



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2025 – 02:49 PM EDT

PDB ID : 4WYE  
Title : Crystal structure of 7,8-diaminopelargonic acid synthase (BioA) from Mycobacterium tuberculosis complexed with a DSF fragment hit  
Authors : Dai, R.; Finzel, B.C.  
Deposited on : 2014-11-17  
Resolution : 1.75 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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

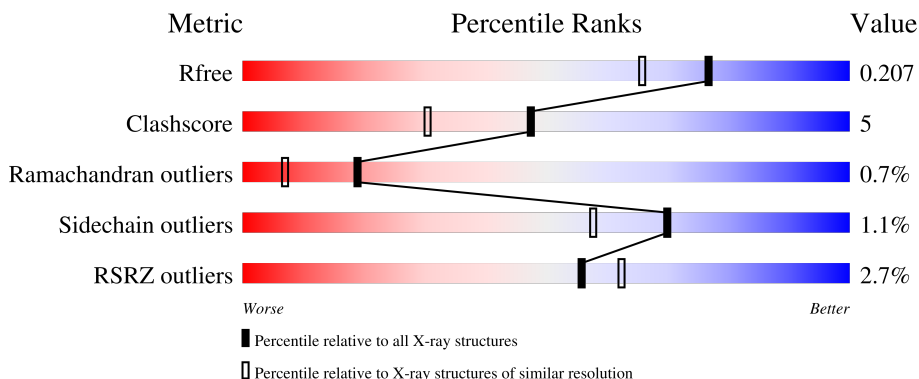
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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	457	
1	B	457	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7296 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	429	Total	C	N	O	S	0	18	0
			3316	2124	575	594	23			
1	B	429	Total	C	N	O	S	0	26	0
			3337	2132	582	601	22			

There are 40 discrepancies between the modelled and reference sequences:

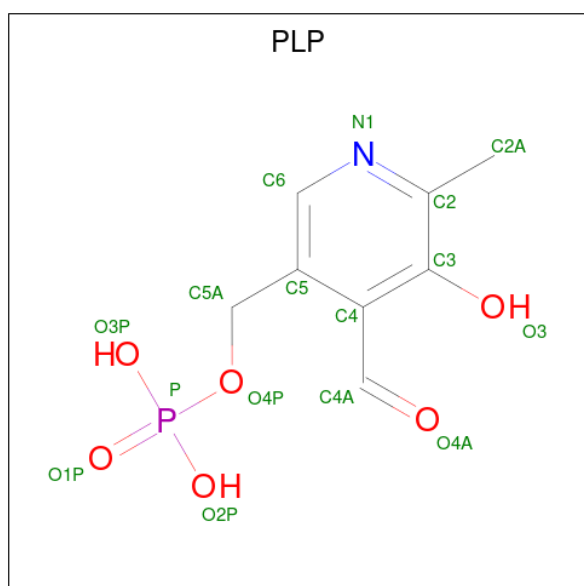
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WQ81
A	-18	GLY	-	expression tag	UNP P9WQ81
A	-17	SER	-	expression tag	UNP P9WQ81
A	-16	SER	-	expression tag	UNP P9WQ81
A	-15	HIS	-	expression tag	UNP P9WQ81
A	-14	HIS	-	expression tag	UNP P9WQ81
A	-13	HIS	-	expression tag	UNP P9WQ81
A	-12	HIS	-	expression tag	UNP P9WQ81
A	-11	HIS	-	expression tag	UNP P9WQ81
A	-10	HIS	-	expression tag	UNP P9WQ81
A	-9	SER	-	expression tag	UNP P9WQ81
A	-8	SER	-	expression tag	UNP P9WQ81
A	-7	GLY	-	expression tag	UNP P9WQ81
A	-6	LEU	-	expression tag	UNP P9WQ81
A	-5	VAL	-	expression tag	UNP P9WQ81
A	-4	PRO	-	expression tag	UNP P9WQ81
A	-3	ARG	-	expression tag	UNP P9WQ81
A	-2	GLY	-	expression tag	UNP P9WQ81
A	-1	SER	-	expression tag	UNP P9WQ81
A	0	HIS	-	expression tag	UNP P9WQ81
B	-19	MET	-	initiating methionine	UNP P9WQ81
B	-18	GLY	-	expression tag	UNP P9WQ81
B	-17	SER	-	expression tag	UNP P9WQ81
B	-16	SER	-	expression tag	UNP P9WQ81

