



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2017 – 02:15 PM EDT

PDB ID : 5IJG
Title : Crystal structure of O-acetylhomoserine sulphydrolase from Brucella melitensis at 2.0 Å resolution
Authors : Boyko, K.M.; Nikolaeva, A.Y.; Koolikova, V.V.; Kotlov, M.I.; Demidkina, T.V.; Popov, V.O.
Deposited on : 2016-03-02
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

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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029077

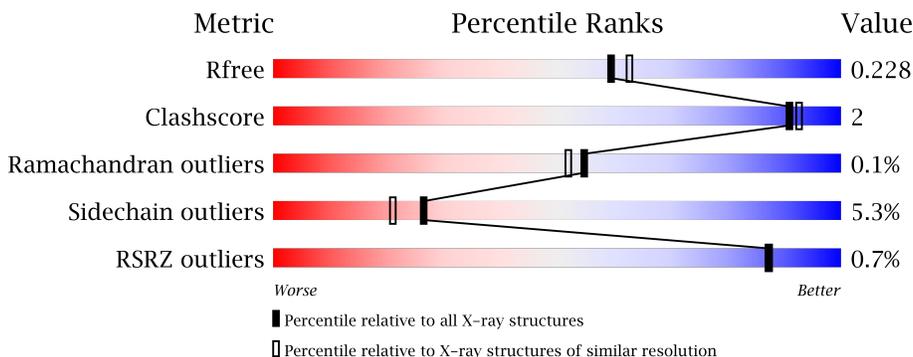
1 Overall quality at a glance

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))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 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	427	
1	B	427	

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
3	GOL	B	502	-	-	-	X

2 Entry composition [i](#)

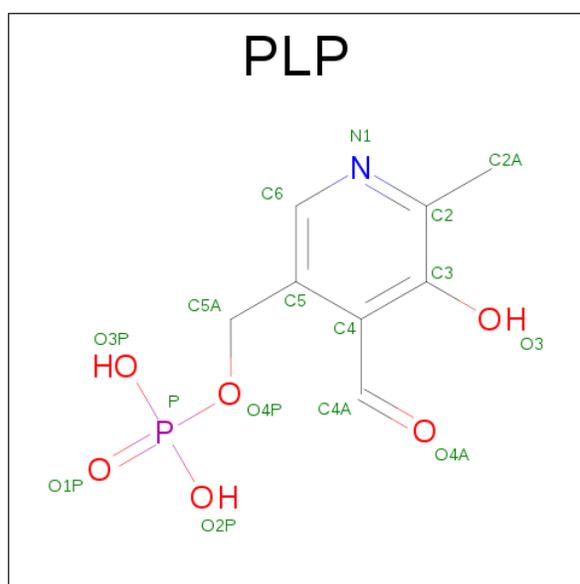
There are 4 unique types of molecules in this entry. The entry contains 6131 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cys/Met metabolism pyridoxal-phosphate-dependent enzyme.

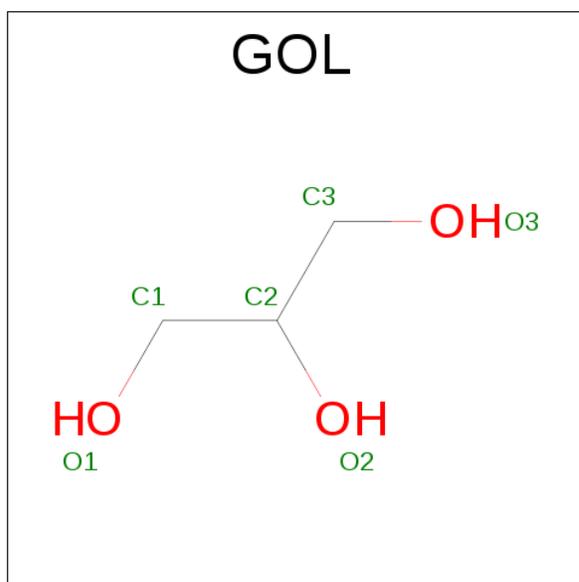
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	353	Total 2616	C 1652	N 452	O 504	S 8	0	3	0
1	B	403	Total 2992	C 1897	N 516	O 572	S 7	0	6	0

