



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 09:26 AM EDT

PDB ID : 4A0F  
Title : Structure of selenomethionine substituted bifunctional DAPA aminotransferase-dethiobiotin synthetase from *Arabidopsis thaliana* in its apo form.  
Authors : Cobessi, D.; Dumas, R.; Pautre, V.; Meinguet, C.; Ferrer, J.L.; Alban, C.  
Deposited on : 2011-09-09  
Resolution : 2.71 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

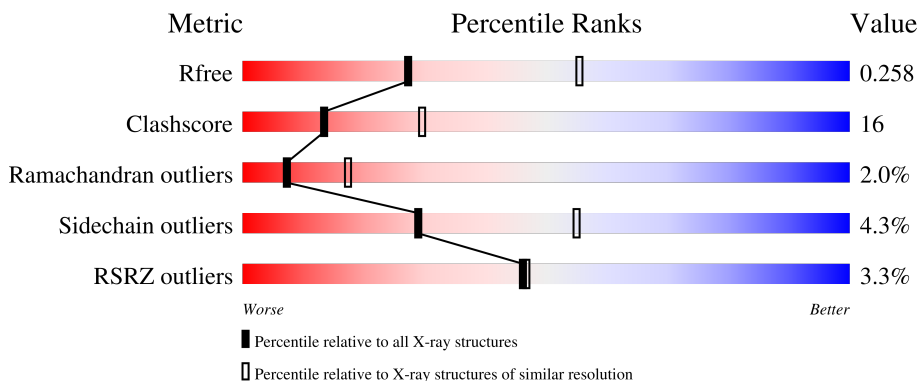
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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))
$R_{free}$	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	B	831	

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	SO4	B	1810	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11317 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	746	Total	C	N	O	S	Se	0	1	0
			5568	3562	937	1037	16	16			
1	B	750	Total	C	N	O	S	Se	0	0	0
			5619	3598	944	1046	16	15			

There are 42 discrepancies between the modelled and reference sequences:

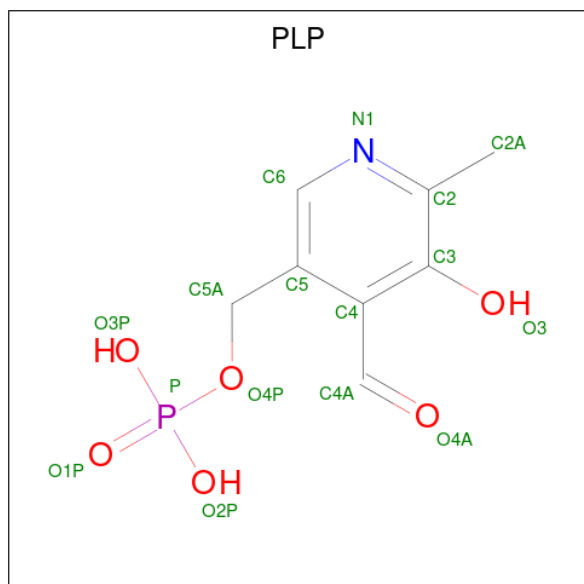
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	expression tag	UNP B0F481
A	-18	SER	-	expression tag	UNP B0F481
A	-17	SER	-	expression tag	UNP B0F481
A	-16	HIS	-	expression tag	UNP B0F481
A	-15	HIS	-	expression tag	UNP B0F481
A	-14	HIS	-	expression tag	UNP B0F481
A	-13	HIS	-	expression tag	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	MSE	-	expression tag	UNP B0F481
A	326	TYR	PHE	engineered mutation	UNP B0F481
B	-19	GLY	-	expression tag	UNP B0F481
B	-18	SER	-	expression tag	UNP B0F481
B	-17	SER	-	expression tag	UNP B0F481

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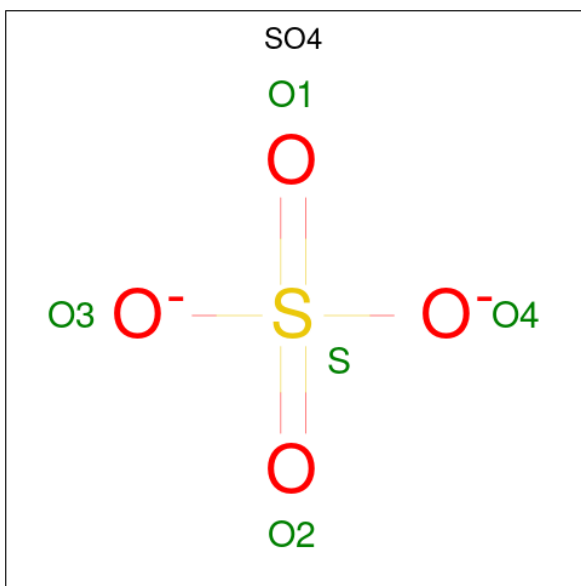
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP B0F481
B	-15	HIS	-	expression tag	UNP B0F481
B	-14	HIS	-	expression tag	UNP B0F481
B	-13	HIS	-	expression tag	UNP B0F481
B	-12	HIS	-	expression tag	UNP B0F481
B	-11	HIS	-	expression tag	UNP B0F481
B	-10	SER	-	expression tag	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	MSE	-	expression tag	UNP B0F481
B	326	TYR	PHE	engineered mutation	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 SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	30	Total	O	0	0
			30	30		



