wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:48 PM BST

PDB ID	:	3J67
EMDB ID:	:	EMD-5757
Title	:	Structural mechanism of the dynein powerstroke (post-powerstroke state)
Authors	:	Lin, J.; Okada, K.; Raytchev, M.; Smith, M.C.; Nicastro, D.
Deposited on	:	2013-12-22
Resolution	:	34.00 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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

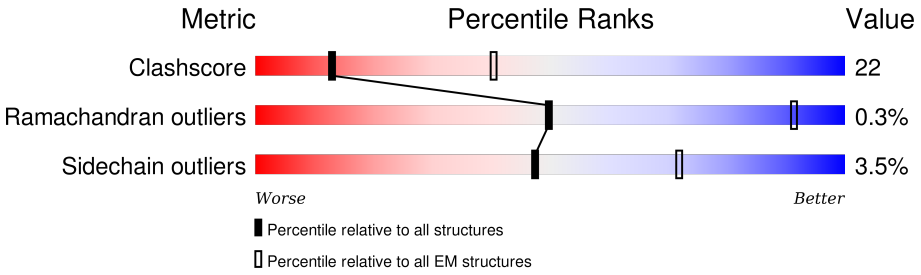
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 34.00 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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	2286	64% 33%

2 Entry composition (i)

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.

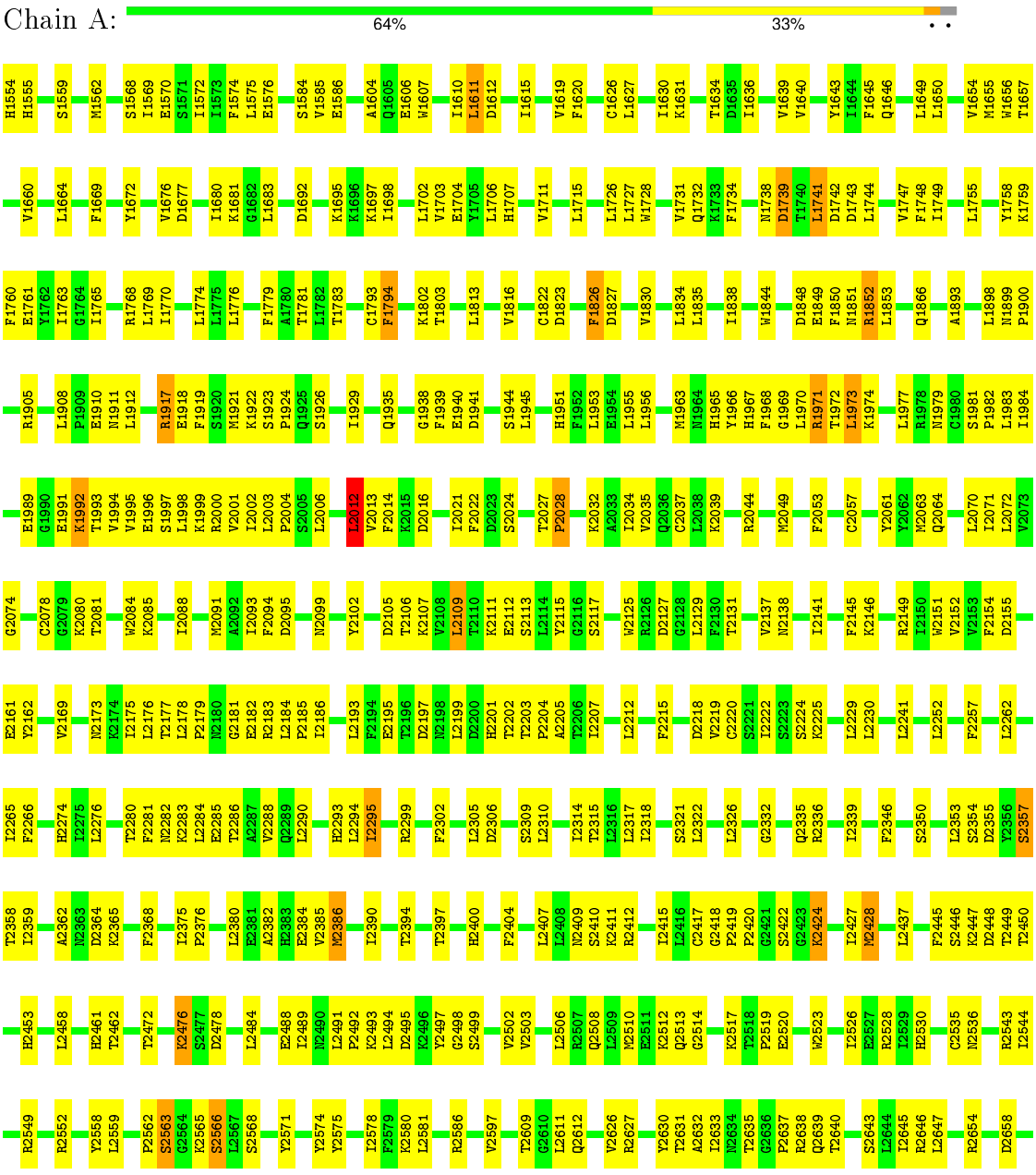
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2245	18105	11610	3004	3403	88	0	0

