



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 08:38 AM EST

PDB ID : 1B9H  
Title : CRYSTAL STRUCTURE OF 3-AMINO-5-HYDROXYBENZOIC ACID  
(AHBA) SYNTHASE  
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Deposited on : 1999-02-11  
Resolution : 2.00 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

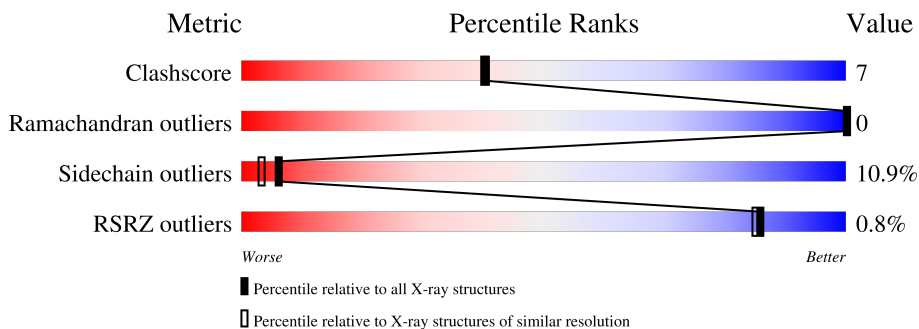
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

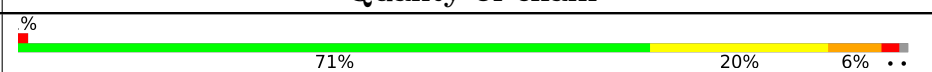
The reported resolution of this entry is 2.00 Å.

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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  $\leq 5\%$ . 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	388	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3171 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.

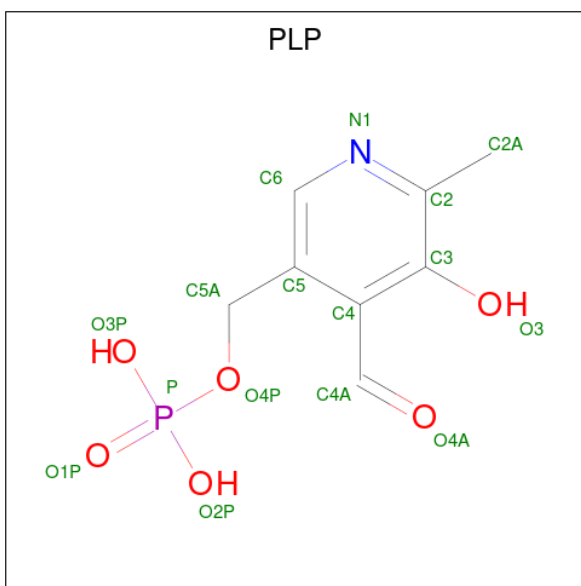
- Molecule 1 is a protein called PROTEIN (3-AMINO-5-HYDROXYBENZOIC ACID SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	2940	1839	539	549	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	ALA	GLY	REMARK 999	UNP O52552
A	262	ARG	PRO	REMARK 999	UNP O52552

