



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 05:20 AM EST

PDB ID : 2DKB
Title : DIALKYLGLYCINE DECARBOXYLASE STRUCTURE: BIFUNCTIONAL
ACTIVE SITE AND ALKALI METAL BINDING SITES
Authors : Toney, M.D.; Hohenester, E.; Jansonius, J.N.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (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)	:	rb-20030345

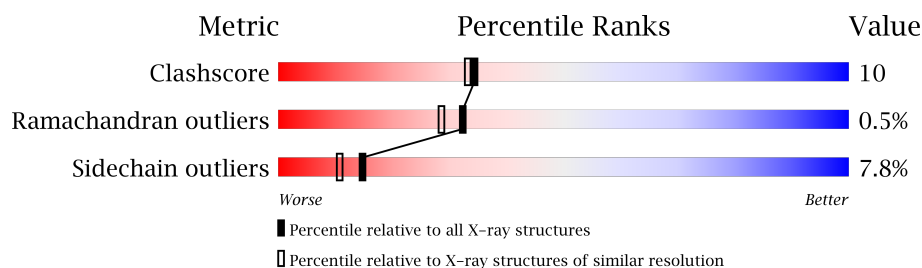
1 Overall quality at a glance

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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	433	 73% 22% .

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			

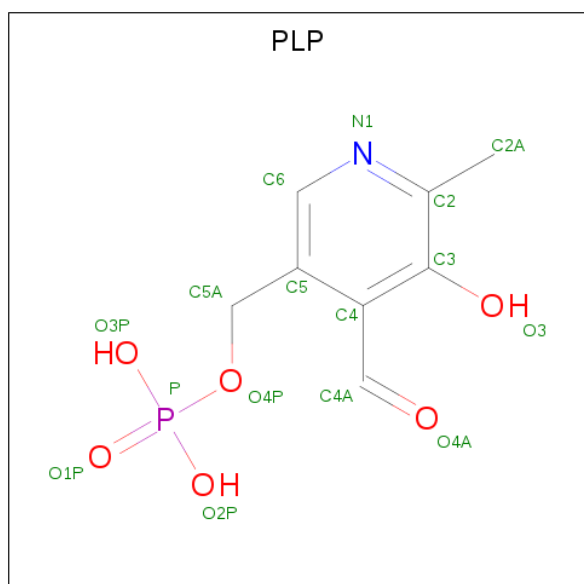
There are 2 discrepancies between the modelled and reference sequences:

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 (three-letter code: NA) (formula: Na).

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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: 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 (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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.

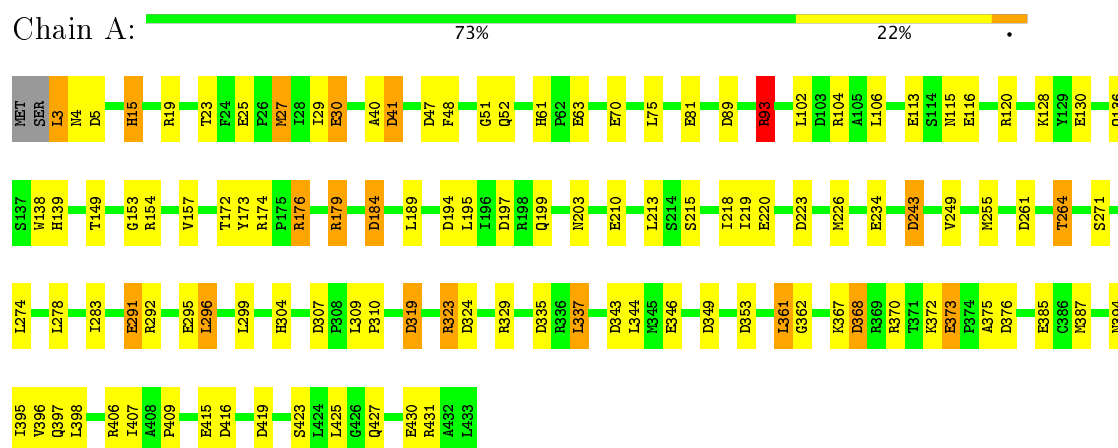
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	229	Total	O	0	0
			229	229		

3 Residue-property plots [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 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: 2,2-DIALKYLGLYCINE DECARBOXYLASE (PYRUVATE)



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: NA, MES, 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	0.90	19/3309 (0.6%)	1.34	50/4478 (1.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	GLY	C-N	-7.70	1.16	1.34
1	A	52	GLN	C-N	-7.21	1.17	1.34
1	A	210	GLU	CD-OE2	6.67	1.32	1.25
1	A	220	GLU	CD-OE1	6.60	1.32	1.25
1	A	234	GLU	CD-OE1	6.30	1.32	1.25
1	A	385	GLU	CD-OE1	5.71	1.31	1.25
1	A	113	GLU	CD-OE1	5.50	1.31	1.25
1	A	415	GLU	CD-OE1	5.48	1.31	1.25
1	A	291	GLU	CD-OE1	5.38	1.31	1.25
1	A	81	GLU	CD-OE2	5.36	1.31	1.25
1	A	295	GLU	CD-OE2	5.36	1.31	1.25
1	A	116	GLU	CD-OE1	5.34	1.31	1.25
1	A	373	GLU	CD-OE1	5.29	1.31	1.25
1	A	70	GLU	CD-OE2	5.25	1.31	1.25
1	A	346	GLU	CD-OE2	5.25	1.31	1.25
1	A	130	GLU	CD-OE2	5.14	1.31	1.25
1	A	30	GLU	CD-OE2	5.08	1.31	1.25
1	A	430	GLU	CD-OE2	5.08	1.31	1.25
1	A	25	GLU	CD-OE1	5.03	1.31	1.25