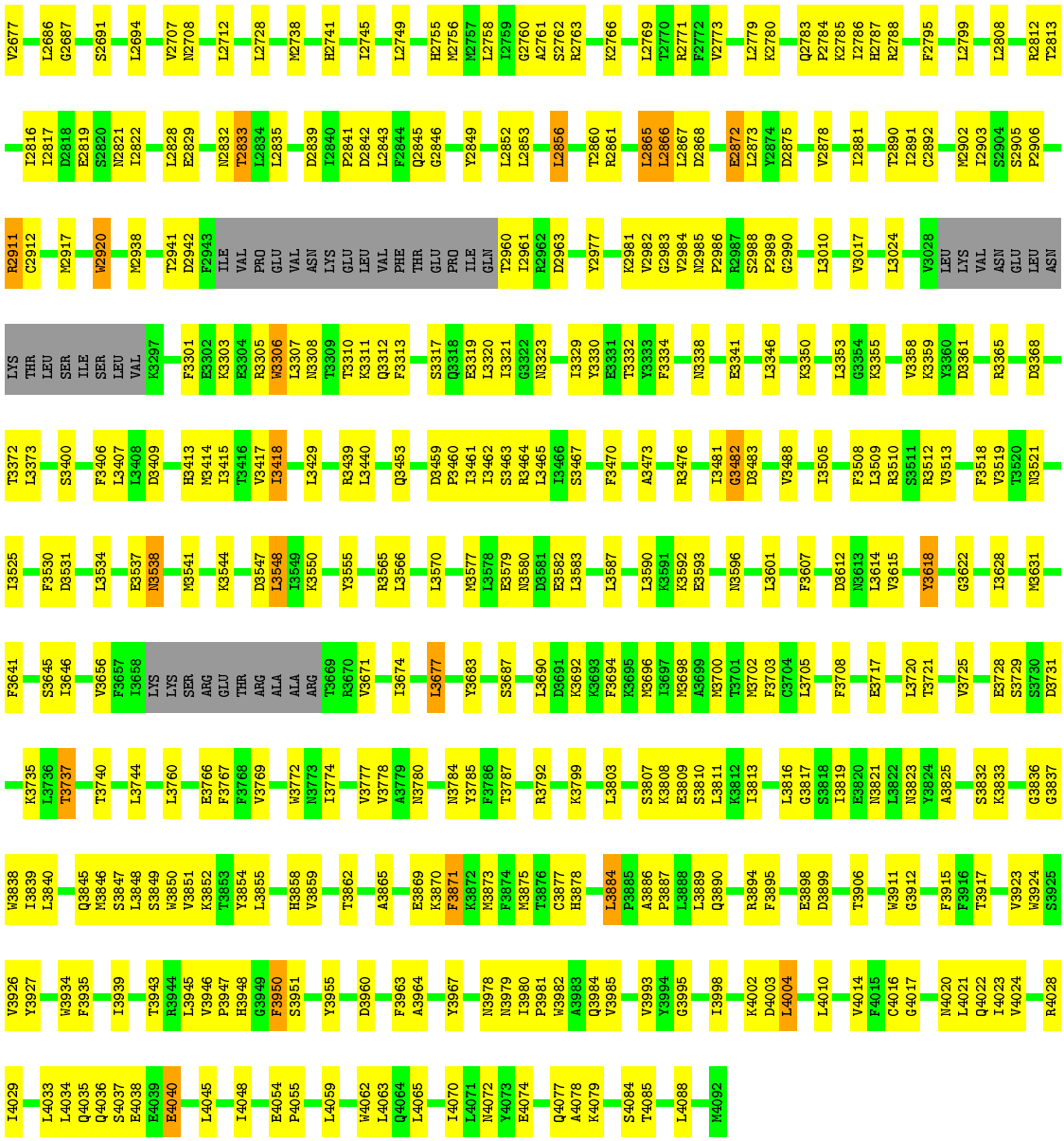
3 Residue-property plots (i)

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

Chain A:




