



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 08:33 pm GMT

PDB ID : 1K8Z
Title : CRYSTAL STRUCTURE OF THE TRYPTOPHAN SYNTHASE BETA-SER178PRO MUTANT COMPLEXED WITH N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID
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Deposited on : 2001-10-26
Resolution : 1.70 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

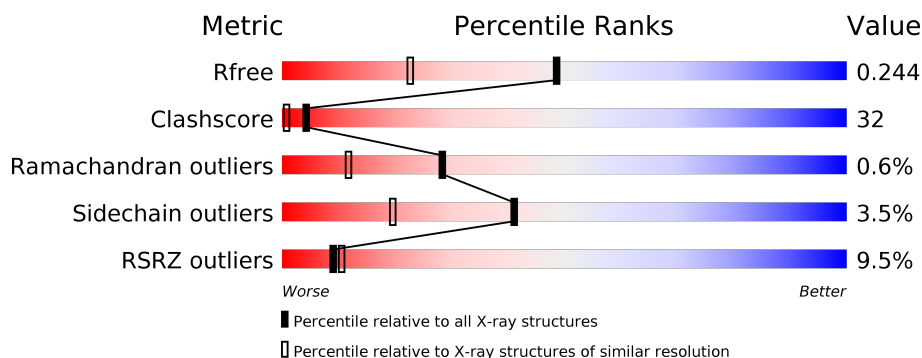
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	268	
2	B	396	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5352 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 TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	2	0
			1955	1248	334	365	8			

- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	1	0
			2987	1877	527	564	19			

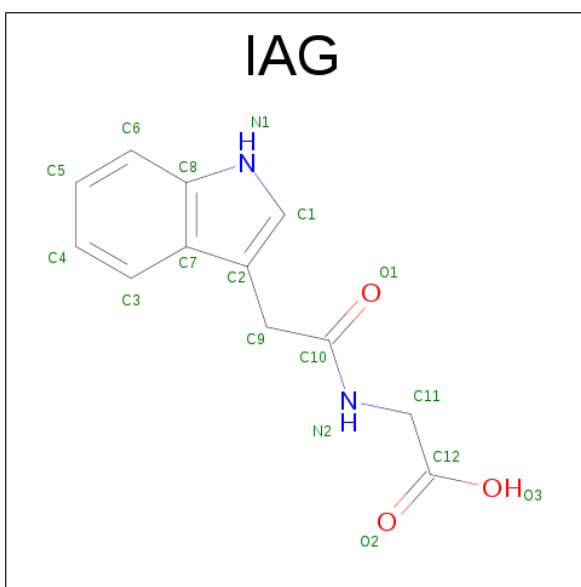
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	SER	ARG	CLONING ARTIFACT	UNP P0A2K1
B	178	PRO	SER	ENGINEERED	UNP P0A2K1

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

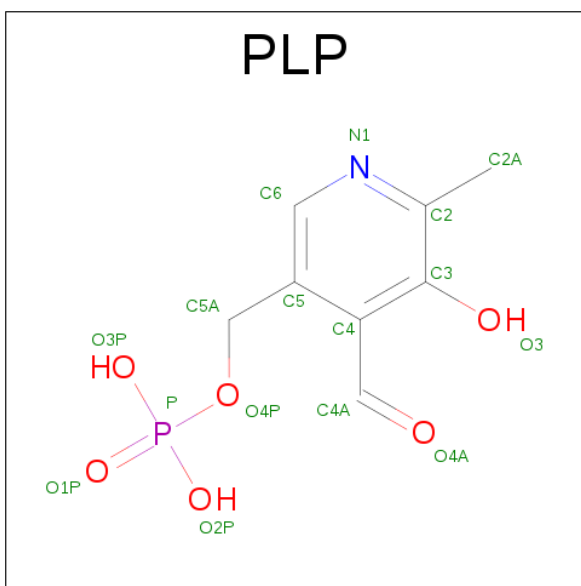
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID (three-letter code: IAG) (formula: C₁₂H₁₂N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	12	2	3		

