wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:59 PM GMT

PDB ID	:	3VKH
Title	:	X-ray structure of a functional full-length dynein motor domain
Authors	:	Kon, T.; Oyama, T.; Shimo-Kon, R.; Suto, K.; Kurisu, G.
Deposited on	:	2011-11-16
Resolution	:	3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

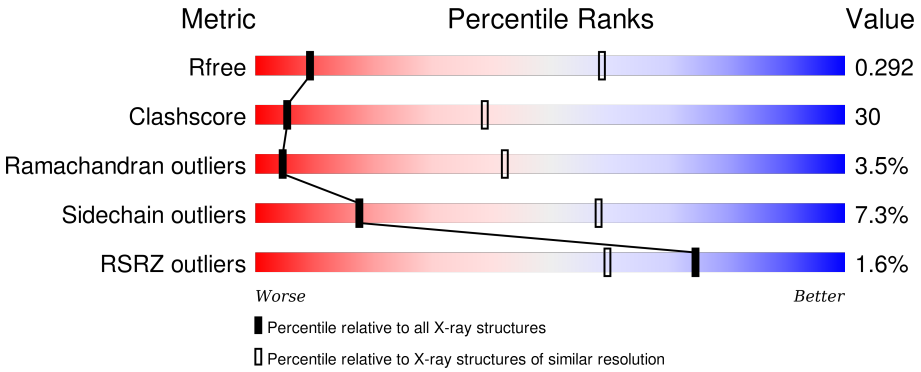
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3367	2% 42% 42% 6% 10%
1	B	3367	% 46% 37% • 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	A	9001	-	-	-	X
2	ADP	B	9007	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 45974 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	A	3042	Total	C	N	O	S	0	0	0
			23374	14951	3955	4368	100			
1	B	2908	Total	C	N	O	S	0	0	0
			22384	14307	3792	4190	95			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	EXPRESSION TAG	UNP P34036
A	1365	THR	-	EXPRESSION TAG	UNP P34036
A	1366	ARG	-	EXPRESSION TAG	UNP P34036
A	1367	HIS	-	EXPRESSION TAG	UNP P34036
A	1368	HIS	-	EXPRESSION TAG	UNP P34036
A	1369	HIS	-	EXPRESSION TAG	UNP P34036
A	1370	HIS	-	EXPRESSION TAG	UNP P34036
A	1371	HIS	-	EXPRESSION TAG	UNP P34036
A	1372	HIS	-	EXPRESSION TAG	UNP P34036
A	1373	GLY	-	EXPRESSION TAG	UNP P34036
A	1374	GLY	-	EXPRESSION TAG	UNP P34036
A	1375	GLY	-	EXPRESSION TAG	UNP P34036
A	1376	ASP	-	EXPRESSION TAG	UNP P34036
A	1377	TYR	-	EXPRESSION TAG	UNP P34036
A	1378	LYS	-	EXPRESSION TAG	UNP P34036
A	1379	ASP	-	EXPRESSION TAG	UNP P34036
A	1380	ASP	-	EXPRESSION TAG	UNP P34036
A	1381	ASP	-	EXPRESSION TAG	UNP P34036
A	1382	ASP	-	EXPRESSION TAG	UNP P34036
A	1383	LYS	-	EXPRESSION TAG	UNP P34036
A	1384	GLY	-	EXPRESSION TAG	UNP P34036
A	1385	GLY	-	EXPRESSION TAG	UNP P34036
A	1386	GLY	-	EXPRESSION TAG	UNP P34036
A	1387	LYS	-	EXPRESSION TAG	UNP P34036
B	1364	MET	-	EXPRESSION TAG	UNP P34036

