



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 02:32 PM EST

PDB ID : 5G4I
Title : PLP-dependent phospholyase A1RDF1 from *Arthrobacter aurescens* TC1
Authors : Cuetos, A.; Tuan, A.N.; Mangas Sanchez, J.; Grogan, G.
Deposited on : 2016-05-13
Resolution : 1.50 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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-20028442

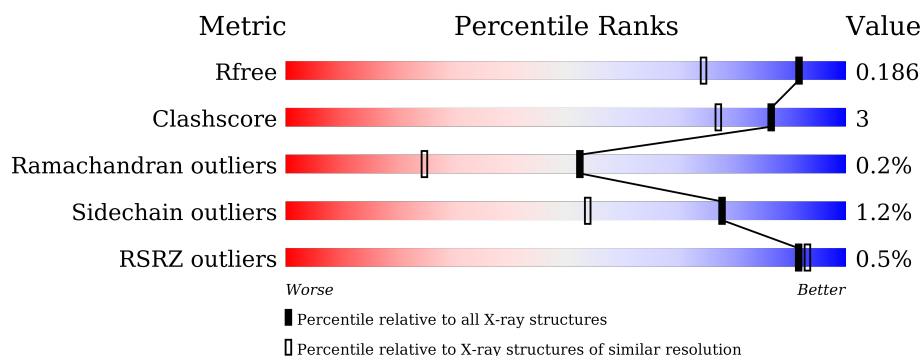
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.50 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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.

Mol	Chain	Length	Quality of chain
1	A	446	 85% 9% • 5%
1	B	446	 88% 6% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	A	1441	-	-	-	X
2	PLP	B	1440	-	-	-	X
3	PO4	A	1442	-	-	-	X
3	PO4	B	1442	-	-	-	X
4	ACT	A	1443	-	-	X	-
4	ACT	B	1445	-	-	X	-
5	B3P	A	1445	-	-	-	X

2 Entry composition [i](#)

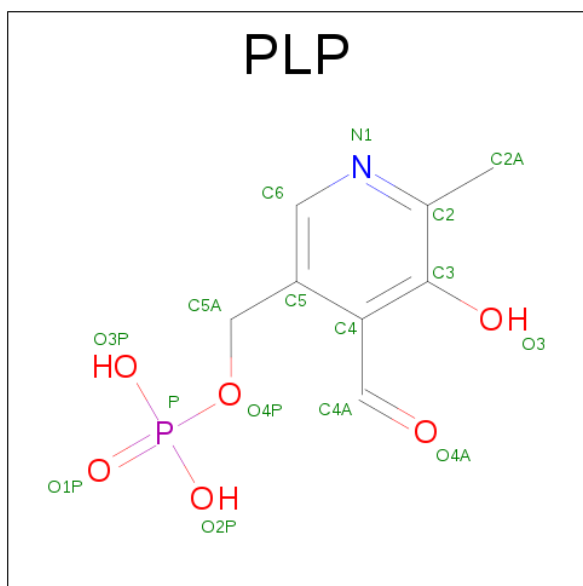
There are 6 unique types of molecules in this entry. The entry contains 7107 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOLYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	5	0
			3198	2031	554	604	9			
1	B	422	Total	C	N	O	S	0	1	0
			3158	2006	550	593	9			

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



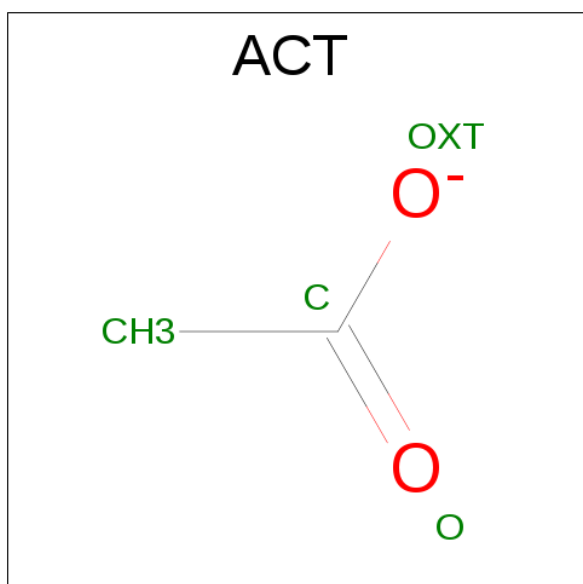
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO₄) (formula: O₄P).



