



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:00 am GMT

PDB ID : 3TAT  
Title : TYROSINE AMINOTRANSFERASE FROM E. COLI  
Authors : Ko, T.P.; Yang, W.Z.; Wu, S.P.; Tsai, H.; Yuan, H.S.  
Deposited on : 1998-08-12  
Resolution : 3.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

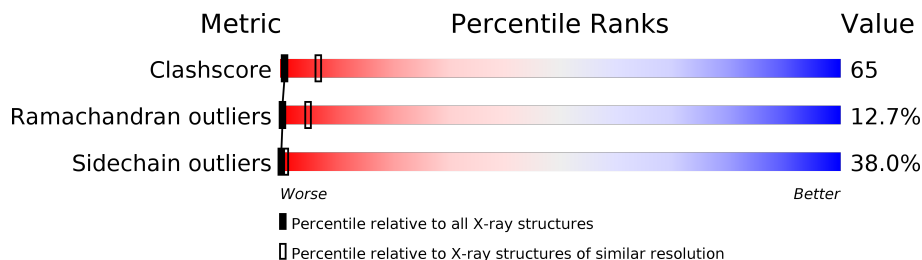
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	397	
1	B	397	
1	C	397	
1	D	397	
1	E	397	
1	F	397	

## 2 Entry composition [i](#)

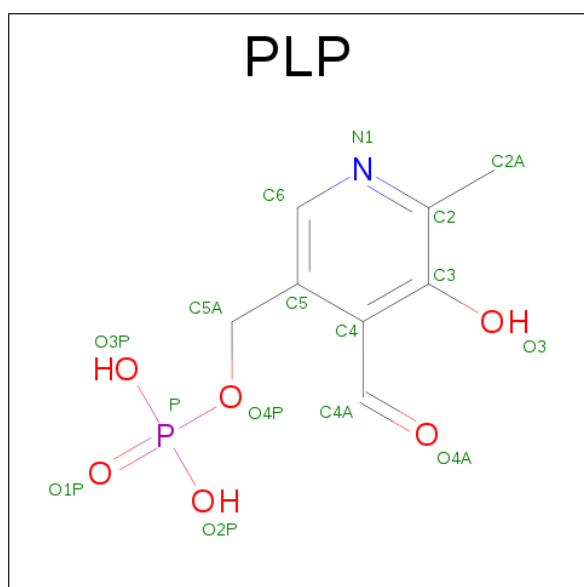
There are 2 unique types of molecules in this entry. The entry contains 18480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TYROSINE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3065	1950	528	571	16			
1	B	397	Total	C	N	O	S	0	0	0
			3065	1950	528	571	16			
1	C	397	Total	C	N	O	S	0	0	0
			3065	1950	528	571	16			
1	D	397	Total	C	N	O	S	0	0	0
			3065	1950	528	571	16			
1	E	397	Total	C	N	O	S	0	0	0
			3065	1950	528	571	16			
1	F	397	Total	C	N	O	S	0	0	0
			3065	1950	528	571	16			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



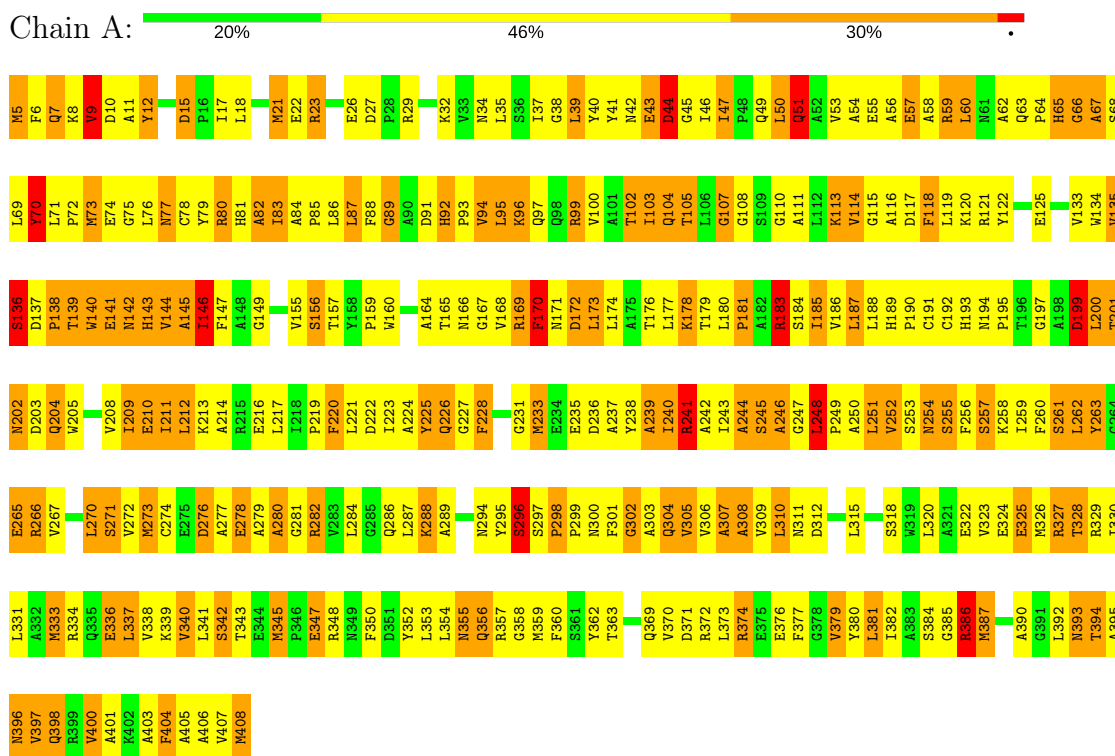
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

