Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:35 pm BST

PDB ID	:	1EG5
Title	:	NIFS-LIKE PROTEIN
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Deposited on	:	2000-02-13
Resolution	:	2.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

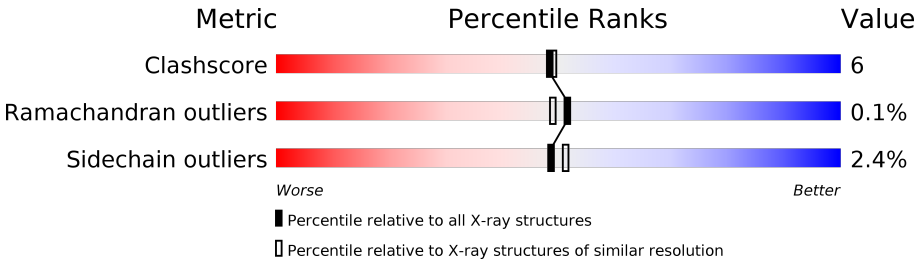
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	384	80% 13% • 5%
1	B	384	84% 10% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6012 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.

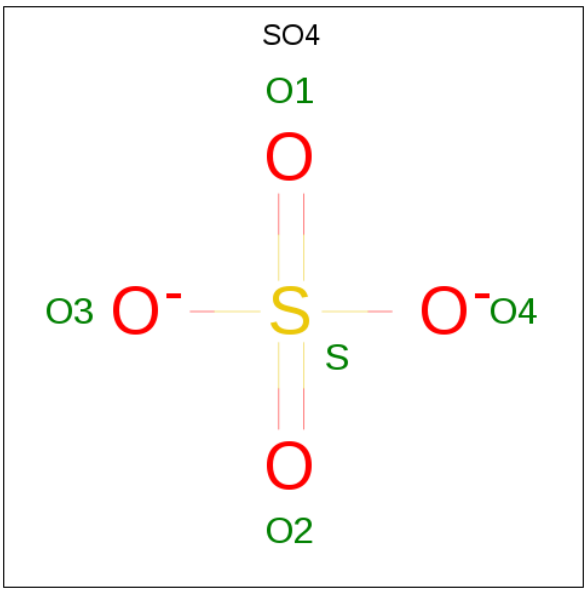
- Molecule 1 is a protein called AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	Se	0	0	0
			2853	1817	492	531	2	11			
1	B	365	Total	C	N	O	S	Se	0	0	0
			2864	1823	496	532	2	11			

There are 24 discrepancies between the modelled and reference sequences:

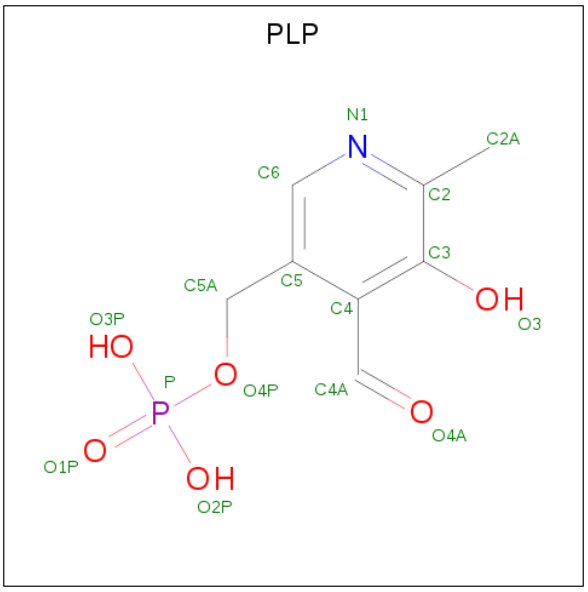
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
A	21	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
A	38	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
A	46	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
A	106	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
A	111	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
A	146	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
A	251	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
A	265	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
A	277	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
A	332	ARG	SER	SEE REMARK 999	UNP Q9X218
A	338	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
B	21	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
B	38	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
B	46	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
B	106	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
B	111	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
B	146	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
B	251	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
B	265	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
B	277	MSE	MET	MODIFIED RESIDUE	UNP Q9X218
B	332	ARG	SER	SEE REMARK 999	UNP Q9X218
B	338	MSE	MET	MODIFIED RESIDUE	UNP Q9X218