- 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

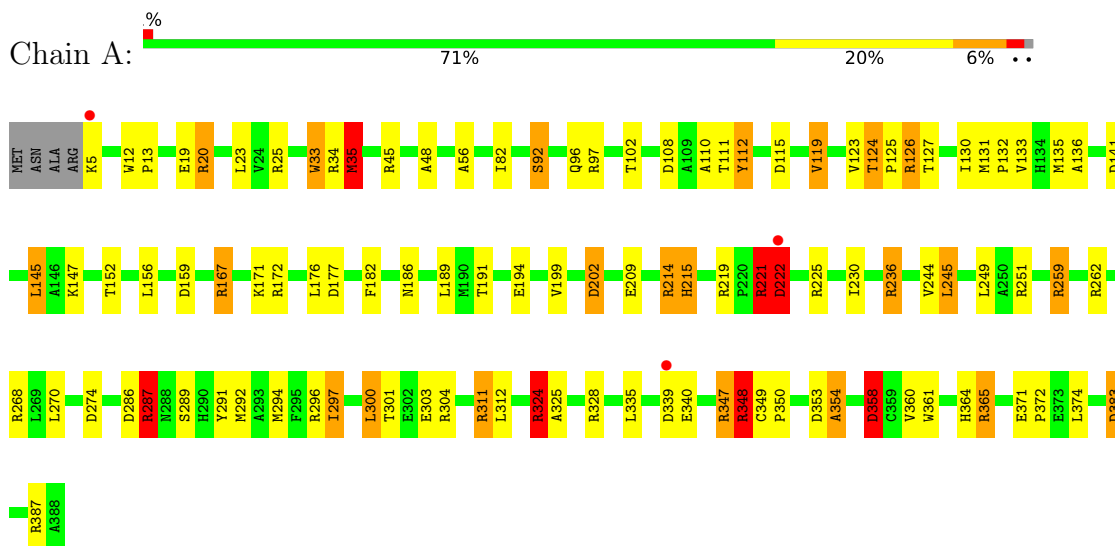
- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	216	Total 216	O 216	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 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.

- Molecule 1: PROTEIN (3-AMINO-5-HYDROXYBENZOIC ACID SYNTHASE)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.70Å 89.70Å 127.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.00 9.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (10.00-2.00) 98.4 (9.97-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	3.80	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.215 , 0.252 0.210 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtrriage
Anisotropy	0.141	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 64.8	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3171	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</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: 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	0.76	0/3005	1.88	76/4083 (1.9%)

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	0	6

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	259	ARG	NE-CZ-NH2	-23.96	108.32	120.30
1	A	259	ARG	NE-CZ-NH1	17.37	128.99	120.30
1	A	311	ARG	NE-CZ-NH2	-16.73	111.94	120.30
1	A	365	ARG	CD-NE-CZ	15.96	145.94	123.60
1	A	287	ARG	NE-CZ-NH1	15.54	128.07	120.30
1	A	365	ARG	NE-CZ-NH2	-15.39	112.61	120.30
1	A	251	ARG	NE-CZ-NH2	-12.73	113.94	120.30
1	A	296	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	A	365	ARG	NH1-CZ-NH2	11.00	131.50	119.40
1	A	34	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	A	97	ARG	NE-CZ-NH2	10.01	125.31	120.30
1	A	221	ARG	CD-NE-CZ	9.54	136.96	123.60
1	A	141	ASP	CB-CG-OD1	9.52	126.87	118.30
1	A	214	ARG	NE-CZ-NH2	-9.51	115.54	120.30
1	A	347	ARG	CD-NE-CZ	9.39	136.75	123.60
1	A	383	ASP	CB-CG-OD2	-9.37	109.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	365	ARG	NE-CZ-NH1	-8.87	115.87	120.30
1	A	304	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	358	ASP	CB-CA-C	-8.57	93.25	110.40
1	A	34	ARG	CD-NE-CZ	8.55	135.56	123.60
1	A	222	ASP	CB-CG-OD1	-8.38	110.76	118.30
1	A	311	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	328	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	A	303	GLU	OE1-CD-OE2	-8.17	113.50	123.30
1	A	167	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	A	268	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	A	194	GLU	OE1-CD-OE2	-7.65	114.12	123.30
1	A	172	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	A	287	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	387	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	141	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	A	311	ARG	CB-CG-CD	7.18	130.28	111.60
1	A	176	LEU	CA-C-N	7.15	132.94	117.20
1	A	45	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	214	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	221	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	177	ASP	N-CA-CB	-6.78	98.40	110.60
1	A	287	ARG	CD-NE-CZ	6.71	133.00	123.60
1	A	202	ASP	CB-CG-OD1	-6.70	112.27	118.30
1	A	324	ARG	N-CA-CB	-6.61	98.70	110.60
1	A	324	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	348	ARG	CD-NE-CZ	6.55	132.77	123.60
1	A	225	ARG	CD-NE-CZ	6.52	132.73	123.60
1	A	20	ARG	CD-NE-CZ	-6.50	114.50	123.60
1	A	19	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	A	274	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	182	PHE	CB-CG-CD2	-6.18	116.47	120.80
1	A	202	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	202	ASP	OD1-CG-OD2	6.08	134.85	123.30
1	A	172	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	339	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	324	ARG	CG-CD-NE	-5.89	99.44	111.80
1	A	225	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	A	296	ARG	CD-NE-CZ	5.81	131.73	123.60
1	A	347	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	145	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	251	ARG	CD-NE-CZ	5.59	131.42	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	251	ARG	NH1-CZ-NH2	5.50	125.45	119.40
1	A	296	ARG	NH1-CZ-NH2	-5.47	113.38	119.40
1	A	358	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	A	215	HIS	CA-CB-CG	5.43	122.83	113.60
1	A	286	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	292	MET	CG-SD-CE	5.31	108.70	100.20
1	A	35	MET	CA-CB-CG	5.27	122.27	113.30
1	A	268	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	A	25	ARG	CD-NE-CZ	5.23	130.92	123.60
1	A	209	GLU	OE1-CD-OE2	5.19	129.53	123.30
1	A	219	ARG	CD-NE-CZ	5.18	130.85	123.60
1	A	20	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	110	ALA	N-CA-CB	-5.14	102.90	110.10
1	A	236	ARG	CD-NE-CZ	-5.13	116.41	123.60
1	A	25	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	176	LEU	CA-C-O	-5.08	109.44	120.10
1	A	354	ALA	N-CA-CB	-5.07	103.00	110.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	THR	Mainchain
1	A	244	VAL	Mainchain
1	A	297	ILE	Mainchain
1	A	301	THR	Mainchain
1	A	312	LEU	Mainchain
1	A	358	ASP	Mainchain

