



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 12:38 AM UTC

PDB ID : 9OT6 / pdb_00009ot6
EMDB ID : EMD-70826
Title : Cryo-EM structure of the PI4KA complex bound to an EFR3 interfering nanobody (F3IN)
Authors : Shaw, A.L.; Suresh, S.; Yip, C.K.; Burke, J.E.
Deposited on : 2025-05-26
Resolution : 3.54 Å (reported)
Based on initial models : ., 9BAX

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

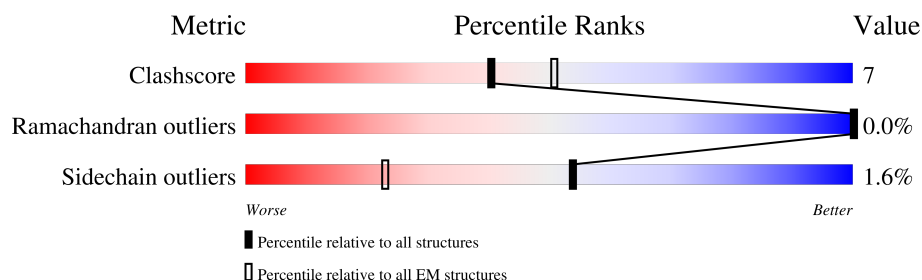
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.54 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	2104	67% 14% 18%
1	B	2104	67% 15% 18%
2	C	165	48% 14% 37%
2	H	165	50% 12% 37%
3	D	843	58% 11% 30%
3	F	843	58% 12% 30%
4	E	308	67% 14% 18%
4	G	308	67% 14% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 42678 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Phosphatidylinositol 4-kinase alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1724	Total	C	N	O	S	0	0
			13842	8951	2305	2489	97		
1	B	1724	Total	C	N	O	S	0	0
			13842	8951	2305	2489	97		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42356
A	0	SER	-	expression tag	UNP P42356
B	-1	GLY	-	expression tag	UNP P42356
B	0	SER	-	expression tag	UNP P42356

- Molecule 2 is a protein called EFR3 interfering Nanobody (F3IN).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	104	Total	C	N	O	S	0	0
			811	511	141	154	5		
2	H	104	Total	C	N	O	S	0	0
			811	511	141	154	5		

- Molecule 3 is a protein called Tetratricopeptide repeat protein 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	592	Total	C	N	O	S	0	0
			4676	2983	811	855	27		
3	F	592	Total	C	N	O	S	0	0
			4676	2983	811	855	27		

