



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2023 – 09:35 AM EDT

PDB ID : 2Z1Y  
Title : Crystal structure of LysN, alpha-aminoacidase aminotransferase (complexed with N-(5'-phosphopyridoxyl)-L-leucine), from *Thermus thermophilus* HB27  
Authors : Tomita, T.; Miyazaki, T.; Miyagawa, T.; Fushinobu, S.; Kuzuyama, T.; Nishiyama, M.  
Deposited on : 2007-05-16  
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

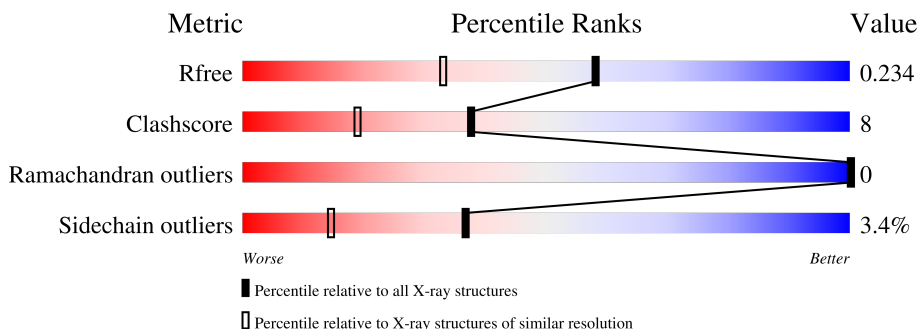
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	397	 84% 13% ..
1	B	397	 87% 11% ..

## 2 Entry composition [i](#)

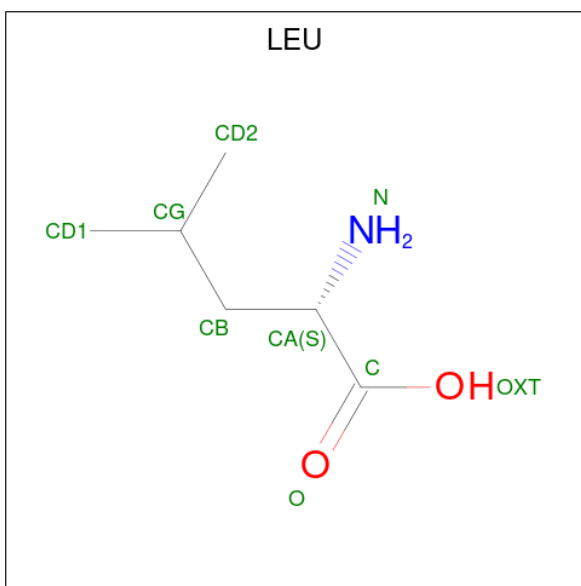
There are 3 unique types of molecules in this entry. The entry contains 6148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-aminodipate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	389	Total 3029	C 1944	N 533	O 544	S 8	0	0	0
1	B	394	Total 3071	C 1970	N 542	O 551	S 8	0	0	0

- Molecule 2 is LEUCINE (three-letter code: LEU) (formula:  $C_6H_{13}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 9	C 6	N 1	O 2	0	0
2	B	1	Total 9	C 6	N 1	O 2	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).




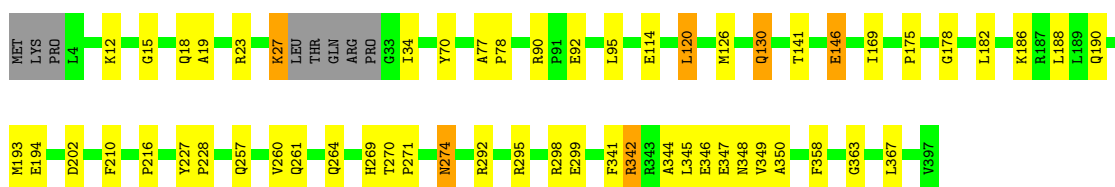
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0
3	B	1	15	8	1	5	1	0	0

### 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. 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. 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.

