Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:25 PM GMT

PDB ID	:	1ART
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:

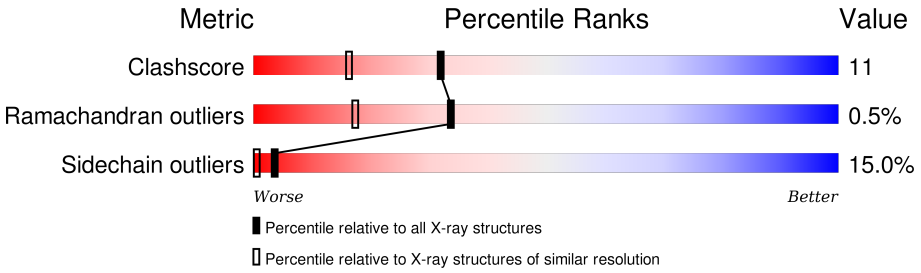
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 <=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	65% 26% 8% •

2 Entry composition

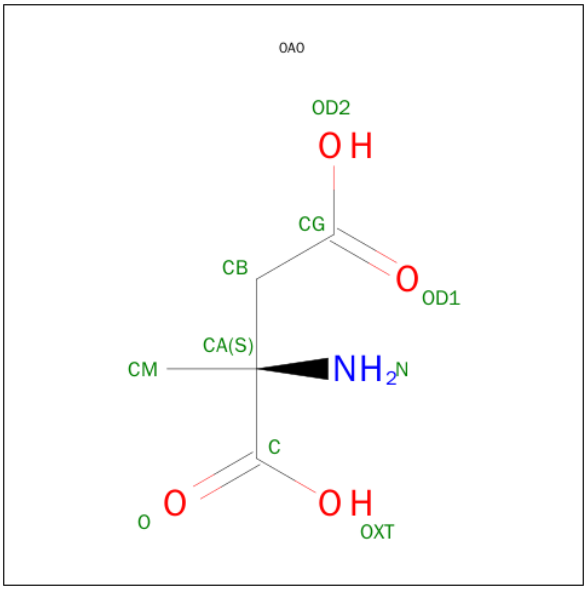
There are 3 unique types of molecules in this entry. The entry contains 3226 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: 0A0, PLP) (formula: $C_5H_9NO_4$, $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	2	Total	C	N	O	P	0	0
			25	13	2	9	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		

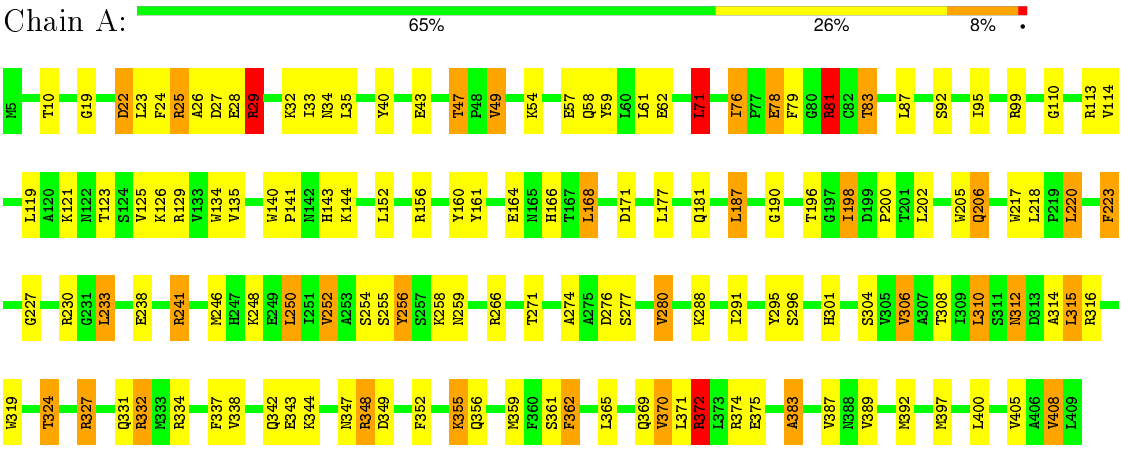
3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