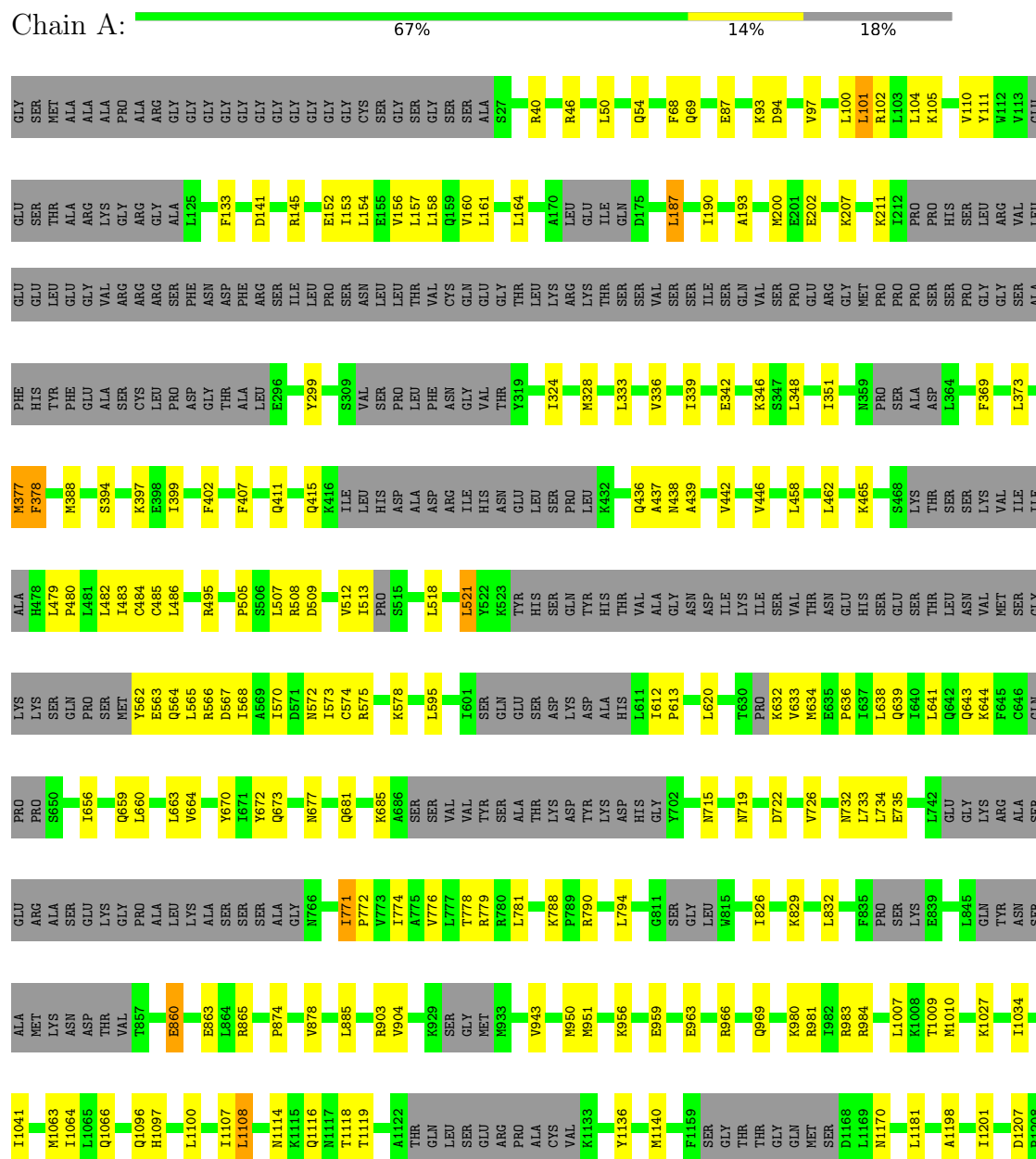
- Molecule 4 is a protein called Hyccin.

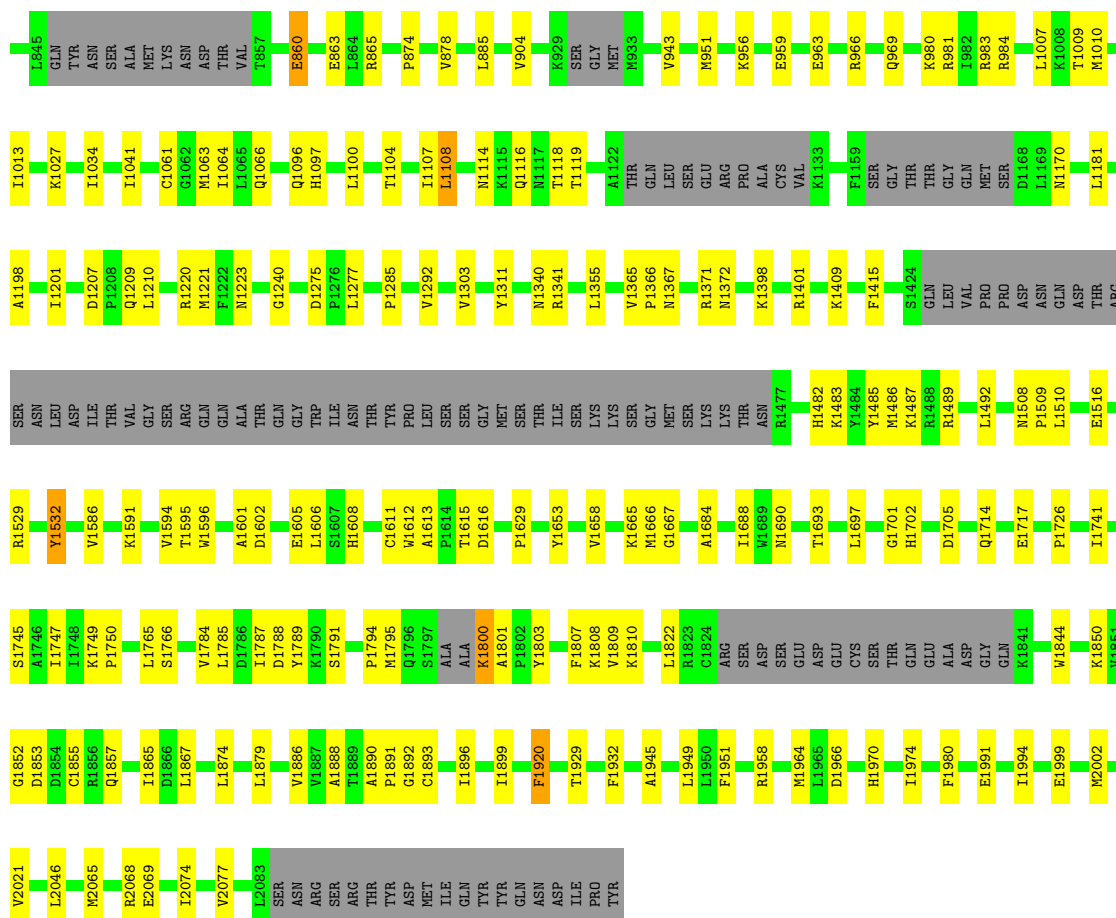
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	252	Total 2010	C 1309	N 323	O 366	S 12	0	0
4	G	252	Total 2010	C 1309	N 323	O 366	S 12	0	0

