



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:28 AM UTC

PDB ID : 2DKB / pdb_00002dkb
Title : DIALKYLGLYCINE DECARBOXYLASE STRUCTURE: BIFUNCTIONAL
ACTIVE SITE AND ALKALI METAL BINDING SITES
Authors : Toney, M.D.; Hohenester, E.; Jansonius, J.N.
Deposited on : 1994-07-12
Resolution : 2.10 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

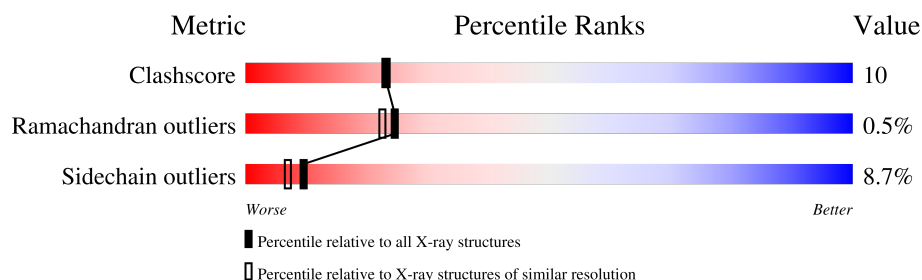
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	433	 75% 21% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3510 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 2,2-DIALKYLGLYCINE DECARBOXYLASE (PYRUVATE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	232	0	0
			3252	2051	576	607	18			

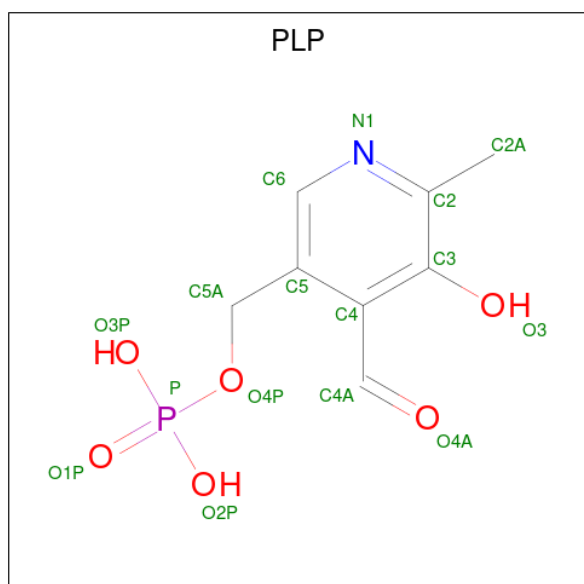
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	HIS	GLN	conflict	UNP P16932
A	81	GLU	GLY	conflict	UNP P16932

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

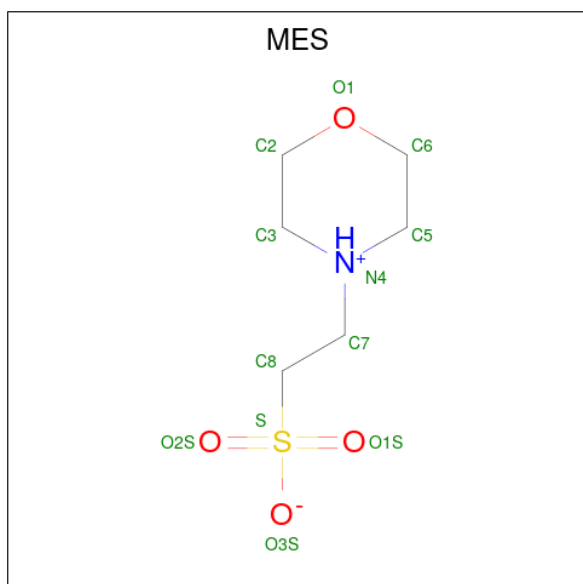
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	3	0
			12	6	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	229	Total	O	0	0
			229	229		

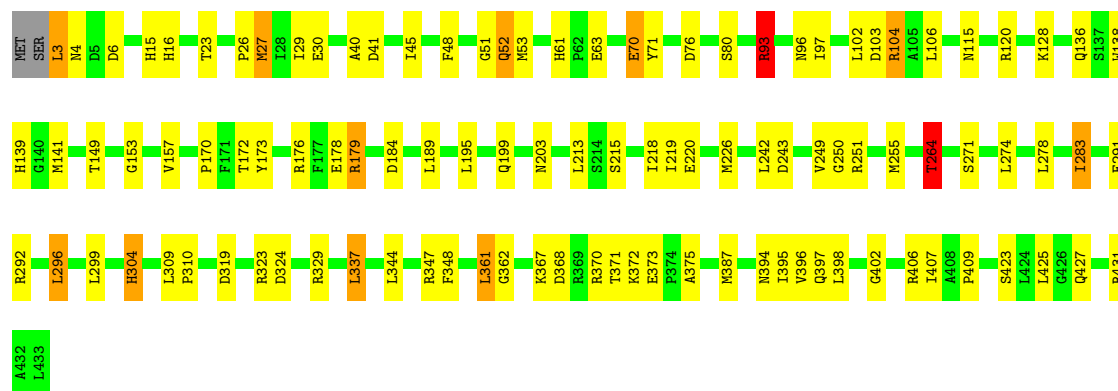
3 Residue-property plots

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: 2,2-DIALKYLGLYCINE DECARBOXYLASE (PYRUVATE)