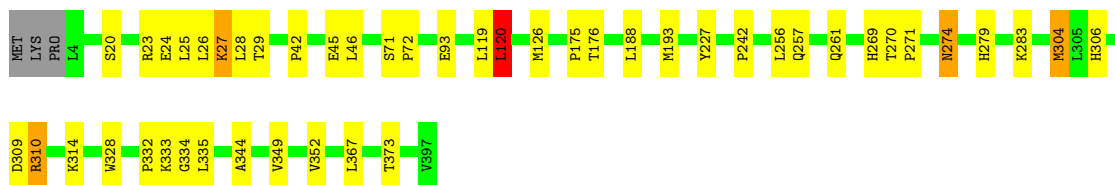
- Molecule 1: Alpha-aminodipate aminotransferase

Chain A:  84% 13% ..



- Molecule 1: Alpha-aminodipate aminotransferase

Chain B:  87% 11% ..



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.11Å 62.23Å 107.44Å 90.00° 116.34° 90.00°	Depositor
Resolution (Å)	36.83 – 1.75 36.83 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (36.83-1.75) 99.7 (36.83-1.75)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 1.75Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.180 , 0.217 0.233 , 0.234	Depositor DCC
$R_{free}$ test set	4097 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 33.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6148	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.51	0/3093	0.71	0/4178
1	B	0.51	0/3137	0.72	1/4240 (0.0%)
All	All	0.51	0/6230	0.71	1/8418 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	LEU	CA-CB-CG	5.65	128.30	115.30

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	3029	0	3089	59	0
1	B	3071	0	3136	49	0
2	A	9	0	10	0	0
2	B	9	0	10	1	0
3	A	15	0	6	0	0
3	B	15	0	6	0	0
All	All	6148	0	6257	96	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 8.

