



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:38 PM GMT

PDB ID : 4A0R
Title : Structure of bifunctional DAPA aminotransferase-DTB synthetase from *Arabidopsis thaliana* bound to dethiobiotin (DTB).
Authors : Cobessi, D.; Dumas, R.; Pautre, V.; Meinguet, C.; Ferrer, J.L.; Alban, C.
Deposited on : 2011-09-12
Resolution : 2.68 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

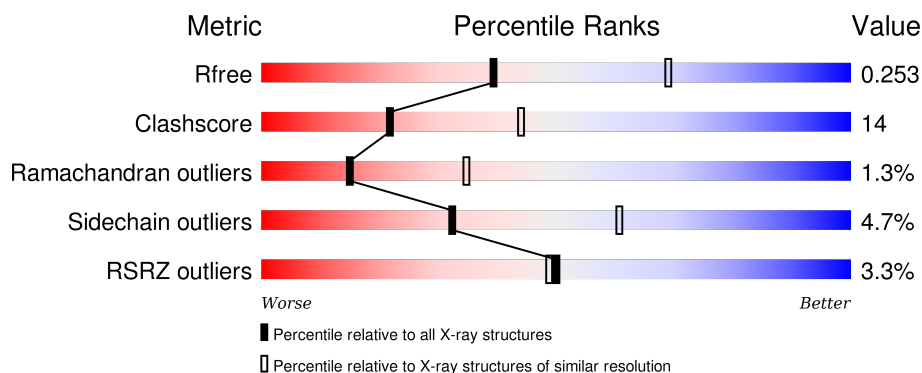
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	831	<div> <div>3%</div> <div>67%</div> <div>22%</div> <div>9%</div> </div>
1	B	831	<div> <div>3%</div> <div>64%</div> <div>23%</div> <div>10%</div> </div>

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	TLA	B	1809	-	-	X	-
4	DTB	A	1811	-	-	-	X
4	DTB	B	1808	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11693 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 ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOAT E AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	755	Total	C	N	O	S	0	2	0
			5788	3703	974	1079	32			
1	B	748	Total	C	N	O	S	0	2	0
			5704	3652	961	1059	32			

There are 40 discrepancies between the modelled and reference sequences:

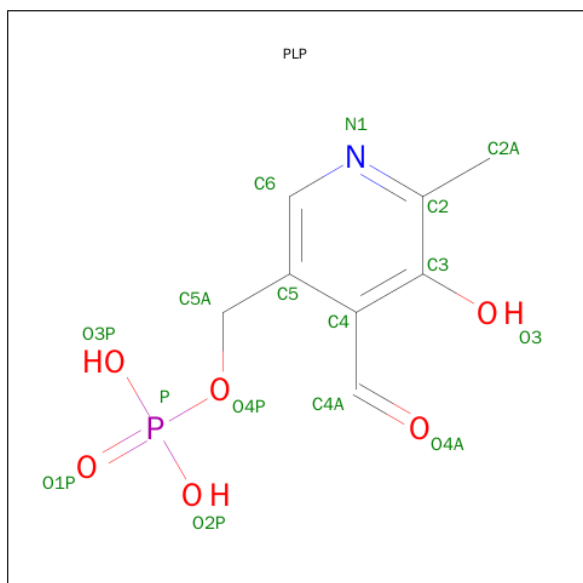
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	EXPRESSION TAG	UNP B0F481
A	-18	SER	-	EXPRESSION TAG	UNP B0F481
A	-17	SER	-	EXPRESSION TAG	UNP B0F481
A	-16	HIS	-	EXPRESSION TAG	UNP B0F481
A	-15	HIS	-	EXPRESSION TAG	UNP B0F481
A	-14	HIS	-	EXPRESSION TAG	UNP B0F481
A	-13	HIS	-	EXPRESSION TAG	UNP B0F481
A	-12	HIS	-	EXPRESSION TAG	UNP B0F481
A	-11	HIS	-	EXPRESSION TAG	UNP B0F481
A	-10	SER	-	EXPRESSION TAG	UNP B0F481
A	-9	SER	-	EXPRESSION TAG	UNP B0F481
A	-8	GLY	-	EXPRESSION TAG	UNP B0F481
A	-7	LEU	-	EXPRESSION TAG	UNP B0F481
A	-6	VAL	-	EXPRESSION TAG	UNP B0F481
A	-5	PRO	-	EXPRESSION TAG	UNP B0F481
A	-4	ARG	-	EXPRESSION TAG	UNP B0F481
A	-3	GLY	-	EXPRESSION TAG	UNP B0F481
A	-2	SER	-	EXPRESSION TAG	UNP B0F481
A	-1	HIS	-	EXPRESSION TAG	UNP B0F481
A	0	MET	-	EXPRESSION TAG	UNP B0F481
B	-19	GLY	-	EXPRESSION TAG	UNP B0F481
B	-18	SER	-	EXPRESSION TAG	UNP B0F481
B	-17	SER	-	EXPRESSION TAG	UNP B0F481
B	-16	HIS	-	EXPRESSION TAG	UNP B0F481