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.70Å 152.70Å 86.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3510	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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, MES, NA

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	1.07	2/3309 (0.1%)	1.50	25/4478 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	GLY	C-N	-12.39	1.16	1.33
1	A	52	GLN	C-N	-11.22	1.17	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	GLY	O-C-N	-9.79	109.98	122.70
1	A	71	TYR	N-CA-C	7.59	119.64	111.36
1	A	348	PHE	N-CA-C	7.19	120.64	109.07
1	A	264	THR	CB-CA-C	6.72	117.58	109.31
1	A	70	GLU	N-CA-CB	6.36	119.42	109.94
1	A	251	ARG	N-CA-C	6.22	118.85	111.33
1	A	6	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	283	ILE	N-CA-CB	6.01	121.84	111.39
1	A	304	HIS	N-CA-C	5.93	119.48	112.72
1	A	16	HIS	N-CA-C	5.80	121.11	112.94
1	A	93	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	A	402	GLY	N-CA-C	-5.61	103.82	112.85
1	A	220	GLU	CB-CA-C	-5.52	100.75	109.80
1	A	103	ASP	N-CA-C	5.51	120.88	114.04
1	A	370	ARG	N-CA-CB	5.39	117.99	110.07
1	A	26	PRO	N-CA-CB	5.35	106.40	102.81
1	A	96	ASN	N-CA-C	5.27	117.94	111.82
1	A	250	GLY	N-CA-C	5.21	122.28	115.40
1	A	80	SER	N-CA-C	5.20	118.41	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	HIS	CB-CA-C	-5.20	99.22	109.67
1	A	76	ASP	N-CA-C	5.16	118.86	111.02
1	A	51	GLY	CA-C-N	5.12	131.31	121.54
1	A	51	GLY	C-N-CA	5.12	131.31	121.54
1	A	170	PRO	CB-CA-C	-5.07	106.04	111.56
1	A	93	ARG	CG-CD-NE	-5.01	100.98	112.00

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	3252	0	3276	63	0
2	A	2	0	0	0	0
3	A	15	0	6	1	0
4	A	12	0	13	0	0
5	A	229	0	0	12	0
All	All	3510	0	3295	63	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 10.

