



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:55 PM UTC

PDB ID : 1K8Z / pdb_00001k8z
Title : CRYSTAL STRUCTURE OF THE TRYPTOPHAN SYNTHASE BETA-SER178PRO MUTANT COMPLEXED WITH N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID
Authors : Weyand, M.; Schlichting, I.; Marabotti, A.; Mozzarelli, A.
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

<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

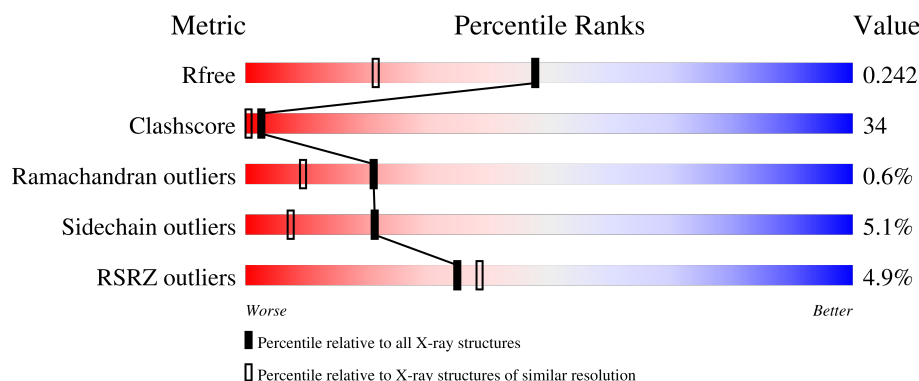
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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	268	4% 9% 67% 18% • •
2	B	396	6% • 65% 29% • •

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	IAG	A	501	-	X	-	-
5	PLP	B	502	-	X	-	-

2 Entry composition [i](#)

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			

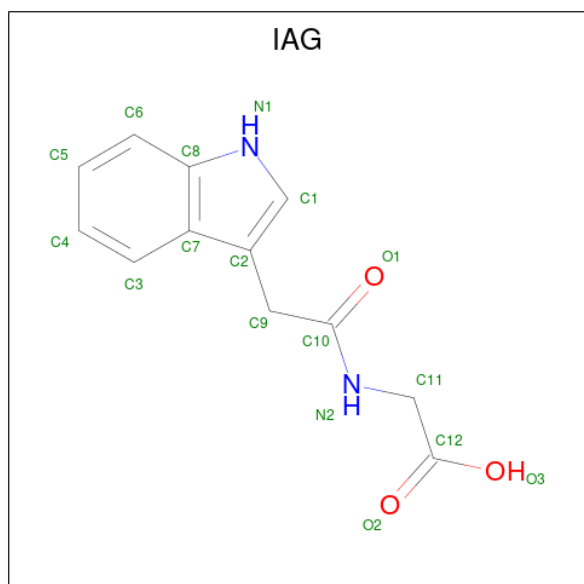
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

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 mutation	UNP P0A2K1

- Molecule 3 is N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID (CCD ID: IAG) (formula: $C_{12}H_{12}N_2O_3$).

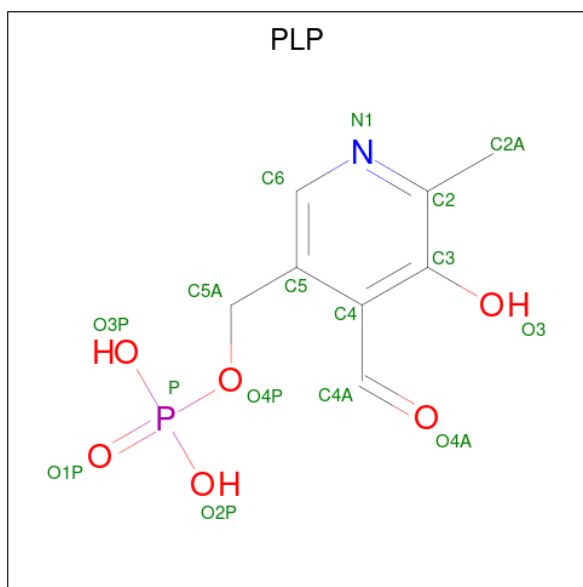


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	12	2	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