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	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	117	Total	O	0	0
			117	117		
4	B	138	Total	O	0	0
			138	138		

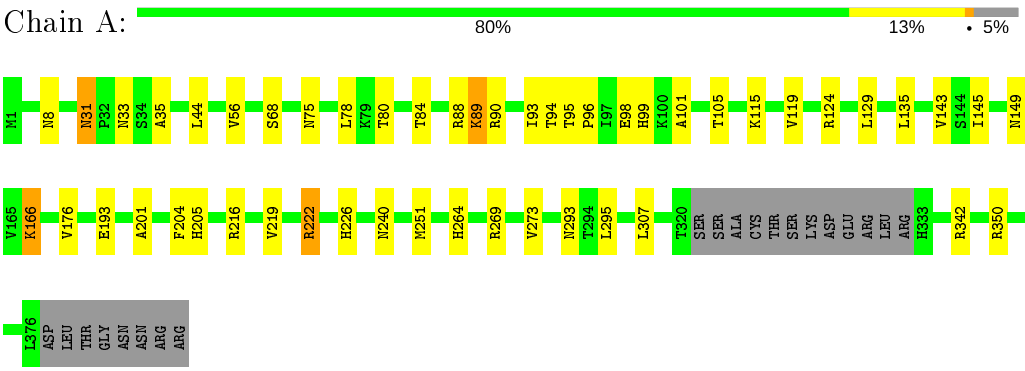
3 Residue-property plots (i)

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. 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.

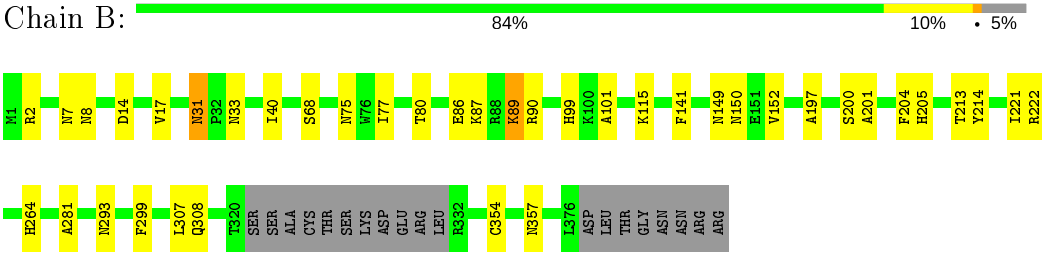
- Molecule 1: AMINOTRANSFERASE

Chain A:



- Molecule 1: AMINOTRANSFERASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	114.11Å 114.11Å 156.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.92 – 2.00	Depositor
% Data completeness (in resolution range)	98.2 (35.92-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6012	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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: SO4, 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	0.50	0/2890	0.65	0/3880
1	B	0.54	0/2901	0.65	0/3894
All	All	0.52	0/5791	0.65	0/7774

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

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	2853	0	2940	43	0
1	B	2864	0	2953	33	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	15	0	6	0	0
3	B	15	0	6	0	0
4	A	117	0	0	2	0
4	B	138	0	0	2	0
All	All	6012	0	5905	70	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 6.