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. 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. 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.

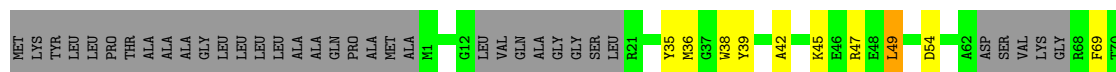
- Molecule 1: Phosphatidylinositol 4-kinase alpha





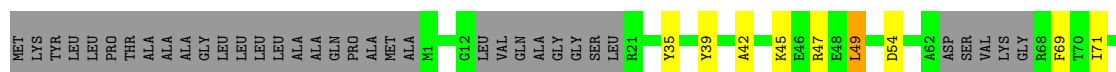
- Molecule 2: EFR3 interfering Nanobody (F3IN)

Chain C: 48% 14% 37%



- Molecule 2: EFR3 interfering Nanobody (F3IN)

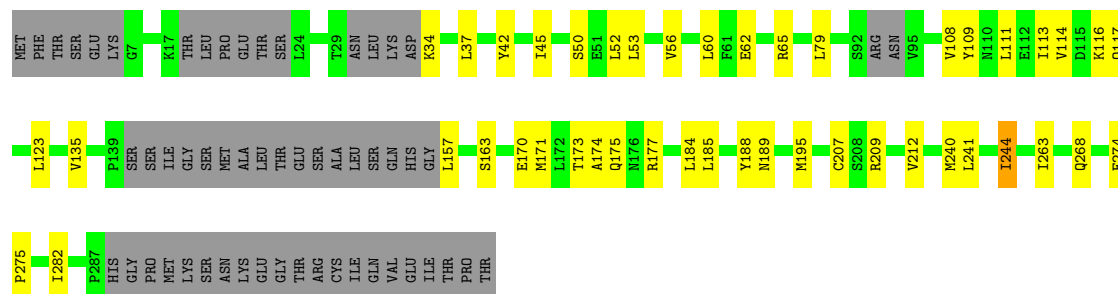
Chain H: 50% 12% 37%



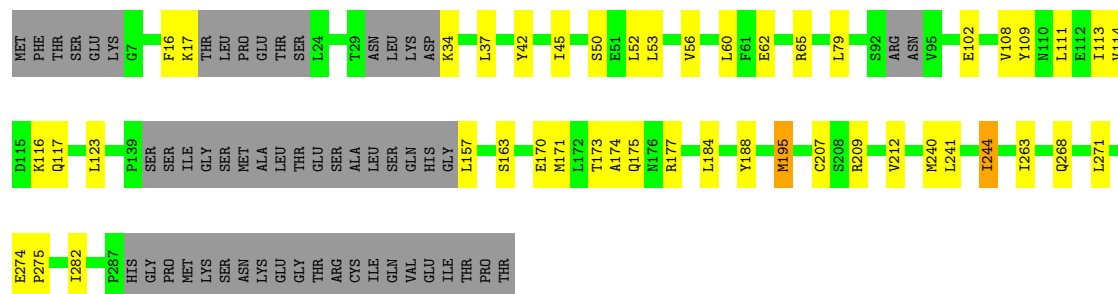
- Molecule 3: Tetratricopeptide repeat protein 7B



• Molecule 4: Hyccin



• Molecule 4: Hyccin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	282982	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

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	0.10	0/14149	0.26	0/19141
1	B	0.10	0/14149	0.26	0/19141
2	C	0.11	0/826	0.33	0/1116
2	H	0.11	0/826	0.33	0/1116
3	D	0.09	0/4762	0.25	0/6443
3	F	0.09	0/4762	0.25	0/6443
4	E	0.10	0/2058	0.28	0/2793
4	G	0.10	0/2058	0.28	0/2793
All	All	0.10	0/43590	0.26	0/58986

There are no bond length outliers.

There are no bond angle outliers.

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	13842	0	13974	193	0
1	B	13842	0	13974	197	0
2	C	811	0	771	20	0
2	H	811	0	771	15	0
3	D	4676	0	4734	66	0
3	F	4676	0	4734	68	0
4	E	2010	0	2017	27	0
4	G	2010	0	2017	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	42678	0	42992	598	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 7.

The worst 5 of 598 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:H:92:THR:HA	2:H:120:VAL:O	1.73	0.88
2:C:92:THR:HA	2:C:120:VAL:O	1.73	0.88
3:F:378:GLN:HB3	3:F:381:MET:HE1	1.56	0.88
3:D:378:GLN:HB3	3:D:381:MET:HE1	1.56	0.87
3:D:347:ARG:HG3	3:D:349:PRO:HD3	1.66	0.76

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 PDB entries followed by that with respect to all EM entries.

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	1676/2104 (80%)	1605 (96%)	70 (4%)	1 (0%)	48	79
1	B	1676/2104 (80%)	1605 (96%)	70 (4%)	1 (0%)	48	79
2	C	96/165 (58%)	91 (95%)	5 (5%)	0	100	100
2	H	96/165 (58%)	91 (95%)	5 (5%)	0	100	100
3	D	580/843 (69%)	571 (98%)	9 (2%)	0	100	100
3	F	580/843 (69%)	571 (98%)	9 (2%)	0	100	100
4	E	242/308 (79%)	232 (96%)	10 (4%)	0	100	100
4	G	242/308 (79%)	233 (96%)	9 (4%)	0	100	100
All	All	5188/6840 (76%)	4999 (96%)	187 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1980	PHE
1	B	1980	PHE

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 PDB entries followed by that with respect to all EM entries.

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	1527/1842 (83%)	1505 (99%)	22 (1%)	59	71
1	B	1527/1842 (83%)	1506 (99%)	21 (1%)	59	71
2	C	82/129 (64%)	80 (98%)	2 (2%)	43	64
2	H	82/129 (64%)	80 (98%)	2 (2%)	43	64
3	D	494/712 (69%)	484 (98%)	10 (2%)	48	67
3	F	494/712 (69%)	484 (98%)	10 (2%)	48	67
4	E	227/277 (82%)	224 (99%)	3 (1%)	61	72
4	G	227/277 (82%)	224 (99%)	3 (1%)	61	72
All	All	4660/5920 (79%)	4587 (98%)	73 (2%)	54	70

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	244	ILE
2	H	49	LEU
3	F	350	GLU
3	F	576	LEU
1	B	200	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	276	GLN
3	F	763	HIS
2	H	119	GLN

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Mol	Chain	Res	Type
1	B	438	ASN
1	B	91	GLN

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-70826. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.