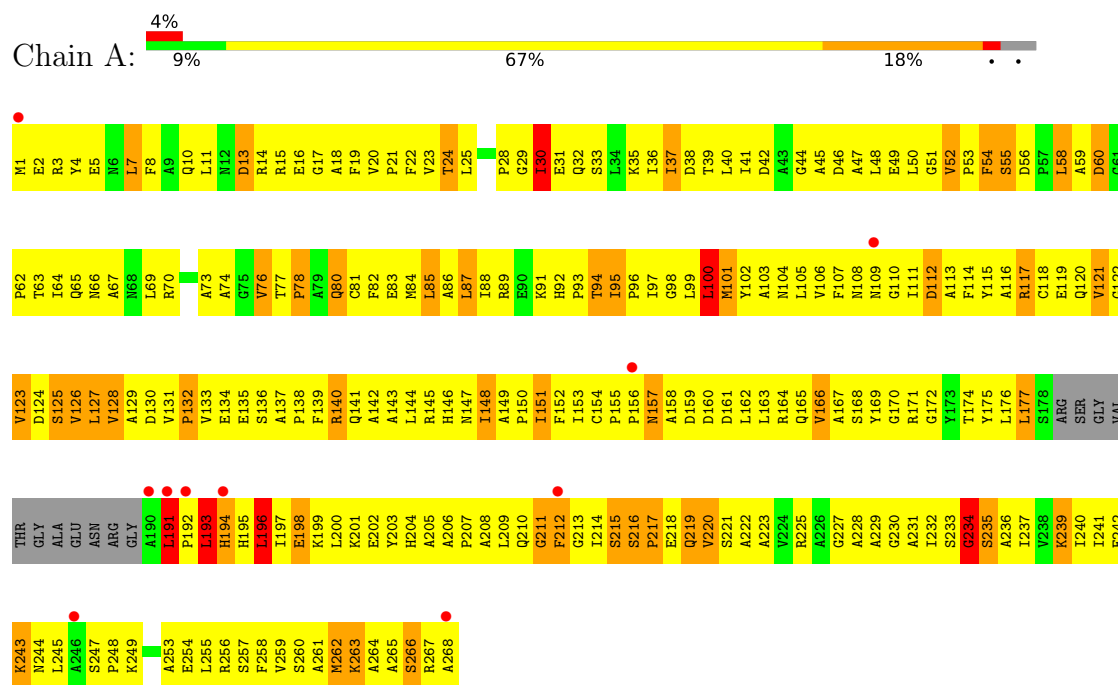
- Molecule 6 is water.

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

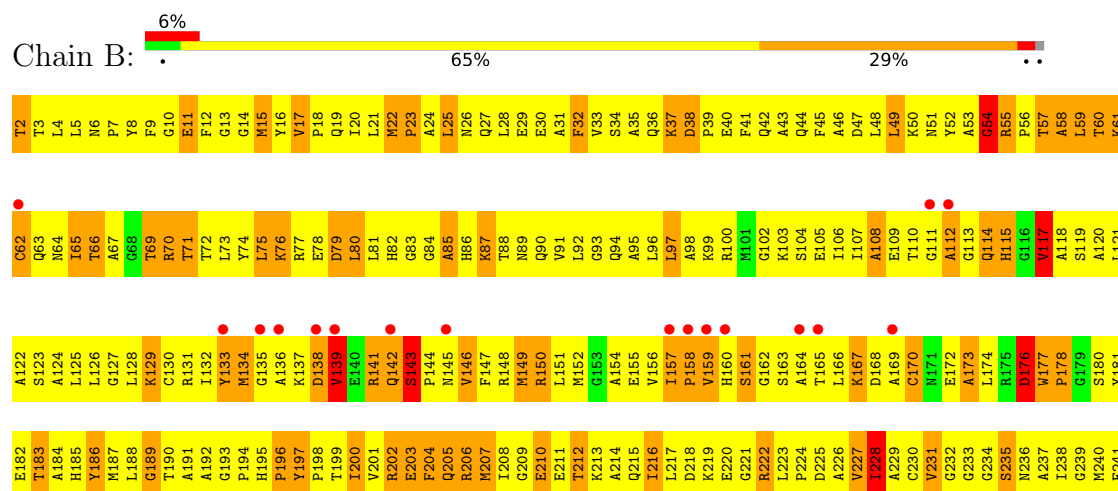
3 Residue-property plots

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: TRYPTOPHAN SYNTHASE ALPHA CHAIN



• Molecule 2: TRYPTOPHAN SYNTHASE BETA CHAIN



A242	A302	K362
D243	G303	R363
F244	I304	E364
I245	D305	Q365
N246	F306	P366
D247	P307	E367
T248	S308	K368
S249	V309	E369
V250	G310	Q370
G251	F311	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	Y325	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
I278	T338	
Y279	L339	
F280	C340	
G281	R341	
M282	H342	
K283	E343	
A284	G344	
P285	I345	
M286	I346	
M287	P347	
Q288	A348	
T289	L349	
A290	E350	
D291	S351	
G292	S352	
Q293	H353	
I294	A354	
E295	L355	
E296	A356	
S297	H357	
Y298	A358	
S299	L359	
I300	K360	
S301	M361	