All (70) 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:226:HIS:H	1:B:75:ASN:HD21	1.15	0.90
1:A:75:ASN:HD21	1:B:226:HIS:H	1.19	0.86
1:B:31:ASN:HD22	1:B:33:ASN:H	1.25	0.82
1:A:31:ASN:HD22	1:A:33:ASN:H	1.29	0.78
1:A:226:HIS:H	1:B:75:ASN:ND2	1.85	0.75
1:A:150:ASN:HD22	1:A:150:ASN:H	1.35	0.74
1:B:31:ASN:HD21	1:B:33:ASN:HD22	1.35	0.73
1:A:99:HIS:HD2	1:A:101:ALA:H	1.35	0.73
1:A:149:ASN:HD22	1:A:152:VAL:H	1.37	0.73
1:B:99:HIS:HD2	1:B:101:ALA:H	1.37	0.72
1:B:149:ASN:HD22	1:B:152:VAL:H	1.39	0.71
1:A:75:ASN:ND2	1:B:226:HIS:H	1.91	0.68
1:A:8:ASN:HD21	1:A:293:ASN:HD21	1.38	0.67
1:A:99:HIS:CD2	1:A:101:ALA:H	2.13	0.66
1:A:150:ASN:H	1:A:150:ASN:ND2	1.96	0.63
1:B:8:ASN:HD21	1:B:293:ASN:HD21	1.46	0.62
1:B:99:HIS:CD2	1:B:101:ALA:H	2.17	0.62
1:A:264:HIS:HE1	1:A:357:ASN:O	1.83	0.62
1:B:90:ARG:NH2	1:B:115:LYS:HE3	2.15	0.61
1:A:90:ARG:HH22	1:A:115:LYS:HE3	1.67	0.59
1:B:31:ASN:ND2	1:B:33:ASN:H	2.01	0.58
1:A:8:ASN:ND2	1:A:293:ASN:HD21	2.02	0.58
1:A:369:ILE:O	1:A:373:LEU:HG	2.03	0.57
1:B:264:HIS:HE1	1:B:357:ASN:O	1.87	0.57
1:A:269:ARG:O	1:A:273:VAL:HG23	2.06	0.56
1:A:350:ARG:HD2	4:A:606:HOH:O	2.06	0.55
1:A:31:ASN:HD21	1:A:33:ASN:HD22	1.52	0.54
1:A:31:ASN:ND2	1:A:33:ASN:H	1.99	0.54
1:B:8:ASN:ND2	1:B:293:ASN:HD21	2.06	0.54
1:A:90:ARG:NH2	1:A:115:LYS:HE3	2.24	0.53
1:B:205:HIS:HE1	4:B:607:HOH:O	1.90	0.53
1:B:31:ASN:HD21	1:B:33:ASN:ND2	2.06	0.53
1:A:205:HIS:HE1	4:A:608:HOH:O	1.92	0.52
1:A:31:ASN:HD21	1:A:33:ASN:ND2	2.08	0.52
1:B:150:ASN:HD22	1:B:150:ASN:H	1.59	0.52
1:A:119:VAL:HG22	1:A:135:LEU:HD12	1.92	0.51
1:A:129:LEU:HD22	1:A:164:ILE:HD12	1.93	0.51
1:A:80:THR:O	1:A:84:THR:HG23	2.12	0.50
1:B:150:ASN:H	1:B:150:ASN:ND2	2.10	0.49
1:A:93:ILE:HB	1:A:143:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:THR:HB	1:A:222:ARG:HB2	1.94	0.48
1:B:281:ALA:HB2	1:B:299:PHE:CZ	2.48	0.48
1:A:216:ARG:O	1:A:219:VAL:HG22	2.13	0.47
1:A:273:VAL:HG22	1:A:295:LEU:HD11	1.97	0.47
1:A:166:LYS:HB2	1:A:166:LYS:NZ	2.30	0.46
1:A:149:ASN:ND2	1:A:152:VAL:H	2.07	0.46
1:A:31:ASN:C	1:A:31:ASN:HD22	2.18	0.46
1:A:88:ARG:O	1:A:89:LYS:HD2	2.16	0.45
1:A:193:GLU:HA	1:A:216:ARG:NH1	2.32	0.45
1:B:149:ASN:ND2	1:B:152:VAL:H	2.10	0.44
1:B:89:LYS:HB3	1:B:141:PHE:CD2	2.53	0.43
1:B:90:ARG:HH22	1:B:115:LYS:HE3	1.81	0.43
1:B:80:THR:HB	1:B:222:ARG:HB2	2.00	0.43
1:B:77:ILE:HD11	1:B:213:THR:HG23	2.00	0.43
1:B:89:LYS:HB3	1:B:141:PHE:HD2	1.84	0.43
1:A:35:ALA:HB3	1:B:308:GLN:HE22	1.83	0.43
1:A:56:VAL:HG11	1:A:251:MSE:HG2	2.01	0.42
1:B:40:ILE:HD11	4:B:723:HOH:O	2.19	0.42
1:B:86:GLU:O	1:B:87:LYS:HB2	2.20	0.42
1:B:7:ASN:CG	1:B:354:CYS:HB3	2.40	0.41
1:A:94:THR:OG1	1:A:98:GLU:HG3	2.20	0.41
1:B:14:ASP:HB3	1:B:17:VAL:HG23	2.02	0.41
1:B:201:ALA:HA	1:B:204:PHE:CZ	2.55	0.41
1:A:201:ALA:HA	1:A:204:PHE:CZ	2.55	0.41
1:A:78:LEU:HB2	1:A:105:THR:HG21	2.03	0.41
1:B:197:ALA:HB3	1:B:214:TYR:HB3	2.02	0.41
1:A:68:SER:CB	1:B:68:SER:HB3	2.51	0.41
1:A:145:ILE:O	1:A:176:VAL:HA	2.20	0.41
1:A:95:THR:HB	1:A:96:PRO:HD2	2.02	0.40
1:A:342:ARG:HH21	1:A:342:ARG:HG2	1.86	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	360/384 (94%)	345 (96%)	15 (4%)	0	100 100
1	B	361/384 (94%)	347 (96%)	13 (4%)	1 (0%)	41 37
All	All	721/768 (94%)	692 (96%)	28 (4%)	1 (0%)	51 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	221	ILE

