



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:11 PM UTC

PDB ID : 7AI4 / pdb_00007ai4
Title : Crystal structure of the KLC1-TPR domain truncated from its nonTPR region ([A1-B6]-Delta-nonTPR fragment)
Authors : Menetrey, J.; Llinas, P.
Deposited on : 2020-09-26
Resolution : 2.79 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

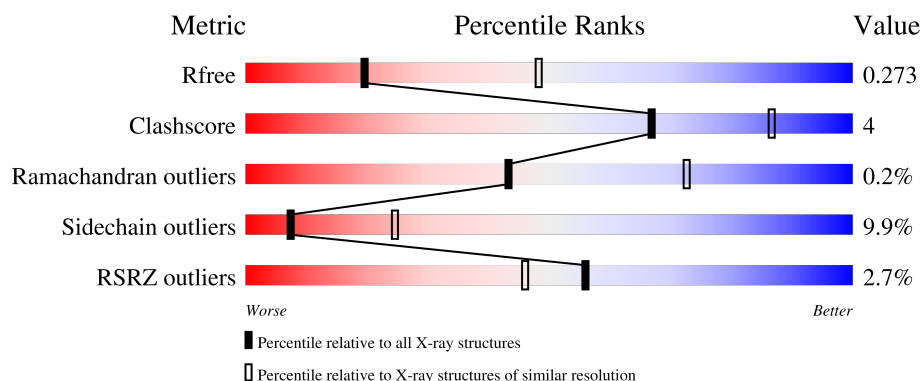
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	293	 69% 13% • 17%
1	B	293	 68% 11% • 20%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3501 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 Isoform C of Kinesin light chain 1, Isoform C of Kinesin light chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1842	1160	322	355	5			
1	B	235	Total	C	N	O	S	0	0	0
			1659	1039	299	316	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MET	-	initiating methionine	UNP Q07866
A	176	ARG	-	expression tag	UNP Q07866
A	177	SER	-	expression tag	UNP Q07866
A	178	GLU	-	expression tag	UNP Q07866
A	179	THR	-	expression tag	UNP Q07866
A	180	MET	-	expression tag	UNP Q07866
A	181	SER	-	expression tag	UNP Q07866
A	182	TYR	-	expression tag	UNP Q07866
A	183	TYR	-	expression tag	UNP Q07866
A	184	HIS	-	expression tag	UNP Q07866
A	185	HIS	-	expression tag	UNP Q07866
A	186	HIS	-	expression tag	UNP Q07866
A	187	HIS	-	expression tag	UNP Q07866
A	188	HIS	-	expression tag	UNP Q07866
A	189	HIS	-	expression tag	UNP Q07866
A	190	ASP	-	expression tag	UNP Q07866
A	191	TYR	-	expression tag	UNP Q07866
A	192	ASP	-	expression tag	UNP Q07866
A	193	ILE	-	expression tag	UNP Q07866
A	194	PRO	-	expression tag	UNP Q07866
A	195	THR	-	expression tag	UNP Q07866
A	196	THR	-	expression tag	UNP Q07866
A	197	GLU	-	expression tag	UNP Q07866
A	198	ASN	-	expression tag	UNP Q07866

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	LEU	-	expression tag	UNP Q07866
A	200	TYR	-	expression tag	UNP Q07866
A	201	PHE	-	expression tag	UNP Q07866
A	202	GLN	-	expression tag	UNP Q07866
A	203	GLY	-	expression tag	UNP Q07866
A	204	ALA	-	expression tag	UNP Q07866
A	205	MET	-	expression tag	UNP Q07866
A	454	GLY	-	linker	UNP Q07866
A	455	GLY	-	linker	UNP Q07866
A	456	GLY	-	linker	UNP Q07866
A	457	GLY	-	linker	UNP Q07866
A	458	SER	-	linker	UNP Q07866
B	175	MET	-	initiating methionine	UNP Q07866
B	176	ARG	-	expression tag	UNP Q07866
B	177	SER	-	expression tag	UNP Q07866
B	178	GLU	-	expression tag	UNP Q07866
B	179	THR	-	expression tag	UNP Q07866
B	180	MET	-	expression tag	UNP Q07866
B	181	SER	-	expression tag	UNP Q07866
B	182	TYR	-	expression tag	UNP Q07866
B	183	TYR	-	expression tag	UNP Q07866
B	184	HIS	-	expression tag	UNP Q07866
B	185	HIS	-	expression tag	UNP Q07866
B	186	HIS	-	expression tag	UNP Q07866
B	187	HIS	-	expression tag	UNP Q07866
B	188	HIS	-	expression tag	UNP Q07866
B	189	HIS	-	expression tag	UNP Q07866
B	190	ASP	-	expression tag	UNP Q07866
B	191	TYR	-	expression tag	UNP Q07866
B	192	ASP	-	expression tag	UNP Q07866
B	193	ILE	-	expression tag	UNP Q07866
B	194	PRO	-	expression tag	UNP Q07866
B	195	THR	-	expression tag	UNP Q07866
B	196	THR	-	expression tag	UNP Q07866
B	197	GLU	-	expression tag	UNP Q07866
B	198	ASN	-	expression tag	UNP Q07866
B	199	LEU	-	expression tag	UNP Q07866
B	200	TYR	-	expression tag	UNP Q07866
B	201	PHE	-	expression tag	UNP Q07866
B	202	GLN	-	expression tag	UNP Q07866
B	203	GLY	-	expression tag	UNP Q07866
B	204	ALA	-	expression tag	UNP Q07866

Continued on next page...

