



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 08:54 am BST

PDB ID : 1MLZ
Title : Crystal Structure of 7,8-Diaminopelargonic Acid Synthase in complex with the trans-isomer of amiclennomycin.
Authors : Sandmark, J.; Mann, S.; Marquet, A.; Schneider, G.
Deposited on : 2002-09-02
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

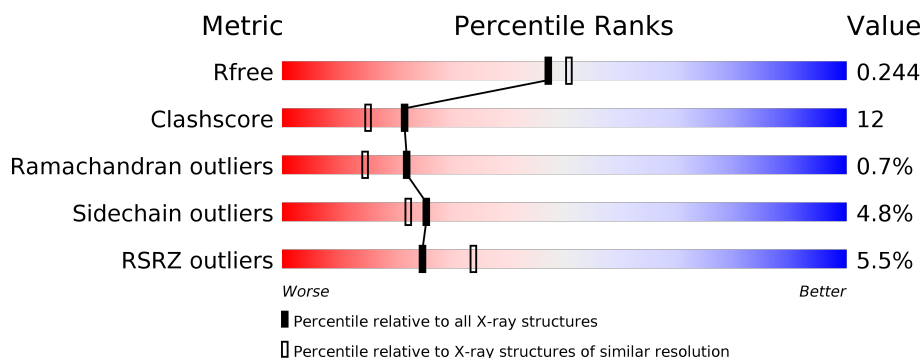
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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	429	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div></div> </div> </div>
1	B	429	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div></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
2	TZA	B	531	-	-	X	-
4	PLP	B	530	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7013 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.

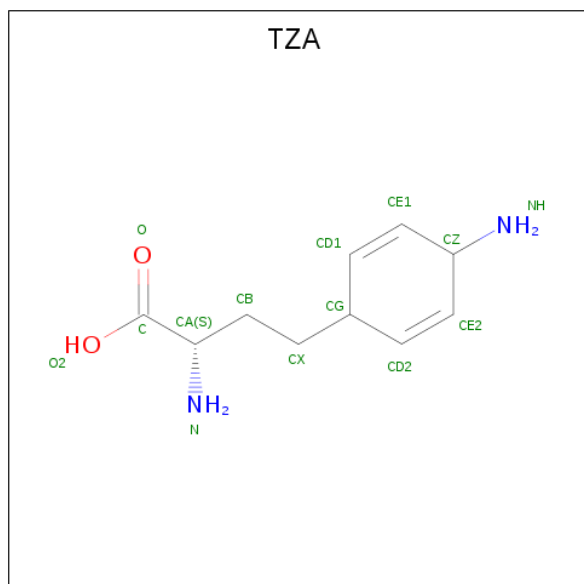
- Molecule 1 is a protein called 7,8-diamino-pelargonic acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	102	1	0
			3299	2093	576	598	32			
1	B	428	Total	C	N	O	S	96	5	0
			3330	2121	578	599	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	LEU	TRP	SEE REMARK 999	UNP P12995
B	14	LEU	TRP	SEE REMARK 999	UNP P12995

- Molecule 2 is TRANS-AMICLENOMYCIN (three-letter code: TZA) (formula: C₁₀H₁₆N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	10	2	2		

Continued on next page...

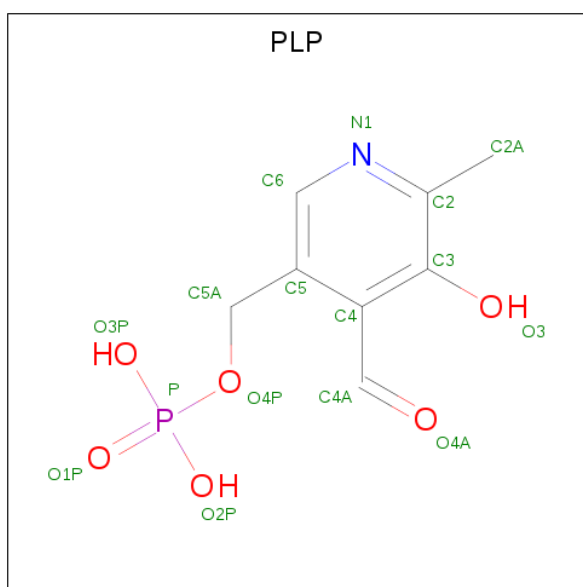
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	10	2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

