



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 15, 2026 – 01:33 pm BST

PDB ID : 28IY / pdb_000028iy
Title : Crystal structure of the TPR domain of KLC1 in complex with the C-terminal peptide of JIP1 at 2.13 Angstrom resolution
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Deposited on : 2026-02-02
Resolution : 2.13 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

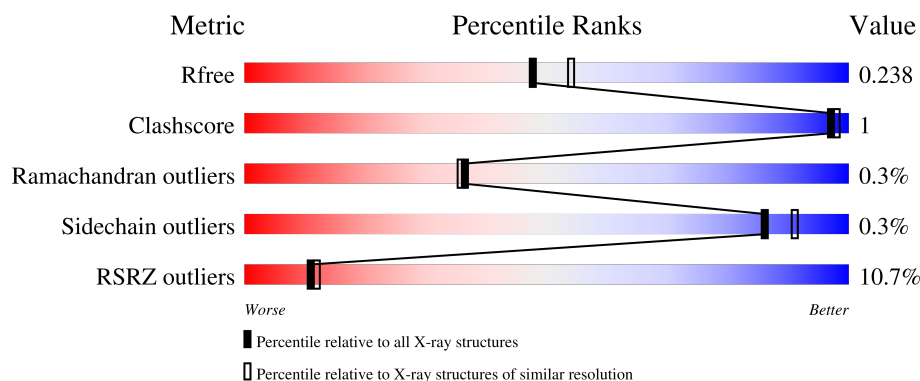
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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 $\leq 5\%$. 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	370	11% 72% • 25%
2	F	121	2% 90% • • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6569 atoms, of which 3251 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 Kinesin light chain,C-Jun-amino-terminal kinase-interacting protein 1 isoform X2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	277	Total	C	H	N	O	S	2416	24	0
			4825	1508	2416	433	459	9			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	GLY	-	expression tag	UNP Q5UE59
A	169	SER	-	expression tag	UNP Q5UE59
A	170	HIS	-	expression tag	UNP Q5UE59
A	171	MET	-	expression tag	UNP Q5UE59
A	671	THR	-	linker	UNP Q5UE59
A	672	GLY	-	linker	UNP Q5UE59
A	673	SER	-	linker	UNP Q5UE59
A	674	THR	-	linker	UNP Q5UE59
A	675	GLY	-	linker	UNP Q5UE59
A	676	SER	-	linker	UNP Q5UE59
A	677	THR	-	linker	UNP Q5UE59
A	678	GLY	-	linker	UNP Q5UE59
A	679	SER	-	linker	UNP Q5UE59
A	680	THR	-	linker	UNP Q5UE59
A	681	GLY	-	linker	UNP Q5UE59
A	682	SER	-	linker	UNP Q5UE59
A	683	THR	-	linker	UNP Q5UE59
A	684	GLY	-	linker	UNP Q5UE59
A	685	SER	-	linker	UNP Q5UE59
A	686	THR	-	linker	UNP Q5UE59
A	687	GLY	-	linker	UNP Q5UE59
A	688	SER	-	linker	UNP Q5UE59
A	689	THR	-	linker	UNP Q5UE59
A	690	GLY	-	linker	UNP Q5UE59
A	691	SER	-	linker	UNP Q5UE59
A	692	THR	-	linker	UNP Q5UE59

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Chain	Residue	Modelled	Actual	Comment	Reference
A	693	GLY	-	linker	UNP Q5UE59
A	694	SER	-	linker	UNP Q5UE59
A	695	THR	-	linker	UNP Q5UE59
A	696	GLY	-	linker	UNP Q5UE59
A	697	SER	-	linker	UNP Q5UE59
A	698	THR	-	linker	UNP Q5UE59
A	699	GLY	-	linker	UNP Q5UE59
A	700	SER	-	linker	UNP Q5UE59

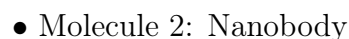
- Molecule 2 is a protein called Nanobody.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	114	Total	C	H	N	O	S	835	0	0
			1708	547	835	149	172	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	F	11	Total	O	0	0
			11	11		

● Molecule 1: Kinesin light chain,C-Jun-amino-terminal kinase-interacting protein 1 isoform X2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.58Å 89.55Å 51.33Å 90.00° 100.56° 90.00°	Depositor
Resolution (Å)	68.34 – 2.13 68.34 – 2.13	Depositor EDS
% Data completeness (in resolution range)	79.9 (68.34-2.13) 79.9 (68.34-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.12Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.222 , 0.244 0.210 , 0.238	Depositor DCC
R_{free} test set	1075 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	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	0.96	EDS
Total number of atoms	6569	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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 [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	0.70	0/2449	0.96	0/3304
2	F	0.77	1/892 (0.1%)	0.89	1/1207 (0.1%)
All	All	0.72	1/3341 (0.0%)	0.95	1/4511 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	83	MET	SD-CE	-6.27	1.63	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	68	PHE	CA-CB-CG	6.04	119.84	113.80

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	2409	2416	2402	4	0
2	F	873	835	834	2	0
3	A	25	0	0	0	0
3	F	11	0	0	0	0
All	All	3318	3251	3236	6	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 1.

The worst 5 of 6 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)
2:F:83:MET:HE2	2:F:86:LEU:HD21	1.77	0.65
1:A:488:GLU:O	1:A:492:ARG:HG3	2.08	0.54
1:A:346:ALA:HB1	1:A:358:VAL:HG13	1.89	0.54
1:A:425:PRO:HD2	1:A:428:MET:SD	2.56	0.46
2:F:34:MET:HB3	2:F:79:LEU:HD22	2.00	0.43

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	295/370 (80%)	286 (97%)	7 (2%)	2 (1%)	18	15
2	F	112/121 (93%)	111 (99%)	1 (1%)	0	100	100
All	All	407/491 (83%)	397 (98%)	8 (2%)	2 (0%)	36	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212[A]	ARG
1	A	212[B]	ARG

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	253/301 (84%)	252 (100%)	1 (0%)	84	89
2	F	92/99 (93%)	92 (100%)	0	100	100
All	All	345/400 (86%)	344 (100%)	1 (0%)	86	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347	LEU

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

Mol	Chain	Res	Type
2	F	77	ASN
2	F	82	GLN
2	F	84	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 ⓘ

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	277/370 (74%)	1.13	40 (14%) 6 6	17, 39, 64, 75	24 (8%)
2	F	114/121 (94%)	0.27	2 (1%) 67 70	22, 35, 47, 55	0
All	All	391/491 (79%)	0.88	42 (10%) 11 12	17, 37, 62, 75	24 (6%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216[A]	LEU	4.6
1	A	215[A]	THR	4.5
1	A	334	ASP	4.2
1	A	416	PHE	3.5
1	A	207[A]	TYR	3.5

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.