



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 09:42 am 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

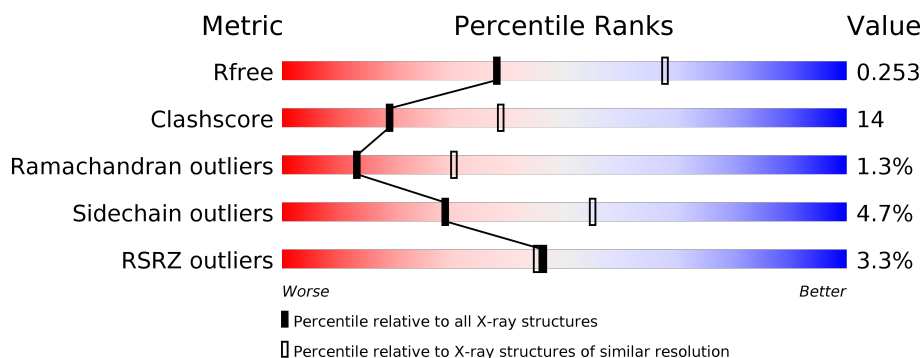
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	111664	3333 (2.70-2.66)
Clashscore	122126	3672 (2.70-2.66)
Ramachandran outliers	120053	3620 (2.70-2.66)
Sidechain outliers	120020	3620 (2.70-2.66)
RSRZ outliers	108989	3248 (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  $\geq 3$ , 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> <div></div> <div>67%</div> <div>22%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	831	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>23%</div> <div>•</div> <div>10%</div> </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	-

## 2 Entry composition [i](#)

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-OXONONANOATE 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:

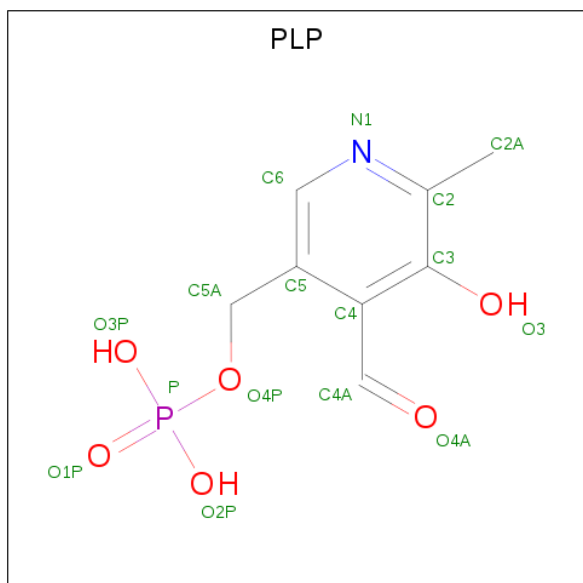
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	expression tag	UNP B0F481
A	-18	SER	-	expression tag	UNP B0F481
A	-17	SER	-	expression tag	UNP B0F481
A	-16	HIS	-	expression tag	UNP B0F481
A	-15	HIS	-	expression tag	UNP B0F481
A	-14	HIS	-	expression tag	UNP B0F481
A	-13	HIS	-	expression tag	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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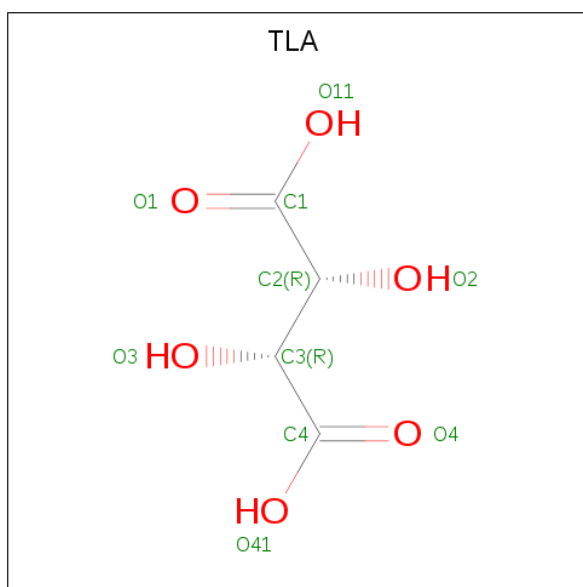
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP B0F481
B	-14	HIS	-	expression tag	UNP B0F481
B	-13	HIS	-	expression tag	UNP B0F481
B	-12	HIS	-	expression tag	UNP B0F481
B	-11	HIS	-	expression tag	UNP B0F481
B	-10	SER	-	expression tag	UNP B0F481
B	-9	SER	-	expression tag	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:  $C_8H_{10}NO_6P$ ).