All (96) 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:23:ARG:HE	1:B:261:GLN:HE22	1.17	0.90
1:A:264:GLN:HE21	1:B:23:ARG:H	1.18	0.87
1:A:34:ILE:HD11	1:A:350:ALA:HB2	1.58	0.84
1:B:257:GLN:HE21	1:B:261:GLN:HE21	1.26	0.82
1:B:333:LYS:HD3	1:B:334:GLY:N	1.94	0.81
1:B:332:PRO:HD2	1:B:335:LEU:HD12	1.69	0.74
1:B:24:GLU:HA	1:B:27:LYS:HE3	1.72	0.72
1:A:274:ASN:H	1:A:274:ASN:HD22	1.35	0.71
1:A:146:GLU:HA	1:A:146:GLU:OE1	1.91	0.69
1:B:274:ASN:H	1:B:274:ASN:HD22	1.41	0.67
1:B:257:GLN:NE2	1:B:261:GLN:HE21	1.92	0.67
1:B:306:HIS:CE1	1:B:310:ARG:HH11	2.13	0.66
1:B:25:LEU:O	1:B:28:LEU:HD22	1.98	0.63
1:A:261:GLN:HE21	1:B:23:ARG:HH21	1.45	0.63
1:A:210:PHE:HA	1:A:298:ARG:NH2	2.15	0.62
1:B:28:LEU:HG	1:B:29:THR:N	2.14	0.62
1:B:314:LYS:N	1:B:314:LYS:HD2	2.15	0.61
1:A:341:PHE:O	1:A:345:LEU:HD23	2.00	0.61
1:A:23:ARG:HE	1:B:261:GLN:NE2	1.94	0.60
1:A:27:LYS:O	1:A:27:LYS:HD3	2.02	0.60
1:A:92:GLU:H	1:A:92:GLU:CD	2.07	0.58
1:A:190:GLN:O	1:A:194:GLU:HG3	2.03	0.58
1:A:261:GLN:NE2	1:B:23:ARG:HH21	2.00	0.58
1:A:295:ARG:O	1:A:299:GLU:HG3	2.03	0.58
1:B:306:HIS:ND1	1:B:310:ARG:NH1	2.52	0.57
1:A:274:ASN:HD22	1:A:274:ASN:N	2.02	0.57
1:A:19:ALA:HB3	1:A:130:GLN:HE22	1.69	0.57
1:A:90:ARG:HB3	1:A:92:GLU:OE2	2.05	0.57
1:B:269:HIS:HD2	1:B:270:THR:O	1.88	0.55
1:A:146:GLU:OE1	1:A:146:GLU:CA	2.54	0.55
1:A:15:GLY:HA2	1:A:18:GLN:NE2	2.22	0.55
1:B:306:HIS:CE1	1:B:310:ARG:NH1	2.75	0.54
1:A:292:ARG:HG3	1:A:292:ARG:HH21	1.74	0.53
1:A:271:PRO:HG2	1:B:271:PRO:HG2	1.91	0.53
1:B:309:ASP:CB	1:B:310:ARG:HH21	2.22	0.53
1:A:264:GLN:NE2	1:B:23:ARG:H	1.97	0.52
1:B:274:ASN:HD22	1:B:274:ASN:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LYS:HD3	1:A:27:LYS:C	2.29	0.52
1:A:264:GLN:HE22	1:B:20:SER:HA	1.75	0.52
1:B:45:GLU:HG2	1:B:46:LEU:CD1	2.39	0.52
1:B:309:ASP:HB3	1:B:310:ARG:HH21	1.75	0.51
1:A:210:PHE:O	1:A:298:ARG:NH2	2.44	0.51
1:A:269:HIS:HD2	1:A:270:THR:O	1.93	0.50
1:A:95:LEU:HD13	1:A:260:VAL:HG22	1.92	0.50
1:A:90:ARG:NH1	1:A:92:GLU:CG	2.75	0.50
1:A:342:ARG:CG	1:A:342:ARG:HH11	2.25	0.50
1:B:25:LEU:HD21	1:B:352:VAL:HG22	1.93	0.49
1:A:298:ARG:HH21	1:A:298:ARG:HG3	1.77	0.49
1:A:264:GLN:HE21	1:B:23:ARG:N	2.00	0.48
1:B:333:LYS:HD3	1:B:333:LYS:C	2.35	0.48
1:A:182:LEU:HD13	1:A:216:PRO:HD2	1.95	0.47
1:A:344:ALA:HB1	1:A:349:VAL:HG13	1.96	0.47
1:B:344:ALA:HB1	1:B:349:VAL:HG13	1.95	0.47
1:B:193:MET:HG2	1:B:227:TYR:CG	2.49	0.47
1:A:90:ARG:HH12	1:A:92:GLU:HG3	1.79	0.47
1:A:77:ALA:HB3	1:A:78:PRO:HD3	1.97	0.47
1:B:42:PRO:HD2	1:B:242:PRO:HG3	1.97	0.47
1:B:119:LEU:C	1:B:119:LEU:HD13	2.36	0.46
1:A:274:ASN:N	1:A:274:ASN:ND2	2.63	0.46
1:B:279:HIS:O	1:B:283:LYS:HG3	2.16	0.46
1:B:71:SER:HB2	1:B:72:PRO:CD	2.46	0.45
1:A:12:LYS:HE2	1:A:114:GLU:OE1	2.16	0.45
1:A:341:PHE:CZ	1:A:345:LEU:HD21	2.51	0.45
1:A:90:ARG:NH1	1:A:92:GLU:HG3	2.32	0.45
1:A:342:ARG:O	1:A:346:GLU:HG2	2.16	0.45
1:B:176:THR:HA	1:B:328:TRP:HB2	1.99	0.45
1:A:188:LEU:C	1:A:188:LEU:HD13	2.37	0.45
1:A:257:GLN:CD	1:B:23:ARG:HH22	2.20	0.45
1:A:260:VAL:HG11	1:B:23:ARG:CZ	2.46	0.45
1:B:333:LYS:HD3	1:B:334:GLY:H	1.77	0.45
1:B:27:LYS:C	1:B:27:LYS:HD2	2.37	0.45
1:A:210:PHE:HA	1:A:298:ARG:HH22	1.82	0.44
1:A:341:PHE:CE1	1:A:345:LEU:HD21	2.53	0.44
2:B:401:LEU:O	2:B:401:LEU:HG	2.18	0.44
1:A:146:GLU:OE1	1:A:178:GLY:HA2	2.18	0.44
1:A:19:ALA:HB3	1:A:130:GLN:NE2	2.32	0.43
1:A:358:PHE:CE2	1:A:363:GLY:HA3	2.53	0.43
1:A:23:ARG:NE	1:B:261:GLN:HE22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:MET:HG2	1:A:227:TYR:CG	2.53	0.43
1:B:306:HIS:O	1:B:310:ARG:HD2	2.19	0.43
1:B:45:GLU:HG2	1:B:46:LEU:HD12	2.01	0.42
1:B:93:GLU:HA	1:B:256:LEU:HD22	2.02	0.42
1:A:120:LEU:O	1:A:141:THR:HA	2.19	0.42
1:B:309:ASP:HB2	1:B:310:ARG:NH2	2.34	0.42
1:B:119:LEU:HD13	1:B:120:LEU:N	2.35	0.41
1:A:34:ILE:HG23	1:A:34:ILE:O	2.20	0.41
1:B:274:ASN:N	1:B:274:ASN:ND2	2.67	0.41
1:B:304:MET:O	1:B:304:MET:HG3	2.19	0.41
1:A:15:GLY:CA	1:A:18:GLN:NE2	2.83	0.41
1:A:15:GLY:C	1:A:18:GLN:NE2	2.74	0.41
1:A:347:GLU:O	1:A:348:ASN:HB2	2.21	0.41
1:A:169:ILE:HG12	1:A:202:ASP:HB3	2.01	0.41
1:B:188:LEU:C	1:B:188:LEU:HD13	2.40	0.41
1:A:345:LEU:HA	1:A:345:LEU:HD13	1.82	0.41
1:A:182:LEU:HG	1:A:186:LYS:HE2	2.02	0.41
1:A:70:TYR:HB3	1:B:26:LEU:CD2	2.51	0.41