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	157.14Å 85.51Å 78.93Å 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}	0.217 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3226	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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: 0A0, 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	0.90	0/3130	1.69	65/4240 (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	1

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	230	ARG	NE-CZ-NH2	-11.72	114.44	120.30
1	A	81	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	A	140	TRP	CG-CD2-CE3	9.81	142.73	133.90
1	A	134	TRP	CD1-CG-CD2	9.49	113.89	106.30
1	A	266	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	A	25	ARG	NE-CZ-NH1	9.33	124.96	120.30
1	A	129	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	A	217	TRP	CD1-CG-CD2	8.87	113.40	106.30
1	A	372	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	A	134	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	A	374	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	129	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	266	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	246	MET	CG-SD-CE	8.34	113.54	100.20
1	A	140	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	A	319	TRP	CD1-CG-CD2	8.21	112.87	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	288	LYS	CB-CG-CD	-7.95	90.93	111.60
1	A	348	ARG	CB-CG-CD	-7.93	90.98	111.60
1	A	81	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	A	187	LEU	CA-CB-CG	7.30	132.08	115.30
1	A	359	MET	CA-CB-CG	7.29	125.70	113.30
1	A	217	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	140	TRP	CE2-CD2-CG	-7.24	101.50	107.30
1	A	205	TRP	CD1-CG-CD2	7.24	112.09	106.30
1	A	319	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A	241	ARG	NE-CZ-NH2	7.11	123.86	120.30
1	A	78	GLU	CA-CB-CG	6.83	128.43	113.40
1	A	250	LEU	CA-CB-CG	6.77	130.87	115.30
1	A	250	LEU	CB-CA-C	-6.74	97.40	110.20
1	A	140	TRP	CB-CG-CD1	-6.69	118.31	127.00
1	A	217	TRP	CG-CD1-NE1	-6.66	103.44	110.10
1	A	205	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	A	392	MET	CG-SD-CE	-6.51	89.78	100.20
1	A	25	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	256	TYR	CB-CG-CD1	-6.46	117.12	121.00
1	A	374	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	29	ARG	N-CA-CB	6.18	121.72	110.60
1	A	81	ARG	CG-CD-NE	6.13	124.68	111.80
1	A	405	VAL	CG1-CB-CG2	-6.12	101.11	110.90
1	A	332	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	71	LEU	CA-C-N	6.04	128.28	116.20
1	A	58	GLN	CA-CB-CG	-5.98	100.25	113.40
1	A	327	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	280	VAL	CA-CB-CG2	-5.82	102.16	110.90
1	A	316	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	22	ASP	CA-C-N	5.80	129.97	117.20
1	A	241	ARG	CG-CD-NE	5.71	123.80	111.80
1	A	220	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	383	ALA	CB-CA-C	-5.67	101.60	110.10
1	A	140	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	A	343	GLU	CA-CB-CG	5.56	125.63	113.40
1	A	233	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	99	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	134	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	A	71	LEU	O-C-N	-5.47	113.90	123.20
1	A	319	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	A	134	TRP	CB-CG-CD1	-5.25	120.17	127.00
1	A	160	TYR	CB-CG-CD1	-5.24	117.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	217	TRP	CG-CD2-CE3	5.22	138.59	133.90
1	A	134	TRP	CG-CD1-NE1	-5.21	104.89	110.10
1	A	29	ARG	N-CA-C	-5.19	96.99	111.00
1	A	29	ARG	CA-CB-CG	5.15	124.72	113.40
1	A	306	VAL	CG1-CB-CG2	-5.09	102.76	110.90
1	A	198	ILE	CG1-CB-CG2	-5.07	100.26	111.40
1	A	348	ARG	N-CA-CB	-5.02	101.57	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	ARG	Sidechain

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	3069	0	3018	65	0
2	A	25	0	12	0	0
3	A	132	0	0	7	0
All	All	3226	0	3030	65	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 11.

