



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:13 am GMT

PDB ID : 1W7M  
Title : Crystal structure of human kynurenine aminotransferase I in complex with L-Phe  
Authors : Rossi, F.; Han, Q.; Li, J.; Li, J.; Rizzi, M.  
Deposited on : 2004-09-06  
Resolution : 2.70 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

<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

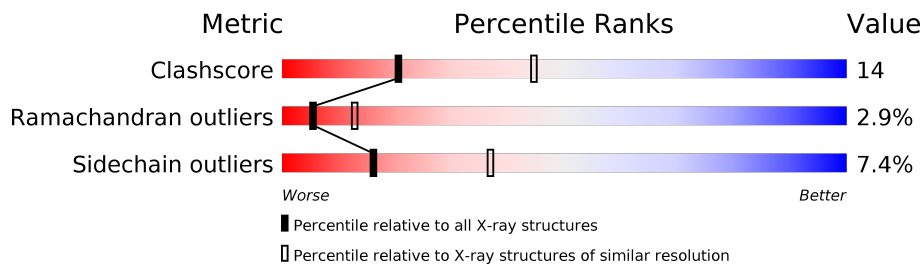
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)

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  $\geq 3$ , 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	422	 <div>69% 25% 5%</div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3550 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.

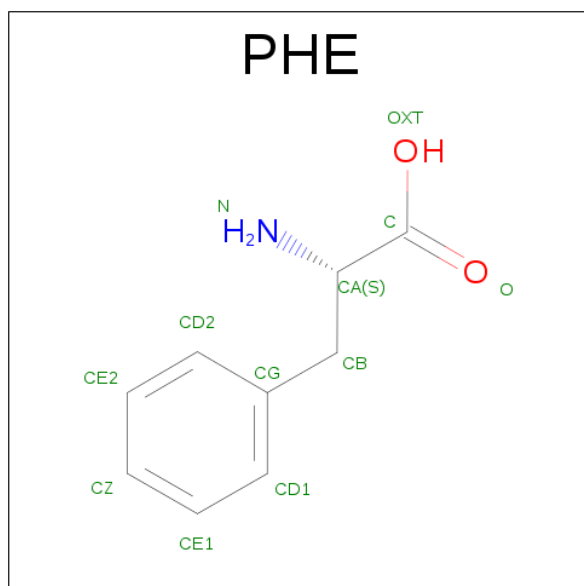
- Molecule 1 is a protein called KYNURENINE--OXOGLUTARATE TRANSAMINASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	415	3321	2146	558	598	19	0	0	0

There is a discrepancy between the modelled and reference sequences:

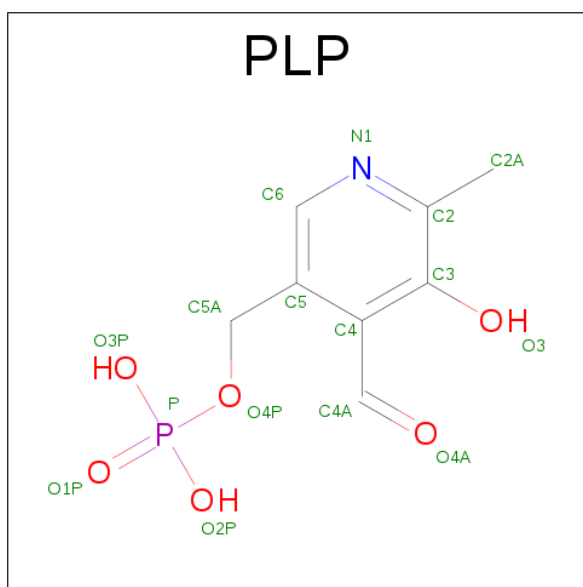
Chain	Residue	Modelled	Actual	Comment	Reference
A	332	LEU	ILE	CONFLICT	UNP Q16773

- Molecule 2 is PHENYLALANINE (three-letter code: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	12	9	1	2	0	0

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.