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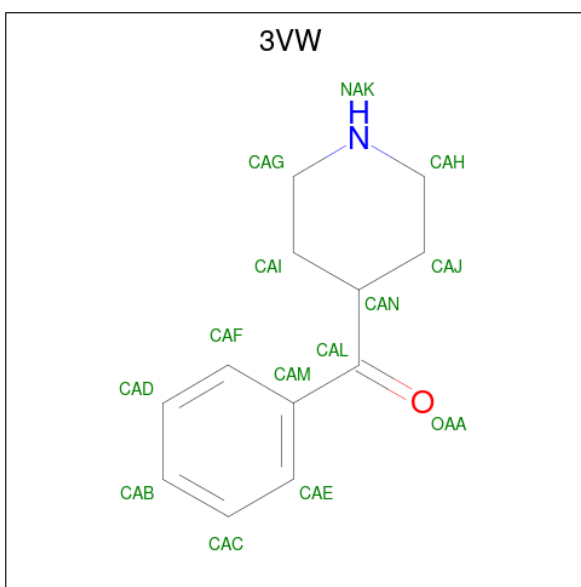
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP P9WQ81
B	-14	HIS	-	expression tag	UNP P9WQ81
B	-13	HIS	-	expression tag	UNP P9WQ81
B	-12	HIS	-	expression tag	UNP P9WQ81
B	-11	HIS	-	expression tag	UNP P9WQ81
B	-10	HIS	-	expression tag	UNP P9WQ81
B	-9	SER	-	expression tag	UNP P9WQ81
B	-8	SER	-	expression tag	UNP P9WQ81
B	-7	GLY	-	expression tag	UNP P9WQ81
B	-6	LEU	-	expression tag	UNP P9WQ81
B	-5	VAL	-	expression tag	UNP P9WQ81
B	-4	PRO	-	expression tag	UNP P9WQ81
B	-3	ARG	-	expression tag	UNP P9WQ81
B	-2	GLY	-	expression tag	UNP P9WQ81
B	-1	SER	-	expression tag	UNP P9WQ81
B	0	HIS	-	expression tag	UNP P9WQ81

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



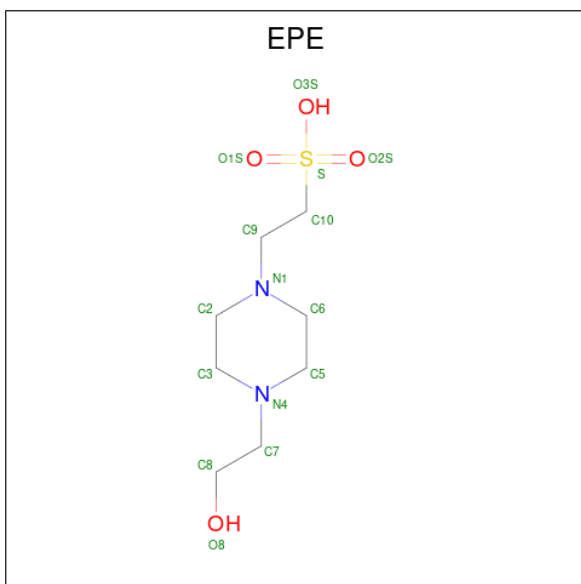
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is phenyl(piperidin-4-yl)methanone (three-letter code: 3VW) (formula:  $C_{12}H_{15}NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	12	1	1		
3	B	1	Total	C	N	O	0	0
			14	12	1	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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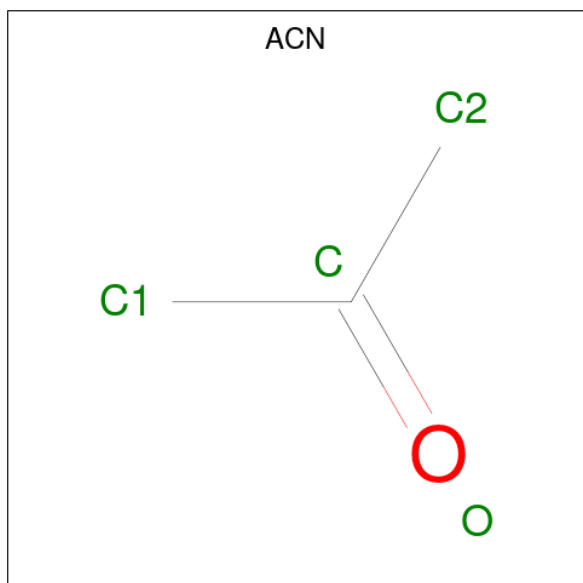
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	15	8	2	4	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is ACETONE (three-letter code: ACN) (formula: C<sub>3</sub>H<sub>6</sub>O).