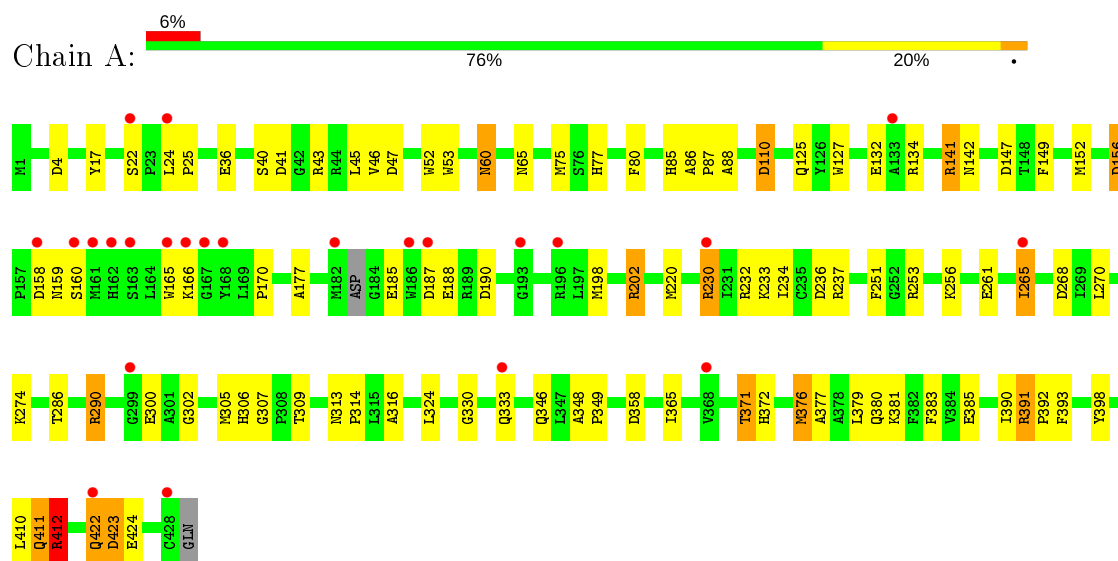
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	165	Total	O	0	0
			165	165		
5	B	159	Total	O	0	0
			159	159		

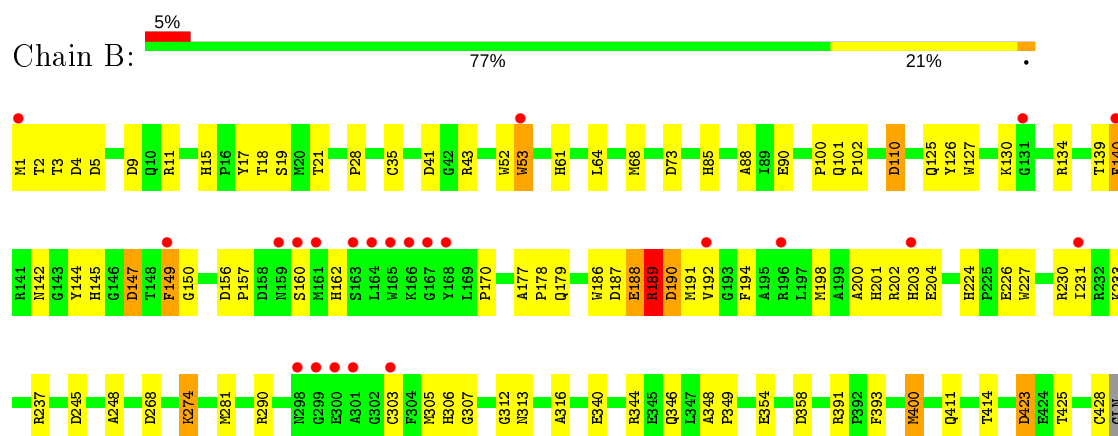
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: 7,8-diamino-pelargonic acid aminotransferase



- Molecule 1: 7,8-diamino-pelargonic acid aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.03Å 55.96Å 116.00Å 90.00° 109.65° 90.00°	Depositor
Resolution (Å)	22.36 – 2.15 19.92 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.5 (22.36-2.15) 98.5 (19.92-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.205 , 0.240 0.211 , 0.244	Depositor DCC
R_{free} test set	2107 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7013	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2364e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TZA, NA, 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	0.75	6/3380 (0.2%)	1.08	20/4586 (0.4%)
1	B	0.99	13/3432 (0.4%)	0.98	21/4658 (0.5%)
All	All	0.88	19/6812 (0.3%)	1.03	41/9244 (0.4%)

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	A	0	2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53[A]	TRP	CG-CD1	25.09	1.71	1.36
1	B	53[B]	TRP	CG-CD1	25.09	1.71	1.36
1	A	385	GLU	CG-CD	13.91	1.72	1.51
1	B	90	GLU	CG-CD	10.75	1.68	1.51
1	A	423	ASP	C-N	7.25	1.50	1.34

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	ASP	O-C-N	-28.26	77.49	122.70
1	A	422	GLN	O-C-N	21.57	157.22	122.70
1	B	53[A]	TRP	CD1-CG-CD2	17.27	120.11	106.30
1	B	53[B]	TRP	CD1-CG-CD2	17.27	120.11	106.30
1	A	422	GLN	CA-C-N	-15.50	83.11	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	422	GLN	Peptide
1	A	423	ASP	Mainchain

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	3299	0	3263	63	2
1	B	3330	0	3278	93	1
2	A	14	0	11	2	0
2	B	14	0	13	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	15	0	6	1	0
4	B	15	0	6	8	0
5	A	165	0	0	1	2
5	B	159	0	0	4	1
All	All	7013	0	6577	153	4

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 12.

