



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:38 AM UTC

PDB ID : 3LDH / pdb_00003ldh
Title : A comparison of the structures of apo dogfish m4 lactate dehydrogenase and its ternary complexes
Authors : White, J.L.; Hackert, M.L.; Buehner, M.; Adams, M.J.; Ford, G.C.; Lentzjunior, P.J.; Smiley, I.E.; Steindel, S.J.; Rossmann, M.G.
Deposited on : 1974-06-06
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

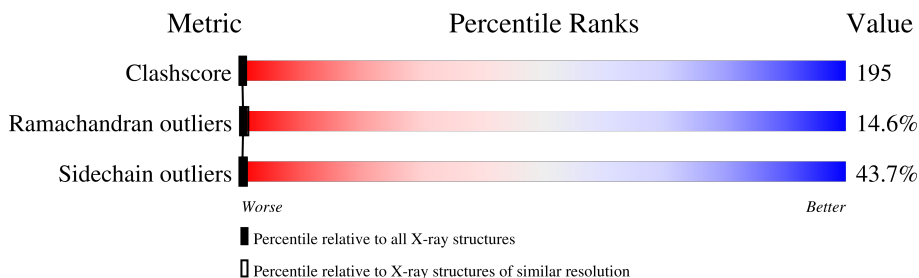
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 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	330	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	A	332	-	-	X	-
3	PYR	A	333	-	X	X	-

2 Entry composition [i](#)

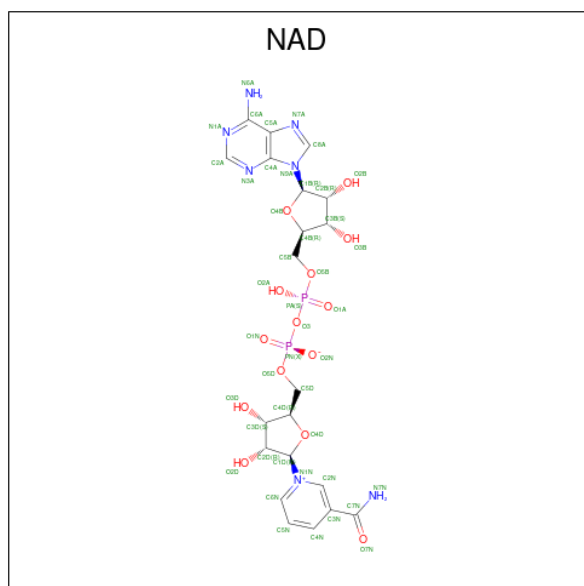
There are 3 unique types of molecules in this entry. The entry contains 2604 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2554	1624	437	474	19			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0

i

Note EDS was not executed.

Chain A:

Category	Count
I302	661
V303	1123
K304	1124
M305	1244
K306	1485
L307	1486
K308	1817
A248	1818
V249	1819
K250	1919
G251	1920
E311	1921
E312	1922
Q313	1923
Q314	1924
L315	1925
Q316	1926
K317	1927
S318	1928
K319	1929
T320	1930
T321	1931
L322	1932
W323	1933
D324	1934
L325	1935
Q326	1936
K327	1937
D328	1938
L329	1939
K330	1940
F331	1941
D242	1261
V243	1262
L244	1263
T245	1264
V246	1265
A247	1266
A248	1267
V249	1268
K250	1269
G251	1270
E252	1271
S253	1272
V254	1273
A255	1274
D256	1275
L257	1276
K258	1277
V259	1278
T260	1279
T261	1280
K262	1281
D263	1282
D264	1283
D265	1284
D266	1285
D267	1286
D268	1287
D269	1288
D270	1289
D271	1290
D272	1291
D273	1292
D274	1293
D275	1294
D276	1295
D277	1296
D278	1297
D279	1298
D280	1299
D281	1300
D282	1301
D283	1302
D284	1303
D285	1304
D286	1305
D287	1306
D288	1307
D289	1308
D290	1309
D291	1310
D292	1311
D293	1312
D294	1313
D295	1314
D296	1315
D297	1316
D298	1317
D299	1318
D300	1319
D301	1320
D302	1321
D303	1322
D304	1323
D305	1324
D306	1325
D307	1326
D308	1327
D309	1328
D310	1329
D311	1330
D312	1331
D313	1332
D314	1333
D315	1334
D316	1335
D317	1336
D318	1337
D319	1338
D320	1339
D321	1340
D322	1341
D323	1342
D324	1343
D325	1344
D326	1345
D327	1346
D328	1347
D329	1348
D330	1349
D331	1350
D332	1351
D333	1352
D334	1353
D335	1354
D336	1355
D337	1356
D338	1357
D339	1358
D340	1359
D341	1360
D342	1361
D343	1362
D344	1363
D345	1364
D346	1365
D347	1366
D348	1367
D349	1368
D350	1369
D351	1370
D352	1371
D353	1372
D354	1373
D355	1374
D356	1375
D357	1376
D358	1377
D359	1378
D360	1379
D361	1380
D362	1381
D363	1382
D364	1383
D365	1384
D366	1385
D367	1386
D368	1387
D369	1388
D370	1389
D371	1390
D372	1391
D373	1392
D374	1393
D375	1394
D376	1395
D377	1396
D378	1397
D379	1398
D380	1399
D381	1400
D382	1401
D383	1402
D384	1403
D385	1404
D386	1405
D387	1406
D388	1407
D38	