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

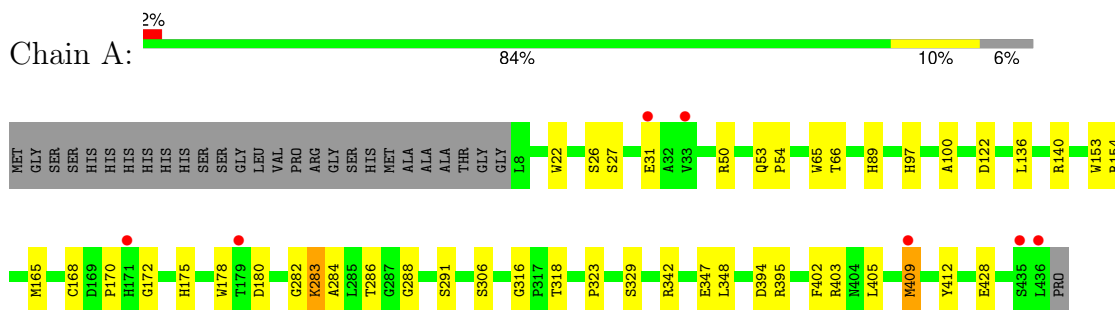
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	287	Total	O	0	1
			288	288		
7	B	257	Total	O	0	1
			258	258		

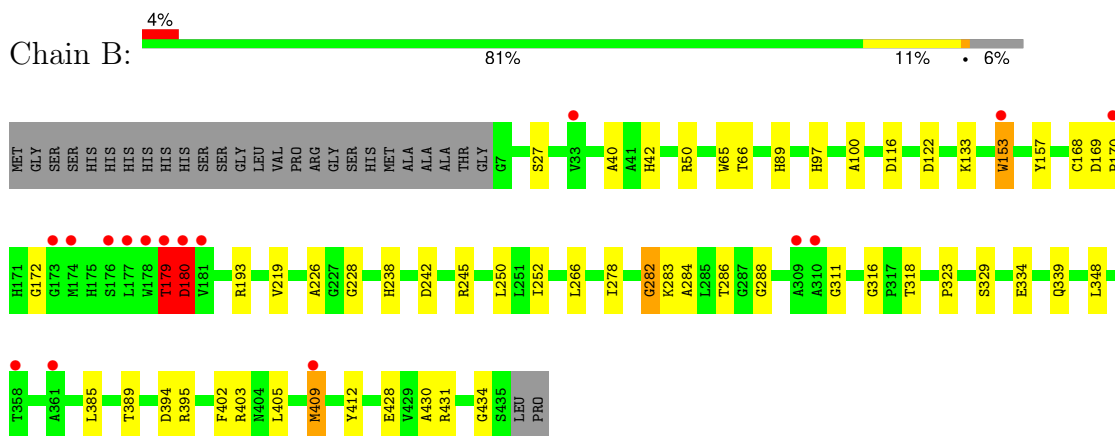
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.69Å 66.25Å 202.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.37 – 1.75 39.37 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.37-1.75) 99.9 (39.37-1.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.174 , 0.206 0.177 , 0.207	Depositor DCC
$R_{free}$ test set	4297 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: 3VW, PLP, ACN, SO4, EPE

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	0.35	0/3449	0.53	0/4713
1	B	0.37	0/3479	0.56	2/4755 (0.0%)
All	All	0.36	0/6928	0.55	2/9468 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	409	MET	CG-SD-CE	-6.48	89.83	100.20
1	B	180	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	179[B]	THR	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	3316	0	3325	33	0
1	B	3337	0	3342	44	0
2	A	15	0	6	1	0
2	B	15	0	6	1	0
3	A	14	0	15	3	0
3	B	14	0	15	2	0
4	A	15	0	17	1	0
4	B	15	0	17	0	0
5	A	5	0	0	0	0
6	B	4	0	6	2	0
7	A	288	0	0	6	0
7	B	258	0	0	11	0
All	All	7296	0	6749	74	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 5.

