



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 17, 2017 – 11:04 AM EDT

PDB ID : 5VLJ  
EMDB ID: : EMD-8706  
Title : Cryo-EM structure of yeast cytoplasmic dynein with Walker B mutation at AAA3 in presence of ATP-VO4  
Authors : Cianfrocco, M.A.; DeSantis, M.E.; Htet, Z.M.; Tran, P.T.; Reck-Peterson, S.L.; Leschziner, A.E.  
Deposited on : unknown  
Resolution : 10.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

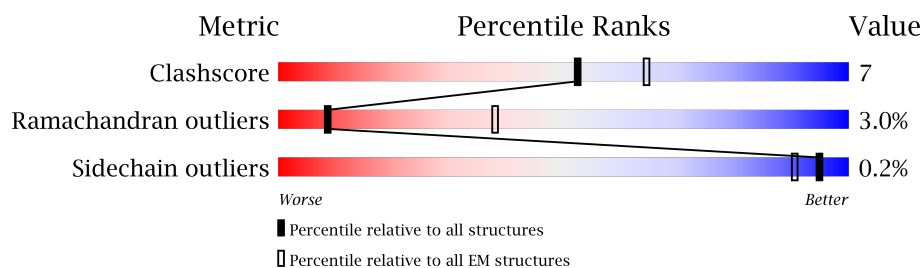
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




The reported resolution of this entry is 10.50 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	2376	
2	B	354	
2	C	354	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 49789 atoms, of which 24885 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 Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2376	Total	C	H	N	O	S	0	0
			38423	12301	19243	3182	3607	90		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1575	PHE	LEU	conflict	UNP P36022
A	1578	SER	PHE	conflict	UNP P36022
A	1668	GLU	GLN	conflict	UNP P36022
A	1777	VAL	ILE	conflict	UNP P36022
A	1984	VAL	ILE	conflict	UNP P36022
A	2936	VAL	ILE	conflict	UNP P36022
A	3343	GLY	ALA	conflict	UNP P36022
A	3444	VAL	ILE	conflict	UNP P36022
A	3556	ARG	LYS	conflict	UNP P36022
A	3742	ASP	ASN	conflict	UNP P36022
A	3895	VAL	PHE	conflict	UNP P36022
A	4072	ASP	ASN	conflict	UNP P36022

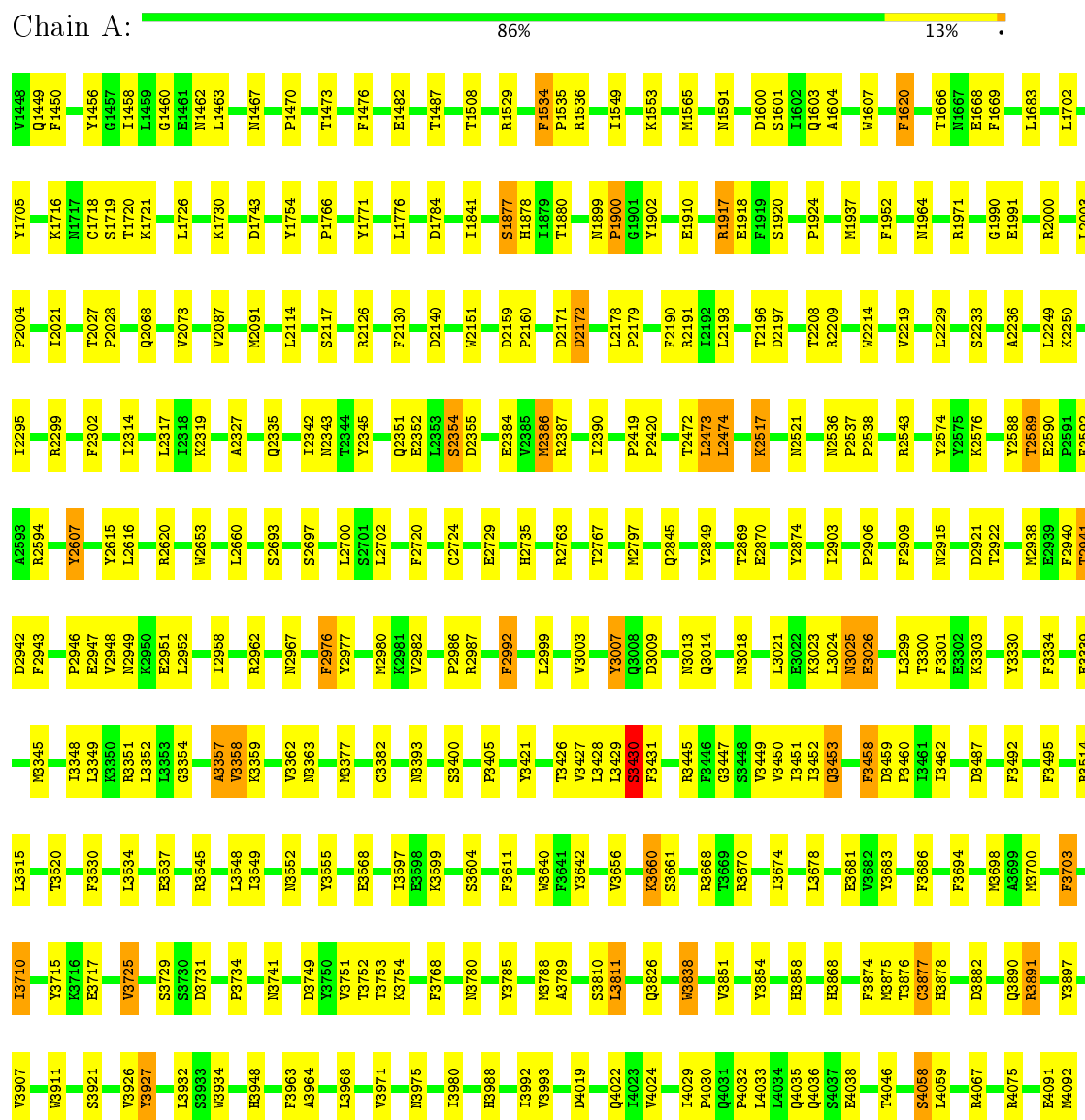
- Molecule 2 is a protein called Nuclear distribution protein PAC1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	354	Total	C	H	N	O	S	0	0
			5683	1831	2821	499	516	16		
2	C	354	Total	C	H	N	O	S	0	0
			5683	1831	2821	499	516	16		

