



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:58 PM UTC

PDB ID : 1G7W / pdb_00001g7w
Title : ASPARTATE AMINOTRANSFERASE ACTIVE SITE MUTANT
N194A/R386L
Authors : Mizuguchi, H.; Hayashi, H.; Okada, K.; Miyahara, I.; Hirotsu, K.;
Kagamiyama, H.
Deposited on : 2000-11-15
Resolution : 2.20 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

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

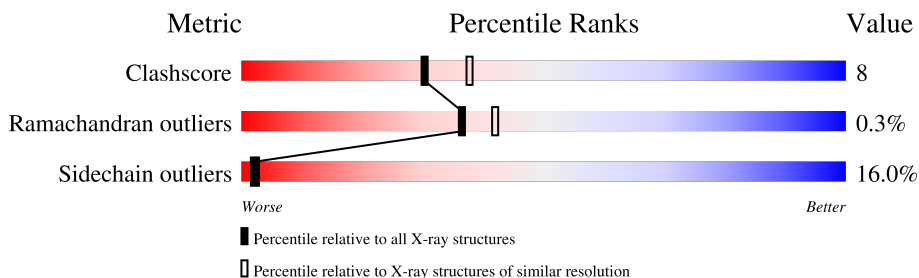
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3266 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.

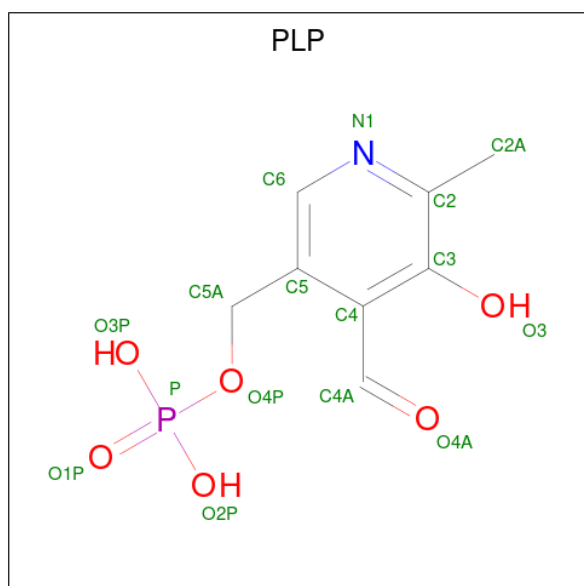
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3063	1935	532	583	13	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	ALA	ASN	engineered mutation	UNP P00509
A	386	LEU	ARG	engineered mutation	UNP P00509

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 3 is water.

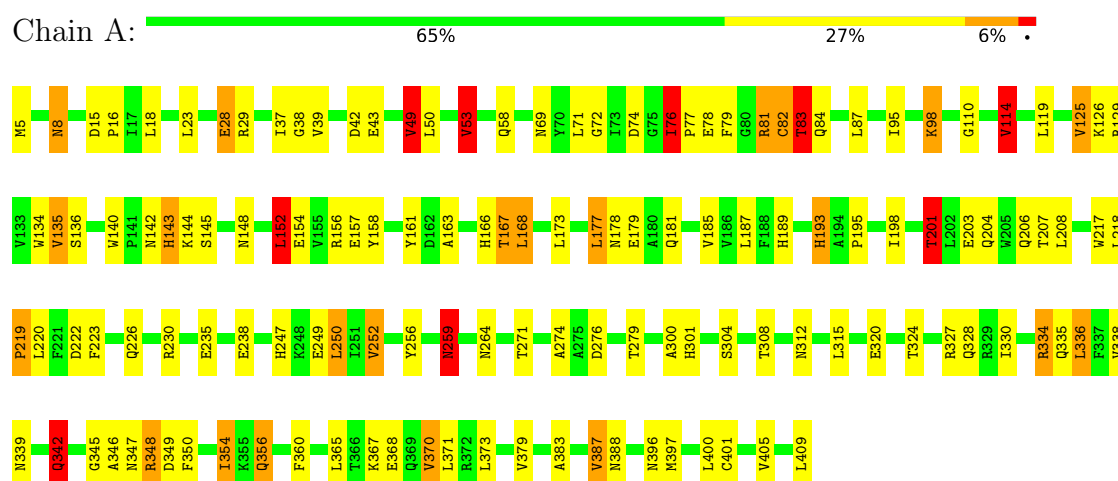
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	188	Total 188	O 188	0	0

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.

Note EDS was not executed.