The worst 5 of 74 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:431:ARG:NH2	7:B:749:HOH:O	2.08	0.85
1:A:122[B]:ASP:OD2	7:A:822:HOH:O	1.99	0.81
1:A:31:GLU:OE1	7:A:837:HOH:O	2.00	0.79
1:A:27[B]:SER:OG	1:B:311[B]:GLY:O	2.01	0.78
1:B:402[B]:PHE:CE2	3:B:501:3VW:H14	2.19	0.78

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	447/457 (98%)	433 (97%)	12 (3%)	2 (0%)	30	16
1	B	453/457 (99%)	440 (97%)	8 (2%)	5 (1%)	12	3
All	All	900/914 (98%)	873 (97%)	20 (2%)	7 (1%)	19	5

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	LYS
1	B	180	ASP
1	B	282[A]	GLY
1	B	282[B]	GLY
1	B	316	GLY

### 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	344/346 (99%)	340 (99%)	4 (1%)	67	54
1	B	347/346 (100%)	340 (98%)	7 (2%)	50	31
All	All	691/692 (100%)	680 (98%)	11 (2%)	70	42

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	179[A]	THR
1	B	179[B]	THR
1	B	238[B]	HIS
1	B	238[A]	HIS
1	B	122[A]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

8 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
4	EPE	B	503	-	15,15,15	0.91	1 (6%)	19,20,20	1.83	3 (15%)
2	PLP	B	502	1	15,15,16	2.76	3 (20%)	21,22,23	1.62	4 (19%)
3	3VW	B	501	-	15,15,15	1.73	1 (6%)	17,19,19	0.92	1 (5%)
3	3VW	A	502	-	15,15,15	1.72	1 (6%)	17,19,19	1.06	0
6	ACN	B	504	-	3,3,3	0.30	0	3,3,3	0.17	0
5	SO4	A	504	-	4,4,4	0.28	0	6,6,6	0.12	0
2	PLP	A	501	1	15,15,16	2.79	3 (20%)	21,22,23	1.80	5 (23%)
4	EPE	A	503	-	15,15,15	0.81	1 (6%)	19,20,20	1.68	4 (21%)

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
4	EPE	B	503	-	-	0/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	B	502	1	-	0/6/6/8	0/1/1/1
3	3VW	B	501	-	-	0/8/16/16	0/2/2/2
3	3VW	A	502	-	-	0/8/16/16	0/2/2/2
2	PLP	A	501	1	-	0/6/6/8	0/1/1/1
4	EPE	A	503	-	-	3/9/19/19	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	PLP	C5-C4	7.19	1.48	1.40
2	A	501	PLP	C5-C4	7.16	1.48	1.40
2	A	501	PLP	C3-C2	6.48	1.47	1.41
3	B	501	3VW	CAM-CAL	-6.48	1.40	1.49
3	A	502	3VW	CAM-CAL	-6.40	1.40	1.49

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	EPE	C5-N4-C3	5.26	120.16	108.84
2	A	501	PLP	C4A-C4-C5	4.90	125.99	120.94
4	A	503	EPE	C5-N4-C3	4.18	117.85	108.84
2	B	502	PLP	O4P-C5A-C5	3.97	116.80	109.36
2	B	502	PLP	C4A-C4-C5	3.66	124.71	120.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	EPE	C10-C9-N1-C6
4	A	503	EPE	N4-C7-C8-O8
4	A	503	EPE	C10-C9-N1-C2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	PLP	1	0
3	B	501	3VW	2	0
3	A	502	3VW	3	0
6	B	504	ACN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PLP	1	0
4	A	503	EPE	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, 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	429/457 (93%)	-0.22	7 (1%) 70 76	7, 18, 33, 63	22 (5%)
1	B	429/457 (93%)	-0.03	16 (3%) 45 52	6, 19, 37, 70	28 (6%)
All	All	858/914 (93%)	-0.13	23 (2%) 56 62	6, 18, 35, 70	50 (5%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	436	LEU	5.3
1	B	179[A]	THR	4.9
1	B	153	TRP	4.3
1	A	409	MET	4.3
1	B	180	ASP	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 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
6	ACN	B	504	4/4	0.80	0.16	26,28,41,43	0
5	SO4	A	504	5/5	0.85	0.12	36,41,48,49	0
3	3VW	A	502	14/14	0.94	0.08	15,17,25,28	0
4	EPE	B	503	15/15	0.96	0.10	21,27,56,66	0
4	EPE	A	503	15/15	0.97	0.08	16,26,39,41	0
3	3VW	B	501	14/14	0.97	0.06	13,20,23,24	0
2	PLP	A	501	15/16	0.98	0.05	10,12,17,19	0
2	PLP	B	502	15/16	0.98	0.05	11,15,19,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.