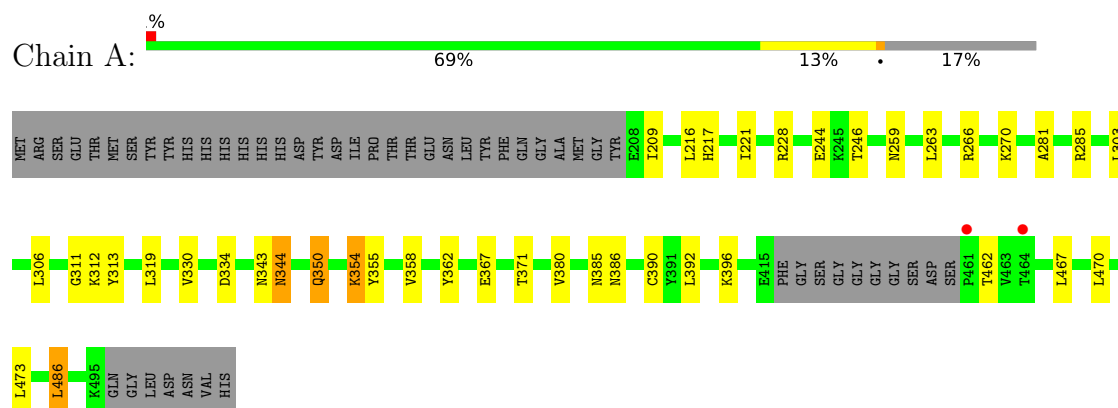
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	205	MET	-	expression tag	UNP Q07866
B	454	GLY	-	linker	UNP Q07866
B	455	GLY	-	linker	UNP Q07866
B	456	GLY	-	linker	UNP Q07866
B	457	GLY	-	linker	UNP Q07866
B	458	SER	-	linker	UNP Q07866

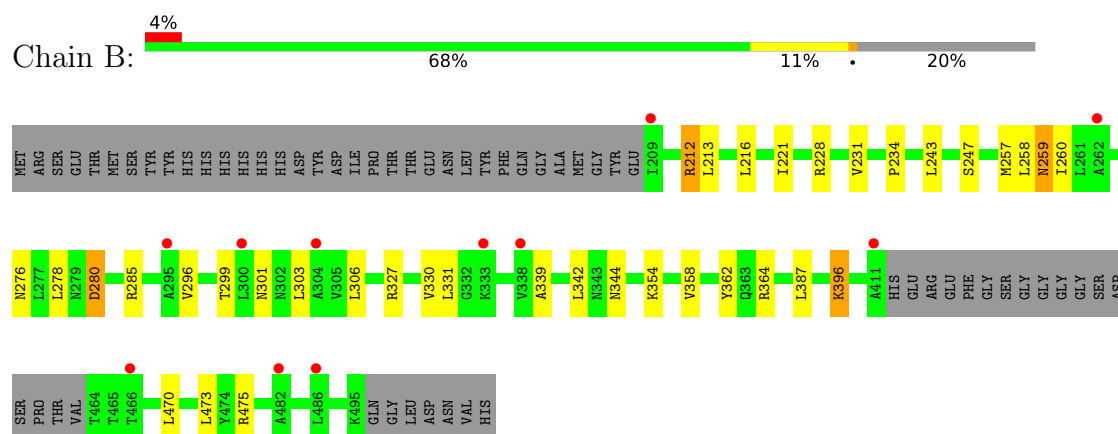
3 Residue-property plots [i](#)

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: Isoform C of Kinesin light chain 1,Isoform C of Kinesin light chain 1



- Molecule 1: Isoform C of Kinesin light chain 1,Isoform C of Kinesin light chain 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.22Å 55.82Å 103.57Å 90.00° 108.51° 90.00°	Depositor
Resolution (Å)	49.11 – 2.79 49.11 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.11-2.79) 99.2 (49.11-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.217 , 0.252 0.234 , 0.273	Depositor DCC
R_{free} test set	834 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	102.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 107.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3501	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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	0.84	0/1870	1.32	12/2541 (0.5%)
1	B	0.79	0/1685	1.21	1/2307 (0.0%)
All	All	0.82	0/3555	1.27	13/4848 (0.3%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ASN	CA-CB-CG	7.19	119.79	112.60
1	A	312	LYS	CA-C-N	5.83	128.09	120.28
1	A	312	LYS	C-N-CA	5.83	128.09	120.28
1	A	343	ASN	CA-C-N	5.75	128.26	120.44
1	A	343	ASN	C-N-CA	5.75	128.26	120.44
1	A	354	LYS	CA-C-N	5.52	128.23	120.28
1	A	354	LYS	C-N-CA	5.52	128.23	120.28
1	A	344	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	270	LYS	CA-C-N	5.19	127.24	120.28
1	A	270	LYS	C-N-CA	5.19	127.24	120.28
1	A	355	TYR	N-CA-C	5.16	117.64	111.71
1	A	396	LYS	CA-C-N	5.04	127.29	120.38
1	A	396	LYS	C-N-CA	5.04	127.29	120.38

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	1842	0	1794	10	0
1	B	1659	0	1478	15	0
All	All	3501	0	3272	25	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 4.