### 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.

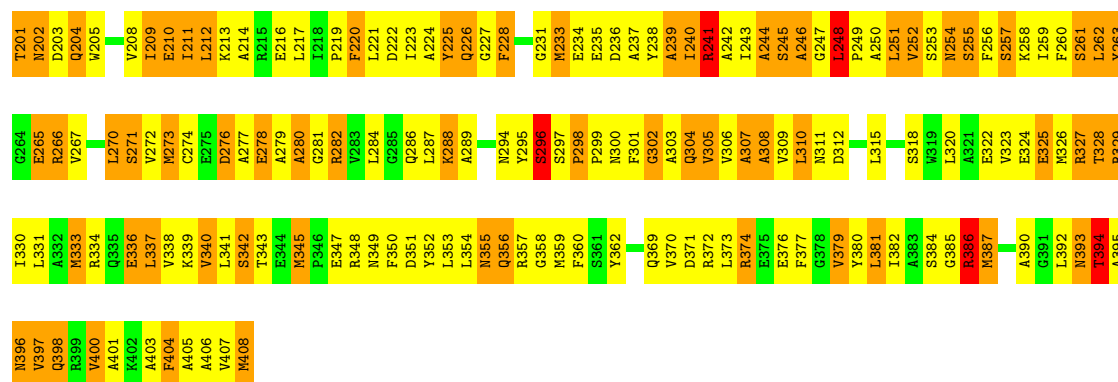
Note EDS was not executed.

#### • Molecule 1: TYROSINE AMINOTRANSFERASE



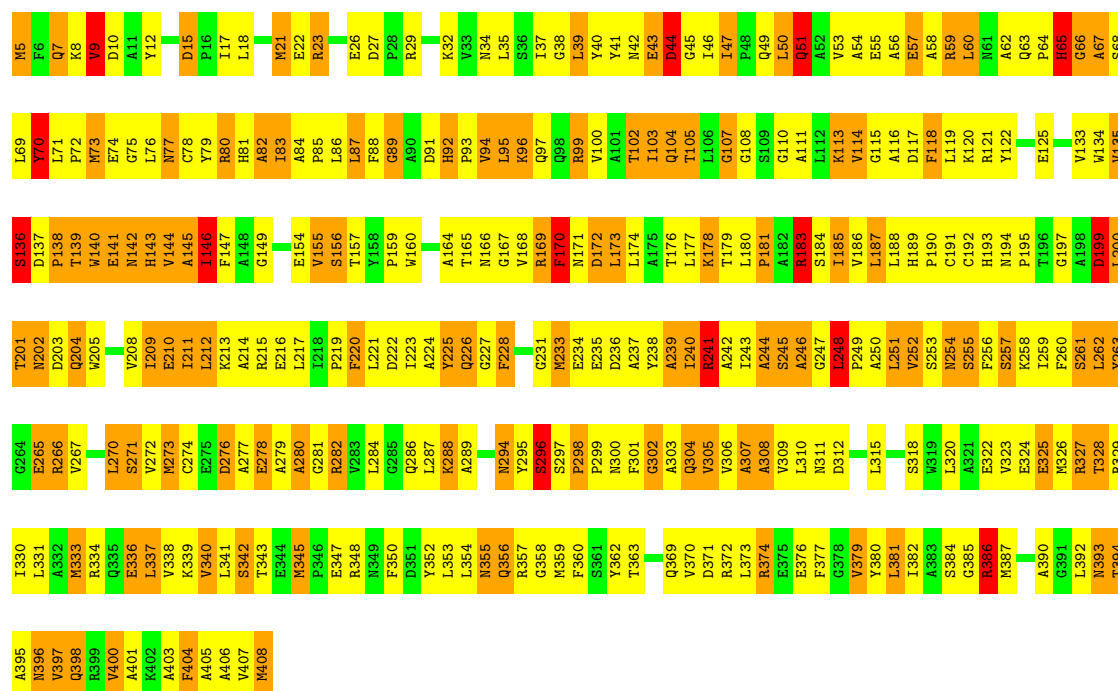
#### • Molecule 1: TYROSINE AMINOTRANSFERASE