All (63) 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:3:LEU:HD12	1:A:4:ASN:H	1.32	0.94
1:A:337:LEU:HD13	1:A:361:LEU:HD23	1.66	0.75
1:A:264:THR:HG21	5:A:608:HOH:O	1.86	0.75
1:A:323:ARG:HD2	1:A:324:ASP:OD1	1.91	0.70
1:A:397:GLN:C	1:A:398:LEU:HD22	2.17	0.69
1:A:45:ILE:HG21	1:A:387:MET:HE1	1.73	0.69
1:A:218:ILE:HD11	1:A:406:ARG:HG2	1.77	0.66
1:A:3:LEU:N	5:A:643:HOH:O	2.29	0.65
1:A:218:ILE:CD1	1:A:406:ARG:HG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:HIS:HE1	1:A:63:GLU:HG3	1.62	0.64
1:A:30:GLU:HG3	1:A:40:ALA:HA	1.81	0.63
1:A:27:MET:HE2	1:A:29:ILE:HD11	1.79	0.62
1:A:3:LEU:HD12	1:A:4:ASN:N	2.09	0.61
1:A:93:ARG:NH2	1:A:319:ASP:OD1	2.27	0.61
1:A:375:ALA:N	5:A:660:HOH:O	2.30	0.60
1:A:45:ILE:CG2	1:A:387:MET:HE1	2.32	0.59
1:A:61:HIS:CE1	1:A:63:GLU:HG3	2.36	0.59
1:A:3:LEU:HA	1:A:41:ASP:OD1	2.03	0.59
1:A:309:LEU:C	1:A:309:LEU:HD23	2.29	0.58
1:A:3:LEU:HD13	1:A:41:ASP:OD2	2.04	0.57
1:A:226:MET:HE1	1:A:242:LEU:HD11	1.88	0.56
1:A:218:ILE:HD11	1:A:406:ARG:HA	1.87	0.56
1:A:398:LEU:HD22	1:A:398:LEU:N	2.20	0.56
1:A:27:MET:CE	1:A:29:ILE:HD11	2.36	0.55
1:A:138:TRP:HB2	1:A:215:SER:HB3	1.88	0.54
1:A:157:VAL:N	5:A:682:HOH:O	2.30	0.53
1:A:27:MET:HE2	1:A:29:ILE:CD1	2.40	0.52
1:A:218:ILE:HD13	1:A:362:GLY:CA	2.41	0.51
1:A:173:TYR:CE1	1:A:372:LYS:HE2	2.47	0.50
1:A:309:LEU:HB3	1:A:310:PRO:HD3	1.93	0.50
1:A:387:MET:HG2	5:A:676:HOH:O	2.12	0.50
1:A:218:ILE:CD1	1:A:406:ARG:HA	2.41	0.49
1:A:176:ARG:HB2	5:A:679:HOH:O	2.12	0.49
1:A:128:LYS:HE2	5:A:633:HOH:O	2.11	0.49
1:A:407:ILE:HG22	1:A:409:PRO:HD3	1.94	0.48
1:A:243:ASP:OD2	3:A:437:PLP:N1	2.47	0.47
1:A:394:ASN:HA	5:A:581:HOH:O	2.15	0.46
1:A:138:TRP:HA	1:A:149:THR:HG23	1.96	0.46
1:A:423:SER:O	1:A:427:GLN:HG3	2.14	0.46
1:A:218:ILE:HD11	1:A:406:ARG:CG	2.46	0.46
1:A:179:ARG:HD2	1:A:184:ASP:OD2	2.16	0.46
1:A:128:LYS:NZ	5:A:686:HOH:O	2.37	0.45
1:A:61:HIS:CE1	1:A:63:GLU:CG	2.99	0.45
1:A:304:HIS:HD2	5:A:544:HOH:O	2.00	0.44
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.80	0.44
1:A:153:GLY:HA2	5:A:715:HOH:O	2.17	0.44
1:A:398:LEU:N	1:A:398:LEU:CD2	2.81	0.44
1:A:218:ILE:O	1:A:218:ILE:HG22	2.18	0.43
1:A:115:ASN:ND2	1:A:139:HIS:HB3	2.34	0.43
1:A:106:LEU:HB3	1:A:283:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HB2	1:A:219:ILE:HB	1.99	0.43
1:A:128:LYS:HG2	1:A:203:ASN:HA	2.02	0.42
1:A:104:ARG:NH2	1:A:291:GLU:OE2	2.46	0.42
1:A:52:GLN:C	1:A:53:MET:HG2	2.43	0.42
1:A:395:ILE:HG12	1:A:396:VAL:N	2.35	0.41
1:A:102:LEU:HD23	1:A:102:LEU:HA	1.89	0.41
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.92	0.41
1:A:218:ILE:HD13	1:A:362:GLY:HA2	2.03	0.41
1:A:195:LEU:O	1:A:199:GLN:HG3	2.21	0.40
1:A:61:HIS:HE1	1:A:63:GLU:CG	2.30	0.40
1:A:172:THR:HG23	5:A:563:HOH:O	2.21	0.40
1:A:27:MET:HE1	1:A:45:ILE:HD13	2.04	0.40
1:A:97:ILE:HD12	1:A:255:MET:HE3	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	429/433 (99%)	413 (96%)	14 (3%)	2 (0%)	24	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	SER
1	A	249	VAL

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	334/336 (99%)	305 (91%)	29 (9%)	9 7

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	23	THR
1	A	27	MET
1	A	48	PHE
1	A	70	GLU
1	A	93	ARG
1	A	104	ARG
1	A	120	ARG
1	A	136	GLN
1	A	141	MET
1	A	178	GLU
1	A	179	ARG
1	A	189	LEU
1	A	264	THR
1	A	274	LEU
1	A	278	LEU
1	A	292	ARG
1	A	296	LEU
1	A	299	LEU
1	A	329	ARG
1	A	337	LEU
1	A	347	ARG
1	A	361	LEU
1	A	367	LYS
1	A	368	ASP
1	A	371	THR
1	A	373	GLU
1	A	425	LEU
1	A	431	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	259	GLN
1	A	304	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	437	1	15,15,16	1.53	3 (20%)	21,22,23	2.37	8 (38%)
4	MES	A	434	-	12,12,12	0.48	0	15,16,16	0.73	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	437	1	-	4/6/6/8	0/1/1/1
4	MES	A	434	-	-	0/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	437	PLP	C4A-C4	-2.88	1.45	1.51
3	A	437	PLP	C3-C2	2.86	1.43	1.41
3	A	437	PLP	C5-C4	2.69	1.43	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	437	PLP	C6-C5-C4	4.85	122.08	118.10
3	A	437	PLP	C2A-C2-C3	4.23	125.75	120.80
3	A	437	PLP	O4P-C5A-C5	3.63	116.16	109.36
3	A	437	PLP	C3-C2-N1	-3.49	116.55	120.96
3	A	437	PLP	C6-N1-C2	3.48	125.51	119.20
3	A	437	PLP	C5-C6-N1	-3.41	118.29	123.83
3	A	437	PLP	C4A-C4-C5	2.74	123.76	120.94
3	A	437	PLP	O3P-P-O4P	2.52	113.25	106.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	437	PLP	C4-C5-C5A-O4P
3	A	437	PLP	C6-C5-C5A-O4P
3	A	437	PLP	C5A-O4P-P-O1P
3	A	437	PLP	C5A-O4P-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	437	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	52:GLN	C	53:MET	N	1.17
1	A	51:GLY	C	52:GLN	N	1.16

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.