Tyr	Ala	S757	L758	Y759	L763	L764	I765	M766	E769	T774	M779	L783	S790	L797	L798	L801	R804	L805	G806	E807	F808	Asn	Arg	Thr																													
L645	M650	V651	P652	T659	D660	A661	V662	F666	S667	G668	D669	S670	K671	L672	L675	S680	A685	M686	G687	C688	T708	S709	Q710	L714	L717	W718	D719	V723	Q724	H729	S730	A731	V737	I738	L741	L746	Lys	Ala	Ala	Asp	Ala	Ser	Asn	Ser	Gly								
H562	Leu	Gln	Val	His	Gly	Val	Arg	Gln	Ser	A573	H574	M575	G576	A577	L578	I579	S487	P488	G491	I584	M590	H591	M592	V593	D594	P595	L596	F597	Q598	R599	M600	L601	V602	I610	P611	V612	I613	F614	D615	E616	V617	W622	R623	L624	T628	T629	T630	K636	I639	A643	K644		
K465	V466	I467	R470	H474	L478	G479	A480	M481	E482	A485	P486	S487	P488	G491	W497	R501	P508	T509	V510	S513	N514	G515	I519	S520	F525	Ser	Glu	Ile	Ala	Pro	Glu	Tyr	D449	H450	F452	T536	S537	R538	R546	D547	S556	L559	S560	K561									
G373	P374	L382	A383	R384	E385	M386	G387	Y388	R392	H395	V396	K397	P399	V402	Y403	E411	L414	V417	S428	D429	N430	T433	I437	A438	M441	A442	F443	R444	K445	F446	C447	V448	P449	H450	N451	F452	Cys	Glu	Ala	Thr	Glu	Glu	Lys	His	T462	V463							
L262	V266	L269	D277	F278	G279	D280	D281	L282	V287	F293	L296	K297	M300	V301	L302	A315	K316	L317	V321	P325	V326	T327	K330	H333	T336	V337	I340	F348	S349	K352	D355	N356	S357	S360	Q361	A367	S368	W369	Q372														
V138	E139	I142	H145	L146	R150	L168	M172	Glu	Cys	Gly	Val	Lys	Ser	Glu	Lys	Ser	D182	L183	L184	C185	L186	V187	P196	L206	F207	R208	P209	F210	R211	G218	D219	G220	R221	L222	G223	G224	I225	I229	E233	K236	L237	D241	L252	P257									
T49	K50	L51	Q58	T59	G60	F61	P62	S67	F71	S72	K73	L74	L79	R80	R81	T85	S86	S88	N89	S90	V91	H93	S94	S95	L96	P97	S101	L104	Asn	Val	Glu	Val	Ser	E110	M113	C114	R119	A127	P128	E129	L130	L131	T134	L135	Y136	A137							
Gly	Ser	Ser	His	His	His	His	His	Ser	Ser	Gly	Leu	Val	Pro	Arg	Gly	Ser	His	Mse	Lys	Ser	Thr	Ser	V5	S6	P7	F8	H9	L10	P11	L12	N13	H14	L18	S21	T24	S25	L26	G27	K28	T29	L30	V31	G34	I35	A36	L41	Q42	Q43	Pro	Ser	Ser	S47	A48



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	233.67Å 75.97Å 88.63Å 90.00° 109.20° 90.00°	Depositor
Resolution (Å)	41.85 – 2.71 41.85 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.85-2.71) 99.2 (41.85-2.71)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.200 , 0.261 0.194 , 0.258	Depositor DCC
$R_{free}$ test set	1990 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11317	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, SO4

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	0.44	0/5681	0.60	1/7722 (0.0%)
1	B	0.45	0/5731	0.60	0/7787
All	All	0.45	0/11412	0.60	1/15509 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	PRO	N-CA-CB	6.07	110.59	103.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5568	0	5367	172	0
1	B	5619	0	5425	206	0
2	A	15	0	6	2	0
2	B	15	0	6	2	0
3	A	10	0	0	1	0
3	B	10	0	0	3	0
4	A	50	0	0	1	0
4	B	30	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11317	0	10804	355	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 16.

