



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:25 PM GMT

PDB ID : 1ARS
Title : X-RAY CRYSTALLOGRAPHIC STUDY OF PYRIDOXAL 5'-
PHOSPHATE-TYPE ASPARTATE AMINOTRANSFERASES FROM
ESCHERICHIA COLI IN OPEN AND CLOSED FORM
Authors : Okamoto, A.; Higuchi, T.; Hirotsu, K.
Deposited on : 1993-08-02
Resolution : 1.80 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

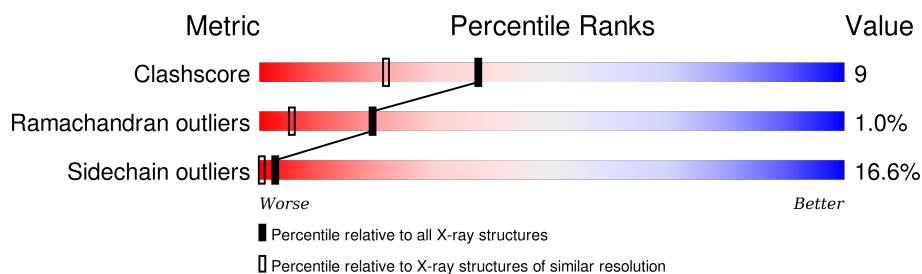
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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	396	 66% 26% 6% •

2 Entry composition [i](#)

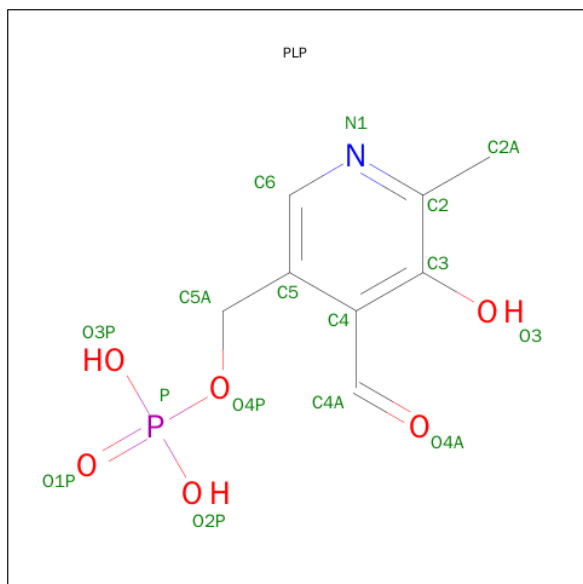
There are 3 unique types of molecules in this entry. The entry contains 3211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3069	1936	536	584	13			

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



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

- Molecule 3 is water.

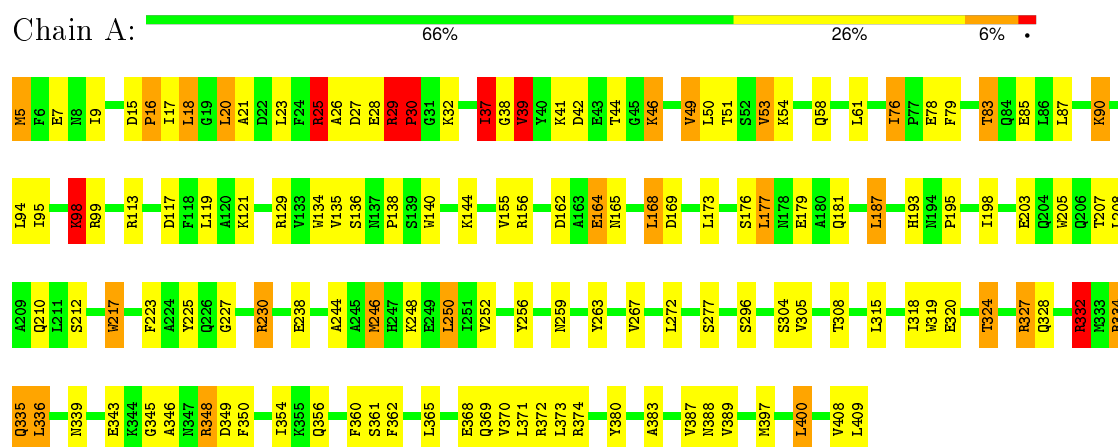
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		