V2677 L2686 G2687 S2691 L2694 V2707 N2708 L2712 L2728 M2738 H2741 I2745 L2749 H2755 M2756 M2757 L2758 I2759 G2760 A2761 S2762 R2763 K2766 L2769 T2770 R2771 F2772 V2773 L2779 K2780 Q2783 P2784 K2785 I2786 H2787 R2788 F2795 L2799 L2808 R2812 T2813
I2816 I2817 D2818 E2819 S2820 N2821 I2822 L2828 E2829 N2832 T2833 L2834 L2835 D2839 I2840 P2841 D2842 L2843 F2844 Q2845 G2846 Y2849 L2852 L2853 L2856 T2860 R2861 L2865 L2866 L2867 D2868 E2872 L2873 Y2874 D2875 V2878 I2881 T2890 I2891 C2892 M2902 I2903 S2904 S2905 P2906
R2911 C2912 M2917 W2920 M2938 T2941 D2942 F2943 ILE VAL PRO GLU VAL ASN LYS GLU LEU VAL PHE THR GLU PRO ILE GLN T2960 I2961 R2962 D2963 Y2977 K2981 V2982 G2983 V2984 N2985 P2986 R2987 S2988 P2989 G2990 L3010 V3017 L3024 V3028 LEU LYS VAL ASN GLU LEU ASN
LYS THR LEU SER ILE SER LEU VAL K3297 F3301 E3302 K3303 E3304 R3305 W3306 L3307 N3308 T3309 T3310 K3311 Q3312 F3313 S3317 Q3318 E3319 L3320 I3321 G3322 N3323 I3329 Y3330 E3331 T3332 Y3333 F3334 N3338 E3341 L3346 K3350 L3353 G3354 K3355 V3358 K3359 Y3360 D3361 R3365 D3368
T3372 L3373 S3400 F3406 L3407 L3408 D3409 H3413 M3414 I3415 T3416 V3417 I3418 L3429 R3439 L3440 Q3453 D3459 P3460 I3461 I3462 S3463 R3464 L3465 I3466 S3467 F3470 A3473 R3476 I3481 G3482 D3483 V3488 I3505 F3508 L3509 R3510 S3511 R3512 V3513 F3518 V3519 T3520 N3521
I3525 F3530 D3531 L3534 E3537 N3538 M3541 K3544 D3547 L3548 I3549 K3550 Y3555 R3565 L3566 L3570 M3577 L3578 E3579 N3580 D3581 E3582 L3583 L3587 L3590 K3591 K3592 E3593 N3596 L3601 F3607 D3612 N3613 L3614 V3615 Y3618 G3622 I3628 M3631
F3641 S3645 I3646 V3656 F3657 I3658 LYS LYS SER ARG GLU THR ARG ALA ALA ARG T3669 R3670 V3671 I3674 L3677 Y3683 S3687 L3690 D3691 K3692 K3693 F3694 K3695 M3696 I3697 M3698 A3699 M3700 T3701 M3702 F3703 C3704 L3705 F3708 E3717 L3720 T3721 V3725 E3728 S3729 S3730 D3731
K3735 L3736 T3737 T3740 L3744 L3760 E3766 F3767 F3768 V3769 W3772 N3773 I3774 V3777 V3778 A3779 N3780 N3784 Y3785 F3786 T3787 R3792 K3799 L3803 S3807 K3808 E3809 S3810 L3811 K3812 I3813 L3816 G3817 S3818 I3819 E3820 N3821 L3822 N3823 Y3824 A3825 S3832 K3833 G3836 G3837
W3838 I3839 L3840 Q3845 M3846 S3847 L3848 S3849 W3850 V3851 K3852 T3853 Y3854 L3855 H3858 V3859 T3862 A3865 E3869 K3870 F3871 K3872 M3873 F3874 M3875 T3876 C3877 H3878 L3884 P3885 A3886 P3887 L3888 L3889 Q3890 R3894 F3895 E3898 D3899 T3906 W3911 G3912 F3915 F3916 T3917 V3923 W3924 S3925
V3926 Y3927 W3934 F3935 I3939 T3943 R3944 L3945 V3946 P3947 H3948 G3949 F3950 S3951 Y3955 D3960 F3963 A3964 Y3967 N3978 N3979 I3980 P3981 W3982 A3983 Q3984 V3985 V3993 Y3994 G3995 I3998 K4002 D4003 L4004 L4010 V4014 F4015 C4016 G4017 N4020 L4021 Q4022 I4023 V4024 R4028
I4029 L4033 L4034 Q4035 Q4036 S4037 E4038 E4039 E4040 L4045 I4048 E4054 P4055 L4059 W4062 L4063 Q4064 L4065 I4070 L4071 N4072 Y4073 E4074 Q4077 A4078 K4079 S4084 T4085 L4088 M4092

4 Experimental information (i)

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 ($e^-/Å^2$)	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	7.51	1.63	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1741	LEU	CB-CG-CD1	8.43	125.33	111.00
1	A	1973	LEU	CB-CG-CD1	-7.36	98.48	111.00
1	A	2872	GLU	OE1-CD-OE2	-7.28	114.56	123.30
1	A	2866	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	1769	LEU	CA-CB-CG	6.05	129.21	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	780	0
All	All	18105	0	18146	780	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 22.

The worst 5 of 780 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	1.20
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:1992:LYS:HG3	1:A:2024:SER:HB2	1.17	1.13
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.25	1.13

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%)	1967 (96%)	72 (4%)	43 74

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2843	LEU
1	A	3301	PHE
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

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.