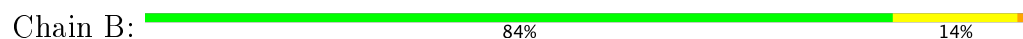
### 3 Residue-property plots

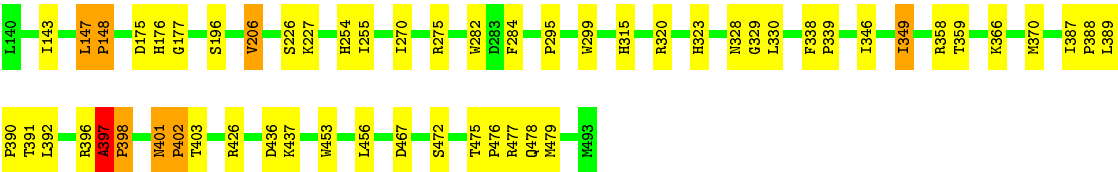
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: Dynein heavy chain, cytoplasmic

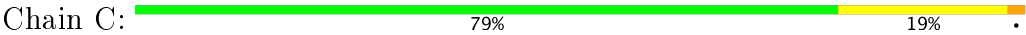


- Molecule 2: Nuclear distribution protein PAC1





● Molecule 2: Nuclear distribution protein PAC1



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	27807	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 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  > 2$	RMSZ	# $ Z  > 2$
1	A	0.82	0/19571	0.83	16/26457 (0.1%)
2	B	0.75	0/2943	0.90	3/4003 (0.1%)
2	C	0.77	1/2943 (0.0%)	0.92	5/4003 (0.1%)
All	All	0.81	1/25457 (0.0%)	0.85	24/34463 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	386	GLU	CG-CD	-5.58	1.43	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3927	TYR	CB-CG-CD1	-8.24	116.06	121.00
1	A	3891	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	A	2000	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	3007	TYR	CB-CG-CD2	-6.61	117.03	121.00
1	A	1917	ARG	NE-CZ-NH1	6.15	123.37	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2236	ALA	Mainchain,Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	2976	PHE	Mainchain,Peptide
1	A	3668	ARG	Mainchain,Peptide
1	A	3921	SER	Mainchain,Peptide
1	A	4058	SER	Mainchain

## 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	19180	19243	19240	239	0
2	B	2862	2821	2820	36	0
2	C	2862	2821	2820	50	0
All	All	24904	24885	24880	325	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 325 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:B:206:VAL:O	2:B:206:VAL:HG12	1.75	0.86
1:A:2159:ASP:O	1:A:2159:ASP:OD1	1.97	0.82
1:A:2903:ILE:HG22	1:A:2903:ILE:O	1.79	0.81
1:A:2952:LEU:HD12	1:A:2952:LEU:O	1.80	0.80
1:A:3725:VAL:HG12	1:A:3725:VAL:O	1.82	0.79

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	2374/2376 (100%)	2113 (89%)	200 (8%)	61 (3%)	6	40
2	B	352/354 (99%)	291 (83%)	47 (13%)	14 (4%)	3	31
2	C	352/354 (99%)	305 (87%)	30 (8%)	17 (5%)	2	28
All	All	3078/3084 (100%)	2709 (88%)	277 (9%)	92 (3%)	9	37

5 of 92 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1600	ASP
1	A	1719	SER
1	A	1766	PRO
1	A	2354	SER
1	A	2517	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 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	2162/2162 (100%)	2155 (100%)	7 (0%)	94	96
2	B	327/327 (100%)	327 (100%)	0	100	100
2	C	327/327 (100%)	327 (100%)	0	100	100
All	All	2816/2816 (100%)	2809 (100%)	7 (0%)	95	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2976	PHE
1	A	3838	TRP
1	A	2992	PHE
1	A	2386	MET
1	A	3703	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3011	GLN
2	C	245	GLN
2	B	230	GLN
1	A	2959	GLN
2	C	230	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 carbohydrates 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.