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: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	155.42Å 87.13Å 79.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.213 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3211	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: 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	0.92	2/3130 (0.1%)	1.71	63/4240 (1.5%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	TRP	CG-CD2	-5.20	1.34	1.43
1	A	230	ARG	CA-CB	-5.02	1.43	1.53

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ARG	NE-CZ-NH1	12.87	126.74	120.30
1	A	334	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	A	334	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	A	29	ARG	CA-CB-CG	10.25	135.96	113.40
1	A	230	ARG	CB-CG-CD	-9.82	86.06	111.60
1	A	332	ARG	NE-CZ-NH1	9.75	125.18	120.30
1	A	327	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	A	230	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	A	140	TRP	CD1-CG-CD2	9.12	113.60	106.30
1	A	156	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	A	134	TRP	CD1-CG-CD2	8.73	113.29	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	A	113	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	A	140	TRP	CE2-CD2-CG	-8.20	100.74	107.30
1	A	29	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	A	37	ILE	CA-C-N	8.05	132.30	116.20
1	A	327	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	140	TRP	CG-CD2-CE3	7.99	141.09	133.90
1	A	319	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	A	29	ARG	NH1-CZ-NH2	-7.76	110.87	119.40
1	A	134	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	A	230	ARG	NH1-CZ-NH2	-7.47	111.18	119.40
1	A	205	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	A	205	TRP	CD1-CG-CD2	7.28	112.12	106.30
1	A	29	ARG	CB-CG-CD	7.03	129.87	111.60
1	A	256	TYR	CB-CG-CD1	-6.98	116.81	121.00
1	A	140	TRP	CB-CG-CD1	-6.83	118.12	127.00
1	A	320	GLU	CA-CB-CG	-6.68	98.70	113.40
1	A	54	LYS	CA-CB-CG	-6.59	98.89	113.40
1	A	29	ARG	CA-C-N	6.58	135.52	117.10
1	A	25	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	A	319	TRP	CE2-CD2-CG	-6.31	102.25	107.30
1	A	187	LEU	CA-CB-CG	6.30	129.80	115.30
1	A	250	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	372	ARG	CA-CB-CG	6.05	126.70	113.40
1	A	217	TRP	CE2-CD2-CG	-6.01	102.49	107.30
1	A	246	MET	N-CA-CB	-5.96	99.87	110.60
1	A	140	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	A	37	ILE	N-CA-C	5.92	126.97	111.00
1	A	129	ARG	CA-CB-CG	5.86	126.28	113.40
1	A	179	GLU	CA-CB-CG	5.79	126.14	113.40
1	A	217	TRP	CA-CB-CG	5.74	124.60	113.70
1	A	374	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	230	ARG	CD-NE-CZ	-5.47	115.94	123.60
1	A	25	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	238	GLU	CA-CB-CG	5.42	125.32	113.40
1	A	332	ARG	CG-CD-NE	5.41	123.15	111.80
1	A	98	LYS	CG-CD-CE	5.36	127.99	111.90
1	A	230	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	349	ASP	CA-C-N	-5.24	105.67	117.20
1	A	37	ILE	O-C-N	-5.23	114.30	123.20
1	A	319	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	A	29	ARG	N-CA-CB	-5.20	101.23	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	TRP	NE1-CE2-CD2	5.20	112.50	107.30
1	A	42	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	135	VAL	CG1-CB-CG2	-5.14	102.67	110.90
1	A	225	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	A	400	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	134	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	A	39	VAL	N-CA-CB	-5.04	100.41	111.50
1	A	30	PRO	N-CA-C	5.00	125.11	112.10
1	A	30	PRO	CA-CB-CG	-5.00	94.50	104.00
1	A	349	ASP	O-C-N	5.00	130.70	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	ARG	Sidechain
1	A	29	ARG	Sidechain

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	3069	0	3016	57	2
2	A	15	0	6	0	0
3	A	127	0	0	3	2
All	All	3211	0	3022	57	3

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 9.

