



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:31 AM UTC

PDB ID : 4WYG / pdb_00004wyg
Title : Crystal structure of 7,8-diaminopelargonic acid synthase (BioA) from Mycobacterium tuberculosis complexed with a fragment hit
Authors : Dai, R.; Finzel, B.C.
Deposited on : 2014-11-17
Resolution : 1.62 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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

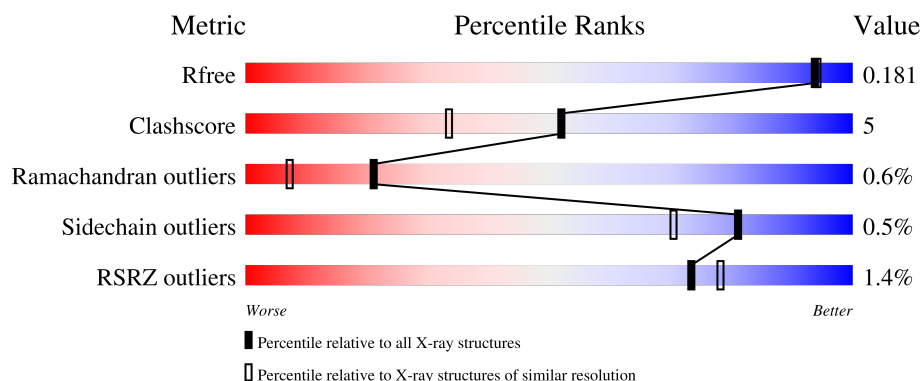
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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}	180053	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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 ≥ 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	85% 9% 6%
1	B	457	2% 84% 10% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7949 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	29	0
			3413	2176	606	610	21			
1	B	429	Total	C	N	O	S	0	35	0
			3448	2197	611	616	24			

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

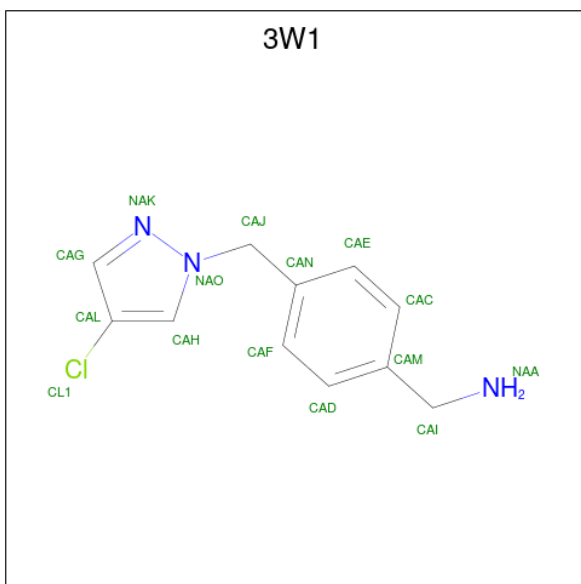
- PLP
-
- The diagram shows the chemical structure of Pyridoxal Phosphate (PLP). It consists of a pyridine ring with a phosphate group at the 3-position and an aldehyde group at the 4-position. The pyridine ring is colored blue, with the nitrogen atom labeled N1. The carbon atoms are labeled C2, C3, C4, C5, and C6. The phosphate group is colored purple, with the phosphorus atom labeled P. The oxygen atoms of the phosphate group are labeled O1P, O2P, O3P, and O4P. The aldehyde group is colored red, with the carbonyl oxygen labeled O4A and the hydroxyl group labeled O3. The hydroxyl group at the 3-position is colored red, with the oxygen labeled O3. The carbon atom of the hydroxyl group is labeled C3A. The carbon atom of the aldehyde group is labeled C4A. The carbon atom of the phosphate group is labeled C5A. The carbon atom of the pyridine ring is labeled C2A. The carbon atom of the pyridine ring is labeled C3. The carbon atom of the pyridine ring is labeled C4. The carbon atom of the pyridine ring is labeled C5. The carbon atom of the pyridine ring is labeled C6.