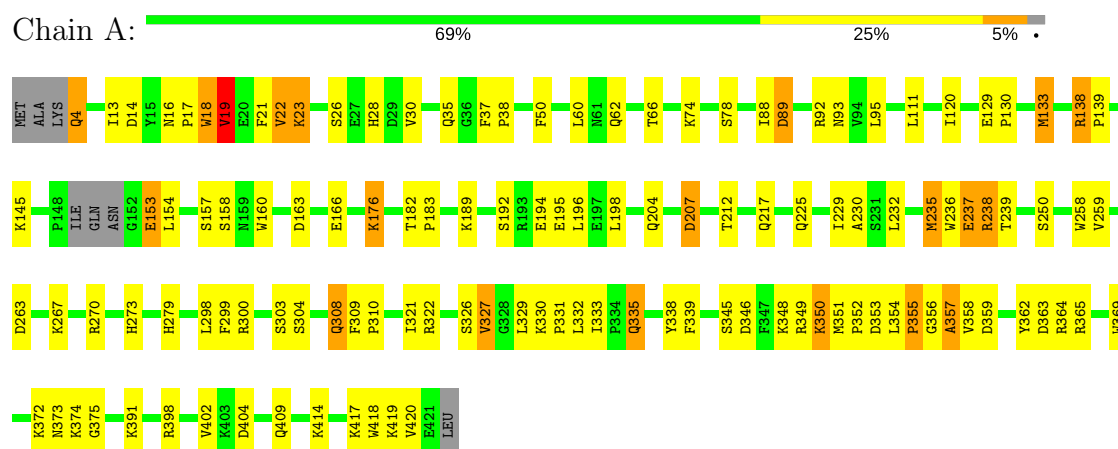
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	202	Total	O	0	0
			202	202		

### 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: KYNURENINE--OXOGLUTARATE TRANSAMINASE I



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.67 Å   145.67 Å   67.23 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	50.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.0 (50.00-2.70)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.176 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	0.91	2/3417 (0.1%)	0.94	13/4637 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	MET	SD-CE	5.75	2.10	1.77
1	A	237	GLU	CG-CD	5.07	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	163	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	207	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	270	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	60	LEU	CB-CG-CD1	-5.76	101.21	111.00
1	A	346	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	270	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	359	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	353	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	404	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	263	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	363	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	259	VAL	CB-CA-C	-5.12	101.68	111.40

There are no chirality outliers.

There are no planarity outliers.

## 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	3321	0	3252	91	0
2	A	12	0	8	1	0
3	A	15	0	6	1	0
4	A	202	0	0	25	0
All	All	3550	0	3266	92	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 14.