All (57) 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:98:LYS:HZ2	1:A:98:LYS:HA	1.45	0.79
1:A:370:VAL:HG21	1:A:383:ALA:HA	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:HB2	1:A:53:VAL:HG13	1.69	0.74
1:A:27:ASP:HB3	1:A:32:LYS:HD3	1.72	0.70
1:A:95:ILE:O	1:A:98:LYS:HD2	1.93	0.68
1:A:20:LEU:HD12	1:A:380:TYR:HD2	1.59	0.68
1:A:203:GLU:O	1:A:207:THR:HG23	1.95	0.67
1:A:304:SER:O	1:A:308:THR:HG23	1.95	0.66
1:A:37:ILE:HD13	1:A:41:LYS:HD2	1.78	0.65
1:A:334:ARG:HH22	1:A:361:SER:HB3	1.64	0.62
1:A:94:LEU:HD11	1:A:244:ALA:HB1	1.82	0.60
1:A:346:ALA:N	1:A:348:ARG:NH1	2.49	0.60
1:A:44:THR:HG22	1:A:46:LYS:HE3	1.84	0.58
1:A:117:ASP:O	1:A:121:LYS:HG2	2.04	0.58
1:A:335:GLN:HA	1:A:354:ILE:HD11	1.86	0.56
1:A:348:ARG:HB2	1:A:350:PHE:CD2	2.41	0.55
1:A:49:VAL:HG23	1:A:53:VAL:HG22	1.89	0.54
1:A:164:GLU:HG3	1:A:165:ASN:N	2.22	0.54
1:A:168:LEU:HD21	1:A:173:LEU:HD12	1.89	0.54
1:A:90:LYS:H	1:A:90:LYS:HD2	1.73	0.53
1:A:136:SER:OG	1:A:193:HIS:HE1	1.91	0.53
1:A:76:ILE:HD11	1:A:78:GLU:HB2	1.90	0.53
1:A:212:SER:HA	1:A:217:TRP:CD1	2.43	0.53
1:A:17:ILE:HG13	1:A:18:LEU:N	2.24	0.53
1:A:324:THR:HB	1:A:327:ARG:NH2	2.24	0.52
1:A:328:GLN:O	1:A:332:ARG:HD3	2.10	0.51
1:A:227:GLY:O	1:A:327:ARG:HD3	2.11	0.51
1:A:308:THR:HB	3:A:504:HOH:O	2.10	0.50
1:A:38:GLY:HA2	1:A:360:PHE:CZ	2.47	0.50
1:A:334:ARG:HG2	1:A:389:VAL:HG11	1.93	0.49
1:A:79:PHE:O	1:A:83:THR:HG23	2.11	0.49
1:A:356:GLN:NE2	1:A:361:SER:HB2	2.26	0.49
1:A:98:LYS:NZ	1:A:98:LYS:HA	2.22	0.49
1:A:144:LYS:HA	1:A:155:VAL:HG21	1.95	0.49
1:A:85:GLU:HG2	1:A:90:LYS:HA	1.94	0.48
1:A:336:LEU:HB3	1:A:397:MET:HE3	1.96	0.48
1:A:58:GLN:HE22	1:A:61:LEU:HD23	1.79	0.47
1:A:37:ILE:HD12	1:A:39:VAL:O	2.15	0.47
1:A:324:THR:HB	1:A:327:ARG:HH22	1.80	0.47
1:A:38:GLY:HA2	1:A:360:PHE:HZ	1.79	0.46
1:A:27:ASP:HB2	3:A:539:HOH:O	2.15	0.46
1:A:51:THR:HG23	3:A:433:HOH:O	2.15	0.46
1:A:373:LEU:CD1	1:A:408:VAL:HG21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ALA:O	1:A:25:ARG:HG2	2.16	0.45
1:A:17:ILE:HG13	1:A:18:LEU:H	1.82	0.44
1:A:53:VAL:HB	1:A:305:VAL:HG11	1.99	0.44
1:A:15:ASP:HA	1:A:16:PRO:HD2	1.85	0.43
1:A:346:ALA:HB3	1:A:348:ARG:CZ	2.49	0.43
1:A:369:GLN:NE2	1:A:409:LEU:HA	2.34	0.42
1:A:138:PRO:HG3	1:A:362:PHE:HE2	1.83	0.42
1:A:28:GLU:HG3	1:A:29:ARG:CZ	2.49	0.42
1:A:162:ASP:HB2	1:A:169:ASP:HB2	2.00	0.42
1:A:38:GLY:N	1:A:388:ASN:HD22	2.19	0.41
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.90	0.41
1:A:348:ARG:HE	1:A:350:PHE:HD2	1.68	0.41
1:A:39:VAL:HG22	1:A:263:TYR:CE1	2.56	0.40
1:A:318:ILE:HD13	1:A:318:ILE:HG21	1.92	0.40