## 5.2 Too-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 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	2940	0	2859	42	0
2	A	15	0	6	0	0
3	A	216	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3171	0	2865	42	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 7.

All (42) 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:124:THR:HG22	1:A:126:ARG:H	1.25	0.98
1:A:135:MET:HG3	1:A:294:MET:HE1	1.55	0.88
1:A:92:SER:HB3	1:A:102:THR:HG21	1.71	0.71
1:A:133:VAL:HG22	1:A:159:ASP:HB3	1.75	0.68
1:A:236:ARG:NH1	3:A:601:HOH:O	2.24	0.60
1:A:124:THR:HG23	1:A:125:PRO:HD2	1.85	0.59
1:A:135:MET:HG3	1:A:294:MET:CE	2.29	0.58
1:A:112:TYR:CD2	1:A:294:MET:HE3	2.39	0.58
1:A:262:ARG:HB3	1:A:374:LEU:HD11	1.86	0.58
1:A:291:TYR:O	1:A:364:HIS:HB3	2.04	0.57
1:A:297:ILE:HB	1:A:300:LEU:HD22	1.85	0.57
1:A:189:LEU:HD22	1:A:259:ARG:NH2	2.20	0.57
1:A:348:ARG:HG3	1:A:348:ARG:HH11	1.70	0.57
1:A:112:TYR:HD2	1:A:294:MET:HE3	1.71	0.54
1:A:371:GLU:HB2	1:A:372:PRO:HD3	1.90	0.53
1:A:96:GLN:NE2	3:A:430:HOH:O	2.41	0.52
1:A:167:ARG:HB2	1:A:287:ARG:HB3	1.90	0.52
1:A:349:CYS:N	1:A:350:PRO:CD	2.74	0.51
1:A:12:TRP:CG	1:A:13:PRO:HA	2.48	0.49
1:A:82:ILE:HD12	1:A:127:THR:HG21	1.93	0.49
1:A:33:TRP:CE2	1:A:35:MET:HB2	2.48	0.49
1:A:262:ARG:HB3	1:A:374:LEU:CD1	2.43	0.47
1:A:136:ALA:HB2	1:A:294:MET:CE	2.45	0.46
1:A:221:ARG:NH1	1:A:222:ASP:OD2	2.48	0.46
1:A:48:ALA:HB2	1:A:56:ALA:HB2	1.97	0.46
1:A:214:ARG:HG2	1:A:230:ILE:HD12	1.98	0.45
1:A:119:VAL:O	1:A:123:VAL:HG23	2.17	0.44
1:A:360:VAL:HG12	1:A:361:TRP:N	2.33	0.44
1:A:48:ALA:HB2	1:A:56:ALA:CB	2.48	0.43
1:A:324:ARG:HD2	3:A:491:HOH:O	2.19	0.43
1:A:123:VAL:HG11	1:A:152:THR:HG21	2.01	0.43
1:A:371:GLU:N	1:A:372:PRO:HD2	2.34	0.43
1:A:20:ARG:HH11	1:A:20:ARG:HD2	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ALA:HB2	1:A:294:MET:HE1	2.00	0.42
1:A:124:THR:HG22	1:A:126:ARG:N	2.10	0.42
1:A:131:MET:HA	1:A:132:PRO:HD2	1.96	0.41
1:A:324:ARG:O	1:A:325:ALA:C	2.58	0.41
1:A:115:ASP:O	1:A:119:VAL:HG12	2.21	0.41
1:A:354:ALA:O	1:A:358:ASP:HB2	2.20	0.41
1:A:108:ASP:HB3	1:A:111:THR:OG1	2.20	0.40
1:A:186:ASN:HA	1:A:191:THR:OG1	2.21	0.40
1:A:130:ILE:HB	1:A:156:LEU:HD23	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	382/388 (98%)	371 (97%)	11 (3%)	0	<b>100</b> <b>100</b>