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	1
			30	16	4	8	2		

- Molecule 4 is 1-{4-[(4-chloro-1H-pyrazol-1-yl)methyl]phenyl}methanamine (CCD ID: 3W1) (formula: C₁₁H₁₂ClN₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	1
			45	33	3	9		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	0	1
			30	22	2	6		
4	B	1	Total	C	Cl	N	0	0
			15	11	1	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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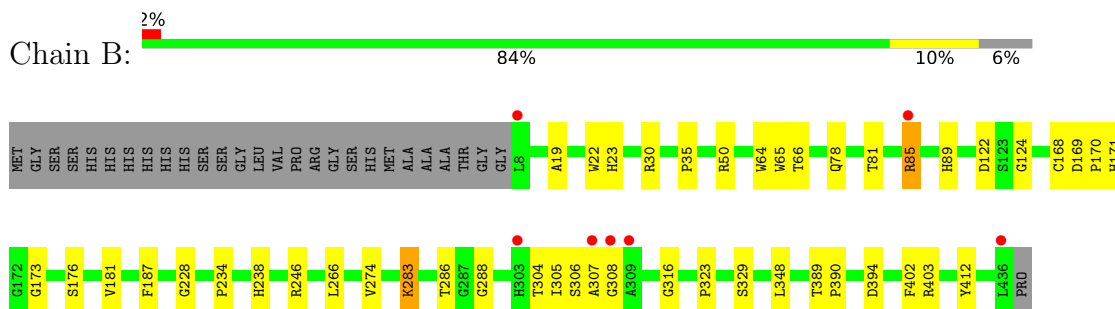
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	455	Total	O	0	0
			455	455		
6	B	424	Total	O	0	0
			424	424		

- 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, α , β , γ	63.12Å 66.43Å 205.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.40 – 1.62 46.40 – 1.62	Depositor EDS
% Data completeness (in resolution range)	96.1 (46.40-1.62) 96.1 (46.40-1.62)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.14 (at 1.62Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.151 , 0.180 0.152 , 0.181	Depositor DCC
R_{free} test set	5320 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7949	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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, 0.333 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: PLP, 3W1, EDO, 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	0.43	0/3534	0.68	0/4827
1	B	0.41	0/3568	0.69	0/4871
All	All	0.42	0/7102	0.68	0/9698

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3413	0	3431	28	0
1	B	3448	0	3447	43	0
2	A	15	0	6	0	0
2	B	15	0	6	2	0
3	A	15	0	17	0	0
3	B	30	0	34	0	0
4	A	45	0	36	1	0
4	B	45	0	36	7	0
5	A	16	0	24	3	0
5	B	28	0	42	8	0
6	A	455	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	424	0	0	12	0
All	All	7949	0	7079	73	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 73 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)
4:B:503[A]:3W1:H2	6:B:672:HOH:O	1.57	1.01
4:A:503[B]:3W1:H2	6:A:703:HOH:O	1.62	0.97
1:B:305[A]:ILE:O	6:B:862:HOH:O	1.93	0.84
1:A:113:ALA:H	5:A:507:EDO:H21	1.45	0.80
1:B:246:ARG:HH11	5:B:510:EDO:H21	1.52	0.73

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	456/457 (100%)	444 (97%)	10 (2%)	2 (0%)	30	14
1	B	463/457 (101%)	441 (95%)	19 (4%)	3 (1%)	21	7
All	All	919/914 (100%)	885 (96%)	29 (3%)	5 (0%)	21	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	LYS
1	B	283	LYS
1	A	316	GLY

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Mol	Chain	Res	Type
1	B	228	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	355/346 (103%)	353 (99%)	2 (1%)	78	66
1	B	356/346 (103%)	353 (99%)	3 (1%)	73	59
All	All	711/692 (103%)	706 (99%)	5 (1%)	81	62