All (3) 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)
3:A:437:HOH:O	3:A:495:HOH:O[6_555]	1.37	0.83
1:A:5:MET:SD	1:A:368:GLU:CG[6_555]	1.65	0.55
1:A:368:GLU:OE2	3:A:462:HOH:O[6_554]	2.19	0.01

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	394/396 (100%)	373 (95%)	17 (4%)	4 (1%)	19 5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	345	GLY
1	A	26	ALA
1	A	16	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	320/320 (100%)	267 (83%)	53 (17%)	3 0

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	7	GLU
1	A	9	ILE
1	A	18	LEU
1	A	20	LEU
1	A	23	LEU
1	A	25	ARG
1	A	29	ARG
1	A	30	PRO
1	A	37	ILE
1	A	39	VAL
1	A	46	LYS
1	A	49	VAL
1	A	53	VAL
1	A	76	ILE
1	A	83	THR
1	A	87	LEU
1	A	90	LYS
1	A	98	LYS
1	A	99	ARG
1	A	119	LEU
1	A	164	GLU
1	A	168	LEU

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Mol	Chain	Res	Type
1	A	176	SER
1	A	177	LEU
1	A	181	GLN
1	A	187	LEU
1	A	195	PRO
1	A	198	ILE
1	A	208	LEU
1	A	210	GLN
1	A	223	PHE
1	A	246	MET
1	A	248	LYS
1	A	250	LEU
1	A	252	VAL
1	A	259	ASN
1	A	267	VAL
1	A	272	LEU
1	A	277	SER
1	A	296	SER
1	A	315	LEU
1	A	324	THR
1	A	332	ARG
1	A	335	GLN
1	A	336	LEU
1	A	339	ASN
1	A	343	GLU
1	A	348	ARG
1	A	365	LEU
1	A	371	LEU
1	A	387	VAL
1	A	400	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	69	ASN
1	A	84	GLN
1	A	166	HIS
1	A	181	GLN
1	A	193	HIS
1	A	226	GLN
1	A	247	HIS

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Mol	Chain	Res	Type
1	A	259	ASN
1	A	335	GLN
1	A	356	GLN
1	A	357	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 carbohydrates 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	413	1	15,15,16	2.00	1 (6%)	21,22,23	2.26	4 (19%)

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	413	1	-	0/6/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	413	PLP	C3-C2	-6.70	1.36	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	413	PLP	O3P-P-O4P	-2.44	99.55	106.56
2	A	413	PLP	O2P-P-O1P	2.34	118.11	110.58
2	A	413	PLP	C5A-C5-C4	2.70	125.23	121.65
2	A	413	PLP	O4P-C5A-C5	8.14	122.45	108.99

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 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.