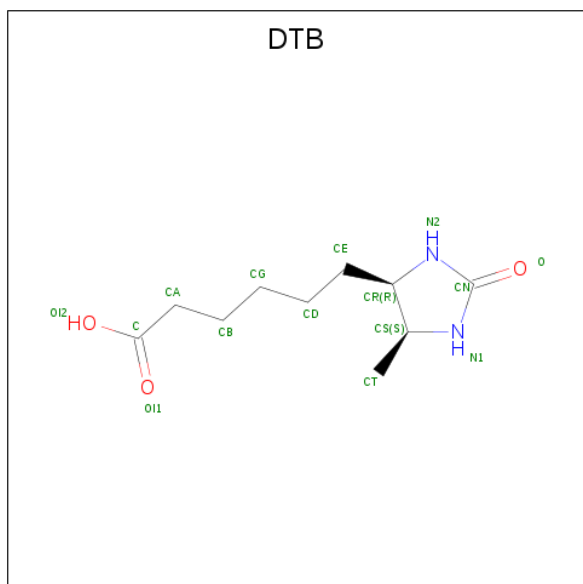
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- 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		

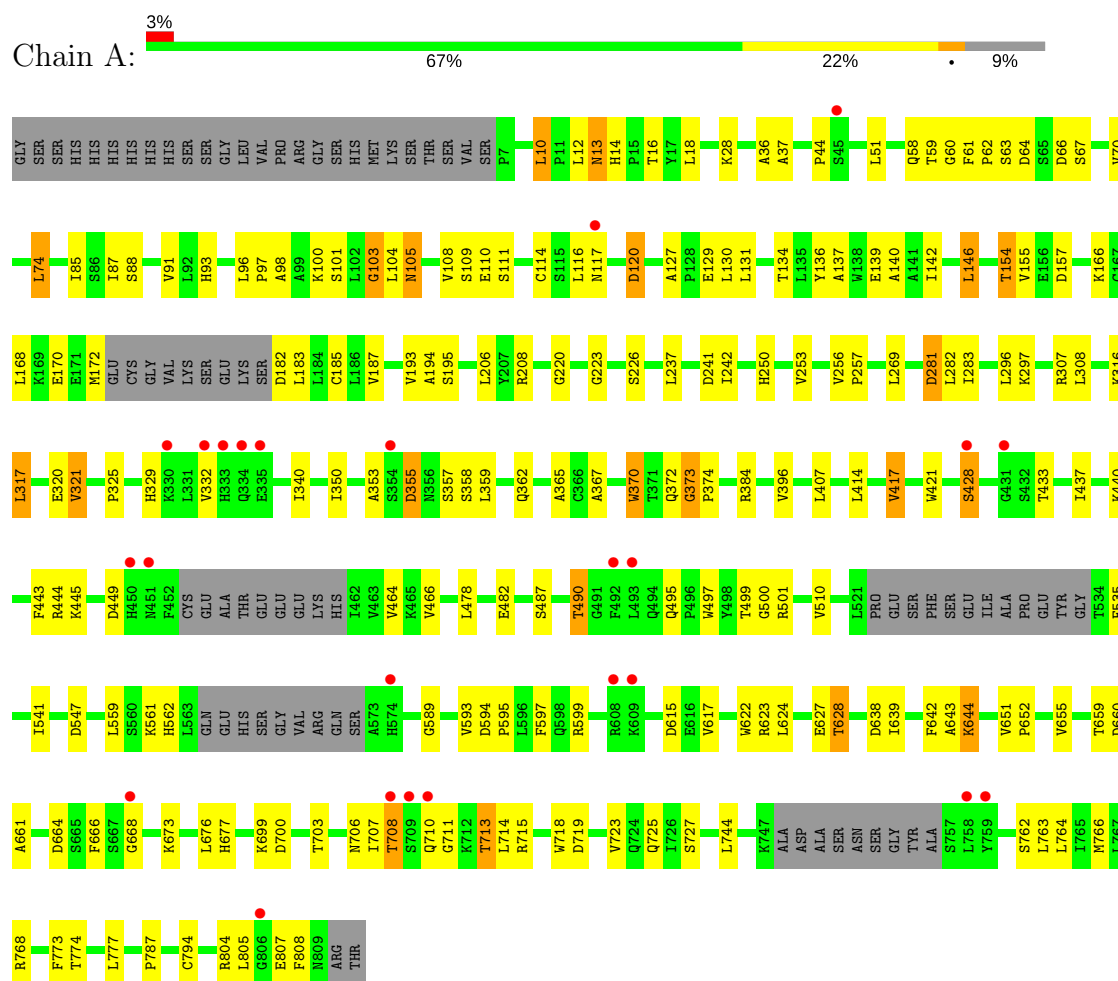
- Molecule 5 is water.

