



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:43 PM UTC

PDB ID : 1PJB / pdb_00001pjb
Title : L-ALANINE DEHYDROGENASE
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Deposited on : 1998-06-05
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
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

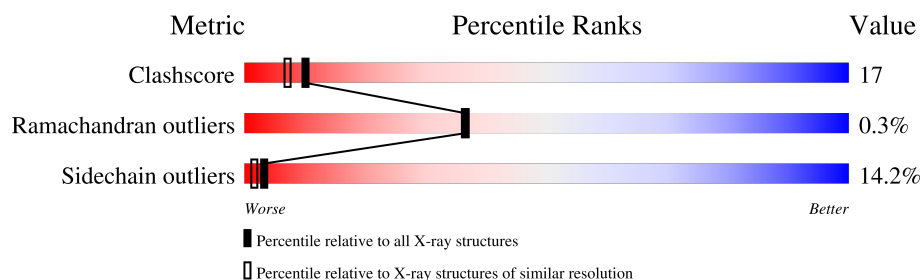
1 Overall quality at a glance

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	361	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2814 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 L-ALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2715	1730	467	509	9			

- Molecule 2 is water.

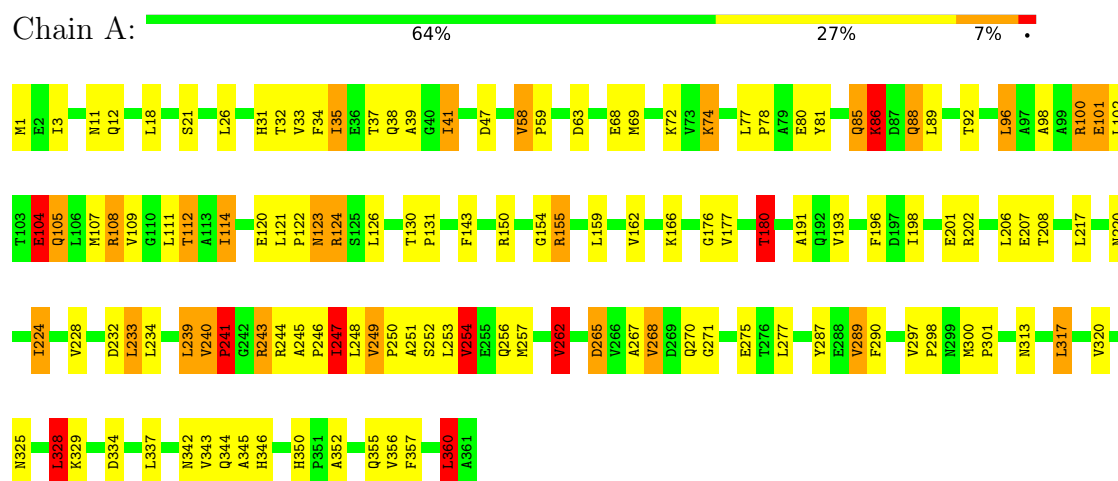
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	99	Total	O	0	0
			99	99		

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: L-ALANINE DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	123.10Å 123.10Å 184.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	86.0 (30.00-2.10)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.190 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2814	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.41	17/2765 (0.6%)	1.16	20/3766 (0.5%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	VAL	CA-CB	8.46	1.65	1.54
1	A	265	ASP	CA-C	-6.81	1.44	1.52
1	A	268	VAL	CA-CB	6.78	1.61	1.54
1	A	92	THR	CA-CB	6.72	1.63	1.53
1	A	177	VAL	CA-CB	6.41	1.61	1.54
1	A	247	ILE	N-CA	-5.94	1.39	1.46
1	A	88	GLN	CB-CG	-5.93	1.34	1.52
1	A	88	GLN	CA-C	-5.80	1.45	1.53
1	A	268	VAL	N-CA	5.62	1.53	1.46
1	A	114	ILE	CA-CB	-5.61	1.47	1.54
1	A	208	THR	CA-CB	5.52	1.62	1.53
1	A	154	GLY	C-O	-5.39	1.17	1.23
1	A	320	VAL	CA-CB	-5.27	1.48	1.54
1	A	180	THR	CA-CB	5.20	1.61	1.53
1	A	289	VAL	CA-CB	5.11	1.61	1.54
1	A	191	ALA	CA-CB	5.04	1.61	1.53
1	A	104	GLU	CA-C	-5.03	1.46	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	LYS	N-CA-C	10.43	123.70	111.71
1	A	41	ILE	N-CA-C	10.00	122.03	110.62
1	A	360	LEU	N-CA-C	-7.70	104.03	113.50
1	A	268	VAL	N-CA-C	7.23	117.95	110.36
1	A	232	ASP	N-CA-C	-7.09	104.26	113.12
1	A	249	VAL	N-CA-C	6.47	114.56	108.15
1	A	248	LEU	N-CA-C	-6.39	105.61	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	VAL	N-CA-C	6.08	117.52	108.46
1	A	240	VAL	CA-C-N	5.90	127.22	119.84
1	A	240	VAL	C-N-CA	5.90	127.22	119.84
1	A	193	VAL	N-CA-C	5.79	116.81	108.48
1	A	328	LEU	N-CA-C	5.57	119.55	112.87
1	A	155	ARG	N-CA-CB	-5.49	101.28	110.39
1	A	96	LEU	N-CA-C	5.48	117.25	111.28
1	A	33	VAL	N-CA-C	5.45	115.75	108.11
1	A	275	GLU	N-CA-C	5.40	117.59	111.11
1	A	102	LEU	N-CA-C	-5.34	105.36	111.07
1	A	241	PRO	N-CA-C	5.08	122.94	112.47
1	A	254	VAL	N-CA-C	5.04	117.35	111.05
1	A	268	VAL	N-CA-CB	5.02	116.08	110.51