The worst 5 of 355 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:21:SER:HB2	1:A:28:LYS:HD3	1.41	1.01
1:B:21:SER:HB2	1:B:28:LYS:HD3	1.41	1.00
1:A:510:VAL:HB	1:A:592:MSE:HE2	1.48	0.96
1:B:510:VAL:HB	1:B:592:MSE:HE2	1.51	0.91
1:B:766:MSE:HE2	1:B:804:ARG:HD2	1.57	0.86

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	733/831 (88%)	669 (91%)	50 (7%)	14 (2%)	8	18
1	B	734/831 (88%)	672 (92%)	46 (6%)	16 (2%)	6	15
All	All	1467/1662 (88%)	1341 (91%)	96 (6%)	30 (2%)	7	17

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	LEU
1	A	357	SER
1	B	222	LEU
1	B	357	SER

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Mol	Chain	Res	Type
1	B	730	SER

### 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	575/688 (84%)	552 (96%)	23 (4%)	31	58
1	B	583/688 (85%)	556 (95%)	27 (5%)	27	52
All	All	1158/1376 (84%)	1108 (96%)	50 (4%)	29	55

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	183	LEU
1	B	356	ASN
1	B	790	SER
1	B	206	LEU
1	B	321	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	HIS
1	B	450	HIS
1	B	484	GLN
1	B	574	HIS

### 5.3.3 RNA ⓘ

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 monosaccharides 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	1.83	2 (13%)	21,22,23	1.83	5 (23%)
3	SO4	A	1809	-	4,4,4	0.33	0	6,6,6	0.28	0
3	SO4	B	1809	-	4,4,4	0.35	0	6,6,6	0.21	0
2	PLP	B	1644	1	15,15,16	1.89	3 (20%)	21,22,23	1.73	4 (19%)
3	SO4	B	1810	-	4,4,4	0.36	0	6,6,6	0.31	0
3	SO4	A	1810	-	4,4,4	0.26	0	6,6,6	0.45	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 Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	B	1644	1	-	5/6/6/8	0/1/1/1
2	PLP	A	1644	1	-	5/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1644	PLP	O3-C3	-5.67	1.23	1.36
2	B	1644	PLP	O3-C3	-5.44	1.24	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1644	PLP	C2-N1	2.98	1.39	1.33
2	B	1644	PLP	C6-N1	2.47	1.39	1.34
2	A	1644	PLP	C2-N1	2.43	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1644	PLP	O4P-C5A-C5	6.13	120.84	109.36
2	B	1644	PLP	O4P-C5A-C5	5.77	120.16	109.36
2	B	1644	PLP	C6-C5-C4	2.65	120.27	118.10
2	B	1644	PLP	O3P-P-O4P	-2.65	99.77	106.67
2	A	1644	PLP	O3P-P-O4P	-2.59	99.91	106.67

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1644	PLP	C4-C5-C5A-O4P
2	A	1644	PLP	C6-C5-C5A-O4P
2	A	1644	PLP	C5A-O4P-P-O2P
2	A	1644	PLP	C5A-O4P-P-O3P
2	B	1644	PLP	C4-C5-C5A-O4P

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1644	PLP	2	0
3	A	1809	SO4	1	0
2	B	1644	PLP	2	0
3	B	1810	SO4	3	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	731/831 (87%)	-0.03	30 (4%) 37 36	28, 54, 95, 119	0
1	B	735/831 (88%)	-0.06	18 (2%) 59 60	27, 56, 89, 114	0
All	All	1466/1662 (88%)	-0.04	48 (3%) 46 47	27, 55, 92, 119	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	551	LEU	5.8
1	A	449	ASP	4.6
1	A	574	HIS	4.2
1	A	762	SER	4.2
1	A	512	LEU	4.1

### 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 monosaccharides 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	SO4	B	1810	5/5	0.89	0.25	57,64,91,114	5
3	SO4	A	1809	5/5	0.93	0.22	48,57,85,89	5
3	SO4	B	1809	5/5	0.95	0.17	52,63,81,83	5
3	SO4	A	1810	5/5	0.96	0.21	31,34,44,57	5
2	PLP	B	1644	15/16	0.97	0.21	34,47,56,60	0
2	PLP	A	1644	15/16	0.98	0.20	44,48,58,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.