



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:46 PM BST

PDB ID : 3J68  
EMDB ID: : EMD-5758  
Title : Structural mechanism of the dynein powerstroke (pre-powerstroke state)  
Authors : Lin, J.; Okada, K.; Raytchev, M.; Smith, M.C.; Nicastro, D.  
Deposited on : 2013-12-23  
Resolution : 30.00 Å(reported)  
Based on PDB ID : 4AKI

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

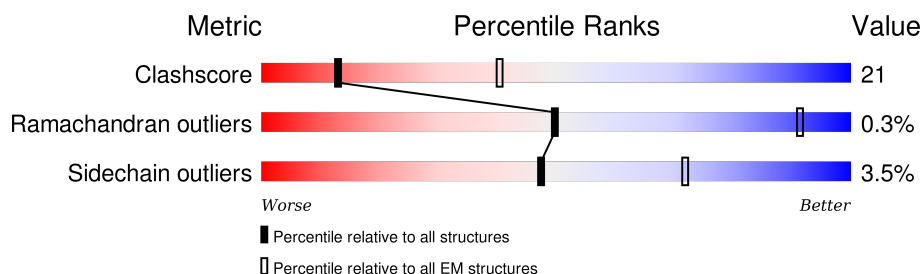
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


The reported resolution of this entry is 30.00 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	2286	 64% 32% . .

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18105 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.

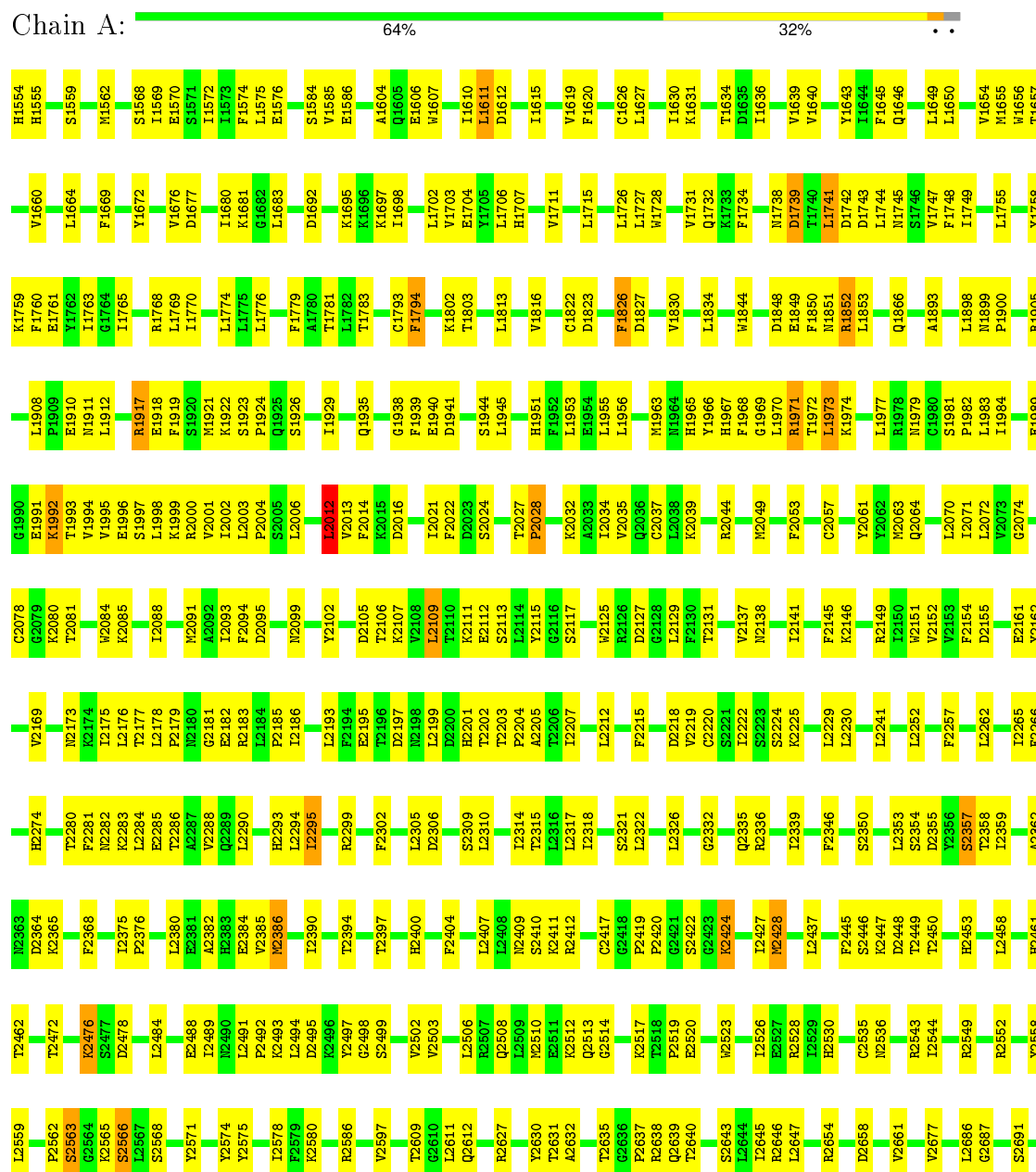
- Molecule 1 is a protein called Dynein motor domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2245	18105	11610	3004	3403	88	0	0