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	293/296 (99%)	261 (89%)	32 (11%)	<b>6</b> <b>3</b>

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	23	LEU
1	A	33	TRP
1	A	35	MET
1	A	92	SER
1	A	112	TYR
1	A	119	VAL
1	A	126	ARG
1	A	145	LEU
1	A	147	LYS
1	A	171	LYS
1	A	199	VAL
1	A	202	ASP
1	A	215	HIS
1	A	221	ARG
1	A	222	ASP
1	A	245	LEU
1	A	249	LEU
1	A	270	LEU
1	A	287	ARG
1	A	289	SER
1	A	300	LEU
1	A	311	ARG
1	A	324	ARG
1	A	335	LEU
1	A	340	GLU
1	A	347	ARG
1	A	348	ARG
1	A	353	ASP
1	A	358	ASP
1	A	365	ARG
1	A	383	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	364	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	389	1	15,15,16	1.90	7 (46%)	20,22,23	2.30	5 (25%)

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	389	1	-	3/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	389	PLP	C3-C2	-3.42	1.37	1.40
2	A	389	PLP	C2A-C2	2.83	1.55	1.50
2	A	389	PLP	C2-N1	2.72	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	389	PLP	C3-C4	2.51	1.45	1.40
2	A	389	PLP	O4P-C5A	-2.40	1.36	1.45
2	A	389	PLP	O3-C3	-2.24	1.31	1.37
2	A	389	PLP	P-O3P	-2.02	1.47	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	389	PLP	O4P-C5A-C5	5.99	120.76	109.35
2	A	389	PLP	C5A-C5-C6	-3.91	112.94	119.37
2	A	389	PLP	C2A-C2-C3	3.63	125.37	120.89
2	A	389	PLP	C6-C5-C4	3.33	120.78	118.16
2	A	389	PLP	C3-C4-C5	-2.94	115.56	118.74

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	389	PLP	C4-C5-C5A-O4P
2	A	389	PLP	C6-C5-C5A-O4P
2	A	389	PLP	C5A-O4P-P-O2P

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	384/388 (98%)	-0.62	3 (0%) 86 85	18, 32, 52, 84	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	ASP	4.1
1	A	5	LYS	3.3
1	A	222	ASP	2.3

### 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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	PLP	A	389	15/16	0.98	0.05	18,23,33,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.