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



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

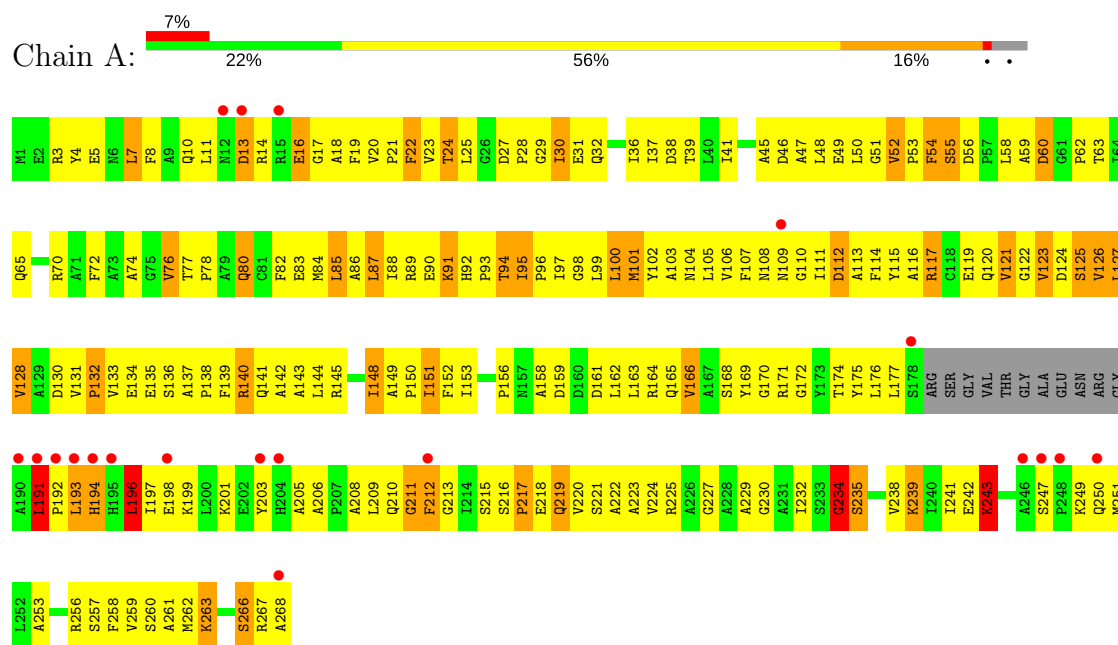
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	129	Total 129	O 129	0	0
6	B	248	Total 248	O 248	0	0

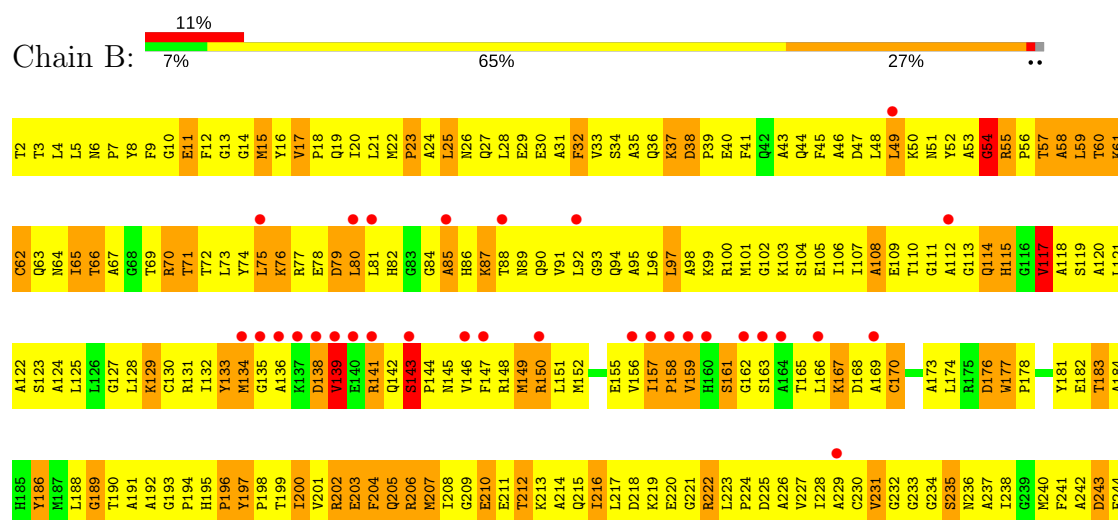
3 Residue-property plots

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: TRYPTOPHAN SYNTHASE ALPHA CHAIN



• Molecule 2: TRYPTOPHAN SYNTHASE BETA CHAIN



I245	D305	Q365
N246	F306	P366
D247	P307	E367
T248	S308	K368
S249	V309	E369
V250	G310	Q370
G251	P311	L371
L252	Q312	L372
I253	H313	V373
G254	A314	V374
V255	Y315	N375
E256	L316	L376
P257	N317	S377
G258	S318	G378
G259	I319	R379
H260	G320	G380
G261	R321	D381
I262	A322	K382
E263	D323	D383
T264	Y324	I384
G265	V325	F385
E266	S326	T386
H267	I327	V387
G268	T328	H388
A269	D329	D389
P270	D330	I390
L271	E331	L391
K272	A332	K392
H273	L333	A393
G274	E334	R394
R275	A335	G395
V276	F336	GLU
G277	K337	ILE
	T338	
I278	L339	
Y279	C340	
F280	R341	
G281	H342	
M282	E343	
K283	G344	
A284	I345	
P285	T346	
M286	P347	
M287	A348	
Q288	L349	
T289	E350	
A290	S351	
D291	S352	
G292	H353	
Q293	A354	
I294	L355	
E295	A356	
E296	H357	
Y298	A358	
S299	I359	
I300	K360	
S301	H361	
A302	M362	
G303	R363	
L304	E364	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.42Å 61.03Å 67.53Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 43.36 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-1.70) 96.4 (43.36-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.265 0.198 , 0.244	Depositor DCC
R_{free} test set	4065 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.4	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	0.96	EDS
Total number of atoms	5352	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: NA, IAG, 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	3.32	245/2004 (12.2%)	2.86	199/2722 (7.3%)
2	B	4.35	703/3052 (23.0%)	4.01	646/4123 (15.7%)
All	All	3.97	948/5056 (18.8%)	3.60	845/6845 (12.3%)

