



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:11 PM UTC

PDB ID : 1GKX / pdb_00001gkx
Title : Branched-chain alpha-ketoacid dehydrogenase kinase (BCK)
Authors : Machius, M.; Chuang, J.L.; Wynn, R.M.; Tomchick, D.R.; Chuang, D.T.
Deposited on : 2001-08-21
Resolution : 2.30 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

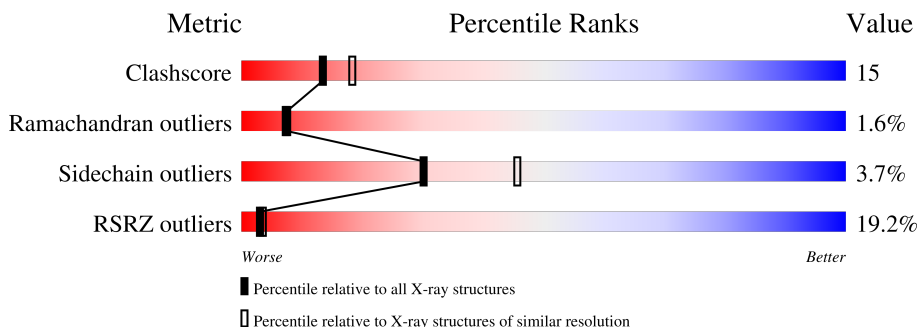
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	388	

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	CL	A	504	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2582 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 [3-METHYL-2-OXOBUTANOATE DEHYDROGENASE [LIPOAMIDE]] KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2491	1586	453	441	11			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cl	0	0
			4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		

- Molecule 1: [3-METHYL-2-OXOBUTANOATE DEHYDROGENASE [LIPOAMIDE]] KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.37Å 129.37Å 73.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.52 – 2.30 48.52 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.0 (48.52-2.30) 94.0 (48.52-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.273 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2582	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.48	1/2545 (0.0%)	0.97	13/3439 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	PRO	C-N	-5.16	1.26	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	PRO	CA-N-CD	-17.89	86.96	112.00
1	A	43	THR	CA-C-N	-9.49	106.51	122.64
1	A	43	THR	C-N-CA	-9.49	106.51	122.64
1	A	42	PRO	N-CA-CB	9.27	112.98	103.25
1	A	67	GLU	N-CA-C	7.32	119.05	111.14
1	A	157	ARG	N-CA-C	-7.05	103.67	111.36
1	A	221	ARG	N-CA-C	-6.41	102.26	110.53
1	A	268	VAL	N-CA-C	-6.31	99.33	108.36
1	A	49	GLY	N-CA-C	5.52	121.22	110.73
1	A	242	ILE	N-CA-C	5.25	115.69	110.23
1	A	278	ASP	N-CA-C	5.12	116.60	108.96
1	A	265	VAL	N-CA-C	5.10	113.50	107.84
1	A	42	PRO	CB-CA-C	-5.08	103.19	111.56

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	2491	0	2527	74	0
2	A	4	0	0	2	0
3	A	87	0	0	2	0
All	All	2582	0	2527	74	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 15.