All (25) 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:350:GLN:HG3	1:A:358:VAL:HG11	1.69	0.74
1:B:278:LEU:HD12	1:B:306:LEU:HD12	1.79	0.64
1:A:217:HIS:CE1	1:A:221:ILE:HD12	2.37	0.59
1:B:327:ARG:HA	1:B:330:VAL:HG12	1.85	0.58
1:B:213:LEU:HD21	1:B:243:LEU:HD11	1.86	0.55
1:A:362:TYR:CZ	1:A:386:ASN:HB3	2.43	0.54
1:B:231:VAL:C	1:B:234:PRO:HD2	2.33	0.52
1:B:330:VAL:HG13	1:B:331:LEU:HG	1.91	0.52
1:B:212:ARG:NH1	1:B:247:SER:OG	2.43	0.51
1:A:392:LEU:HD13	1:A:473:LEU:HD12	1.91	0.51
1:B:257:MET:HA	1:B:260:ILE:HG22	1.93	0.50
1:A:367:GLU:O	1:A:371:THR:HG23	2.12	0.49
1:B:285:ARG:NH1	1:B:299:THR:OG1	2.43	0.49
1:A:467:LEU:HD23	1:A:486:LEU:HD23	1.96	0.48
1:B:285:ARG:HH11	1:B:299:THR:HG1	1.62	0.46
1:B:285:ARG:HB3	1:B:296:VAL:HG22	1.98	0.45
1:B:354:LYS:O	1:B:358:VAL:HG23	2.17	0.44
1:B:362:TYR:HB2	1:B:387:LEU:HD13	2.00	0.44
1:A:470:LEU:HB2	1:A:486:LEU:HD22	2.02	0.42
1:A:303:LEU:HB3	1:A:319:LEU:HD13	2.01	0.42
1:B:258:LEU:HD13	1:B:280:ASP:HB3	2.02	0.41
1:B:339:ALA:HA	1:B:342:LEU:HD12	2.02	0.41
1:B:470:LEU:HD12	1:B:473:LEU:HD23	2.02	0.41
1:A:281:ALA:O	1:A:285:ARG:HG3	2.21	0.41
1:A:311:GLY:HA2	1:A:313:TYR:CZ	2.55	0.41

There are no symmetry-related clashes.

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	239/293 (82%)	234 (98%)	5 (2%)	0	100	100
1	B	231/293 (79%)	217 (94%)	13 (6%)	1 (0%)	30	60
All	All	470/586 (80%)	451 (96%)	18 (4%)	1 (0%)	43	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	LYS

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	183/245 (75%)	164 (90%)	19 (10%)	7	22
1	B	140/245 (57%)	127 (91%)	13 (9%)	8	27
All	All	323/490 (66%)	291 (90%)	32 (10%)	7	24

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	ILE
1	A	216	LEU
1	A	228	ARG
1	A	244	GLU
1	A	246	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	259	ASN
1	A	263	LEU
1	A	266	ARG
1	A	306	LEU
1	A	330	VAL
1	A	334	ASP
1	A	344	ASN
1	A	350	GLN
1	A	354	LYS
1	A	380	VAL
1	A	385	ASN
1	A	390	CYS
1	A	462	THR
1	A	486	LEU
1	B	212	ARG
1	B	216	LEU
1	B	221	ILE
1	B	228	ARG
1	B	259	ASN
1	B	276	ASN
1	B	280	ASP
1	B	301	ASN
1	B	303	LEU
1	B	344	ASN
1	B	364	ARG
1	B	396	LYS
1	B	475	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	ASN
1	A	477	GLN
1	B	341	GLN

5.3.3 RNA ⓘ

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 [i](#)

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

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	243/293 (82%)	0.30	2 (0%) 82 75	71, 97, 124, 132	0
1	B	235/293 (80%)	0.72	11 (4%) 36 29	100, 125, 159, 175	0
All	All	478/586 (81%)	0.51	13 (2%) 56 46	71, 112, 148, 175	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	411	ALA	4.8
1	B	300	LEU	4.3
1	B	304	ALA	4.1
1	B	466	THR	2.8
1	B	486	LEU	2.7
1	B	333	LYS	2.7
1	B	209	ILE	2.7
1	A	461	PRO	2.5
1	B	338	VAL	2.5
1	B	262	ALA	2.4
1	A	464	THR	2.4
1	B	295	ALA	2.1
1	B	482	ALA	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.