



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 10, 2018 – 11:09 PM EST

PDB ID : 6F1V
EMDB ID: : EMD-4170
Title : C terminal region of the dynein heavy chains in the dynein
tail/dynactin/BICDR1 complex
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Deposited on : 2017-11-23
Resolution : 3.40 Å(reported)

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

We welcome your comments at 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-20030736

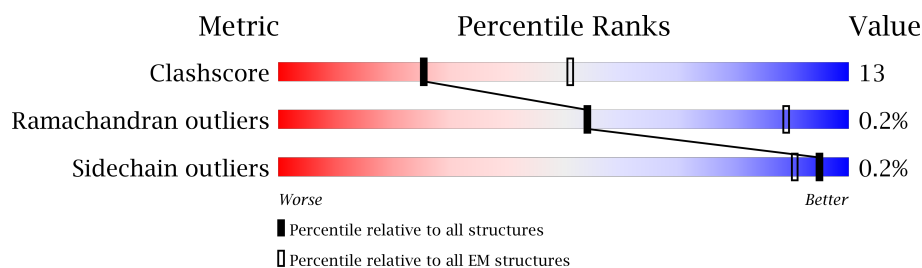
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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 ≥ 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	f	1186	
1	m	1186	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5164 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	f	411	Total	C	N	O	S	0	0
			3363	2131	603	619	10		
1	m	217	Total	C	N	O	S	0	0
			1801	1123	343	328	7		

Chain m: 17% . 82%



LYS	SER	ARG	GLN	GLU	LEU	GLU	GLN	HIS	SER	SER	VAL	ASP	THR	ALA	SER	THR	SER	ASP	ALA	VAL	THR	PHE	ILE	THR	TYR	VAL	GLN	SER	SER	LEU	LYS	ARG	LYS	ILE	LYS	GLN	PHE	GLU	LYS	GLN
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86030	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (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	f	0.56	0/3419	0.87	6/4613 (0.1%)
1	m	0.80	3/1831 (0.2%)	1.02	9/2457 (0.4%)
All	All	0.65	3/5250 (0.1%)	0.93	15/7070 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	m	702	TRP	CB-CG	-6.92	1.37	1.50
1	m	546	TRP	CB-CG	-6.77	1.38	1.50
1	m	702	TRP	CE3-CZ3	-5.41	1.29	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	m	601	ILE	CG1-CB-CG2	-8.35	93.04	111.40
1	m	694	ASN	C-N-CA	8.30	142.44	121.70
1	m	672	GLY	N-CA-C	-7.29	94.88	113.10
1	f	888	LEU	CB-CG-CD2	-7.04	99.03	111.00
1	m	480	ILE	CG1-CB-CG2	-6.89	96.25	111.40
1	f	762	LEU	CA-CB-CG	-6.52	100.30	115.30
1	m	537	ASP	CB-CG-OD1	5.83	123.55	118.30
1	f	733	LEU	CA-CB-CG	5.73	128.49	115.30
1	m	619	LEU	CA-CB-CG	-5.53	102.58	115.30
1	m	568	LEU	CA-CB-CG	-5.50	102.65	115.30
1	f	896	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	m	591	LEU	CA-CB-CG	-5.18	103.38	115.30
1	f	891	HIS	N-CA-C	-5.10	97.23	111.00
1	m	598	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	f	682	LEU	CB-CG-CD1	-5.01	102.49	111.00

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	f	3363	0	3421	0	0
1	m	1801	0	1798	0	0
All	All	5164	0	5219	0	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 13.

There are no clashes within the asymmetric unit.

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	f	409/1186 (34%)	364 (89%)	45 (11%)	0	100	100
1	m	213/1186 (18%)	188 (88%)	24 (11%)	1 (0%)	32	71
All	All	622/2372 (26%)	552 (89%)	69 (11%)	1 (0%)	54	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	m	455	ALA

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	f	366/1056 (35%)	366 (100%)	0	100	100
1	m	191/1056 (18%)	190 (100%)	1 (0%)	91	96
All	All	557/2112 (26%)	556 (100%)	1 (0%)	95	98

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

Mol	Chain	Res	Type
1	m	658	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	f	708	GLN
1	f	731	ASN
1	f	879	ASN
1	f	891	HIS
1	m	453	ASN
1	m	456	HIS
1	m	472	GLN
1	m	529	ASN
1	m	589	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.