All (74) 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:255:MET:HE1	1:A:265:VAL:HG21	1.38	1.00
1:A:274:ASN:HD21	1:A:378:GLU:HA	1.39	0.87
1:A:62:ARG:O	1:A:66:GLN:HG2	1.84	0.77
1:A:179:ALA:O	1:A:182:GLU:HG3	1.84	0.76
1:A:302:HIS:HB2	1:A:337:GLY:N	2.03	0.73
1:A:356:LEU:HD22	1:A:366:VAL:HG22	1.72	0.71
1:A:220:PRO:HG3	1:A:255:MET:HE3	1.74	0.70
1:A:67:GLU:HG3	1:A:71:ARG:HE	1.55	0.70
1:A:118:GLU:OE2	1:A:177:HIS:HE1	1.75	0.69
1:A:274:ASN:HD21	1:A:378:GLU:CA	2.07	0.68
1:A:198:LYS:O	1:A:202:GLU:HG3	1.94	0.67
1:A:155:LEU:O	1:A:156:VAL:HG23	1.94	0.66
1:A:244:PRO:O	1:A:248:LYS:HG3	1.97	0.65
1:A:51:SER:HA	1:A:56:HIS:CE1	2.34	0.63
1:A:237:MET:HB3	1:A:238:PRO:HD3	1.81	0.62
1:A:41:THR:HG22	1:A:42:PRO:HD2	1.82	0.62
1:A:344:ARG:O	1:A:348:GLU:HG3	2.00	0.61
1:A:373:ILE:O	1:A:375:GLY:N	2.35	0.59
1:A:41:THR:HB	1:A:44:MET:HG2	1.83	0.59
1:A:57:LEU:HD13	1:A:181:HIS:CE1	2.38	0.58
1:A:93:LEU:O	1:A:97:GLU:HG3	2.04	0.58
1:A:114:ASP:OD1	1:A:116:ALA:HB3	2.05	0.57
1:A:60:SER:OG	1:A:177:HIS:HD2	1.88	0.57
1:A:75:ARG:HA	1:A:75:ARG:CZ	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ARG:HB2	2:A:504:CL:CL	2.42	0.55
1:A:67:GLU:CG	1:A:71:ARG:HE	2.16	0.55
1:A:220:PRO:CG	1:A:255:MET:HE3	2.36	0.55
1:A:144:ARG:HG2	1:A:144:ARG:HH11	1.72	0.55
1:A:50:ARG:O	1:A:50:ARG:HG3	2.08	0.53
1:A:146:SER:O	1:A:150:ILE:HG12	2.08	0.53
1:A:42:PRO:C	1:A:44:MET:N	2.65	0.52
1:A:39:ARG:HD3	1:A:191:ILE:HD13	1.91	0.52
1:A:122:CYS:O	1:A:126:ARG:HG3	2.09	0.52
1:A:171:ARG:HD2	2:A:504:CL:CL	2.47	0.51
1:A:75:ARG:HG2	1:A:99:TYR:CE2	2.46	0.51
1:A:220:PRO:HG3	1:A:255:MET:CE	2.38	0.51
1:A:51:SER:HA	1:A:56:HIS:ND1	2.26	0.50
1:A:141:GLU:O	1:A:145:GLU:HG3	2.12	0.50
1:A:373:ILE:HG22	1:A:374:ASP:OD1	2.13	0.49
1:A:42:PRO:C	1:A:44:MET:H	2.21	0.49
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.78	0.49
1:A:84:PHE:CZ	1:A:88:CYS:SG	3.06	0.49
1:A:359:LEU:HD12	1:A:359:LEU:N	2.28	0.48
1:A:377:GLU:HG2	1:A:378:GLU:H	1.78	0.48
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.12	0.48
1:A:210:ARG:HH11	1:A:210:ARG:HG3	1.79	0.47
1:A:166:SER:HB2	3:A:2005:HOH:O	2.13	0.47
1:A:222:VAL:HG22	1:A:268:VAL:HB	1.97	0.46
1:A:58:LEU:O	1:A:62:ARG:HG3	2.14	0.46
1:A:340:LEU:N	1:A:341:PRO:HD2	2.30	0.46
1:A:185:PRO:O	1:A:186:ASP:HB2	2.16	0.46
1:A:38:VAL:HG12	1:A:38:VAL:O	2.15	0.46
1:A:254:THR:HG22	1:A:255:MET:HE2	1.98	0.46
1:A:121:TYR:O	1:A:125:VAL:HG23	2.16	0.45
1:A:198:LYS:HD2	1:A:228:VAL:HB	1.97	0.45
1:A:276:ASP:HB3	1:A:376:ARG:HB2	1.98	0.45
1:A:289:GLY:HA2	1:A:364:THR:OG1	2.17	0.45
1:A:167:ARG:HH11	1:A:167:ARG:HG2	1.83	0.44
1:A:299:MET:HE2	1:A:344:ARG:NE	2.33	0.43
1:A:144:ARG:HG2	1:A:144:ARG:NH1	2.33	0.43
1:A:48:SER:OG	1:A:188:VAL:HG11	2.18	0.43
1:A:39:ARG:CD	1:A:191:ILE:HD13	2.48	0.43
1:A:377:GLU:HG2	1:A:378:GLU:N	2.33	0.43
1:A:231:ARG:NH1	3:A:2045:HOH:O	2.52	0.43
1:A:176:HIS:HA	1:A:190:ILE:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:HG2	1:A:221:ARG:HH11	1.85	0.42
1:A:247:LEU:HD21	1:A:270:ILE:HD11	2.02	0.42
1:A:147:ARG:HA	1:A:150:ILE:HG12	2.02	0.41
1:A:160:LEU:HD23	1:A:160:LEU:HA	1.90	0.41
1:A:195:LEU:O	1:A:231:ARG:HA	2.20	0.41
1:A:196:SER:HB3	1:A:199:LYS:HB2	2.03	0.41
1:A:150:ILE:HD12	1:A:156:VAL:HG21	2.01	0.41
1:A:100:ILE:O	1:A:104:GLN:HG3	2.20	0.41
1:A:44:MET:HE1	1:A:169:GLY:HA2	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	304/388 (78%)	282 (93%)	17 (6%)	5 (2%)	7 7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	156	VAL
1	A	374	ASP
1	A	51	SER
1	A	43	THR