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 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-1.70) 96.3 (20.00-1.70)	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	CNS, REFMAC	Depositor
R, R_{free}	0.209 , 0.265 0.200 , 0.242	Depositor DCC
R_{free} test set	4065 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.9	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	0.95	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 [i](#)

5.1 Standard geometry [i](#)

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	4.41	408/2004 (20.4%)	3.42	359/2722 (13.2%)
2	B	5.82	1056/3052 (34.6%)	4.73	1017/4123 (24.7%)
All	All	5.31	1464/5056 (29.0%)	4.26	1376/6845 (20.1%)

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 1464 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	THR	CA-CB	-24.91	1.19	1.53
1	A	52	VAL	CA-C	23.08	1.73	1.52
2	B	70	ARG	CA-C	22.13	1.81	1.53
2	B	361	MET	SD-CE	-21.34	1.26	1.79
2	B	61	LYS	N-CA	21.27	1.72	1.46

The worst 5 of 1376 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	254	GLY	O-C-N	-23.61	105.43	123.61
2	B	375	ASN	CA-C-O	20.99	143.04	120.58
2	B	368	LYS	O-C-N	20.15	148.35	122.96
2	B	328	THR	O-C-N	20.00	145.34	122.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	353	HIS	O-C-N	-19.79	99.59	122.15

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	1961	89	0
2	B	2987	0	2964	252	0
3	A	17	0	11	1	0
4	B	1	0	0	0	0
5	B	15	0	7	1	0
6	A	129	0	0	2	0
6	B	248	0	0	2	0
All	All	5352	0	4943	339	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 34.

The worst 5 of 339 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:CG1	2:B:278:ILE:CD1	1.74	1.64
2:B:129:LYS:CD	2:B:129:LYS:CG	1.75	1.63
1:A:52:VAL:CB	1:A:52:VAL:CG1	1.75	1.63
1:A:126:VAL:CB	1:A:126:VAL:CG1	1.75	1.63

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	16	5
2	B	393/396 (99%)	371 (94%)	20 (5%)	2 (0%)	24	12
All	All	648/664 (98%)	621 (96%)	23 (4%)	4 (1%)	21	9

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

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%)	192 (95%)	11 (5%)	20	6
2	B	309/310 (100%)	294 (95%)	15 (5%)	22	8
All	All	512/518 (99%)	486 (95%)	26 (5%)	21	7

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	141	ARG
2	B	176	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	390	ILE
2	B	161	SER
2	B	207	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	A	219	GLN
2	B	246	ASN
1	A	109	ASN
1	A	10	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 oligosaccharides 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	$\# Z > 2$
3	IAG	A	501	-	18,18,18	2.63	9 (50%)	24,24,24	6.69	14 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PLP	B	502	2	15,15,16	3.71	12 (80%)	21,22,23	2.93	6 (28%)

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
3	IAG	A	501	-	-	2/9/9/9	0/2/2/2
5	PLP	B	502	2	-	0/6/6/8	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)
5	B	502	PLP	P-O4P	-6.92	1.38	1.60
5	B	502	PLP	C2A-C2	6.04	1.59	1.50
3	A	501	IAG	C7-C2	-5.66	1.34	1.44
5	B	502	PLP	C3-C2	-5.57	1.35	1.41
5	B	502	PLP	P-O3P	-4.47	1.38	1.54

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	IAG	C8-N1-C1	18.16	125.24	109.08
3	A	501	IAG	C2-C1-N1	-15.45	93.35	110.31
3	A	501	IAG	C7-C8-N1	-11.99	97.53	107.52
3	A	501	IAG	C7-C2-C1	9.54	115.92	106.16
3	A	501	IAG	C6-C8-N1	9.16	145.41	130.74

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	IAG	N2-C10-C9-C2
3	A	501	IAG	O1-C10-C9-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	6
1	A	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	65:ILE	C	66:THR	N	1.19
1	B	321:ARG	C	322:ALA	N	1.19
1	B	332:ALA	C	333:LEU	N	1.19
1	B	343:GLU	C	344:GLY	N	1.19
1	B	362:MET	C	363:ARG	N	1.19

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%)	0.26	10 (3%)	43 47	13, 26, 48, 78	2 (0%)
2	B	394/396 (99%)	0.15	22 (5%)	30 33	11, 19, 42, 73	1 (0%)
All	All	651/664 (98%)	0.19	32 (4%)	35 38	11, 22, 44, 78	3 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	159	VAL	6.5
1	A	268	ALA	5.5
2	B	395	GLY	4.7
1	A	190	ALA	4.2
2	B	385	PHE	3.9

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
3	IAG	A	501	17/17	0.84	0.10	22,35,50,52	0
5	PLP	B	502	15/16	0.98	0.06	15,18,28,30	0
4	NA	B	503	1/1	0.99	0.06	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.