



## Full wwPDB EM Validation Report ⓘ

Apr 6, 2025 – 01:47 AM JST

PDB ID : 9IVK / pdb\_00009ivk  
EMDB ID : EMD-60929  
Title : cryo-EM structure of a tmFAP  
Authors : Sun, K.; Zhu, J.Y.; Liang, M.F.; Lu, P.L.  
Deposited on : 2024-07-23  
Resolution : 2.74 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

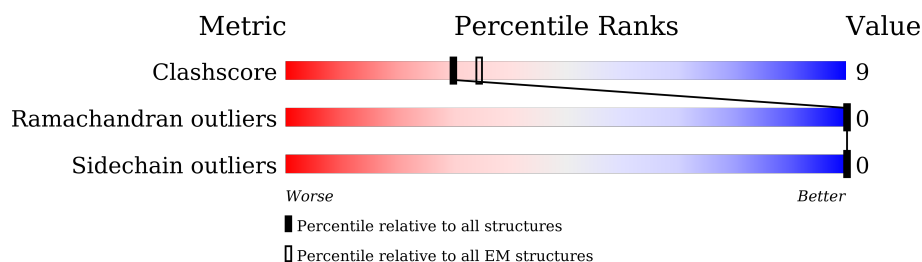
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.74 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	285	
2	H	229	
3	L	214	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4077 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 HBC599 membrane protein binder.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	278	Total	C	N	O	S	0	0
			2271	1487	360	419	5		

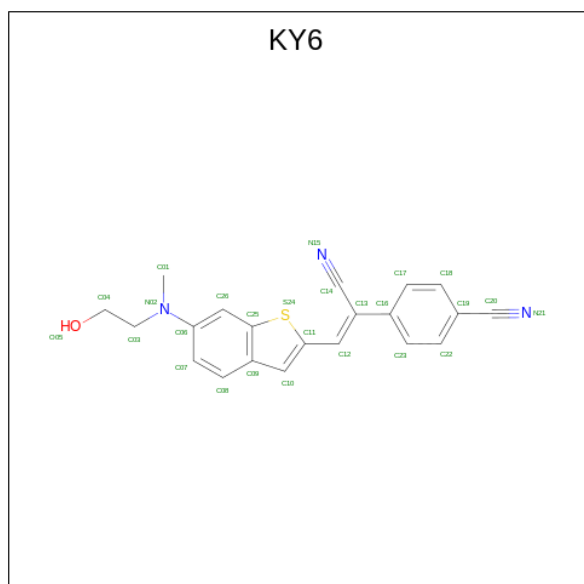
- Molecule 2 is a protein called Heavy chain, Fab fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	122	Total	C	N	O	S	4	0
			958	612	158	184	4		

- Molecule 3 is a protein called Light Chain, Fab fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	1	0
			822	520	133	165	4		

- Molecule 4 is 4-[(Z)-1-cyano-2-{6-[(2-hydroxyethyl)(methyl)amino]-1-benzothiophen-2-yl}ethenyl]benzonitrile (CCD ID: KY6) (formula: C<sub>21</sub>H<sub>17</sub>N<sub>3</sub>OS).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
4	A	1	26	21	3	1	1	0



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	453223	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)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KY6

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	0.37	0/2302	0.53	0/3091
2	H	0.30	0/999	0.52	0/1361
3	L	0.31	0/843	0.51	0/1145
All	All	0.34	0/4144	0.53	0/5597

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	2271	0	2382	55	0
2	H	958	0	902	13	0
3	L	822	0	802	6	0
4	A	26	0	0	6	0
All	All	4077	0	4086	73	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 9.