• Molecule 1: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.94Å 89.33Å 79.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	86.4 (10.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.217 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3266	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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	0.89	11/3124 (0.4%)	1.71	62/4233 (1.5%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	VAL	CA-CB	6.89	1.63	1.54
1	A	189	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	143	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	247	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	301	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	193	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	53	VAL	CA-CB	5.80	1.62	1.54
1	A	166	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	76	ILE	CA-CB	5.51	1.61	1.54
1	A	114	VAL	CA-CB	5.26	1.61	1.54
1	A	83	THR	CA-CB	5.11	1.61	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	GLN	OE1-CD-NE2	-9.76	112.84	122.60
1	A	276	ASP	CA-CB-CG	8.38	120.98	112.60
1	A	126	LYS	N-CA-C	-8.12	103.97	114.04
1	A	259	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	A	201	THR	N-CA-CB	-7.57	99.54	110.36
1	A	347	ASN	CA-C-O	7.56	130.40	121.11
1	A	356	GLN	OE1-CD-NE2	-7.51	115.09	122.60
1	A	349	ASP	N-CA-C	-7.44	95.05	107.32
1	A	301	HIS	N-CA-C	7.42	120.02	111.11
1	A	334	ARG	NE-CZ-NH2	7.40	125.86	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	A	125	VAL	N-CA-CB	7.27	120.22	110.26
1	A	300	ALA	N-CA-C	7.12	119.04	111.28
1	A	259	ASN	CA-CB-CG	7.08	119.68	112.60
1	A	167	THR	CA-CB-OG1	-6.96	99.16	109.60
1	A	312	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	A	301	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	A	125	VAL	CB-CA-C	-6.69	101.83	111.34
1	A	69	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	A	37	ILE	N-CA-C	6.54	121.57	112.35
1	A	342	GLN	CG-CD-NE2	6.54	126.20	116.40
1	A	349	ASP	CA-CB-CG	-6.50	106.10	112.60
1	A	42	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	74	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	226	GLN	OE1-CD-NE2	-6.26	116.34	122.60
1	A	143	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	A	148	ASN	OD1-CG-ND2	-5.95	116.65	122.60
1	A	264	ASN	CA-CB-CG	5.92	118.52	112.60
1	A	58	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	A	259	ASN	CB-CG-ND2	5.86	125.19	116.40
1	A	388	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	A	339	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	A	71	LEU	N-CA-C	-5.80	103.05	110.53
1	A	396	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	350	PHE	N-CA-C	-5.73	105.87	112.92
1	A	82	CYS	CA-C-O	-5.71	114.50	120.55
1	A	178	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	A	167	THR	N-CA-CB	-5.64	102.77	111.46
1	A	142	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	334	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	A	342	GLN	CB-CG-CD	5.59	122.11	112.60
1	A	140	TRP	CA-C-N	5.53	124.99	119.24
1	A	140	TRP	C-N-CA	5.53	124.99	119.24
1	A	226	GLN	CG-CD-NE2	5.52	124.69	116.40
1	A	69	ASN	CB-CG-ND2	5.51	124.67	116.40
1	A	301	HIS	CB-CG-ND1	5.48	130.92	122.70
1	A	81	ARG	CB-CG-CD	5.46	123.86	111.30
1	A	217	TRP	CG-CD2-CE3	5.45	139.35	133.90
1	A	167	THR	CA-CB-CG2	5.42	119.71	110.50
1	A	148	ASN	CA-CB-CG	5.36	117.96	112.60
1	A	347	ASN	O-C-N	5.32	129.22	122.84
1	A	328	GLN	OE1-CD-NE2	-5.29	117.31	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	VAL	N-CA-C	-5.27	100.30	107.99
1	A	72	GLY	N-CA-C	-5.22	104.53	112.51
1	A	189	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	A	387	VAL	N-CA-CB	-5.15	103.00	111.44
1	A	15	ASP	CA-C-N	5.11	126.22	119.84
1	A	15	ASP	C-N-CA	5.11	126.22	119.84
1	A	219	PRO	CB-CA-C	5.11	117.09	111.11
1	A	327	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	A	134	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	A	152	LEU	N-CA-C	-5.01	101.06	109.24