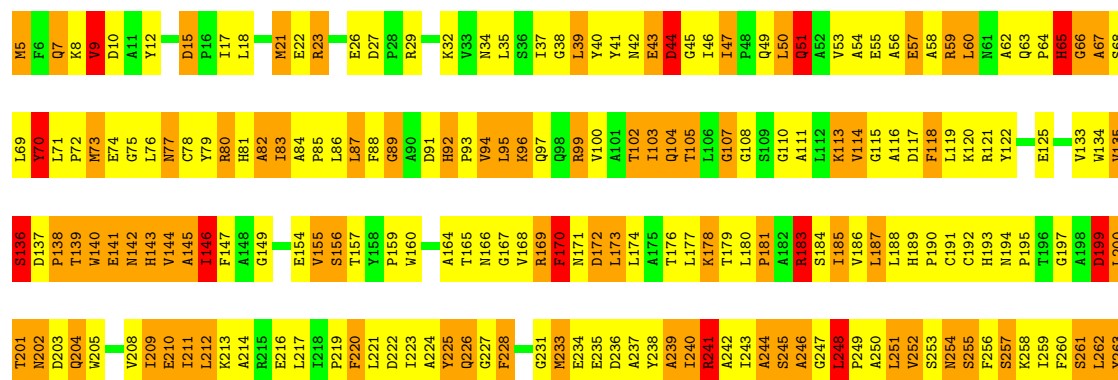
## • Molecule 1: TYROSINE AMINOTRANSFERASE

Chain C: 20% 47% 29%



## • Molecule 1: TYROSINE AMINOTRANSFERASE

Chain D: 21% 46% 30%





I330	A395
I331	N396
A332	V397
N333	Q398
R334	R399
Q335	V400
E336	A401
L337	K402
V338	A403
K339	F404
V340	A405
L341	A406
S342	V407
T343	M408
E344	
N345	
P346	
E347	
R348	
R349	
F350	
D351	
Y352	
L353	
L354	
N355	
Q356	
R357	
G358	
N359	
F360	
S361	
Y362	
T363	
Q369	
V370	
D371	
R372	
L373	
R374	
E375	
E376	
F377	
G378	
V379	
Y380	
L381	
L382	
A383	
S384	
G385	
R386	
N387	
A390	
G391	
L392	
N393	
T394	



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.58Å 126.58Å 156.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.50	Depositor
% Data completeness (in resolution range)	88.5 (30.00-3.50)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.213 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

## 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: 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	0.38	0/3130	0.59	0/4248
1	B	0.38	0/3130	0.59	0/4248
1	C	0.38	0/3130	0.59	0/4248
1	D	0.38	0/3130	0.59	0/4248
1	E	0.38	0/3130	0.59	0/4248
1	F	0.38	0/3130	0.59	0/4248
All	All	0.38	0/18780	0.59	0/25488

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 [i](#)

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	3065	0	3034	408	0
1	B	3065	0	3034	407	9
1	C	3065	0	3034	410	1
1	D	3065	0	3034	405	0
1	E	3065	0	3034	414	8
1	F	3065	0	3034	413	0
2	A	15	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	7	1	0
2	C	15	0	7	1	0
2	D	15	0	7	1	0
2	E	15	0	7	1	0
2	F	15	0	7	1	0
All	All	18480	0	18246	2397	9

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 65.