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2715	0	2775	95	0
2	A	99	0	0	2	0
All	All	2814	0	2775	95	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 17.

All (95) 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:228:VAL:HG13	1:A:257:MET:HE2	1.38	1.00
1:A:58:VAL:CG1	1:A:63:ASP:HB2	1.93	0.99
1:A:35:ILE:HD11	1:A:39:ALA:HB3	1.45	0.98
1:A:58:VAL:HG11	1:A:63:ASP:HB2	1.50	0.94
1:A:228:VAL:CG1	1:A:257:MET:HE2	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:HG12	1:A:69:MET:HE2	1.57	0.85
1:A:123:ASN:OD1	1:A:123:ASN:N	2.09	0.84
1:A:244:ARG:HG2	1:A:271:GLY:HA3	1.62	0.82
1:A:86:LYS:HG3	1:A:109:VAL:O	1.78	0.82
1:A:155:ARG:NH1	2:A:416:HOH:O	1.84	0.80
1:A:81:TYR:CE2	1:A:105:GLN:HG3	2.15	0.79
1:A:81:TYR:CD2	1:A:105:GLN:HG3	2.20	0.77
1:A:18:LEU:HA	1:A:313:ASN:HD21	1.50	0.76
1:A:58:VAL:HG13	1:A:63:ASP:HB2	1.67	0.74
1:A:37:THR:HG22	1:A:38:GLN:HE21	1.53	0.71
1:A:176:GLY:O	1:A:180:THR:HG23	1.91	0.71
1:A:100:ARG:HD3	1:A:104:GLU:OE2	1.92	0.69
1:A:35:ILE:HD11	1:A:39:ALA:CB	2.20	0.69
1:A:265:ASP:CB	1:A:277:LEU:HD23	2.24	0.67
1:A:120:GLU:HB2	1:A:126:LEU:CD2	2.25	0.67
1:A:120:GLU:HB2	1:A:126:LEU:HD23	1.78	0.66
1:A:345:ALA:O	1:A:346:HIS:HB2	1.97	0.65
1:A:334:ASP:HB3	1:A:337:LEU:HB2	1.79	0.64
1:A:1:MET:H1	1:A:31:HIS:HD2	1.45	0.63
1:A:1:MET:N	1:A:31:HIS:HD2	1.96	0.63
1:A:180:THR:HG21	1:A:202:ARG:HH21	1.63	0.63
1:A:265:ASP:HB2	1:A:277:LEU:HD23	1.82	0.62
1:A:31:HIS:CE1	1:A:325:ASN:OD1	2.54	0.61
1:A:107:MET:O	1:A:346:HIS:HD2	1.83	0.60
1:A:58:VAL:HG13	1:A:59:PRO:HD2	1.82	0.60
1:A:228:VAL:CG1	1:A:257:MET:CE	2.79	0.60
1:A:233:LEU:HD23	1:A:262:VAL:HG22	1.84	0.59
1:A:35:ILE:CD1	1:A:39:ALA:HB3	2.28	0.59
1:A:107:MET:O	1:A:346:HIS:CD2	2.56	0.58
1:A:220:ASN:O	1:A:224:ILE:HG13	2.02	0.58
1:A:265:ASP:HB2	1:A:277:LEU:CD2	2.34	0.58
1:A:313:ASN:O	1:A:317:LEU:HB2	2.04	0.57
1:A:265:ASP:HB3	1:A:277:LEU:HD23	1.86	0.56
1:A:180:THR:CG2	1:A:202:ARG:HH21	2.19	0.55
1:A:247:ILE:N	1:A:247:ILE:HD13	2.20	0.55
1:A:58:VAL:HG11	1:A:63:ASP:CB	2.30	0.54
1:A:86:LYS:HE2	1:A:109:VAL:HA	1.89	0.54
1:A:120:GLU:HG3	1:A:124:ARG:HA	1.90	0.54
1:A:31:HIS:HE1	1:A:325:ASN:OD1	1.89	0.53
1:A:85:GLN:H	1:A:88:GLN:NE2	2.07	0.53
1:A:11:ASN:O	1:A:12:GLN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:SER:O	1:A:256:GLN:HG3	2.10	0.51
1:A:265:ASP:CB	1:A:277:LEU:CD2	2.87	0.51
1:A:245:ALA:HB1	1:A:246:PRO:HD2	1.93	0.51
1:A:251:ALA:HA	1:A:254:VAL:HG13	1.93	0.51
1:A:37:THR:HG23	1:A:47:ASP:OD2	2.11	0.50
1:A:143:PHE:HE2	1:A:300:MET:HG2	1.76	0.50
1:A:96:LEU:C	1:A:98:ALA:H	2.19	0.50
1:A:342:ASN:HA	1:A:350:HIS:HB2	1.95	0.49
1:A:180:THR:HG21	1:A:202:ARG:NH2	2.27	0.49
1:A:317:LEU:HD23	1:A:317:LEU:HA	1.59	0.49
1:A:243:ARG:NH2	1:A:244:ARG:HH21	2.11	0.48
1:A:300:MET:N	1:A:301:PRO:CD	2.76	0.48
1:A:77:LEU:HB3	1:A:78:PRO:HD2	1.96	0.48
1:A:121:LEU:HB3	1:A:122:PRO:HD2	1.96	0.48
1:A:328:LEU:HD21	1:A:344:GLN:OE1	2.14	0.48
1:A:101:GLU:O	1:A:105:GLN:HB2	2.15	0.47
1:A:130:THR:N	1:A:131:PRO:CD	2.76	0.47
1:A:352:ALA:O	1:A:356:VAL:HG23	2.15	0.47
1:A:357:PHE:HB3	1:A:360:LEU:HD22	1.97	0.46
1:A:32:THR:HG23	1:A:34:PHE:CE1	2.50	0.46
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.63	0.46
1:A:360:LEU:HD12	1:A:360:LEU:HA	1.72	0.46
1:A:85:GLN:O	1:A:88:GLN:HG3	2.16	0.45
1:A:345:ALA:O	1:A:346:HIS:CB	2.62	0.45
1:A:240:VAL:HA	1:A:241:PRO:HD3	1.67	0.45
1:A:72:LYS:HB3	1:A:72:LYS:HE3	1.77	0.44
1:A:58:VAL:CG1	1:A:63:ASP:CB	2.80	0.44
1:A:105:GLN:HA	1:A:108:ARG:HG3	2.00	0.44
1:A:112:THR:HA	1:A:343:VAL:O	2.18	0.44
1:A:180:THR:HG21	1:A:206:LEU:HD21	1.98	0.44
1:A:300:MET:HB2	1:A:301:PRO:HD3	2.00	0.43
1:A:196:PHE:HA	1:A:217:LEU:O	2.19	0.43
1:A:277:LEU:HA	1:A:287:TYR:OH	2.17	0.42
1:A:289:VAL:O	1:A:290:PHE:HB2	2.18	0.42
1:A:34:PHE:CD1	1:A:34:PHE:N	2.87	0.42
1:A:150:ARG:NH1	2:A:387:HOH:O	2.52	0.42
1:A:297:VAL:HA	1:A:298:PRO:HD3	1.76	0.42
1:A:74:LYS:HA	1:A:74:LYS:HD2	1.34	0.42
1:A:357:PHE:HB3	1:A:360:LEU:CD2	2.49	0.42
1:A:1:MET:H1	1:A:31:HIS:CD2	2.33	0.41
1:A:89:LEU:HA	1:A:89:LEU:HD23	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LEU:HD12	1:A:267:ALA:CA	2.50	0.41
1:A:120:GLU:OE2	1:A:124:ARG:HG3	2.21	0.41
1:A:86:LYS:CG	1:A:109:VAL:O	2.61	0.41
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.94	0.41
1:A:247:ILE:N	1:A:247:ILE:CD1	2.80	0.41
1:A:249:VAL:HA	1:A:250:PRO:HD2	1.82	0.41
1:A:77:LEU:HB3	1:A:78:PRO:CD	2.51	0.40
1:A:239:LEU:HD12	1:A:267:ALA:HA	2.04	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	359/361 (99%)	343 (96%)	15 (4%)	1 (0%)	36	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	PRO