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	3063	0	3013	51	0
2	A	15	0	7	0	0
3	A	188	0	0	4	0
All	All	3266	0	3020	51	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 (51) 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:81:ARG:NH1	1:A:82:CYS:SG	2.43	0.92
1:A:335:GLN:HA	1:A:354:ILE:HD11	1.66	0.76
1:A:76:ILE:HG21	3:A:446:HOH:O	1.85	0.76
1:A:125:VAL:HG11	1:A:185:VAL:HG23	1.65	0.76
1:A:203:GLU:HA	1:A:206:GLN:HE21	1.62	0.65
1:A:370:VAL:HG21	1:A:383:ALA:HA	1.81	0.62
1:A:81:ARG:CZ	1:A:82:CYS:SG	2.88	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:HB2	1:A:53:VAL:HG13	1.84	0.60
1:A:304:SER:O	1:A:308:THR:HG23	2.04	0.58
1:A:252:VAL:HG13	1:A:271:THR:HB	1.84	0.58
1:A:320:GLU:O	1:A:324:THR:HG23	2.03	0.57
1:A:168:LEU:HD21	1:A:173:LEU:HD12	1.86	0.57
1:A:49:VAL:HG23	1:A:53:VAL:HG22	1.87	0.55
1:A:346:ALA:H	1:A:348:ARG:HD2	1.72	0.55
1:A:348:ARG:HH22	1:A:405:VAL:HG22	1.71	0.54
1:A:274:ALA:HB1	1:A:279:THR:HG23	1.88	0.54
1:A:95:ILE:O	1:A:98:LYS:HD2	2.07	0.53
1:A:135:VAL:HG22	1:A:187:LEU:HD23	1.91	0.53
1:A:219:PRO:HG2	1:A:250:LEU:HB2	1.90	0.53
1:A:336:LEU:HB3	1:A:397:MET:HE3	1.91	0.52
1:A:81:ARG:NE	1:A:82:CYS:SG	2.82	0.52
1:A:125:VAL:HG13	3:A:604:HOH:O	2.09	0.51
1:A:38:GLY:HA2	1:A:360:PHE:HZ	1.78	0.49
1:A:201:THR:HG22	1:A:204:GLN:H	1.78	0.49
1:A:346:ALA:HB3	1:A:348:ARG:CZ	2.43	0.48
1:A:129:ARG:HD3	1:A:154:GLU:HB2	1.94	0.48
1:A:136:SER:OG	1:A:193:HIS:HE1	1.97	0.48
1:A:198:ILE:HD13	1:A:356:GLN:HG2	1.97	0.47
1:A:158:TYR:HB3	1:A:177:LEU:HD13	1.96	0.47
1:A:84:GLN:HE22	1:A:98:LYS:NZ	2.13	0.47
1:A:28:GLU:HG2	1:A:29:ARG:HE	1.79	0.47
1:A:203:GLU:O	1:A:207:THR:HG23	2.14	0.47
1:A:330:ILE:O	1:A:334:ARG:HG3	2.17	0.45
1:A:401:CYS:O	1:A:405:VAL:HG23	2.16	0.45
1:A:76:ILE:HA	1:A:77:PRO:HD3	1.80	0.44
1:A:129:ARG:HD2	1:A:156:ARG:HG2	1.99	0.44
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.88	0.43
1:A:110:GLY:O	1:A:114:VAL:HG13	2.18	0.43
1:A:79:PHE:O	1:A:83:THR:HG23	2.19	0.43
1:A:187:LEU:HD11	1:A:222:ASP:HB2	2.00	0.43
1:A:143:HIS:HB2	3:A:595:HOH:O	2.19	0.42
1:A:29:ARG:HG3	3:A:530:HOH:O	2.19	0.42
1:A:338:VAL:HG21	1:A:354:ILE:HD13	2.02	0.42
1:A:161:TYR:CE2	1:A:163:ALA:HA	2.55	0.42
1:A:28:GLU:HG2	1:A:29:ARG:HH11	1.85	0.41
1:A:348:ARG:H	1:A:348:ARG:HG2	1.69	0.41
1:A:342:GLN:HE21	1:A:342:GLN:N	2.19	0.41
1:A:135:VAL:O	1:A:157:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:O	1:A:238:GLU:HB2	2.20	0.41
1:A:256:TYR:HA	1:A:259:ASN:HD21	1.86	0.41
1:A:342:GLN:HA	1:A:348:ARG:HD3	2.03	0.40

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	394/396 (100%)	379 (96%)	14 (4%)	1 (0%)	36	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	GLY

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	319/319 (100%)	268 (84%)	51 (16%)	2	2

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	8	ASN
1	A	16	PRO
1	A	18	LEU
1	A	23	LEU
1	A	28	GLU
1	A	39	VAL
1	A	43	GLU
1	A	49	VAL
1	A	53	VAL
1	A	76	ILE
1	A	78	GLU
1	A	83	THR
1	A	87	LEU
1	A	98	LYS
1	A	114	VAL
1	A	119	LEU
1	A	135	VAL
1	A	144	LYS
1	A	145	SER
1	A	152	LEU
1	A	167	THR
1	A	168	LEU
1	A	177	LEU
1	A	179	GLU
1	A	181	GLN
1	A	195	PRO
1	A	201	THR
1	A	208	LEU
1	A	218	LEU
1	A	220	LEU
1	A	223	PHE
1	A	230	ARG
1	A	249	GLU
1	A	250	LEU
1	A	252	VAL
1	A	259	ASN
1	A	315	LEU
1	A	336	LEU
1	A	342	GLN
1	A	348	ARG
1	A	354	ILE
1	A	365	LEU

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Mol	Chain	Res	Type
1	A	367	LYS
1	A	368	GLU
1	A	370	VAL
1	A	371	LEU
1	A	373	LEU
1	A	387	VAL
1	A	400	LEU
1	A	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	69	ASN
1	A	84	GLN
1	A	165	ASN
1	A	166	HIS
1	A	178	ASN
1	A	193	HIS
1	A	206	GLN
1	A	247	HIS
1	A	259	ASN
1	A	342	GLN
1	A	347	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	413	1	15,15,16	1.49	3 (20%)	21,22,23	1.43	2 (9%)

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	413	1	-	0/6/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	413	PLP	C3-C2	-2.98	1.37	1.41
2	A	413	PLP	C5-C4	-2.62	1.37	1.40
2	A	413	PLP	P-O3P	-2.21	1.46	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	413	PLP	O4P-C5A-C5	4.73	118.22	109.36
2	A	413	PLP	C5-C6-N1	-2.04	120.51	123.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.