:B:32:GLU:OE1	1:B:47:HIS:HD2	2.01	0.43
1:B:171:ARG:HD2	3:B:688:HOH:O	2.18	0.43
1:A:82:LEU:HD22	1:A:115:THR:HB	2.01	0.43
1:A:25:GLN:HE22	1:A:98:ARG:HB2	1.83	0.42
1:B:22:ARG:HD2	1:B:93:ARG:HB3	2.02	0.42
1:B:186:ILE:HB	1:B:235:GLU:HB2	2.01	0.42
1:B:86:HIS:HD2	3:B:608:HOH:O	2.03	0.42
1:B:2:TYR:H	1:B:80:ASN:ND2	2.10	0.41
1:A:153:VAL:HB	1:B:100:HIS:O	2.21	0.41
1:A:249:ILE:HD12	1:A:250:GLU:HB2	2.03	0.41
1:A:101:GLN:HB2	1:B:157:GLN:NE2	2.37	0.40
1:B:88:TYR:O	1:B:113:GLY:HA2	2.22	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	275/282 (98%)	263 (96%)	12 (4%)	0	100	100
1	B	275/282 (98%)	265 (96%)	10 (4%)	0	100	100
All	All	550/564 (98%)	528 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	247/252 (98%)	239 (97%)	8 (3%)	34	20
1	B	247/252 (98%)	243 (98%)	4 (2%)	55	46
All	All	494/504 (98%)	482 (98%)	12 (2%)	43	31

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	A	101	GLN
1	A	116	LYS
1	A	153	VAL
1	A	156	LYS
1	A	197	ASN
1	A	199	MET
1	A	223	ILE

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Mol	Chain	Res	Type
1	B	95	THR
1	B	197	ASN
1	B	236	LEU
1	B	257	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	25	GLN
1	A	70	HIS
1	A	80	ASN
1	A	86	HIS
1	A	157	GLN
1	A	172	ASN
1	A	173	ASN
1	A	182	ASN
1	A	197	ASN
1	A	269	GLN
1	B	6	ASN
1	B	25	GLN
1	B	45	ASN
1	B	47	HIS
1	B	80	ASN
1	B	86	HIS
1	B	157	GLN
1	B	173	ASN
1	B	197	ASN

### 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 oligosaccharides 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	B	285	-	16,16,16	1.59	5 (31%)	20,23,23	1.79	4 (20%)
2	PLP	A	285	-	16,16,16	1.66	3 (18%)	20,23,23	1.28	4 (20%)

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	B	285	-	-	3/8/8/8	0/1/1/1
2	PLP	A	285	-	-	0/8/8/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	285	PLP	C4-C4A	4.42	1.56	1.46
2	B	285	PLP	C2A-C2	2.61	1.54	1.50
2	B	285	PLP	C4-C4A	2.51	1.52	1.46
2	B	285	PLP	C4-C5	-2.43	1.38	1.42
2	B	285	PLP	C2-N1	2.35	1.38	1.33
2	A	285	PLP	C2-N1	2.31	1.38	1.33
2	B	285	PLP	C6-N1	2.23	1.39	1.34
2	A	285	PLP	C3-C2	-2.07	1.38	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	285	PLP	O4A-C4A-C4	-5.25	112.37	124.80
2	B	285	PLP	O2P-P-O4P	-2.97	98.92	106.67
2	B	285	PLP	C3-C4-C5	2.54	120.32	118.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	285	PLP	O3P-P-O1P	2.37	120.05	110.83
2	A	285	PLP	O4A-C4A-C4	-2.17	119.66	124.80
2	A	285	PLP	O2P-P-O4P	-2.17	101.02	106.67
2	A	285	PLP	O3P-P-O1P	2.12	119.09	110.83
2	A	285	PLP	C5-C6-N1	-2.05	120.50	123.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	285	PLP	C3-C4-C4A-O4A
2	B	285	PLP	C5-C4-C4A-O4A
2	B	285	PLP	C5A-O4P-P-O1P

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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.