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

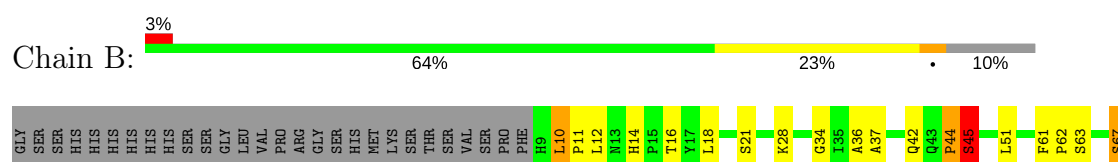
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE



#### • Molecule 1: ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE





ASP	K644	E540	D449	V321	L168	L74
ALA	L645	I541	F542	H329	M172	R80
SER	L646	T647	CYS	V332	GLU	
ASN	L647	G648	ALA	V332	CYS	I85
GLY	G649	S556	THR	I340	GLY	S86
TYR	M650	A557	GLU	I340	VAL	I87
ALA	V651	Y558	GLU	I350	LYS	S88
SER	P652	L559	GLU	I350	VAL	N89
L758	L653	S560	GLU	S354	SER	S90
Y759	A654	K561	LYS	D355	GLU	V91
A760	V655	H562	HIS	V356	LYS	
S761	T656	L563	I462	S357	SER	L92
L762	L657	L563	V463	S357	D182	H93
L763	A658	Q564	V464	S258	L183	S94
L764	T659	GLU	K465	L359	L184	S94
L765	D660	HIS	V466	Q362	C185	S95
L766	D660	SER	L478	Q362	L186	L96
M766	V662	GLY	E482	GLY	V187	P97
L767	F663	VAL	E482	A365		A98
R768	D664	ARG	E482		G191	A99
	S665	GLN		W370	G191	K100
F773	F666	SER	S487	T371	G192	S101
R775	S667	A573	P488	Q372	A194	L102
P776	G668	H574	Y489	G373	GLY	GLY
L777	D669	V575	T490	P374	LEU	LEU
			G491		ASN	ASN
			F492	L382	VAL	VAL
P787	H677	G689	L493		Y207	GLJ
			Q494		R208	GLJ
Y802	K699	V593	Q494	V396	P209	VAL
R803	D700	D594	Q495	M397	L222	SER
R804		P595	P496	F398		GLU
L805	T703	L596	W497	P399		SER
G806		F597			I225	G112
E807	T708	Q598	R501	L407	S226	M113
PHE	S709	R599	G502	K408	D241	
ASN	Q710		V510	L414	I242	L116
ARG	G711	M607				D120
THR	K712	R608	N514	V417	V256	
	T713	K609	G515	W421	P257	A127
	L714	F614	S516	V421	L269	L130
			V517			
D719	D719	V617	P522	R424	D281	T134
E720	E720	F618			L282	L135
E721	E721	T619	F525	S428	I283	Y136
L722	L722		S526	T433	E284	
V723	V723	R623	S526		F293	E139
Q724	Q724	L624	GLU	I437		
Q725	Q725	G625	ILE		L296	L146
S728	S728	V626	ALA		K297	
H729	H729	E627	PRO	K440		E151
S730	S730	T628	GLU	M441	A153	N152
			TYR	A442	A153	
V737	V737	P637	GLY	F443	T154	
		D638	T534	R444	V155	
L744	L744	I639	F535	V445	E156	
				F446	D157	
K747	K747	F642	R538	C447		
A748	A748	A643	D539	V448	E322	M163