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	153	TRP
1	B	85[A]	ARG
1	B	85[B]	ARG
1	B	85[C]	ARG

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 ⓘ

22 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	3W1	A	503[B]	-	15,16,16	2.76	4 (26%)	18,21,21	1.19	3 (16%)
4	3W1	B	503[C]	-	15,16,16	2.73	4 (26%)	18,21,21	2.31	5 (27%)
5	EDO	B	504	-	3,3,3	0.43	0	2,2,2	0.46	0
4	3W1	A	503[A]	-	15,16,16	2.64	5 (33%)	18,21,21	2.85	5 (27%)
2	PLP	A	501	1	15,15,16	2.74	3 (20%)	21,22,23	1.53	3 (14%)
5	EDO	B	510	-	3,3,3	0.45	0	2,2,2	0.16	0
4	3W1	B	503[A]	-	15,16,16	3.19	4 (26%)	18,21,21	1.23	3 (16%)
5	EDO	B	509	-	3,3,3	0.40	0	2,2,2	0.35	0
5	EDO	B	508	-	3,3,3	0.41	0	2,2,2	0.34	0
5	EDO	A	506	-	3,3,3	0.44	0	2,2,2	0.33	0
3	EPE	B	502[B]	-	15,15,15	0.87	1 (6%)	19,20,20	1.53	3 (15%)
4	3W1	B	506	-	15,16,16	2.63	4 (26%)	18,21,21	1.86	4 (22%)
5	EDO	B	505	-	3,3,3	0.42	0	2,2,2	0.05	0
2	PLP	B	501	1	15,15,16	2.79	3 (20%)	21,22,23	1.91	6 (28%)
5	EDO	A	505	-	3,3,3	0.31	0	2,2,2	0.50	0
5	EDO	A	504	-	3,3,3	0.40	0	2,2,2	0.26	0
5	EDO	A	507	-	3,3,3	0.50	0	2,2,2	0.18	0
3	EPE	B	502[A]	-	15,15,15	0.86	1 (6%)	19,20,20	1.48	3 (15%)
3	EPE	A	502	-	15,15,15	0.93	1 (6%)	19,20,20	1.46	4 (21%)
5	EDO	B	507	-	3,3,3	0.42	0	2,2,2	0.22	0
4	3W1	A	503[C]	-	15,16,16	2.33	4 (26%)	18,21,21	1.63	4 (22%)
5	EDO	B	511	-	3,3,3	0.42	0	2,2,2	0.55	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
4	3W1	A	503[B]	-	-	0/6/6/6	0/2/2/2
4	3W1	B	503[C]	-	-	1/6/6/6	0/2/2/2
5	EDO	B	504	-	-	0/1/1/1	-
4	3W1	A	503[A]	-	-	0/6/6/6	0/2/2/2
2	PLP	A	501	1	-	2/6/6/8	0/1/1/1
5	EDO	B	510	-	-	0/1/1/1	-
4	3W1	B	503[A]	-	-	0/6/6/6	0/2/2/2
5	EDO	B	509	-	-	0/1/1/1	-
5	EDO	B	508	-	-	1/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
3	EPE	B	502[B]	-	-	1/9/19/19	0/1/1/1
4	3W1	B	506	-	-	1/6/6/6	0/2/2/2
5	EDO	B	505	-	-	1/1/1/1	-
2	PLP	B	501	1	-	2/6/6/8	0/1/1/1
5	EDO	A	505	-	-	0/1/1/1	-
5	EDO	A	504	-	-	1/1/1/1	-
5	EDO	A	507	-	-	1/1/1/1	-
3	EPE	B	502[A]	-	-	0/9/19/19	0/1/1/1
3	EPE	A	502	-	-	1/9/19/19	0/1/1/1
5	EDO	B	507	-	-	0/1/1/1	-
4	3W1	A	503[C]	-	-	0/6/6/6	0/2/2/2
5	EDO	B	511	-	-	1/1/1/1	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503[A]	3W1	NAO-NAK	-9.87	1.17	1.36
4	A	503[B]	3W1	NAO-NAK	-7.74	1.21	1.36
2	B	501	PLP	C5-C4	7.32	1.48	1.40
2	A	501	PLP	C5-C4	7.29	1.48	1.40
4	B	506	3W1	CAJ-CAN	-7.07	1.38	1.51