All (65) 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:372:ARG:HD2	1:A:408:VAL:HG22	1.67	0.77
1:A:312:ASN:ND2	1:A:315:LEU:H	1.91	0.67
1:A:143:HIS:HB2	1:A:144:LYS:HD3	1.78	0.65
1:A:123:THR:HG22	1:A:125:VAL:H	1.62	0.65
1:A:76:ILE:HD13	1:A:79:PHE:H	1.63	0.63
1:A:78:GLU:HG3	3:A:541:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:O	1:A:29:ARG:HB3	2.00	0.61
1:A:356:GLN:NE2	1:A:361:SER:HA	2.16	0.60
1:A:202:LEU:HD13	1:A:238:GLU:HG2	1.84	0.59
1:A:23:LEU:HB2	3:A:540:HOH:O	2.01	0.59
1:A:337:PHE:HD1	1:A:397:MET:HE1	1.68	0.58
1:A:352:PHE:HA	1:A:355:LYS:HE2	1.85	0.58
1:A:327:ARG:HG2	1:A:331:GLN:HE21	1.67	0.58
1:A:370:VAL:HG21	1:A:383:ALA:HA	1.86	0.58
1:A:141:PRO:O	1:A:144:LYS:HG2	2.05	0.57
1:A:40:TYR:O	1:A:47:THR:HB	2.04	0.57
1:A:356:GLN:HE22	1:A:362:PHE:H	1.51	0.56
1:A:166:HIS:HB3	3:A:511:HOH:O	2.06	0.55
1:A:190:GLY:HA3	1:A:223:PHE:CD1	2.42	0.55
1:A:375:GLU:HG2	3:A:464:HOH:O	2.06	0.55
1:A:92:SER:HB3	1:A:95:ILE:HD12	1.88	0.55
1:A:338:VAL:O	1:A:342:GLN:HG2	2.07	0.54
1:A:19:GLY:O	1:A:22:ASP:HB3	2.08	0.54
1:A:371:LEU:O	1:A:375:GLU:HG3	2.08	0.53
1:A:312:ASN:HD22	1:A:315:LEU:H	1.55	0.53
1:A:57:GLU:OE2	1:A:301:HIS:HE1	1.93	0.52
1:A:356:GLN:HE22	1:A:361:SER:HA	1.76	0.51
1:A:327:ARG:O	1:A:331:GLN:HG3	2.11	0.51
1:A:24:PHE:CE1	1:A:34:ASN:HB2	2.47	0.50
1:A:29:ARG:O	1:A:32:LYS:HG3	2.13	0.49
1:A:314:ALA:HB3	3:A:429:HOH:O	2.13	0.49
1:A:71:LEU:HB2	3:A:524:HOH:O	2.12	0.49
1:A:334:ARG:HB3	1:A:389:VAL:HG11	1.95	0.49
1:A:306:VAL:O	1:A:310:LEU:HB2	2.12	0.49
1:A:304:SER:O	1:A:308:THR:HG23	2.12	0.49
1:A:227:GLY:O	1:A:327:ARG:HD3	2.12	0.48
1:A:397:MET:CE	1:A:400:LEU:HD22	2.43	0.48
1:A:312:ASN:HD21	1:A:314:ALA:HB3	1.79	0.47
1:A:202:LEU:O	1:A:206:GLN:HG2	2.13	0.47
1:A:33:ILE:HG22	1:A:35:LEU:HD13	1.96	0.47
1:A:83:THR:HB	1:A:256:TYR:OH	2.16	0.46
1:A:49:VAL:HG22	1:A:54:LYS:HG2	1.97	0.46
1:A:119:LEU:O	1:A:123:THR:HB	2.15	0.45
1:A:143:HIS:CB	1:A:144:LYS:HD3	2.47	0.45
1:A:81:ARG:HG3	1:A:81:ARG:HH11	1.82	0.45
1:A:144:LYS:N	1:A:144:LYS:HD3	2.32	0.44
1:A:223:PHE:O	1:A:254:SER:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:SER:HA	1:A:280:VAL:HG12	1.99	0.43
1:A:252:VAL:HG13	1:A:271:THR:HB	2.00	0.42
1:A:324:THR:HB	1:A:327:ARG:NH2	2.34	0.42
1:A:312:ASN:HD22	1:A:315:LEU:N	2.16	0.42
1:A:27:ASP:HB3	1:A:32:LYS:HD3	2.01	0.42
1:A:59:TYR:O	1:A:62:GLU:HG2	2.19	0.42
1:A:349:ASP:HB3	3:A:537:HOH:O	2.20	0.41
1:A:291:ILE:HG23	1:A:295:TYR:CE1	2.55	0.41
1:A:144:LYS:N	1:A:144:LYS:CD	2.83	0.41
1:A:274:ALA:HB3	1:A:280:VAL:HB	2.03	0.41
1:A:196:THR:O	1:A:198:ILE:HD12	2.19	0.41
1:A:161:TYR:CE1	1:A:198:ILE:HD13	2.56	0.41
1:A:87:LEU:O	1:A:241:ARG:NH1	2.54	0.41
1:A:168:LEU:HD11	1:A:200:PRO:HG3	2.02	0.41
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.78	0.40
1:A:25:ARG:HG3	1:A:26:ALA:N	2.34	0.40
1:A:110:GLY:O	1:A:114:VAL:HG13	2.21	0.40
1:A:369:GLN:HG2	1:A:408:VAL:HG13	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	394/396 (100%)	371 (94%)	21 (5%)	2 (0%)	34 17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	43	GLU