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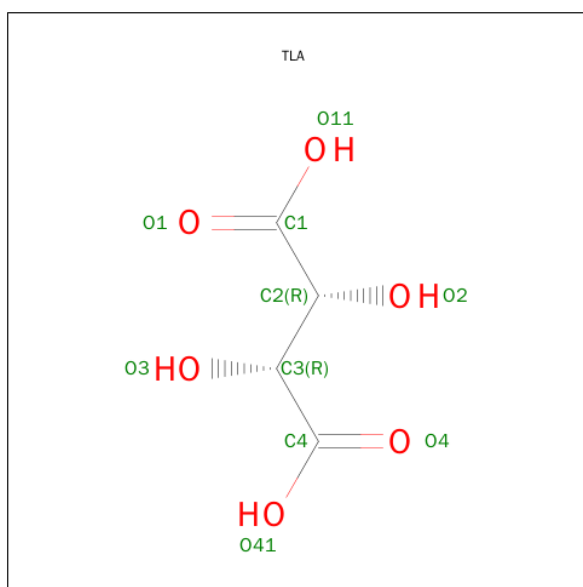
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	EXPRESSION TAG	UNP B0F481
B	-14	HIS	-	EXPRESSION TAG	UNP B0F481
B	-13	HIS	-	EXPRESSION TAG	UNP B0F481
B	-12	HIS	-	EXPRESSION TAG	UNP B0F481
B	-11	HIS	-	EXPRESSION TAG	UNP B0F481
B	-10	SER	-	EXPRESSION TAG	UNP B0F481
B	-9	SER	-	EXPRESSION TAG	UNP B0F481
B	-8	GLY	-	EXPRESSION TAG	UNP B0F481
B	-7	LEU	-	EXPRESSION TAG	UNP B0F481
B	-6	VAL	-	EXPRESSION TAG	UNP B0F481
B	-5	PRO	-	EXPRESSION TAG	UNP B0F481
B	-4	ARG	-	EXPRESSION TAG	UNP B0F481
B	-3	GLY	-	EXPRESSION TAG	UNP B0F481
B	-2	SER	-	EXPRESSION TAG	UNP B0F481
B	-1	HIS	-	EXPRESSION TAG	UNP B0F481
B	0	MET	-	EXPRESSION TAG	UNP B0F481

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



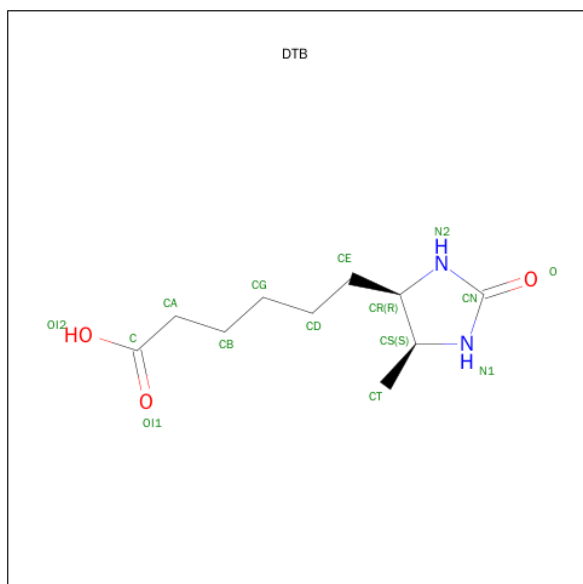
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is 6-(5-METHYL-2-OXO-IMIDAZOLIDIN-4-YL)-HEXANOIC ACID (three-letter code: DTB) (formula: $C_{10}H_{18}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	10	2	3		