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	289/289 (100%)	248 (86%)	41 (14%)	3 1

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	26	LEU
1	A	35	ILE
1	A	41	ILE
1	A	58	VAL
1	A	68	GLU
1	A	74	LYS
1	A	80	GLU
1	A	85	GLN
1	A	86	LYS
1	A	100	ARG
1	A	101	GLU
1	A	104	GLU
1	A	105	GLN
1	A	108	ARG
1	A	111	LEU
1	A	112	THR
1	A	114	ILE
1	A	123	ASN
1	A	124	ARG
1	A	166	LYS
1	A	180	THR
1	A	198	ILE
1	A	201	GLU
1	A	207	GLU
1	A	224	ILE
1	A	233	LEU
1	A	234	LEU
1	A	239	LEU
1	A	243	ARG
1	A	247	ILE
1	A	253	LEU
1	A	254	VAL
1	A	262	VAL
1	A	268	VAL
1	A	270	GLN
1	A	317	LEU
1	A	328	LEU

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Mol	Chain	Res	Type
1	A	329	LYS
1	A	355	GLN
1	A	360	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	38	GLN
1	A	88	GLN
1	A	105	GLN
1	A	142	GLN
1	A	282	HIS
1	A	313	ASN
1	A	346	HIS
1	A	355	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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.