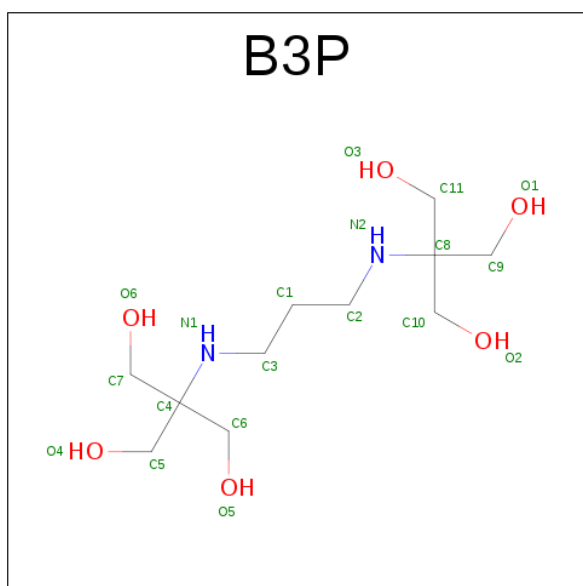
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	415	Total	O	0	0
			415	415		
6	B	250	Total	O	0	0
			250	250		

- Molecule 1: PHOSPHOLYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.94Å 97.18Å 124.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.55 – 1.50 65.41 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (76.55-1.50) 99.3 (65.41-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.153 , 0.175 0.166 , 0.186	Depositor DCC
R_{free} test set	7218 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7107	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ACT, B3P, 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	1.36	12/3278 (0.4%)	1.36	38/4458 (0.9%)
1	B	1.21	2/3225 (0.1%)	1.23	19/4388 (0.4%)
All	All	1.29	14/6503 (0.2%)	1.30	57/8846 (0.6%)

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	GLU	CD-OE1	-11.27	1.13	1.25
1	A	371	ILE	C-N	-11.15	1.08	1.34
1	A	432	GLU	CD-OE2	-8.05	1.16	1.25
1	A	432	GLU	CG-CD	7.94	1.63	1.51
1	A	235	GLU	CD-OE2	-7.63	1.17	1.25
1	A	108	ASP	CB-CG	-7.33	1.36	1.51
1	A	235	GLU	CG-CD	6.71	1.62	1.51
1	A	372	ASP	CB-CG	-6.07	1.39	1.51
1	A	112	GLU	CB-CG	-5.64	1.41	1.52
1	B	61	TYR	CE2-CZ	-5.43	1.31	1.38
1	A	279	MET	SD-CE	-5.41	1.47	1.77
1	B	143	SER	CB-OG	-5.33	1.35	1.42
1	A	346	ARG	CZ-NH1	5.26	1.39	1.33
1	A	275	GLU	CD-OE2	5.11	1.31	1.25