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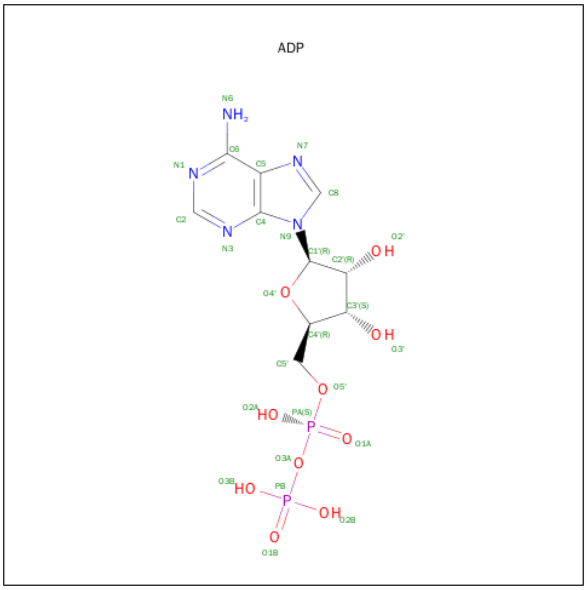
Chain	Residue	Modelled	Actual	Comment	Reference
B	1365	THR	-	EXPRESSION TAG	UNP P34036
B	1366	ARG	-	EXPRESSION TAG	UNP P34036
B	1367	HIS	-	EXPRESSION TAG	UNP P34036
B	1368	HIS	-	EXPRESSION TAG	UNP P34036
B	1369	HIS	-	EXPRESSION TAG	UNP P34036
B	1370	HIS	-	EXPRESSION TAG	UNP P34036
B	1371	HIS	-	EXPRESSION TAG	UNP P34036
B	1372	HIS	-	EXPRESSION TAG	UNP P34036
B	1373	GLY	-	EXPRESSION TAG	UNP P34036
B	1374	GLY	-	EXPRESSION TAG	UNP P34036
B	1375	GLY	-	EXPRESSION TAG	UNP P34036
B	1376	ASP	-	EXPRESSION TAG	UNP P34036
B	1377	TYR	-	EXPRESSION TAG	UNP P34036
B	1378	LYS	-	EXPRESSION TAG	UNP P34036
B	1379	ASP	-	EXPRESSION TAG	UNP P34036
B	1380	ASP	-	EXPRESSION TAG	UNP P34036
B	1381	ASP	-	EXPRESSION TAG	UNP P34036
B	1382	ASP	-	EXPRESSION TAG	UNP P34036
B	1383	LYS	-	EXPRESSION TAG	UNP P34036
B	1384	GLY	-	EXPRESSION TAG	UNP P34036
B	1385	GLY	-	EXPRESSION TAG	UNP P34036
B	1386	GLY	-	EXPRESSION TAG	UNP P34036
B	1387	LYS	-	EXPRESSION TAG	UNP P34036

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



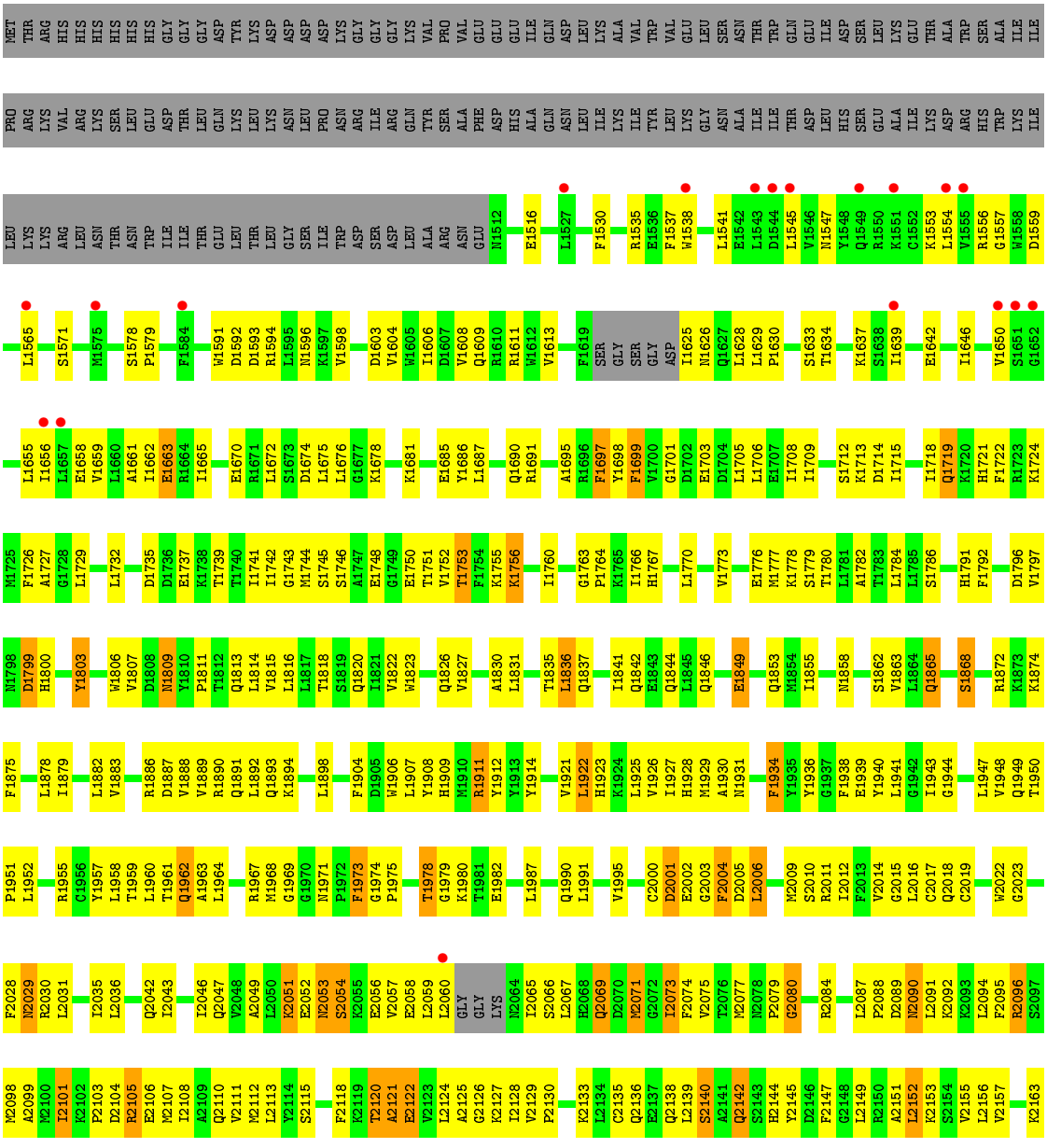
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

