



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:24 PM UTC

PDB ID : 4UY9 / pdb_00004uy9
Title : Structure of MLK1 kinase domain with leucine zipper 1
Authors : Read, J.A.; Brassington, C.; Pollard, H.K.; Phillips, C.; Green, I.; Overmann, R.; Collier, M.
Deposited on : 2014-08-29
Resolution : 2.81 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

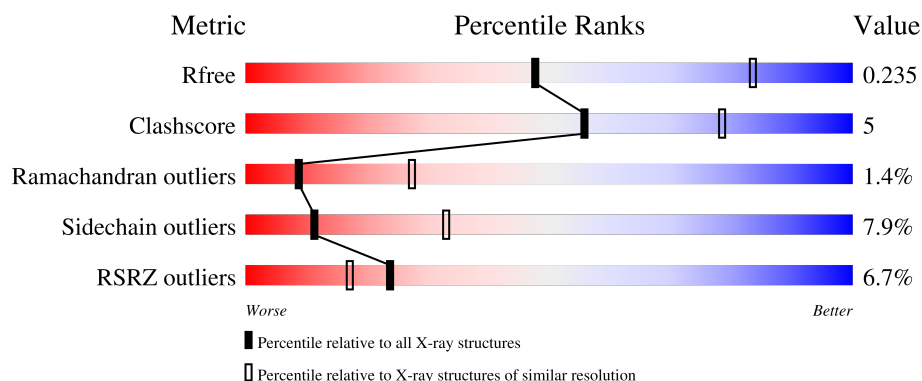
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	323	3% 78% 17% ..
1	B	323	10% 78% 17% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4964 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 MITOGEN-ACTIVATED PROTEIN KINASE KINASE KINASE 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	1	0
			2424	1558	420	431	15			
1	B	315	Total	C	N	O	S	0	0	0
			2371	1524	402	431	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	GLY	-	expression tag	UNP P80192
B	134	GLY	-	expression tag	UNP P80192

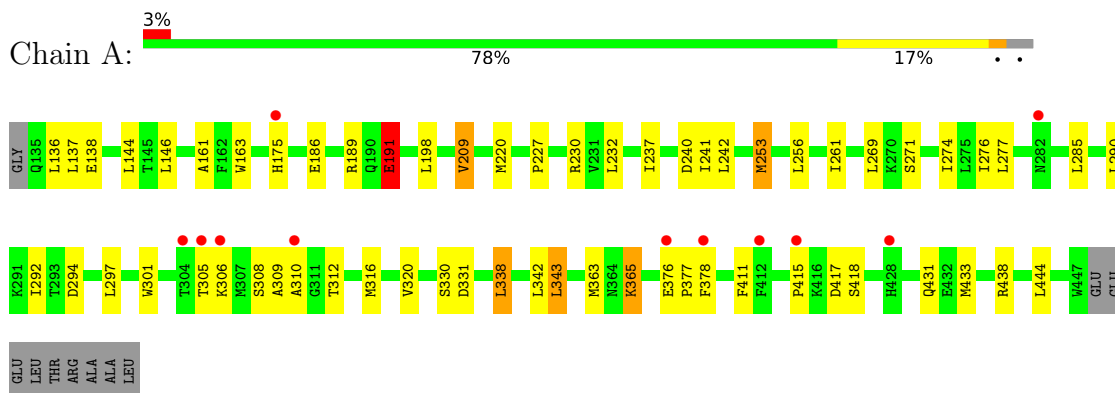
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	89	Total	O	0	0
			89	89		
2	B	80	Total	O	0	0
			80	80		

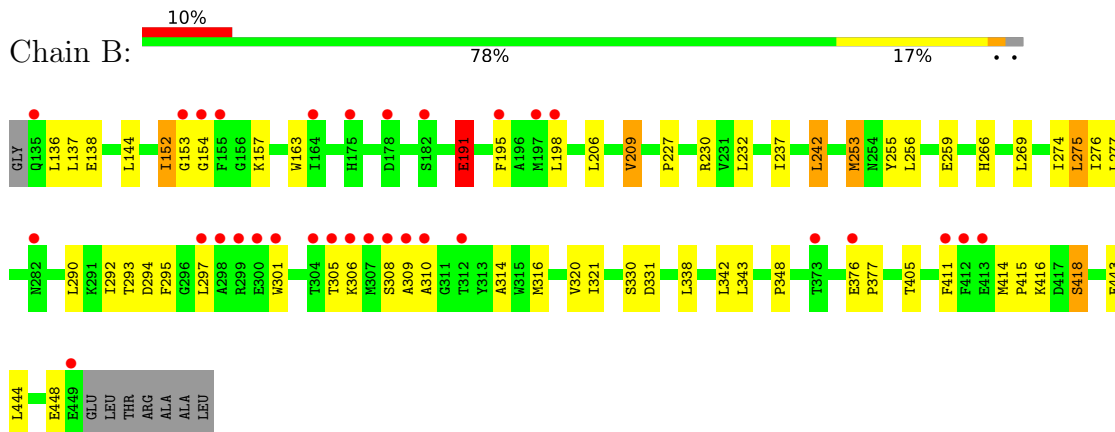
3 Residue-property plots

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 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.