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	ARG	NE-CZ-NH1	-23.57	108.51	120.30
1	A	346	ARG	NE-CZ-NH2	-23.41	108.59	120.30
1	A	346	ARG	NE-CZ-NH1	23.16	131.88	120.30
1	B	414	ARG	NE-CZ-NH2	21.05	130.82	120.30
1	A	235	GLU	OE1-CD-OE2	-15.18	105.08	123.30
1	A	413	MET	CG-SD-CE	14.96	124.14	100.20
1	B	240	ARG	NE-CZ-NH1	9.73	125.17	120.30
1	B	240	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	A	235	GLU	CG-CD-OE1	8.94	136.18	118.30
1	A	339	ASP	CB-CG-OD1	8.84	126.26	118.30
1	A	372	ASP	CB-CA-C	-8.73	92.94	110.40
1	A	108	ASP	CB-CA-C	-8.41	93.58	110.40
1	A	346	ARG	CD-NE-CZ	8.36	135.30	123.60
1	A	372	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	A	333	ASP	CB-CG-OD1	7.99	125.49	118.30
1	B	339	ASP	CB-CG-OD1	7.84	125.36	118.30
1	A	132	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	24	TYR	CB-CG-CD1	7.62	125.57	121.00
1	B	283	MET	CG-SD-CE	-7.62	88.02	100.20
1	A	172	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	A	372	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	307	MET	CG-SD-CE	-7.32	88.49	100.20
1	A	144	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	18	ASP	CB-CG-OD2	7.25	124.83	118.30
1	B	397	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	B	414	ARG	CB-CG-CD	7.21	130.34	111.60
1	A	348	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	414	ARG	CD-NE-CZ	-7.04	113.74	123.60
1	A	348	ARG	CG-CD-NE	-7.00	97.10	111.80
1	B	333	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	144	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	76	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	113	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	108	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	B	172	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	A	414	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	B	414	ARG	CG-CD-NE	6.31	125.05	111.80
1	A	355	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	333	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	355	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	330	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	371	ILE	C-N-CA	5.88	136.39	121.70
1	B	346	ARG	NE-CZ-NH1	5.79	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	264	MET	CG-SD-CE	-5.75	91.00	100.20
1	B	300	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	22	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	23	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	283	MET	CG-SD-CE	5.44	108.90	100.20
1	B	24	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	A	178	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	365	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	365	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	172	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
1	B	144	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	144	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	B	199	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	372	ASP	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	3198	0	3160	13	0
1	B	3158	0	3113	19	0
2	A	15	0	6	0	0
2	B	15	0	7	0	0
3	A	5	0	0	0	0
3	B	20	0	0	1	0
4	A	8	0	6	4	0
4	B	4	0	3	2	0
5	A	19	0	26	0	0
6	A	415	0	0	4	0
6	B	250	0	0	4	0
All	All	7107	0	6321	35	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 3.

All (35) 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:B:414:ARG:HH11	1:B:414:ARG:HG2	1.11	1.13
1:B:414:ARG:HH11	1:B:414:ARG:CG	1.53	1.10
1:B:414:ARG:NH1	1:B:414:ARG:CG	2.31	0.88
1:A:300[A]:ASP:OD2	1:A:304:ARG:NH1	2.10	0.85
1:B:300:ASP:OD2	1:B:304:ARG:NH1	2.13	0.81
1:B:368:PHE:CE2	1:B:414:ARG:HD3	2.15	0.81
1:B:414:ARG:NH1	1:B:414:ARG:HG2	1.92	0.80
1:A:420:GLY:H	1:A:423:HIS:HD2	1.30	0.80
1:B:420:GLY:H	1:B:423:HIS:HD2	1.30	0.76
1:A:134:HIS:HD2	1:A:301:GLU:OE1	1.76	0.68
1:A:164:HIS:HD2	4:A:1443:ACT:OXT	1.75	0.67
1:B:134:HIS:HD2	1:B:301:GLU:OE1	1.78	0.67
1:B:164:HIS:HD2	4:B:1445:ACT:O	1.81	0.64
1:B:414:ARG:HD2	6:B:2033:HOH:O	1.98	0.64
1:B:420:GLY:H	1:B:423:HIS:CD2	2.15	0.62
1:A:420:GLY:H	1:A:423:HIS:CD2	2.16	0.60
1:A:404:VAL:HG13	1:A:412:LYS:HE3	1.87	0.56
1:B:164:HIS:CD2	4:B:1445:ACT:O	2.58	0.56
4:A:1444:ACT:H1	6:A:2354:HOH:O	2.07	0.54
4:A:1443:ACT:H3	6:A:2231:HOH:O	2.07	0.54
1:B:79:TYR:CZ	1:B:83:LEU:HD11	2.46	0.52
1:A:346:ARG:HD2	6:A:2371:HOH:O	2.09	0.51
1:A:300[B]:ASP:CG	6:A:2154:HOH:O	2.49	0.50
1:B:234:ILE:HB	3:B:1442:PO4:O1	2.11	0.49
1:B:368:PHE:CD2	1:B:414:ARG:HD3	2.47	0.49
1:B:113:ARG:HB3	1:B:299:LEU:HD13	1.95	0.47
1:A:113:ARG:HB3	1:A:299:LEU:HD13	1.98	0.46
1:A:412:LYS:C	1:A:413:MET:HG3	2.36	0.45
1:B:331:GLN:NE2	6:B:2222:HOH:O	2.50	0.44
1:A:369[B]:PHE:CD2	1:A:413:MET:HE2	2.53	0.44
1:B:189:VAL:HG23	6:B:2144:HOH:O	2.20	0.41
1:A:369[B]:PHE:HE2	1:A:413:MET:HE3	1.85	0.41
4:A:1443:ACT:H2	6:B:2034:HOH:O	2.21	0.41
1:A:369[B]:PHE:CE2	1:A:413:MET:HE3	2.56	0.40
1:B:79:TYR:CE2	1:B:83:LEU:HD11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	426/446 (96%)	412 (97%)	13 (3%)	1 (0%)	52	25
1	B	421/446 (94%)	410 (97%)	10 (2%)	1 (0%)	52	25
All	All	847/892 (95%)	822 (97%)	23 (3%)	2 (0%)	52	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	LYS
1	B	281	LYS