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.50Å 134.50Å 85.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2604	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PYR, NAD, ACE

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	1.25	31/2600 (1.2%)	2.00	130/3515 (3.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	TRP	NE1-CE2	-8.63	1.27	1.37
1	A	150	TRP	NE1-CE2	-8.61	1.27	1.37
1	A	249	TRP	NE1-CE2	-8.59	1.27	1.37
1	A	323	TRP	NE1-CE2	-8.56	1.28	1.37
1	A	203	TRP	NE1-CE2	-8.56	1.28	1.37

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	VAL	N-CA-C	-24.52	84.61	112.80
1	A	220	TYR	N-CA-C	18.75	150.74	110.80
1	A	250	LYS	N-CA-C	-18.42	90.91	113.20
1	A	291	CYS	N-CA-C	-14.40	87.18	109.07
1	A	227	GLY	N-CA-C	-13.27	95.62	113.27

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Sidechain
1	A	159	ARG	Sidechain
1	A	171	ARG	Sidechain
1	A	173	ARG	Sidechain

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	2554	0	2601	1016	1107
2	A	44	0	25	52	22
3	A	6	0	0	10	0
All	All	2604	0	2626	1021	1107

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 195.

The worst 5 of 1021 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:123:ILE:HG22	1:A:127:ILE:CD1	1.25	1.57
1:A:281:ILE:HG21	1:A:285:VAL:CG2	1.34	1.53
1:A:289:LEU:CD2	1:A:290:PRO:HD2	1.35	1.52
1:A:123:ILE:CG2	1:A:127:ILE:HD11	1.39	1.52
1:A:199:VAL:HG13	1:A:231:TRP:CZ2	1.44	1.50

The worst 5 of 1107 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:CD1	1:A:129:LYS:C[16_555]	0.17	2.03
1:A:119:ILE:C	1:A:252:CYS:CA[4_555]	0.20	2.00
1:A:33:GLY:CA	1:A:52:VAL:CG1[16_555]	0.21	1.99
1:A:211:LEU:CG	1:A:321:THR:CA[3_545]	0.21	1.99
1:A:99:GLY:C	1:A:244:LEU:CA[4_555]	0.22	1.98

5.3 Torsion angles

5.3.1 Protein backbone

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	328/330 (99%)	184 (56%)	96 (29%)	48 (15%)	0 0

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	30	ASP
1	A	31	ALA
1	A	70	SER
1	A	76	ALA

5.3.2 Protein sidechains

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	286/286 (100%)	161 (56%)	125 (44%)	0 0

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	ILE
1	A	306	LYS
1	A	197	ASP
1	A	299	HIS
1	A	321	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	A	301	ASN
1	A	194	GLN
1	A	295	ASN
1	A	166	ASN

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](#)

2 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	PYR	A	333	-	5,5,5	6.20	4 (80%)	3,6,6	4.16	3 (100%)
2	NAD	A	332	-	46,48,48	2.66	17 (36%)	64,73,73	2.62	17 (26%)

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	PYR	A	333	-	-	0/4/4/4	-
2	NAD	A	332	-	-	6/30/62/62	0/5/5/5

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	333	PYR	CB-CA	9.18	1.68	1.50
2	A	332	NAD	C4N-C3N	8.38	1.52	1.39
3	A	333	PYR	O3-CA	8.21	1.41	1.23
2	A	332	NAD	C5N-C4N	5.97	1.49	1.38
2	A	332	NAD	C2N-N1N	5.63	1.41	1.35