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	320/320 (100%)	272 (85%)	48 (15%)	3 0

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	29	ARG
1	A	47	THR
1	A	49	VAL
1	A	61	LEU
1	A	71	LEU
1	A	76	ILE
1	A	81	ARG
1	A	83	THR
1	A	113	ARG
1	A	121	LYS
1	A	126	LYS
1	A	135	VAL
1	A	152	LEU
1	A	156	ARG
1	A	164	GLU
1	A	168	LEU
1	A	171	ASP
1	A	181	GLN
1	A	187	LEU
1	A	206	GLN
1	A	218	LEU
1	A	220	LEU
1	A	223	PHE
1	A	233	LEU
1	A	248	LYS
1	A	250	LEU
1	A	252	VAL
1	A	255	SER
1	A	258	LYS

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Mol	Chain	Res	Type
1	A	259	ASN
1	A	276	ASP
1	A	296	SER
1	A	310	LEU
1	A	312	ASN
1	A	315	LEU
1	A	324	THR
1	A	332	ARG
1	A	344	LYS
1	A	347	ASN
1	A	348	ARG
1	A	355	LYS
1	A	362	PHE
1	A	365	LEU
1	A	370	VAL
1	A	372	ARG
1	A	387	VAL
1	A	408	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	166	HIS
1	A	247	HIS
1	A	259	ASN
1	A	286	GLN
1	A	301	HIS
1	A	312	ASN
1	A	331	GLN
1	A	356	GLN

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)

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	413	2	15,15,16	1.82	1 (6%)	21,22,23	1.34	4 (19%)
2	0A0	A	414	2	0,9,9	0.00	-	1,13,13	3.77	1 (100%)

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	2	-	0/6/6/8	0/1/1/1
2	0A0	A	414	2	-	0/2/11/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	413	PLP	C3-C2	-5.56	1.36	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	414	0A0	CM-CA-CB	-3.77	105.77	111.02
2	A	413	PLP	C5-C6-N1	-2.66	119.24	123.86
2	A	413	PLP	O2P-P-O4P	-2.61	99.05	106.56
2	A	413	PLP	O4P-P-O1P	2.05	112.36	107.14
2	A	413	PLP	C6-C5-C4	2.39	120.18	118.15

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

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.