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	335/361 (93%)	331 (99%)	4 (1%)	78	54
1	B	326/361 (90%)	322 (99%)	4 (1%)	78	54
All	All	661/722 (92%)	653 (99%)	8 (1%)	78	54

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	MET
1	A	346	ARG
1	A	368	PHE
1	A	408	ASP

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Mol	Chain	Res	Type
1	B	143	SER
1	B	368	PHE
1	B	386	LEU
1	B	408	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	118	ASN
1	A	134	HIS
1	A	137	ASN
1	A	164	HIS
1	A	331	GLN
1	A	423	HIS
1	B	93	ASN
1	B	118	ASN
1	B	134	HIS
1	B	137	ASN
1	B	164	HIS
1	B	254	GLN
1	B	287	HIS
1	B	331	GLN
1	B	423	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

11 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	1441	1	15,15,16	3.66	3 (20%)	21,22,23	1.24	1 (4%)
3	PO4	A	1442	-	4,4,4	1.54	1 (25%)	6,6,6	0.47	0
4	ACT	A	1443	-	0,3,3	0.00	-	0,3,3	0.00	-
4	ACT	A	1444	-	0,3,3	0.00	-	0,3,3	0.00	-
5	B3P	A	1445	-	18,18,18	3.10	7 (38%)	17,23,23	1.89	6 (35%)
2	PLP	B	1440	1	15,15,16	3.86	7 (46%)	21,22,23	2.14	9 (42%)
3	PO4	B	1441	-	4,4,4	1.41	1 (25%)	6,6,6	0.33	0
3	PO4	B	1442	-	4,4,4	1.56	1 (25%)	6,6,6	0.41	0
3	PO4	B	1443	-	4,4,4	0.79	0	6,6,6	0.27	0
3	PO4	B	1444	-	4,4,4	0.27	0	6,6,6	0.26	0
4	ACT	B	1445	-	0,3,3	0.00	-	0,3,3	0.00	-