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	332	NAD	C5N-C4N-C3N	-10.57	109.97	120.36
2	A	332	NAD	C6N-N1N-C1D	8.65	136.71	119.73
2	A	332	NAD	C2N-N1N-C1D	-6.42	104.97	119.13
2	A	332	NAD	O7N-C7N-C3N	-5.71	112.62	119.60
3	A	333	PYR	O3-CA-CB	-5.62	107.17	119.77

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	332	NAD	C5B-O5B-PA-O1A
2	A	332	NAD	C5B-O5B-PA-O2A
2	A	332	NAD	C5B-O5B-PA-O3
2	A	332	NAD	PA-O3-PN-O5D
2	A	332	NAD	O4B-C4B-C5B-O5B

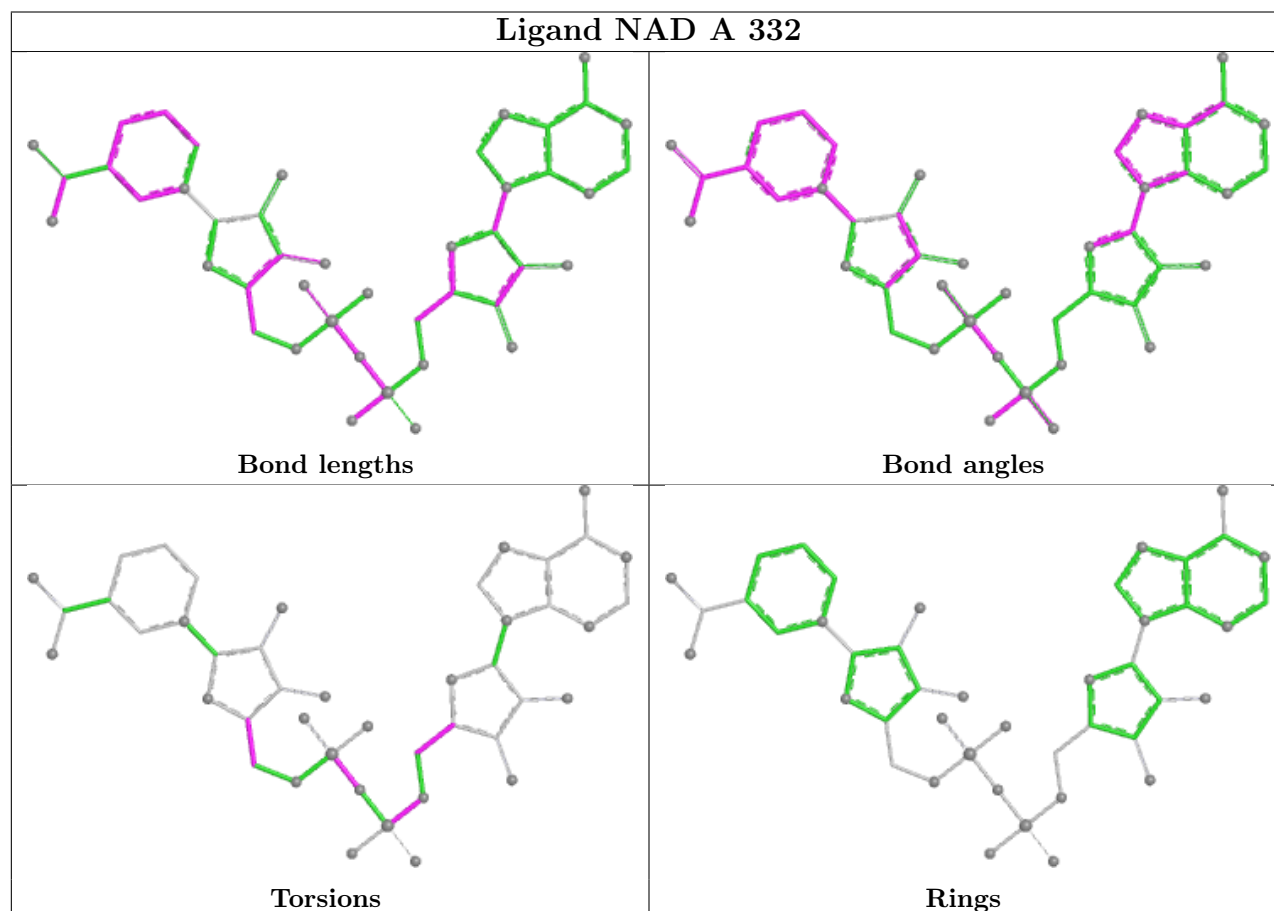
There are no ring outliers.

2 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	333	PYR	10	0
2	A	332	NAD	52	22

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.