• Molecule 1: MITOGEN-ACTIVATED PROTEIN KINASE KINASE KINASE 9



• Molecule 1: MITOGEN-ACTIVATED PROTEIN KINASE KINASE KINASE 9



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.93Å 96.93Å 416.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	77.87 – 2.81 77.87 – 2.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (77.87-2.81) 100.0 (77.87-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.187 , 0.228 0.198 , 0.235	Depositor DCC
R_{free} test set	1494 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4964	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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

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	0.88	1/2485 (0.0%)	1.41	7/3383 (0.2%)
1	B	0.90	1/2430 (0.0%)	1.43	10/3318 (0.3%)
All	All	0.89	2/4915 (0.0%)	1.42	17/6701 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	MET	SD-CE	-6.06	1.64	1.79
1	B	253	MET	SD-CE	-5.82	1.65	1.79

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	GLU	N-CA-C	-11.06	93.86	109.24
1	A	376	GLU	CA-C-O	-8.78	113.59	119.29
1	A	376	GLU	N-CA-C	-8.14	93.90	108.47
1	B	376	GLU	CA-C-O	-6.96	114.17	119.32
1	B	331	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	331	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	416	LYS	CA-C-N	6.30	129.05	120.54
1	B	416	LYS	C-N-CA	6.30	129.05	120.54
1	A	240	ASP	CA-CB-CG	6.24	118.84	112.60
1	B	154	GLY	CA-C-N	6.08	129.26	120.38
1	B	154	GLY	C-N-CA	6.08	129.26	120.38
1	A	191	GLU	CB-CG-CD	5.48	121.91	112.60
1	B	191	GLU	CB-CG-CD	5.45	121.86	112.60
1	B	405	THR	CA-C-N	5.13	127.48	120.46
1	B	405	THR	C-N-CA	5.13	127.48	120.46
1	A	241	ILE	CA-C-N	5.10	127.07	120.44
1	A	241	ILE	C-N-CA	5.10	127.07	120.44

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	2424	0	2349	19	0
1	B	2371	0	2226	25	0
2	A	89	0	0	1	0
2	B	80	0	0	0	0
All	All	4964	0	4575	44	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 5.

All (44) 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:191:GLU:HG2	1:A:301:TRP:CD1	2.03	0.94
1:A:237:ILE:HG13	1:A:285:LEU:HD13	1.56	0.87
1:B:191:GLU:HG3	1:B:301:TRP:CD1	2.20	0.77
1:A:175:HIS:HA	2:A:2011:HOH:O	1.97	0.64
1:A:253:MET:HE2	1:A:292:ILE:HD13	1.81	0.62
1:B:136:LEU:HD11	1:B:209:VAL:HG22	1.83	0.59
1:B:253:MET:HE2	1:B:292:ILE:HD13	1.83	0.59
1:B:152:ILE:HG12	1:B:157:LYS:HG2	1.86	0.57
1:A:363:MET:HB2	1:A:365:LYS:HD3	1.89	0.54
1:B:415:PRO:HG2	1:B:418:SER:HB2	1.89	0.53
1:B:191:GLU:CG	1:B:301:TRP:CD1	2.91	0.53
1:A:343:LEU:HD21	1:A:378:PHE:CD1	2.45	0.52
1:B:314:ALA:HB1	1:B:348:PRO:HB2	1.91	0.51
1:A:186:GLU:HG3	1:A:189:ARG:NH2	2.26	0.51
1:A:144:LEU:HD23	1:A:163:TRP:HB2	1.92	0.50
1:B:414:MET:HE2	1:B:418:SER:HB3	1.93	0.50
1:B:144:LEU:HD23	1:B:163:TRP:HB2	1.93	0.50
1:B:316:MET:HE2	1:B:321:ILE:HG12	1.95	0.49
1:B:152:ILE:HD13	1:B:153:GLY:H	1.78	0.49
1:B:255:TYR:HA	1:B:259:GLU:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:MET:HE3	1:B:320:VAL:HG12	1.95	0.48
1:B:198:LEU:HD11	1:B:297:LEU:HD21	1.96	0.47
1:A:232:LEU:HD21	1:A:342:LEU:HD23	1.97	0.47
1:B:237:ILE:HG13	1:B:242:LEU:HD12	1.97	0.46
1:A:415:PRO:HG2	1:A:418:SER:HB2	1.98	0.45
1:B:266:HIS:CD2	1:B:295:PHE:HB3	2.51	0.45
1:A:316:MET:HE3	1:A:320:VAL:HG12	1.98	0.45
1:A:136:LEU:HD11	1:A:209:VAL:HG22	1.99	0.45
1:B:232:LEU:HD21	1:B:342:LEU:HD23	1.98	0.45
1:B:237:ILE:HD11	1:B:242:LEU:HG	1.98	0.44
1:B:237:ILE:CG1	1:B:242:LEU:HD12	2.49	0.43
1:B:306:LYS:C	1:B:308:SER:H	2.28	0.42
1:B:227:PRO:HG2	1:B:230:ARG:HG3	2.03	0.41
1:A:198:LEU:HD11	1:A:297:LEU:HD21	2.01	0.41
1:A:276:ILE:HG13	1:A:290:LEU:HD22	2.02	0.41
1:B:276:ILE:HG13	1:B:290:LEU:HD22	2.02	0.41
1:A:306:LYS:C	1:A:308:SER:H	2.28	0.41
1:B:275:LEU:HD22	1:B:293:THR:HG21	2.03	0.41
1:B:269:LEU:HD11	1:B:274:ILE:HD11	2.02	0.41
1:A:146:LEU:HD23	1:A:161:ALA:HB2	2.03	0.41
1:B:195:PHE:HB3	1:B:206:LEU:HD22	2.02	0.40
1:A:271:SER:N	1:A:338:LEU:HD11	2.37	0.40
1:A:227:PRO:HG2	1:A:230:ARG:HG3	2.04	0.40
1:A:269:LEU:HD11	1:A:274:ILE:HD11	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	312/323 (97%)	300 (96%)	7 (2%)	5 (2%)	7 24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	313/323 (97%)	302 (96%)	7 (2%)	4 (1%)	9	29
All	All	625/646 (97%)	602 (96%)	14 (2%)	9 (1%)	9	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	PRO
1	B	377	PRO
1	A	310	ALA
1	A	309	ALA
1	A	411	PHE
1	B	309	ALA
1	B	310	ALA
1	B	411	PHE
1	A	417	ASP