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	1441	1	-	0/6/6/8	0/1/1/1
3	PO4	A	1442	-	-	0/0/0/0	0/0/0/0
4	ACT	A	1443	-	-	0/0/0/0	0/0/0/0
4	ACT	A	1444	-	-	0/0/0/0	0/0/0/0
5	B3P	A	1445	-	-	0/28/28/28	0/0/0/0
2	PLP	B	1440	1	-	0/6/6/8	0/1/1/1
3	PO4	B	1441	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1442	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1443	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1444	-	-	0/0/0/0	0/0/0/0
4	ACT	B	1445	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1445	B3P	C5-C4	-4.80	1.49	1.53
3	A	1442	PO4	P-O1	-2.93	1.41	1.53
3	B	1442	PO4	P-O3	-2.66	1.45	1.53
3	B	1441	PO4	P-O2	-2.65	1.45	1.53
2	B	1440	PLP	C2-N1	-2.33	1.29	1.33
2	B	1440	PLP	P-O3P	-2.16	1.47	1.54
2	B	1440	PLP	C5A-C5	2.11	1.56	1.51
5	A	1445	B3P	C6-C4	2.22	1.55	1.53
5	A	1445	B3P	O2-C10	2.70	1.50	1.42
5	A	1445	B3P	C3-N1	2.74	1.51	1.46
2	B	1440	PLP	C6-C5	2.92	1.43	1.37
5	A	1445	B3P	O5-C6	3.13	1.52	1.42
2	B	1440	PLP	C3-C4	3.38	1.47	1.40
2	A	1441	PLP	C3-C4	3.70	1.48	1.40
2	B	1440	PLP	C5-C4	4.13	1.45	1.40
5	A	1445	B3P	C7-C4	4.54	1.57	1.53
2	A	1441	PLP	C5-C4	6.92	1.48	1.40
5	A	1445	B3P	C9-C8	9.45	1.61	1.53
2	A	1441	PLP	C3-C2	11.47	1.48	1.40
2	B	1440	PLP	C3-C2	12.73	1.49	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1440	PLP	C3-C4-C5	-4.44	113.47	118.68
2	B	1440	PLP	O2P-P-O4P	-3.64	96.10	106.72
5	A	1445	B3P	C11-C8-C10	-3.51	103.71	110.16
2	B	1440	PLP	P-O4P-C5A	-3.37	112.99	120.79
5	A	1445	B3P	C10-C8-C9	-3.22	104.25	110.16
5	A	1445	B3P	O3-C11-C8	-2.94	105.18	111.47
2	B	1440	PLP	C5A-C5-C4	-2.86	117.77	121.63
5	A	1445	B3P	O2-C10-C8	-2.70	105.68	111.47
5	A	1445	B3P	C7-C4-C5	-2.04	106.41	110.16
2	B	1440	PLP	O3-C3-C2	2.07	120.57	117.53
5	A	1445	B3P	C11-C8-C9	2.14	114.08	110.16
2	B	1440	PLP	O2P-P-O1P	2.30	118.12	110.63
2	B	1440	PLP	C4A-C4-C5	2.33	123.29	120.90
2	B	1440	PLP	C6-C5-C4	2.49	120.24	118.12
2	B	1440	PLP	O4P-P-O1P	2.54	113.46	107.08
2	A	1441	PLP	O3-C3-C2	2.54	121.26	117.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1443	ACT	3	0
4	A	1444	ACT	1	0
3	B	1442	PO4	1	0
4	B	1445	ACT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	371:ILE	C	372:ASP	N	1.08

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, 95th 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 ²)	Q<0.9
1	A	423/446 (94%)	-0.16	0	100 100	9, 14, 27, 47	0
1	B	422/446 (94%)	-0.16	4 (0%)	85 87	10, 17, 32, 57	0
All	All	845/892 (94%)	-0.16	4 (0%)	91 93	9, 15, 31, 57	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	439	PRO	3.9
1	B	379	SER	3.3
1	B	377	ASP	2.9
1	B	376	SER	2.4

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, 95th 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(\AA^2)	Q<0.9
2	PLP	A	1441	15/16	0.95	0.13	10.69	12,16,22,23	0
2	PLP	B	1440	15/16	0.97	0.12	5.38	13,17,21,21	0
3	PO4	B	1442	5/5	0.97	0.19	3.30	31,37,47,60	0
3	PO4	A	1442	5/5	0.97	0.13	2.30	28,29,36,43	0
5	B3P	A	1445	19/19	0.93	0.12	2.21	14,19,32,34	0
3	PO4	B	1441	5/5	0.96	0.11	0.77	30,31,38,41	0
3	PO4	B	1444	5/5	0.88	0.26	-	47,57,62,64	0
4	ACT	B	1445	4/4	0.79	0.16	-	16,21,34,35	0
4	ACT	A	1444	4/4	0.80	0.16	-	34,37,39,39	0
3	PO4	B	1443	5/5	0.93	0.11	-	50,53,60,65	0
4	ACT	A	1443	4/4	0.85	0.13	-	16,20,31,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.