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	A	51	GLY	O-C-N	-7.95	109.98	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	A	368	ASP	CB-CG-OD1	-7.24	111.78	118.30
1	A	47	ASP	CB-CG-OD1	-7.13	111.88	118.30
1	A	419	ASP	CB-CG-OD1	7.13	124.72	118.30
1	A	41	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	335	ASP	CB-CG-OD1	-6.84	112.14	118.30
1	A	174	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	A	5	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	197	ASP	CB-CG-OD1	6.48	124.13	118.30
1	A	335	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	376	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	323	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	419	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	A	343	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	368	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	197	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	194	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	93	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	223	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	A	226	MET	CG-SD-CE	-6.11	90.43	100.20
1	A	47	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	349	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	A	89	ASP	CB-CG-OD1	6.06	123.76	118.30
1	A	89	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	416	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	A	5	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	319	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	307	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	376	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	176	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	A	343	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	261	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	15	HIS	CB-CA-C	-5.59	99.22	110.40
1	A	194	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	184	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	307	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	349	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	223	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	353	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	416	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	323	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	226	MET	CA-CB-CG	-5.19	104.47	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	93	ARG	CG-CD-NE	-5.15	100.98	111.80
1	A	370	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	243	ASP	CB-CG-OD2	-5.12	113.70	118.30
1	A	19	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	A	41	ASP	CB-CG-OD1	5.06	122.85	118.30

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	3275	58	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	3294	58	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 (58) 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: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
1:A:397:GLN:C	1:A:398:LEU:HD22	2.17	0.65
1:A:61:HIS:HE1	1:A:63:GLU:HG3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:HG3	1:A:40:ALA:HA	1.81	0.63
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: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:128:LYS:NZ	5:A:686:HOH:O	2.37	0.57
1:A:3:LEU:HD13	1:A:41:ASP:OD2	2.04	0.57
1:A:218:ILE:HD11	1:A:406:ARG:HA	1.87	0.56
1:A:398:LEU:N	1:A:398:LEU:HD22	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:309:LEU:C	1:A:309:LEU:HD23	2.29	0.53
1:A:157:VAL:N	5:A:682:HOH:O	2.30	0.53
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:27:MET:HE2	1:A:29:ILE:HD11	1.96	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:27:MET:HE1	1:A:29:ILE:HD11	1.97	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:HA	1:A:296:LEU:HD12	1.80	0.44
1:A:153:GLY:HA2	5:A:715:HOH:O	2.17	0.44
1:A:398:LEU:CD2	1:A:398:LEU:N	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:344:LEU:HD23	1.92	0.41
1:A:218:ILE:HD13	1:A:362:GLY:HA2	2.03	0.41
1:A:27:MET:HE2	1:A:29:ILE:CD1	2.50	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

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%)	32	28

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%)	308 (92%)	26 (8%)	15	11

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	15	HIS
1	A	23	THR
1	A	27	MET
1	A	48	PHE
1	A	75	LEU
1	A	93	ARG
1	A	120	ARG
1	A	136	GLN
1	A	179	ARG
1	A	189	LEU
1	A	255	MET
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	361	LEU
1	A	367	LYS
1	A	368	ASP
1	A	373	GLU
1	A	425	LEU
1	A	431	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

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

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	MES	A	434	-	12,12,12	0.48	0	14,16,16	0.84	0
3	PLP	A	437	1	15,15,16	1.75	3 (20%)	20,22,23	2.32	8 (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
4	MES	A	434	-	-	0/6/14/14	0/1/1/1
3	PLP	A	437	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)
3	A	437	PLP	C4A-C4	-2.85	1.45	1.51
3	A	437	PLP	C5-C4	2.63	1.43	1.40
3	A	437	PLP	C3-C2	4.61	1.43	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	437	PLP	C5-C6-N1	-3.30	118.29	123.87
3	A	437	PLP	C3-C2-N1	-3.19	116.55	120.75
3	A	437	PLP	O3P-P-O4P	2.45	113.25	106.73
3	A	437	PLP	C4A-C4-C5	2.87	123.76	120.86
3	A	437	PLP	C6-N1-C2	3.25	125.51	119.26
3	A	437	PLP	O4P-C5A-C5	3.40	116.16	109.32
3	A	437	PLP	C2A-C2-C3	4.01	125.75	120.96
3	A	437	PLP	C6-C5-C4	4.67	122.08	118.18

There are no chirality outliers.

There are no torsion outliers.

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.