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	271/340 (80%)	261 (96%)	10 (4%)	30	45

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	75	ARG
1	A	124	LEU
1	A	151	GLU
1	A	155	LEU
1	A	173	LEU
1	A	182	GLU
1	A	206	ASP
1	A	298	VAL
1	A	303	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	120	GLN
1	A	177	HIS
1	A	249	ASN
1	A	274	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	308/388 (79%)	1.21	59 (19%) 3 3	38, 61, 111, 133	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	VAL	12.5
1	A	40	LEU	10.3
1	A	303	PHE	6.8
1	A	155	LEU	6.7
1	A	42	PRO	6.7
1	A	41	THR	5.6
1	A	377	GLU	5.4
1	A	43	THR	5.4
1	A	376	ARG	5.2
1	A	53	ASP	5.0
1	A	158	TYR	4.5
1	A	156	VAL	4.5
1	A	241	TYR	4.2
1	A	45	MET	4.2
1	A	378	GLU	4.2
1	A	138	LEU	3.3
1	A	214	HIS	3.3
1	A	337	GLY	3.2
1	A	374	ASP	3.1
1	A	298	VAL	3.0
1	A	47	TYR	3.0
1	A	50	ARG	2.9
1	A	54	GLY	2.9
1	A	154	LYS	2.9
1	A	48	SER	2.9
1	A	185	PRO	2.8
1	A	51	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	55	SER	2.8
1	A	180	LEU	2.8
1	A	338	PHE	2.8
1	A	302	HIS	2.7
1	A	300	ASP	2.7
1	A	88	CYS	2.7
1	A	162	LYS	2.6
1	A	157	ARG	2.6
1	A	115	GLN	2.5
1	A	297	ARG	2.5
1	A	153	GLU	2.5
1	A	46	LEU	2.4
1	A	148	LYS	2.4
1	A	296	ASP	2.4
1	A	210	ARG	2.4
1	A	373	ILE	2.4
1	A	44	MET	2.4
1	A	301	TYR	2.4
1	A	144	ARG	2.4
1	A	344	ARG	2.4
1	A	375	GLY	2.3
1	A	184	LYS	2.3
1	A	356	LEU	2.3
1	A	104	GLN	2.3
1	A	147	ARG	2.2
1	A	252	ARG	2.2
1	A	141	GLU	2.2
1	A	59	LYS	2.2
1	A	188	VAL	2.1
1	A	52	GLN	2.1
1	A	116	ALA	2.0
1	A	139	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	A	501	1/1	0.83	0.43	110,110,110,110	0
2	CL	A	503	1/1	0.87	0.27	110,110,110,110	0
2	CL	A	504	1/1	0.91	0.14	90,90,90,90	0
2	CL	A	502	1/1	0.92	0.19	103,103,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.