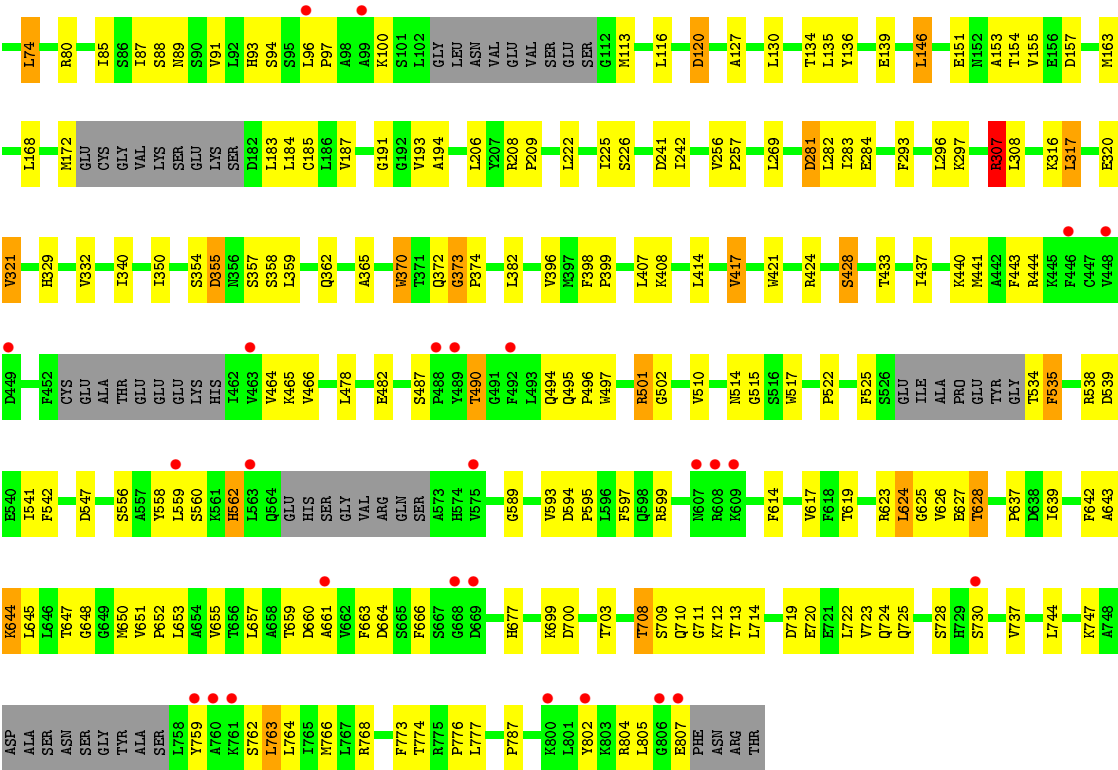
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			15	10	2	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	51	Total	O	0	0
			51	51		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.67Å 76.63Å 79.84Å 90.00° 108.02° 90.00°	Depositor
Resolution (Å)	40.44 – 2.68 40.72 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.44-2.68) 99.5 (40.72-2.68)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.184 , 0.259 0.184 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 65.7	EDS
Estimated twinning fraction	0.027 for -h+k-l,-l,-k 0.005 for -h-k-l,l,k 0.023 for -h-2*l,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39935 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11693	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: DTB, TLA, 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	0.48	1/5922 (0.0%)	0.64	3/8050 (0.0%)
1	B	0.48	2/5836 (0.0%)	0.65	3/7938 (0.0%)
All	All	0.48	3/11758 (0.0%)	0.64	6/15988 (0.0%)

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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	ARG	CZ-NH1	-11.03	1.18	1.33
1	A	307	ARG	CZ-NH1	-9.79	1.20	1.33
1	B	307	ARG	CZ-NH2	-5.56	1.25	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	NE-CZ-NH2	17.58	129.09	120.30
1	B	307	ARG	NE-CZ-NH2	16.14	128.37	120.30
1	B	307	ARG	NH1-CZ-NH2	-8.37	110.19	119.40
1	A	44	PRO	N-CA-CB	6.33	110.90	103.30
1	A	307	ARG	NH1-CZ-NH2	-5.93	112.87	119.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	45	SER	Peptide

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	5788	0	5697	161	0
1	B	5704	0	5585	181	0
2	A	15	0	6	1	0
2	B	15	0	6	1	0
3	A	10	0	3	3	0
3	B	10	0	4	4	0
4	A	15	0	17	2	0
4	B	15	0	17	5	0
5	A	70	0	0	1	0
5	B	51	0	0	2	0
All	All	11693	0	11335	321	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 14.