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	1
2	B	0	1
All	All	0	2

The worst 5 of 948 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	TYR	CE2-CZ	24.33	1.70	1.38
2	B	30	GLU	CD-OE2	20.54	1.48	1.25
2	B	8	TYR	CE1-CZ	19.55	1.64	1.38
2	B	291	ASP	CB-CG	-17.49	1.15	1.51
2	B	16	TYR	CE2-CZ	16.98	1.60	1.38

The worst 5 of 845 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	ARG	NE-CZ-NH1	35.94	138.27	120.30
2	B	291	ASP	CB-CG-OD1	-34.65	87.12	118.30
2	B	55	ARG	NE-CZ-NH2	-29.76	105.42	120.30
1	A	140	ARG	NE-CZ-NH1	-28.07	106.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	222	ARG	NE-CZ-NH2	-26.74	106.93	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	ARG	Peptide
2	B	54	GLY	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	1955	0	1959	85	0
2	B	2987	0	2961	236	0
3	B	1	0	0	0	0
4	A	17	0	11	1	0
5	B	15	0	7	1	0
6	A	129	0	0	3	0
6	B	248	0	0	2	0
All	All	5352	0	4938	319	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 32.

The worst 5 of 319 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)
2:B:235:SER:CA	2:B:235:SER:CB	1.74	1.64
2:B:278:ILE:CD1	2:B:278:ILE:CG1	1.74	1.64
2:B:129:LYS:CG	2:B:129:LYS:CD	1.75	1.63
1:A:52:VAL:CB	1:A:52:VAL:CG1	1.75	1.63
2:B:71:THR:CG2	2:B:71:THR:CB	1.77	1.63

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	255/268 (95%)	250 (98%)	3 (1%)	2 (1%)	22	7
2	B	393/396 (99%)	371 (94%)	20 (5%)	2 (0%)	32	15
All	All	648/664 (98%)	621 (96%)	23 (4%)	4 (1%)	28	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	LEU
1	A	234	GLY
2	B	117	VAL
2	B	139	VAL

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	203/208 (98%)	195 (96%)	8 (4%)	37	15
2	B	309/310 (100%)	299 (97%)	10 (3%)	44	22
All	All	512/518 (99%)	494 (96%)	18 (4%)	41	19

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	65	ILE
2	B	141	ARG

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Mol	Chain	Res	Type
2	B	216	ILE
1	A	243	LYS
1	A	247	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	219	GLN
2	B	246	ASN

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
4	IAG	A	501	-	14,18,18	1.79	4 (28%)	14,24,24	3.30	7 (50%)
5	PLP	B	502	2	15,15,16	3.78	9 (60%)	20,22,23	2.88	5 (25%)

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	IAG	A	501	-	-	0/7/9/9	0/2/2/2
5	PLP	B	502	2	-	0/6/6/8	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	PLP	C3-C2	-7.99	1.35	1.40
5	B	502	PLP	P-O4P	-6.76	1.38	1.60
5	B	502	PLP	P-O3P	-4.05	1.38	1.54
4	A	501	IAG	C3-C7	-3.41	1.35	1.42
4	A	501	IAG	C9-C2	-2.46	1.45	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	IAG	C11-N2-C10	-8.59	108.22	122.35
5	B	502	PLP	C4A-C4-C5	-4.31	116.50	120.86
4	A	501	IAG	C4-C5-C6	-3.92	114.86	120.45
5	B	502	PLP	O4P-P-O1P	-3.52	96.60	106.47
4	A	501	IAG	C9-C10-N2	-3.49	111.29	116.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	IAG	1	0
5	B	502	PLP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	257/268 (95%)	0.51	20 (7%) 14 17	13, 26, 48, 78	0
2	B	394/396 (99%)	0.66	42 (10%) 7 8	11, 19, 42, 73	0
All	All	651/664 (98%)	0.60	62 (9%) 9 10	11, 22, 44, 78	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	ALA	7.2
2	B	159	VAL	6.9
1	A	190	ALA	6.4
2	B	385	PHE	6.3
1	A	191	LEU	5.8

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	IAG	A	501	17/17	0.84	0.15	1.17	22,35,50,52	0
5	PLP	B	502	15/16	0.98	0.12	-0.81	15,18,28,30	0
3	NA	B	503	1/1	0.99	0.09	-1.81	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.