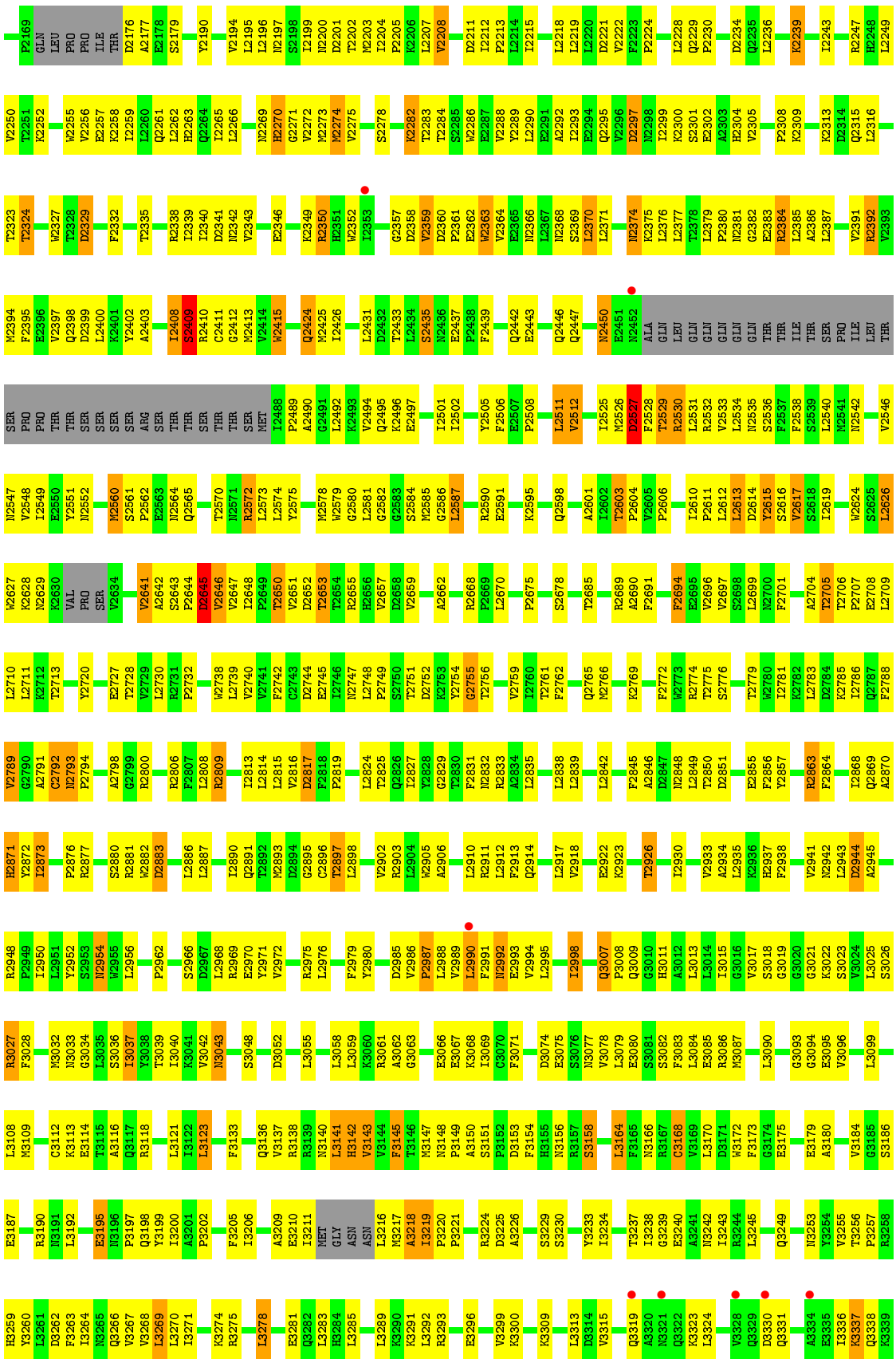
3 Residue-property plots (i)