All (73) 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:33:PHE:HB2	1:A:47:VAL:HG11	1.57	0.86
1:A:239:LYS:HA	1:A:242:LYS:HB2	1.73	0.71
1:A:213:LEU:HD13	1:A:283:ILE:HD13	1.73	0.70
1:A:230:LEU:HD11	1:A:269:ILE:HD12	1.76	0.67
3:L:25:ARG:NH1	3:L:71:ASP:OD2	2.29	0.66
3:L:91:GLN:NE2	3:L:97:LEU:O	2.29	0.65
1:A:93:LEU:HD22	1:A:196:LEU:HD21	1.78	0.64
1:A:230:LEU:CD1	1:A:269:ILE:HD12	2.29	0.62
1:A:5:LEU:HD13	1:A:284:LEU:HD23	1.81	0.62
1:A:41:LYS:NZ	1:A:245:ASN:OD1	2.25	0.62
1:A:86:GLU:OE1	1:A:206:ARG:NH1	2.34	0.61
2:H:102:TRP:CH2	3:L:92:TYR:HB2	2.37	0.60
1:A:131:GLN:NE2	1:A:156:ASP:OD1	2.36	0.58
1:A:9:LEU:HD11	1:A:280:LEU:HD23	1.84	0.58
1:A:212:GLU:OE2	1:A:279:LYS:NZ	2.29	0.58
2:H:43:ALA:HB3	2:H:46:LYS:HB2	1.86	0.58
1:A:266:ALA:HB1	4:A:301:KY6:N15	2.20	0.57
1:A:283:ILE:HG23	1:A:284:LEU:HD12	1.86	0.57
3:L:84:PHE:HB3	3:L:108:ILE:HG12	1.87	0.56
1:A:168:LEU:HD13	1:A:176:GLU:HB3	1.87	0.56
1:A:44:PHE:CZ	1:A:242:LYS:HA	2.41	0.56
2:H:76:ASP:OD1	2:H:78:SER:OG	2.23	0.56
1:A:238:THR:O	1:A:242:LYS:HG3	2.07	0.55
1:A:239:LYS:HG3	1:A:242:LYS:HD3	1.88	0.55
2:H:53:TYR:CE1	2:H:62:SER:HB2	2.41	0.55
1:A:19:VAL:HG11	4:A:301:KY6:C22	2.36	0.54
1:A:31:GLU:O	1:A:35:GLU:HG3	2.05	0.54
1:A:146:PRO:HA	1:A:149:LYS:HD3	1.91	0.53
1:A:76:ILE:HD11	1:A:284:LEU:HD21	1.90	0.53
2:H:64:ALA:HB3	2:H:67:VAL:HG22	1.90	0.53
1:A:234:ALA:HB1	4:A:301:KY6:C06	2.38	0.52
1:A:33:PHE:HE1	1:A:43:GLU:HB3	1.75	0.52
1:A:22:LEU:HD23	1:A:58:SER:OG	2.11	0.52
1:A:26:ASP:HB2	1:A:54:VAL:HG21	1.91	0.51
1:A:69:LEU:HD22	1:A:224:TYR:HD2	1.74	0.51
1:A:72:LEU:HD21	1:A:280:LEU:CD2	2.41	0.51
3:L:67:ARG:HG3	3:L:72:PHE:CE2	2.47	0.50
1:A:52:GLU:O	1:A:56:LEU:HG	2.12	0.49
1:A:238:THR:O	1:A:242:LYS:N	2.45	0.49
2:H:32:VAL:HG22	2:H:37:LEU:HD11	1.94	0.49
2:H:97:TYR:O	2:H:120:GLY:HA2	2.13	0.49
1:A:213:LEU:HD11	1:A:280:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:HG12	1:A:178:GLN:HE22	1.78	0.48
1:A:213:LEU:HD21	1:A:284:LEU:HD11	1.95	0.48
1:A:99:THR:O	1:A:103:ASN:ND2	2.46	0.48
1:A:44:PHE:CD1	1:A:48:ILE:HG13	2.48	0.48
1:A:9:LEU:HD21	1:A:72:LEU:HD11	1.96	0.47
1:A:119:ALA:O	1:A:123:MET:HG3	2.14	0.47
2:H:53:TYR:HE1	2:H:62:SER:HB2	1.80	0.47
1:A:44:PHE:HZ	1:A:242:LYS:HA	1.80	0.47
2:H:32:VAL:HG23	2:H:80:ASN:OD1	2.14	0.47
1:A:6:LYS:HD3	1:A:281:LEU:HD11	1.97	0.47
1:A:72:LEU:HD21	1:A:280:LEU:HD21	1.97	0.46
1:A:48:ILE:C	1:A:50:ILE:N	2.67	0.46
2:H:34:ASP:OD1	2:H:34:ASP:N	2.47	0.46
1:A:280:LEU:O	1:A:284:LEU:HD13	2.16	0.45
1:A:9:LEU:HD21	1:A:72:LEU:CD1	2.47	0.45
2:H:20:SER:HA	2:H:86:MET:O	2.17	0.44
1:A:19:VAL:HG21	4:A:301:KY6:C19	2.48	0.43
1:A:48:ILE:C	1:A:50:ILE:H	2.22	0.43
1:A:38:VAL:HG12	1:A:40:ASP:H	1.83	0.43
1:A:280:LEU:HD12	1:A:284:LEU:HD13	1.99	0.43
1:A:230:LEU:HD11	1:A:269:ILE:CD1	2.45	0.43
4:A:301:KY6:S24	4:A:301:KY6:C14	3.06	0.43
1:A:124:ARG:NE	3:L:93:LEU:O	2.44	0.42
1:A:234:ALA:CB	4:A:301:KY6:C06	2.97	0.42
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.89	0.42
2:H:15:VAL:HG11	2:H:89:LEU:HD13	2.02	0.42
1:A:47:VAL:HG13	1:A:50:ILE:HD12	2.02	0.41
2:H:40:VAL:HG22	2:H:50:TRP:HA	2.00	0.41
1:A:235:LYS:HG3	1:A:239:LYS:NZ	2.35	0.41
1:A:235:LYS:O	1:A:238:THR:HG22	2.21	0.41
1:A:261:VAL:HA	1:A:264:ILE:HG12	2.02	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 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	274/285 (96%)	270 (98%)	4 (2%)	0	100	100
2	H	124/229 (54%)	122 (98%)	2 (2%)	0	100	100
3	L	106/214 (50%)	102 (96%)	4 (4%)	0	100	100
All	All	504/728 (69%)	494 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	241/248 (97%)	241 (100%)	0	100	100
2	H	101/190 (53%)	101 (100%)	0	100	100
3	L	94/189 (50%)	94 (100%)	0	100	100
All	All	436/627 (70%)	436 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	KY6	A	301	-	24,28,28	0.80	0	29,38,38	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	KY6	A	301	-	-	0/17/19/19	0/3/3/3

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.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	KY6	6	0

## 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.