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	385/397 (97%)	375 (97%)	10 (3%)	0	100	100
1	B	392/397 (99%)	383 (98%)	9 (2%)	0	100	100
All	All	777/794 (98%)	758 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	308/316 (98%)	298 (97%)	10 (3%)	39	16
1	B	313/316 (99%)	304 (97%)	9 (3%)	42	19
All	All	621/632 (98%)	602 (97%)	19 (3%)	37	17

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	120	LEU
1	A	126	MET
1	A	130	GLN
1	A	146	GLU
1	A	175	PRO
1	A	228	PRO
1	A	274	ASN
1	A	342	ARG
1	A	367	LEU
1	B	27	LYS
1	B	120	LEU
1	B	126	MET
1	B	175	PRO
1	B	274	ASN
1	B	304	MET
1	B	310	ARG
1	B	367	LEU
1	B	373	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	135	GLN
1	A	261	GLN

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Mol	Chain	Res	Type
1	A	264	GLN
1	A	269	HIS
1	A	274	ASN
1	A	360	ASN
1	B	30	GLN
1	B	101	GLN
1	B	135	GLN
1	B	190	GLN
1	B	261	GLN
1	B	269	HIS
1	B	274	ASN
1	B	360	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

4 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
3	PLP	B	1401	2	15,15,16	1.31	1 (6%)	20,22,23	1.34	3 (15%)
2	LEU	B	401	3	7,8,8	0.78	0	9,10,10	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PLP	A	1400	2	15,15,16	1.28	1 (6%)	20,22,23	1.31	3 (15%)
2	LEU	A	400	3	7,8,8	0.77	0	9,10,10	0.53	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
3	PLP	B	1401	2	-	2/6/6/8	0/1/1/1
2	LEU	B	401	3	-	0/8/8/8	-
3	PLP	A	1400	2	-	3/6/6/8	0/1/1/1
2	LEU	A	400	3	-	1/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1401	PLP	P-O1P	3.23	1.61	1.50
3	A	1400	PLP	P-O1P	3.19	1.60	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1401	PLP	C6-C5-C4	3.39	120.83	118.16
3	A	1400	PLP	C6-C5-C4	3.24	120.71	118.16
3	A	1400	PLP	C3-C4-C5	-2.50	116.03	118.74
3	B	1401	PLP	C3-C4-C5	-2.46	116.09	118.74
3	B	1401	PLP	C5A-C5-C6	-2.33	115.55	119.37
3	A	1400	PLP	C5A-C5-C6	-2.29	115.60	119.37

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1400	PLP	C5A-O4P-P-O2P
3	A	1400	PLP	C5A-O4P-P-O3P
3	B	1401	PLP	C5A-O4P-P-O2P
3	B	1401	PLP	C5A-O4P-P-O3P
3	A	1400	PLP	C5A-O4P-P-O1P
2	A	400	LEU	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	LEU	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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.