All (92) 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:133:MET:CE	1:A:133:MET:SD	2.10	1.40
1:A:326:SER:O	1:A:327:VAL:HG23	1.43	1.15
1:A:4:GLN:HG3	4:A:2002:HOH:O	1.55	1.04
1:A:157:SER:HB2	1:A:335:GLN:NE2	1.76	1.00
1:A:138:ARG:HD3	4:A:2085:HOH:O	1.65	0.96
1:A:89:ASP:H	1:A:93:ASN:HD22	1.10	0.93
1:A:138:ARG:CD	4:A:2085:HOH:O	2.23	0.85
2:A:914:PHE:N	3:A:1247:PLP:C4A	2.39	0.85
1:A:157:SER:HB2	1:A:335:GLN:HE21	1.42	0.83
1:A:138:ARG:HG3	4:A:2073:HOH:O	1.79	0.82
1:A:17:PRO:HG3	4:A:2188:HOH:O	1.82	0.79
1:A:237:GLU:HG2	4:A:2144:HOH:O	1.81	0.79
1:A:89:ASP:H	1:A:93:ASN:ND2	1.80	0.79
1:A:303:SER:HA	1:A:308:GLN:NE2	2.00	0.77
1:A:89:ASP:N	1:A:93:ASN:HD22	1.83	0.76
1:A:157:SER:CB	1:A:335:GLN:NE2	2.48	0.76
1:A:35:GLN:HB3	1:A:37:PHE:CE2	2.22	0.74
1:A:326:SER:O	1:A:327:VAL:CG2	2.32	0.72
1:A:354:LEU:HD23	1:A:355:PRO:HD2	1.72	0.71
1:A:160:TRP:HE1	1:A:332:LEU:HD23	1.55	0.70
1:A:335:GLN:HG3	4:A:2180:HOH:O	1.91	0.69
1:A:157:SER:CB	1:A:335:GLN:HE22	2.04	0.68
1:A:21:PHE:HB3	4:A:2189:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLN:HG2	4:A:2119:HOH:O	1.94	0.68
1:A:160:TRP:O	1:A:189:LYS:HE2	1.95	0.67
1:A:303:SER:HA	1:A:308:GLN:HE21	1.60	0.67
1:A:130:PRO:HG3	4:A:2007:HOH:O	1.98	0.63
1:A:321:ILE:HD13	1:A:333:ILE:HG12	1.81	0.62
1:A:182:THR:HA	1:A:183:PRO:C	2.19	0.62
1:A:17:PRO:HA	4:A:2018:HOH:O	1.99	0.61
1:A:356:GLY:O	1:A:357:ALA:O	2.19	0.61
1:A:327:VAL:O	1:A:327:VAL:HG12	2.00	0.60
1:A:298:LEU:O	1:A:304:SER:HB3	2.04	0.58
1:A:309:PHE:HB3	1:A:310:PRO:HD3	1.86	0.57
1:A:349:ARG:O	1:A:352:PRO:HD3	2.05	0.56
1:A:225:GLN:HG3	4:A:2137:HOH:O	2.05	0.56
1:A:345:SER:HB2	4:A:2183:HOH:O	2.06	0.56
1:A:4:GLN:CG	4:A:2002:HOH:O	2.31	0.56
1:A:166:GLU:HG2	4:A:2103:HOH:O	2.06	0.55
1:A:273:HIS:HD2	4:A:2069:HOH:O	1.90	0.55
1:A:349:ARG:HD3	4:A:2185:HOH:O	2.06	0.54
1:A:22:VAL:O	1:A:22:VAL:CG1	2.55	0.54
1:A:38:PRO:HG3	1:A:250:SER:HB3	1.90	0.54
1:A:22:VAL:HG13	1:A:22:VAL:O	2.08	0.53
1:A:16:ASN:ND2	1:A:18:TRP:HB2	2.24	0.53
1:A:232:LEU:O	1:A:235:MET:HB2	2.09	0.52
1:A:66:THR:O	1:A:273:HIS:HE1	1.92	0.52
1:A:89:ASP:OD2	1:A:92:ARG:HG3	2.09	0.52
1:A:338:TYR:CD1	1:A:402:VAL:HG21	2.44	0.52
1:A:207:ASP:OD1	1:A:238:ARG:NH2	2.42	0.52
1:A:158:SER:HB2	4:A:2094:HOH:O	2.10	0.51
1:A:4:GLN:N	4:A:2001:HOH:O	2.43	0.50
1:A:14:ASP:HB3	4:A:2010:HOH:O	2.12	0.50
1:A:66:THR:O	1:A:273:HIS:CE1	2.65	0.50
1:A:160:TRP:HE1	1:A:332:LEU:CD2	2.23	0.49
1:A:176:LYS:NZ	4:A:2105:HOH:O	2.43	0.49
1:A:194:GLU:HB2	4:A:2115:HOH:O	2.13	0.49
1:A:321:ILE:HD12	4:A:2175:HOH:O	2.13	0.48
1:A:16:ASN:HD21	1:A:18:TRP:HB2	1.78	0.48
1:A:16:ASN:HD22	1:A:19:VAL:HG23	1.79	0.48
1:A:369:TRP:CD1	1:A:373:ASN:ND2	2.81	0.48
1:A:160:TRP:NE1	1:A:332:LEU:HD23	2.26	0.47
1:A:230:ALA:HB2	1:A:239:THR:HG21	1.97	0.47
1:A:369:TRP:NE1	1:A:373:ASN:ND2	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:SER:O	1:A:196:LEU:HG	2.14	0.46
1:A:154:LEU:CD2	1:A:331:PRO:HD2	2.45	0.45
1:A:356:GLY:HA3	1:A:365:ARG:CD	2.46	0.45
1:A:375:GLY:HA3	1:A:414:LYS:HE3	1.98	0.45
1:A:339:PHE:CE1	1:A:398:ARG:NH2	2.85	0.45
1:A:195:GLU:O	1:A:198:LEU:HB3	2.17	0.45
1:A:374:LYS:HD2	1:A:418:TRP:CD1	2.52	0.44
1:A:129:GLU:HB3	1:A:130:PRO:HD3	2.00	0.44
1:A:348:LYS:HG3	1:A:362:TYR:CD2	2.53	0.44
1:A:17:PRO:O	1:A:18:TRP:O	2.34	0.44
1:A:176:LYS:NZ	4:A:2106:HOH:O	2.47	0.43
1:A:21:PHE:C	1:A:23:LYS:H	2.22	0.43
1:A:329:LEU:O	1:A:331:PRO:HD3	2.18	0.43
1:A:111:LEU:O	1:A:176:LYS:HD3	2.18	0.43
1:A:327:VAL:CG1	1:A:327:VAL:O	2.66	0.42
1:A:138:ARG:HD2	4:A:2085:HOH:O	2.03	0.42
1:A:62:GLN:HA	1:A:62:GLN:NE2	2.34	0.42
1:A:207:ASP:HA	1:A:238:ARG:NH2	2.34	0.42
1:A:133:MET:CE	1:A:133:MET:CG	2.95	0.42
1:A:120:ILE:HD12	1:A:139:PRO:HB3	2.01	0.42
1:A:158:SER:HB3	1:A:335:GLN:OE1	2.20	0.42
1:A:356:GLY:HA3	1:A:365:ARG:HD3	2.02	0.41
1:A:229:ILE:O	1:A:232:LEU:HB2	2.20	0.41
1:A:28:HIS:CE1	1:A:372:LYS:HA	2.55	0.41
1:A:95:LEU:O	1:A:258:TRP:HA	2.20	0.41
1:A:322:ARG:HD3	1:A:322:ARG:HH11	1.76	0.41
1:A:88:ILE:HG12	1:A:236:TRP:CH2	2.55	0.41
1:A:299:PHE:O	1:A:300:ARG:HB2	2.21	0.40