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503[A]	3W1	CAJ-NAO-CAH	-7.56	117.77	128.65
4	B	503[C]	3W1	CAJ-NAO-CAH	-6.26	119.64	128.65
4	A	503[A]	3W1	CAJ-NAO-NAK	5.94	131.77	121.04
4	A	503[A]	3W1	CAH-CAL-CL1	-5.48	122.26	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503[C]	3W1	CAJ-NAO-NAK	4.74	129.61	121.04

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PLP	C4-C5-C5A-O4P
2	B	501	PLP	C6-C5-C5A-O4P
5	B	508	EDO	O1-C1-C2-O2
2	A	501	PLP	C6-C5-C5A-O4P
3	A	502	EPE	C8-C7-N4-C5

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503[B]	3W1	1	0
4	B	503[C]	3W1	1	0
5	B	510	EDO	2	0
4	B	503[A]	3W1	1	0
5	B	509	EDO	1	0
5	B	508	EDO	1	0
4	B	506	3W1	5	0
5	B	505	EDO	1	0
2	B	501	PLP	2	0
5	A	505	EDO	1	0
5	A	504	EDO	1	0
5	A	507	EDO	1	0
5	B	507	EDO	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, 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	429/457 (93%)	-0.41	5 (1%) 76 81	5, 14, 26, 49	30 (6%)
1	B	429/457 (93%)	-0.21	7 (1%) 70 75	6, 16, 29, 58	36 (8%)
All	All	858/914 (93%)	-0.31	12 (1%) 73 78	5, 15, 29, 58	66 (7%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307[A]	ALA	7.2
1	B	308[A]	GLY	5.7
1	A	436	LEU	4.1
1	B	436	LEU	3.0
1	A	435	SER	2.8

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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	511	4/4	0.65	0.23	49,51,56,61	0
4	3W1	A	503[B]	15/15	0.76	0.13	10,12,18,26	15
4	3W1	A	503[C]	15/15	0.76	0.13	10,12,15,25	15
4	3W1	B	506	15/15	0.76	0.15	40,43,58,91	0
4	3W1	A	503[A]	15/15	0.76	0.13	10,13,16,22	15
5	EDO	B	507	4/4	0.78	0.17	33,34,37,54	0
5	EDO	A	507	4/4	0.80	0.15	31,32,37,47	0
5	EDO	B	510	4/4	0.82	0.15	27,30,37,47	0
5	EDO	B	504	4/4	0.84	0.11	30,37,49,50	0
5	EDO	A	504	4/4	0.86	0.12	31,31,33,40	0
5	EDO	B	508	4/4	0.87	0.12	28,33,41,42	0
5	EDO	B	509	4/4	0.88	0.24	26,26,37,41	0
5	EDO	A	506	4/4	0.88	0.12	32,32,36,47	0
5	EDO	B	505	4/4	0.88	0.18	24,25,27,39	0
4	3W1	B	503[C]	15/15	0.91	0.08	12,13,20,36	15
4	3W1	B	503[A]	15/15	0.91	0.08	10,14,22,24	15
3	EPE	B	502[A]	15/15	0.93	0.10	14,19,28,32	15
3	EPE	B	502[B]	15/15	0.93	0.10	14,19,28,31	15
5	EDO	A	505	4/4	0.94	0.18	19,22,31,43	0
2	PLP	B	501	15/16	0.97	0.05	7,10,17,17	0
3	EPE	A	502	15/15	0.98	0.07	13,17,41,43	0
2	PLP	A	501	15/16	0.98	0.04	6,9,14,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.