The worst 5 of 2397 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:C:274:CYS:SG	1:D:5:MET:HE1	1.90	1.10
1:D:248:LEU:HB3	1:D:249:PRO:HD3	1.40	1.02
1:C:248:LEU:HB3	1:C:249:PRO:HD3	1.40	1.02
1:B:248:LEU:HB3	1:B:249:PRO:HD3	1.40	1.02
1:E:248:LEU:HB3	1:E:249:PRO:HD3	1.40	1.01

The worst 5 of 9 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:B:349:ASN:CG	1:E:216:GLU:OE1[1_545]	0.69	1.51
1:B:349:ASN:OD1	1:E:216:GLU:OE1[1_545]	0.87	1.33
1:B:349:ASN:OD1	1:E:216:GLU:CD[1_545]	1.22	0.98
1:B:394:THR:CG2	1:C:215:ARG:NH1[1_445]	1.65	0.55
1:B:349:ASN:CG	1:E:216:GLU:CD[1_545]	1.75	0.45

## 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	395/397 (100%)	254 (64%)	91 (23%)	50 (13%)	0	5
1	B	395/397 (100%)	254 (64%)	91 (23%)	50 (13%)	0	5
1	C	395/397 (100%)	254 (64%)	91 (23%)	50 (13%)	0	5
1	D	395/397 (100%)	254 (64%)	91 (23%)	50 (13%)	0	5
1	E	395/397 (100%)	254 (64%)	91 (23%)	50 (13%)	0	5
1	F	395/397 (100%)	254 (64%)	91 (23%)	50 (13%)	0	5
All	All	2370/2382 (100%)	1524 (64%)	546 (23%)	300 (13%)	0	5

5 of 300 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	70	TYR
1	A	141	GLU
1	A	145	ALA
1	A	170	PHE

### 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	316/316 (100%)	196 (62%)	120 (38%)	0	1
1	B	316/316 (100%)	196 (62%)	120 (38%)	0	1
1	C	316/316 (100%)	196 (62%)	120 (38%)	0	1
1	D	316/316 (100%)	196 (62%)	120 (38%)	0	1
1	E	316/316 (100%)	196 (62%)	120 (38%)	0	1
1	F	316/316 (100%)	196 (62%)	120 (38%)	0	1
All	All	1896/1896 (100%)	1176 (62%)	720 (38%)	0	1

5 of 720 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	284	LEU

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Mol	Chain	Res	Type
1	D	156	SER
1	F	228	PHE
1	C	329	ARG
1	D	12	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	254	ASN
1	D	104	GLN
1	F	194	ASN
1	C	311	ASN
1	D	7	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](#)

6 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
2	PLP	A	500	1	15,15,16	2.25	3 (20%)	20,22,23	2.25	4 (20%)
2	PLP	B	500	1	15,15,16	2.24	3 (20%)	20,22,23	2.25	4 (20%)
2	PLP	C	500	1	15,15,16	2.25	3 (20%)	20,22,23	2.26	4 (20%)
2	PLP	D	500	1	15,15,16	2.27	3 (20%)	20,22,23	2.27	4 (20%)
2	PLP	E	500	1	15,15,16	2.25	3 (20%)	20,22,23	2.26	4 (20%)
2	PLP	F	500	1	15,15,16	2.26	3 (20%)	20,22,23	2.25	4 (20%)

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	PLP	A	500	1	-	0/6/6/8	0/1/1/1
2	PLP	B	500	1	-	0/6/6/8	0/1/1/1
2	PLP	C	500	1	-	0/6/6/8	0/1/1/1
2	PLP	D	500	1	-	0/6/6/8	0/1/1/1
2	PLP	E	500	1	-	0/6/6/8	0/1/1/1
2	PLP	F	500	1	-	0/6/6/8	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	PLP	C3-C2	-3.92	1.38	1.40
2	D	500	PLP	C3-C2	-3.90	1.38	1.40
2	E	500	PLP	C3-C2	-3.87	1.38	1.40
2	A	500	PLP	C3-C2	-3.85	1.38	1.40
2	B	500	PLP	C3-C2	-3.84	1.38	1.40

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	PLP	C5A-C5-C6	-3.48	113.35	119.33
2	E	500	PLP	C5A-C5-C6	-3.47	113.36	119.33
2	A	500	PLP	C5A-C5-C6	-3.46	113.39	119.33
2	B	500	PLP	C5A-C5-C6	-3.46	113.39	119.33
2	C	500	PLP	C5A-C5-C6	-3.45	113.39	119.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	PLP	1	0
2	B	500	PLP	1	0
2	C	500	PLP	1	0
2	D	500	PLP	1	0
2	E	500	PLP	1	0
2	F	500	PLP	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.