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	411/422 (97%)	376 (92%)	23 (6%)	12 (3%)	5	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	TRP
1	A	19	VAL
1	A	327	VAL
1	A	350	LYS
1	A	357	ALA
1	A	420	VAL
1	A	153	GLU
1	A	217	GLN
1	A	22	VAL
1	A	351	MET
1	A	13	ILE
1	A	355	PRO

### 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	362/368 (98%)	335 (92%)	27 (8%)	16	36

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	19	VAL
1	A	23	LYS
1	A	26	SER
1	A	30	VAL
1	A	50	PHE
1	A	74	LYS
1	A	78	SER
1	A	138	ARG

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Mol	Chain	Res	Type
1	A	145	LYS
1	A	153	GLU
1	A	176	LYS
1	A	212	THR
1	A	235	MET
1	A	238	ARG
1	A	267	LYS
1	A	279	HIS
1	A	308	GLN
1	A	330	LYS
1	A	335	GLN
1	A	350	LYS
1	A	358	VAL
1	A	364	ARG
1	A	391	LYS
1	A	409	GLN
1	A	417	LYS
1	A	419	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	28	HIS
1	A	62	GLN
1	A	93	ASN
1	A	264	HIS
1	A	273	HIS
1	A	308	GLN
1	A	325	GLN
1	A	335	GLN
1	A	373	ASN
1	A	409	GLN

### 5.3.3 RNA ⓘ

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](#)

2 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	A	1247	1	15,15,16	1.90	3 (20%)	20,22,23	2.29	8 (40%)
2	PHE	A	914	-	8,12,12	5.71	6 (75%)	10,15,15	2.03	4 (40%)

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	A	1247	1	-	0/6/6/8	0/1/1/1
2	PHE	A	914	-	-	0/4/8/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1247	PLP	O3-C3	-5.48	1.24	1.37
3	A	1247	PLP	C3-C2	2.12	1.42	1.40
3	A	1247	PLP	C2-N1	2.69	1.39	1.33
2	A	914	PHE	CD2-CG	6.28	1.51	1.38
2	A	914	PHE	CZ-CE2	6.39	1.53	1.38
2	A	914	PHE	CD1-CG	6.50	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	914	PHE	CZ-CE1	6.60	1.54	1.38
2	A	914	PHE	CE1-CD1	6.67	1.51	1.38
2	A	914	PHE	CE2-CD2	7.07	1.52	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1247	PLP	C5-C6-N1	-3.18	118.50	123.87
2	A	914	PHE	CE2-CD2-CG	-2.43	116.93	120.64
3	A	1247	PLP	C5A-C5-C6	-2.29	115.39	119.33
2	A	914	PHE	CE1-CD1-CG	-2.12	117.41	120.64
2	A	914	PHE	CB-CA-N	-2.04	104.65	112.68
3	A	1247	PLP	O3-C3-C2	2.46	122.94	117.78
3	A	1247	PLP	O3P-P-O2P	2.47	117.58	107.61
3	A	1247	PLP	O2P-P-O1P	2.59	120.62	110.50
3	A	1247	PLP	C2A-C2-C3	3.42	125.05	120.96
2	A	914	PHE	CD2-CG-CD1	4.36	125.07	118.16
3	A	1247	PLP	O4P-C5A-C5	4.54	118.45	109.32
3	A	1247	PLP	C6-C5-C4	5.03	122.38	118.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1247	PLP	1	0
2	A	914	PHE	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

### 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.