The worst 5 of 153 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:188:GLU:OE2	1:A:230:ARG:NH2	1.81	1.13
1:B:53[A]:TRP:CE2	1:B:400:MET:HE1	1.84	1.13
1:B:53[A]:TRP:CD2	1:B:400:MET:CE	2.41	1.04
1:B:274:LYS:HZ3	4:B:530:PLP:C4A	1.76	0.98
1:B:423:ASP:OD1	1:B:425:THR:OG1	1.85	0.94

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LYS:NZ	5:A:3018:HOH:O[2_656]	0.62	1.58
1:B:21:THR:O	1:B:21:THR:O[2_655]	1.48	0.72
5:B:4038:HOH:O	5:B:4038:HOH:O[2_655]	1.83	0.37
1:A:381:LYS:CE	5:A:3018:HOH:O[2_656]	2.08	0.12

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	424/429 (99%)	406 (96%)	14 (3%)	4 (1%)	17	11
1	B	431/429 (100%)	412 (96%)	17 (4%)	2 (0%)	29	22
All	All	855/858 (100%)	818 (96%)	31 (4%)	6 (1%)	22	15

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	GLU
1	A	274	LYS
1	B	274	LYS
1	A	75	MET
1	A	307	GLY

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	344/345 (100%)	324 (94%)	20 (6%)	20	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	348/345 (101%)	334 (96%)	14 (4%)	31	29
All	All	692/690 (100%)	658 (95%)	34 (5%)	25	21

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	MET
1	A	412	ARG
1	B	303	CYS
1	A	410	LEU
1	A	166	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	GLN
1	B	142	ASN
1	B	342	GLN
1	A	335	GLN
1	B	335	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	TZA	B	531	-	9,14,14	6.45	6 (66%)	5,18,18	2.78	4 (80%)
4	PLP	A	430	2	15,15,16	3.36	4 (26%)	20,22,23	1.70	4 (20%)
4	PLP	B	530	-	15,15,16	3.41	4 (26%)	20,22,23	1.63	3 (15%)
2	TZA	A	431	4	9,14,14	6.31	7 (77%)	5,18,18	2.97	4 (80%)

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	TZA	B	531	-	-	1/5/19/19	0/1/1/1
4	PLP	A	430	2	-	0/6/6/8	0/1/1/1
4	PLP	B	530	-	-	1/6/6/8	0/1/1/1
2	TZA	A	431	4	-	2/5/19/19	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	431	TZA	CZ-CE2	-12.35	1.38	1.50
2	B	531	TZA	CZ-CE1	-12.18	1.38	1.50
2	B	531	TZA	CZ-CE2	-11.23	1.39	1.50
2	A	431	TZA	CZ-CE1	-11.02	1.40	1.50
4	A	430	PLP	C3-C2	8.98	1.49	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	431	TZA	CE1-CZ-NH	4.36	123.28	111.21
4	B	530	PLP	C3-C4-C5	-3.73	114.71	118.74
4	A	430	PLP	C6-C5-C4	3.69	121.07	118.16
2	B	531	TZA	CE1-CZ-CE2	3.63	120.80	110.79
4	A	430	PLP	O3P-P-O2P	3.37	120.52	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	431	TZA	C-CA-CB-CX
4	B	530	PLP	C5A-O4P-P-O1P
2	B	531	TZA	CD2-CG-CX-CB
2	A	431	TZA	CD2-CG-CX-CB

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	531	TZA	7	0
4	A	430	PLP	1	0
4	B	530	PLP	8	0
2	A	431	TZA	2	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	423/429 (98%)	0.26	24 (5%)	23 32	20, 33, 54, 70	20 (4%)
1	B	425/429 (99%)	0.30	23 (5%)	25 34	18, 34, 56, 62	22 (5%)
All	All	848/858 (98%)	0.28	47 (5%)	25 34	18, 33, 55, 70	42 (4%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	ALA	6.9
1	A	166	LYS	5.0
1	A	162	HIS	4.8
1	A	163	SER	4.2
1	B	53[A]	TRP	4.2

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, 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(\AA^2)	Q<0.9
2	TZA	B	531	14/14	0.78	0.24	59,60,63,64	0
2	TZA	A	431	14/14	0.86	0.18	34,43,48,49	0
3	NA	A	501	1/1	0.90	0.16	20,20,20,20	0
3	NA	B	502	1/1	0.96	0.27	21,21,21,21	0
4	PLP	A	430	15/16	0.96	0.09	22,24,29,30	0
4	PLP	B	530	15/16	0.97	0.08	22,25,27,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.