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



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

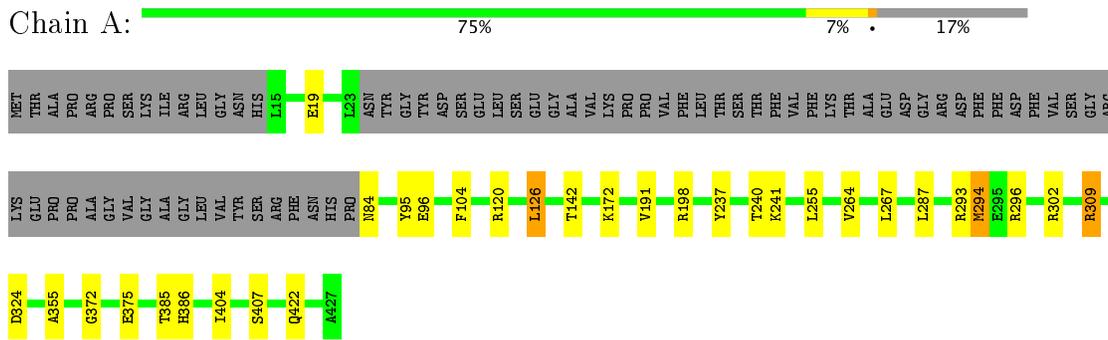
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	262	Total	O	0	0
			262	262		
4	B	225	Total	O	0	0
			225	225		

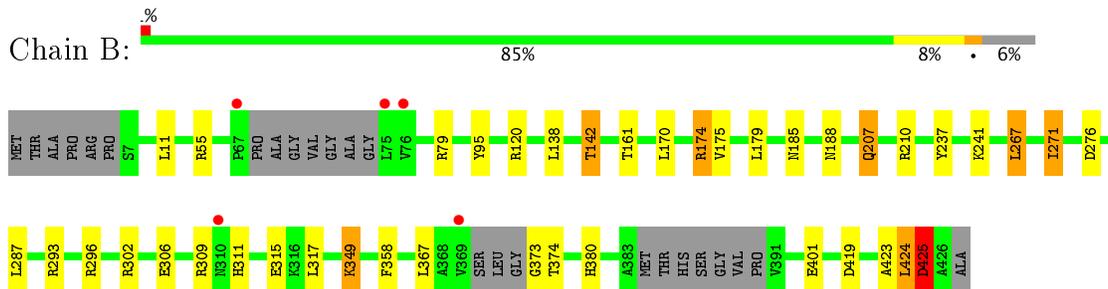
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Cys/Met metabolism pyridoxal-phosphate-dependent enzyme



- Molecule 1: Cys/Met metabolism pyridoxal-phosphate-dependent enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.71Å 109.71Å 110.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.01 – 2.00 95.01 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (95.01-2.00) 99.9 (95.01-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.170 , 0.223 0.177 , 0.228	Depositor DCC
R_{free} test set	2601 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	34.1	Xtrriage
Anisotropy	0.552	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6131	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: GOL, 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	1.05	3/2675 (0.1%)	1.01	9/3633 (0.2%)
1	B	0.85	0/3081	0.98	13/4187 (0.3%)
All	All	0.95	3/5756 (0.1%)	1.00	22/7820 (0.3%)

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
1	B	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	SER	CB-OG	-5.22	1.35	1.42
1	A	375[A]	GLU	CD-OE2	5.04	1.31	1.25
1	A	375[B]	GLU	CD-OE2	5.04	1.31	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	B	276	ASP	CB-CG-OD1	7.43	124.98	118.30
1	B	174	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	B	120	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	210	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	126	LEU	CB-CG-CD2	6.20	121.54	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296[A]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	296[B]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	296[A]	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	B	296[B]	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	296	ARG	CG-CD-NE	-5.99	99.23	111.80
1	B	293	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	302	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	120	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	198	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	293	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	324	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	B	210	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	294	MET	CG-SD-CE	-5.18	91.91	100.20
1	A	198	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	309	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	419	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	TYR	Peptide
1	B	237	TYR	Peptide
1	B	424	LEU	Peptide

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	2616	0	2586	8	0
1	B	2992	0	2883	14	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
3	B	6	0	8	1	0
4	A	262	0	0	1	0
4	B	225	0	0	2	0
All	All	6131	0	5491	22	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 2.

All (22) 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:385:THR:OG1	1:A:386:HIS:HD2	1.77	0.66
1:B:188:ASN:ND2	4:B:602:HOH:O	2.37	0.57
1:B:423:ALA:O	1:B:425:ASP:N	2.40	0.53
1:B:175:VAL:H	1:B:207:GLN:HE22	1.57	0.53
1:B:373:GLY:O	1:B:374:THR:HB	2.08	0.52
1:A:294:MET:HE1	4:A:743:HOH:O	2.08	0.52
1:A:96:GLU:HB2	1:A:255:LEU:HD22	1.93	0.50
1:B:425:ASP:N	1:B:425:ASP:OD1	2.44	0.50
3:B:502:GOL:H12	4:B:693:HOH:O	2.12	0.50
1:A:142:THR:HG21	1:B:271[A]:ILE:HD11	1.93	0.50
1:B:241:LYS:NZ	2:B:501:PLP:O3	2.45	0.50
1:B:311:HIS:CE1	1:B:424:LEU:HD13	2.48	0.48
1:A:355:ALA:HB1	1:A:404:ILE:HD11	1.97	0.46
1:B:267:LEU:CD1	1:B:271[A]:ILE:HD13	2.46	0.46
1:B:315:GLU:HG2	1:B:349:LYS:HG2	2.01	0.42
1:B:380:HIS:HE1	1:B:401:GLU:O	2.03	0.42
1:B:138:LEU:HD12	1:B:142:THR:HG23	2.03	0.41
1:B:302:ARG:NH1	1:B:306:GLU:OE2	2.53	0.41
1:A:241:LYS:NZ	2:A:501:PLP:O3	2.52	0.41
1:A:104:PHE:HZ	1:A:264:VAL:HG12	1.86	0.40
1:A:240:THR:O	1:A:372:GLY:HA2	2.22	0.40
1:B:267:LEU:HD11	1:B:271[A]:ILE:HD13	2.04	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	352/427 (82%)	347 (99%)	5 (1%)	0	100	100
1	B	401/427 (94%)	391 (98%)	9 (2%)	1 (0%)	51	48
All	All	753/854 (88%)	738 (98%)	14 (2%)	1 (0%)	55	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	425	ASP