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.184 , 0.259 0.179 , 0.253	Depositor DCC
$R_{free}$ test set	2000 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 65.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
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
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11693	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

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

### 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	745/831 (90%)	687 (92%)	46 (6%)	12 (2%)	11	24
1	B	736/831 (89%)	696 (95%)	33 (4%)	7 (1%)	17	38
All	All	1481/1662 (89%)	1383 (93%)	79 (5%)	19 (1%)	13	30

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

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%)	28	54
1	B	605/704 (86%)	575 (95%)	30 (5%)	27	52
All	All	1227/1408 (87%)	1167 (95%)	60 (5%)	29	53

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	1.85	3 (20%)	20,22,23	1.67	2 (10%)
3	TLA	A	1810	-	3,9,9	1.97	1 (33%)	6,12,12	3.07	3 (50%)
4	DTB	A	1811	-	12,15,15	0.83	1 (8%)	12,19,19	1.07	1 (8%)
2	PLP	B	1644	1	15,15,16	1.87	3 (20%)	20,22,23	1.74	1 (5%)
4	DTB	B	1808	-	12,15,15	0.83	0	12,19,19	1.73	2 (16%)
3	TLA	B	1809	-	3,9,9	1.72	1 (33%)	6,12,12	2.93	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	-5.83	1.23	1.37
2	A	1644	PLP	O3-C3	-5.73	1.23	1.37
3	A	1810	TLA	O3-C3	-3.33	1.36	1.42
3	B	1809	TLA	O2-C2	-2.57	1.37	1.42
4	A	1811	DTB	CN-N1	-2.15	1.32	1.35

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1810	TLA	C1-C2-C3	-5.84	100.54	113.11
3	B	1809	TLA	C4-C3-C2	-4.90	102.56	113.11
3	B	1809	TLA	C1-C2-C3	-4.80	102.78	113.11
3	A	1810	TLA	C4-C3-C2	-3.91	104.70	113.11
4	B	1808	DTB	CD-CE-CR	-3.73	106.26	113.96

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	755/831 (90%)	-0.02	24 (3%) 47 46	15, 31, 68, 94	0
1	B	748/831 (90%)	-0.03	25 (3%) 46 45	14, 30, 68, 94	0
All	All	1503/1662 (90%)	-0.03	49 (3%) 46 45	14, 31, 68, 94	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	PRO	5.1
1	A	709	SER	3.9
1	B	563	LEU	3.8
1	A	492	PHE	3.7
1	A	451	ASN	3.7

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TLA	B	1809	10/10	0.94	0.16	22,37,47,56	0
3	TLA	A	1810	10/10	0.94	0.16	7,28,39,45	0
4	DTB	B	1808	15/15	0.95	0.20	2,23,45,51	0
4	DTB	A	1811	15/15	0.97	0.18	5,33,64,71	0
2	PLP	A	1644	15/16	0.97	0.21	16,31,39,40	0
2	PLP	B	1644	15/16	0.97	0.18	15,31,36,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.