### 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 errors 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 motor domain



E4039	L3408	F3657	L3409	E3537	L3408	L3408	L2694
E4040	D3409	I3658	D3409	M3538	L3410	D3409	L2707
L4045	S3410	L35	S3410	N3538	S3410	S3410	N2708
L4048	S3411	L3744	S3411	M3541	F3301	F3301	L2712
L4059	K3412	L3760	K3412	K3544	E3302	E3302	L2728
W4062	T3853	E3766	T3853	K3544	K3303	K3303	L2738
L4063	X3854	F3767	X3854	D3547	M3306	M3306	L2749
Q4064	L3855	T3768	L3855	I3548	L3307	L3307	H2755
L4065	H3858	V3769	H3858	I3549	N3308	N3308	M2756
I4070	T3862	W3772	T3862	K3550	T3309	T3309	L2757
L4071	A3865	N3773	A3865	Y3555	K3310	K3310	L2759
N4072	E3869	I3774	E3869	R3565	Q3312	Q3312	A2761
Y4073	K3870	V3777	K3870	L3566	F3313	F3313	S2762
E4074	F3871	A3779	F3871	L3570	S3317	S3317	R2763
Q4077	K3872	N3780	K3872	M3577	Q3318	Q3318	L2822
A4078	F3874	Y3785	F3874	L3578	E3319	E3319	L2828
K4079	M3875	T3786	M3875	E3579	L3320	L3320	E2829
S4084	T3876	F3786	T3876	N3580	G3322	G3322	M2832
T4085	C3877	T3787	C3877	D3581	N3323	N3323	L2833
L4088	H3878	R3792	H3878	E3582	I3329	I3329	T2834
M4092	L3884	D3691	L3884	L3583	Y3330	Y3330	L2835
	P3885	K3692	P3885	L3587	E3331	E3331	L2844
	A3886	K3693	A3886	L3590	T2981	T2981	Y2849
	P3887	F3694	P3887	K3591	V2982	V2982	L2852
	L3888	K3695	L3888	E3593	G2983	G2983	L2853
	L3889	M3696	L3889	E3596	V2984	V2984	L2867
	Q3890	I3697	Q3890	N3596	N2985	N2985	L2868
	R3894	A3698	R3894	G3482	R2987	R2987	E2872
	F3895	M3700	F3895	D3483	S2988	S2988	L2873
	E3896	T3701	E3896	L3601	P2989	P2989	Y2874
	T3906	M3702	T3906	F3607	G2990	G2990	D2875
	W3911	C3704	W3911	D3612	L3010	L3010	Q2783
	G3912	L3705	G3912	K3613	V3017	V3017	P2784
	F3915	F3708	F3915	L3508	L3024	L3024	K2785
	F3916	E3717	F3916	L3509	V3028	V3028	L2786
	T3917	L3720	T3917	S3511	LEU	LEU	H2787
	V3923	T3721	V3923	V3513	VAL	VAL	R2788
	W3924	V3725	W3924	F3518	ASN	ASN	F2795
	S3925	K3833	S3925	V3519	GLU	GLU	L2799
	Y3927	G3836	Y3927	N3521	LEU	LEU	L2808
	W3934	G3837	W3934	M3631	ASN	ASN	R2812
	F3935	S3729	F3935	F3641	LYS	LYS	T2813
	I3939	D3731	I3939	S3645	C2912	C2912	L2816
		Q3845		I3646	LEU	LEU	L2817
		M3846		V3656	THR	THR	D2818
		S3847			LEU	LEU	E2819
					SER	SER	S2820
					LEU	LEU	N2821

## 4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC 0.5	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	6000	Depositor
Maximum defocus (nm)	8000	Depositor
Magnification	13500	Depositor
Image detector	Generic GATAN (2k x 2k)	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	0.59	1/18472 (0.0%)	0.82	12/24968 (0.0%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2872	GLU	CG-CD	7.56	1.63	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1741	LEU	CB-CG-CD1	8.47	125.39	111.00
1	A	1973	LEU	CB-CG-CD1	-7.39	98.44	111.00
1	A	2872	GLU	OE1-CD-OE2	-7.26	114.59	123.30
1	A	2866	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	1769	LEU	CA-CB-CG	6.08	129.28	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1739	ASP	Peptide

## 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	A	18105	0	18146	779	0
All	All	18105	0	18146	779	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 21.

The worst 5 of 779 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:1620:PHE:HD1	1:A:1760:PHE:CZ	1.58	1.22
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.76	1.16
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.59	1.15
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	1.06	1.15
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.18	1.14

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	2237/2286 (98%)	2137 (96%)	93 (4%)	7 (0%)	46 83

5 of 7 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	2990	GLY
1	A	3306	TRP
1	A	3482	GLY
1	A	2519	PRO
1	A	3980	ILE

### 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	2039/2078 (98%)	1968 (96%)	71 (4%)	43 74

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2843	LEU
1	A	2920	TRP
1	A	3950	PHE
1	A	2853	LEU
1	A	2873	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2383	HIS
1	A	2536	ASN
1	A	3890	GLN
1	A	2409	ASN
1	A	2459	HIS

### 5.3.3 RNA ⓘ

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.