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	269/337 (80%)	258 (96%)	11 (4%)	35	31
1	B	303/337 (90%)	283 (93%)	20 (7%)	19	14
All	All	572/674 (85%)	541 (95%)	31 (5%)	26	20

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	84	ASN
1	A	95	TYR
1	A	120	ARG
1	A	126	LEU
1	A	172	LYS
1	A	191	VAL
1	A	267	LEU
1	A	287	LEU
1	A	309	ARG
1	A	422	GLN
1	B	11	LEU
1	B	79	ARG
1	B	95	TYR
1	B	142	THR

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Mol	Chain	Res	Type
1	B	161	THR
1	B	170	LEU
1	B	174	ARG
1	B	179	LEU
1	B	185	ASN
1	B	207	GLN
1	B	267	LEU
1	B	271[A]	ILE
1	B	271[B]	ILE
1	B	287	LEU
1	B	309	ARG
1	B	317	LEU
1	B	349	LYS
1	B	358	PHE
1	B	367	LEU
1	B	425	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	300	ASN
1	A	386	HIS
1	A	422	GLN
1	B	188	ASN
1	B	207	GLN
1	B	300	ASN
1	B	380	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 carbohydrates in this entry.

5.6 Ligand geometry

3 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	501	1	15,15,16	2.25	3 (20%)	20,22,23	1.51	3 (15%)
2	PLP	B	501	1	15,15,16	2.20	3 (20%)	20,22,23	1.95	8 (40%)
3	GOL	B	502	-	5,5,5	0.30	0	5,5,5	0.49	0

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	501	1	-	0/6/6/8	0/1/1/1
2	PLP	B	501	1	-	0/6/6/8	0/1/1/1
3	GOL	B	502	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLP	C2A-C2	-2.44	1.45	1.50
2	B	501	PLP	C4A-C4	-2.27	1.47	1.51
2	A	501	PLP	C4A-C4	-2.21	1.47	1.51
2	B	501	PLP	C3-C4	2.16	1.44	1.40
2	B	501	PLP	C5-C4	6.78	1.48	1.40
2	A	501	PLP	C3-C2	7.37	1.45	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLP	O4P-P-O1P	-2.87	98.42	106.47
2	B	501	PLP	C2A-C2-C3	-2.84	117.57	120.96
2	B	501	PLP	O4P-P-O1P	-2.33	99.95	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLP	C4A-C4-C5	-2.23	118.60	120.86
2	A	501	PLP	O3-C3-C2	2.00	121.97	117.78
2	B	501	PLP	C3-C4-C5	2.21	121.14	118.63
2	B	501	PLP	C2A-C2-N1	2.39	122.67	117.89
2	B	501	PLP	C5A-C5-C6	2.46	123.56	119.33
2	B	501	PLP	C6-N1-C2	2.51	124.10	119.26
2	B	501	PLP	O3P-P-O2P	2.60	118.12	107.61
2	B	501	PLP	O3-C3-C2	3.34	124.77	117.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PLP	1	0
2	B	501	PLP	1	0
3	B	502	GOL	1	0

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, 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	353/427 (82%)	-0.56	0 100 100	26, 37, 53, 64	0
1	B	403/427 (94%)	-0.39	5 (1%) 79 78	27, 44, 65, 86	0
All	All	756/854 (88%)	-0.47	5 (0%) 87 87	26, 40, 62, 86	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	75	LEU	2.6
1	B	76	VAL	2.6
1	B	369	VAL	2.3
1	B	310	ASN	2.2
1	B	67	PRO	2.2

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
3	GOL	B	502	6/6	0.96	0.12	2.47	44,53,57,58	0
2	PLP	B	501	15/16	0.97	0.10	0.13	31,34,38,38	0
2	PLP	A	501	15/16	0.99	0.10	0.06	25,29,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.