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	247/276 (90%)	227 (92%)	20 (8%)	11	32
1	B	232/276 (84%)	214 (92%)	18 (8%)	11	34
All	All	479/552 (87%)	441 (92%)	38 (8%)	11	33

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	138	GLU
1	A	191	GLU
1	A	209	VAL
1	A	220	MET
1	A	242	LEU
1	A	256	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	261	ILE
1	A	277	LEU
1	A	294	ASP
1	A	305	THR
1	A	312	THR
1	A	330	SER
1	A	338	LEU
1	A	343	LEU
1	A	365	LYS
1	A	431	GLN
1	A	433	MET
1	A	438	ARG
1	A	444	LEU
1	B	137	LEU
1	B	138	GLU
1	B	152	ILE
1	B	191	GLU
1	B	209	VAL
1	B	242	LEU
1	B	256	LEU
1	B	275	LEU
1	B	277	LEU
1	B	294	ASP
1	B	305	THR
1	B	330	SER
1	B	338	LEU
1	B	343	LEU
1	B	418	SER
1	B	443	GLU
1	B	444	LEU
1	B	448	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	ASN
1	A	420	HIS
1	B	187	ASN
1	B	254	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](#)

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 [i](#)

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	313/323 (96%)	-0.03	11 (3%)	47 37	42, 69, 114, 129	1 (0%)
1	B	315/323 (97%)	0.27	31 (9%)	13 9	52, 81, 119, 128	0
All	All	628/646 (97%)	0.12	42 (6%)	24 17	42, 76, 117, 129	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	304	THR	5.2
1	B	305	THR	5.1
1	B	306	LYS	5.0
1	B	449	GLU	4.7
1	B	297	LEU	4.5
1	B	310	ALA	4.0
1	B	153	GLY	4.0
1	B	298	ALA	3.9
1	B	175	HIS	3.8
1	A	175	HIS	3.8
1	B	178	ASP	3.7
1	B	155	PHE	3.5
1	B	312	THR	3.5
1	A	306	LYS	3.5
1	B	299	ARG	3.2
1	A	376	GLU	3.2
1	B	376	GLU	3.1
1	B	308	SER	3.0
1	A	310	ALA	2.9
1	B	135	GLN	2.9
1	A	304	THR	2.8
1	A	412	PHE	2.8
1	B	197	MET	2.8
1	B	309	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	305	THR	2.8
1	B	154	GLY	2.8
1	B	282	ASN	2.7
1	A	282	ASN	2.6
1	B	301	TRP	2.6
1	A	428[A]	HIS	2.6
1	A	415	PRO	2.6
1	B	412	PHE	2.6
1	B	182	SER	2.5
1	B	164	ILE	2.4
1	B	373	THR	2.4
1	B	198	LEU	2.4
1	B	300	GLU	2.4
1	A	378	PHE	2.3
1	B	195	PHE	2.3
1	B	411	PHE	2.2
1	B	413	GLU	2.2
1	B	307	MET	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.