The worst 5 of 321 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:522:PRO:HG2	1:B:525:PHE:HD2	1.07	1.13
1:A:12:LEU:HD11	1:A:359:LEU:HG	1.41	1.02
1:B:522:PRO:HG2	1:B:525:PHE:CD2	1.97	1.00
1:A:659:THR:HG22	1:A:661:ALA:H	1.22	1.00
1:B:659:THR:HG22	1:B:661:ALA:H	1.24	0.99

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	745/831 (90%)	687 (92%)	46 (6%)	12 (2%)	12	28
1	B	736/831 (89%)	696 (95%)	33 (4%)	7 (1%)	19	42
All	All	1481/1662 (89%)	1383 (93%)	79 (5%)	19 (1%)	15	35

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	THR
1	B	355	ASP
1	B	490	THR
1	A	373	GLY
1	A	561	LYS

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	622/704 (88%)	592 (95%)	30 (5%)	31	59
1	B	605/704 (86%)	575 (95%)	30 (5%)	30	57
All	All	1227/1408 (87%)	1167 (95%)	60 (5%)	32	58

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	713	THR

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Mol	Chain	Res	Type
1	B	74	LEU
1	B	664	ASP
1	B	10	LEU
1	B	146	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	14	HIS
1	B	514	ASN
1	B	329	HIS
1	A	14	HIS
1	B	362	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](#)

6 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	1644	1	15,15,16	1.84	3 (20%)	21,22,23	1.84	3 (14%)
3	TLA	A	1810	-	3,9,9	1.88	1 (33%)	6,12,12	3.27	3 (50%)
4	DTB	A	1811	-	12,15,15	0.87	1 (8%)	14,19,19	1.18	3 (21%)
2	PLP	B	1644	1	15,15,16	1.87	2 (13%)	21,22,23	1.96	2 (9%)
4	DTB	B	1808	-	12,15,15	0.86	1 (8%)	14,19,19	1.94	2 (14%)
3	TLA	B	1809	-	3,9,9	1.64	1 (33%)	6,12,12	3.13	2 (33%)

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	1644	1	-	0/6/6/8	0/1/1/1
3	TLA	A	1810	-	-	0/4/12/12	0/0/0/0
4	DTB	A	1811	-	-	0/6/20/20	0/1/1/1
2	PLP	B	1644	1	-	0/6/6/8	0/1/1/1
4	DTB	B	1808	-	-	0/6/20/20	0/1/1/1
3	TLA	B	1809	-	-	0/4/12/12	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1644	PLP	O3-C3	-5.78	1.23	1.37
2	A	1644	PLP	O3-C3	-5.68	1.23	1.37
3	A	1810	TLA	O3-C3	-3.18	1.36	1.42
3	B	1809	TLA	O2-C2	-2.45	1.37	1.42
4	A	1811	DTB	CN-N1	-2.27	1.32	1.35

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1810	TLA	C1-C2-C3	-6.25	100.54	113.35
3	B	1809	TLA	C4-C3-C2	-5.26	102.56	113.35
3	B	1809	TLA	C1-C2-C3	-5.16	102.78	113.35
4	B	1808	DTB	CR-N2-CN	-4.24	109.31	112.49
3	A	1810	TLA	C4-C3-C2	-4.22	104.70	113.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1644	PLP	1	0
3	A	1810	TLA	3	0
4	A	1811	DTB	2	0
2	B	1644	PLP	1	0
4	B	1808	DTB	5	0
3	B	1809	TLA	4	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	755/831 (90%)	0.01	24 (3%) 51 50	15, 31, 68, 94	0
1	B	748/831 (90%)	0.00	26 (3%) 48 47	14, 30, 68, 94	0
All	All	1503/1662 (90%)	0.01	50 (3%) 50 49	14, 31, 68, 94	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	PRO	5.2
1	A	709	SER	4.0
1	B	563	LEU	3.8
1	A	492	PHE	3.8
1	A	451	ASN	3.8

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
4	DTB	A	1811	15/15	0.97	0.18	2.78	5,33,64,71	0
4	DTB	B	1808	15/15	0.95	0.21	2.25	2,23,45,51	0
3	TLA	A	1810	10/10	0.94	0.16	0.70	7,28,39,45	0
3	TLA	B	1809	10/10	0.94	0.16	0.21	22,37,47,56	0
2	PLP	A	1644	15/16	0.97	0.21	0.14	16,31,39,40	0
2	PLP	B	1644	15/16	0.97	0.18	-0.32	15,31,36,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.