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	315/322 (98%)	306 (97%)	9 (3%)	42 43
1	B	316/322 (98%)	310 (98%)	6 (2%)	57 61
All	All	631/644 (98%)	616 (98%)	15 (2%)	49 51

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	44	LEU
1	A	89	LYS
1	A	124	ARG
1	A	150	ASN
1	A	166	LYS
1	A	222	ARG
1	A	240	ASN
1	A	307	LEU
1	B	2	ARG
1	B	31	ASN
1	B	89	LYS

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Mol	Chain	Res	Type
1	B	200	SER
1	B	240	ASN
1	B	307	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	8	ASN
1	A	31	ASN
1	A	75	ASN
1	A	99	HIS
1	A	149	ASN
1	A	150	ASN
1	A	205	HIS
1	A	240	ASN
1	A	264	HIS
1	A	308	GLN
1	A	346	GLN
1	B	7	ASN
1	B	8	ASN
1	B	31	ASN
1	B	75	ASN
1	B	99	HIS
1	B	149	ASN
1	B	150	ASN
1	B	205	HIS
1	B	240	ASN
1	B	264	HIS
1	B	308	GLN

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 (i)

There are no carbohydrates 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	A	601	1	15,15,16	1.55	1 (6%)	20,22,23	2.08	5 (25%)
3	PLP	B	600	1	15,15,16	1.60	3 (20%)	20,22,23	1.98	5 (25%)
2	SO4	A	603	-	4,4,4	0.33	0	6,6,6	0.13	0
2	SO4	B	602	-	4,4,4	0.40	0	6,6,6	0.11	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	A	601	1	-	0/6/6/8	0/1/1/1
3	PLP	B	600	1	-	0/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	PLP	C3-C2	-4.04	1.36	1.40
3	B	600	PLP	C3-C2	-4.02	1.36	1.40
3	B	600	PLP	C2A-C2	2.51	1.54	1.50
3	B	600	PLP	P-O3P	-2.06	1.46	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	PLP	O4P-C5A-C5	6.39	121.52	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	600	PLP	O4P-C5A-C5	5.29	119.44	109.35
3	A	601	PLP	O2P-P-O4P	-4.07	95.90	106.73
3	B	600	PLP	O2P-P-O4P	-3.95	96.22	106.73
3	B	600	PLP	C5-C6-N1	-2.81	119.15	123.82
3	B	600	PLP	O3P-P-O1P	2.66	121.09	110.68
3	A	601	PLP	C5-C6-N1	-2.63	119.44	123.82
3	A	601	PLP	O3P-P-O1P	2.53	120.60	110.68
3	B	600	PLP	C6-C5-C4	2.22	119.90	118.16
3	A	601	PLP	C6-C5-C4	2.16	119.86	118.16

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 (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.