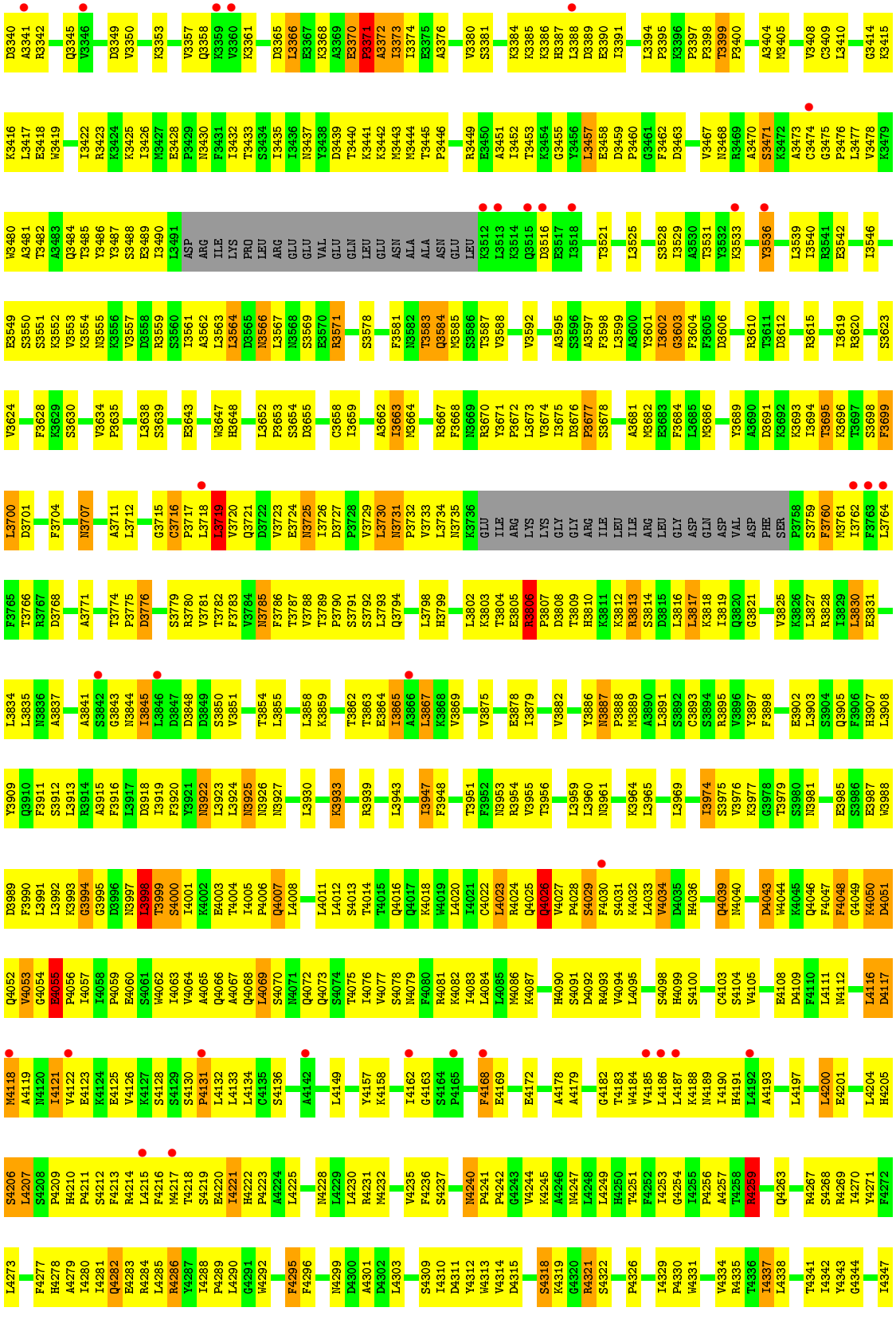
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

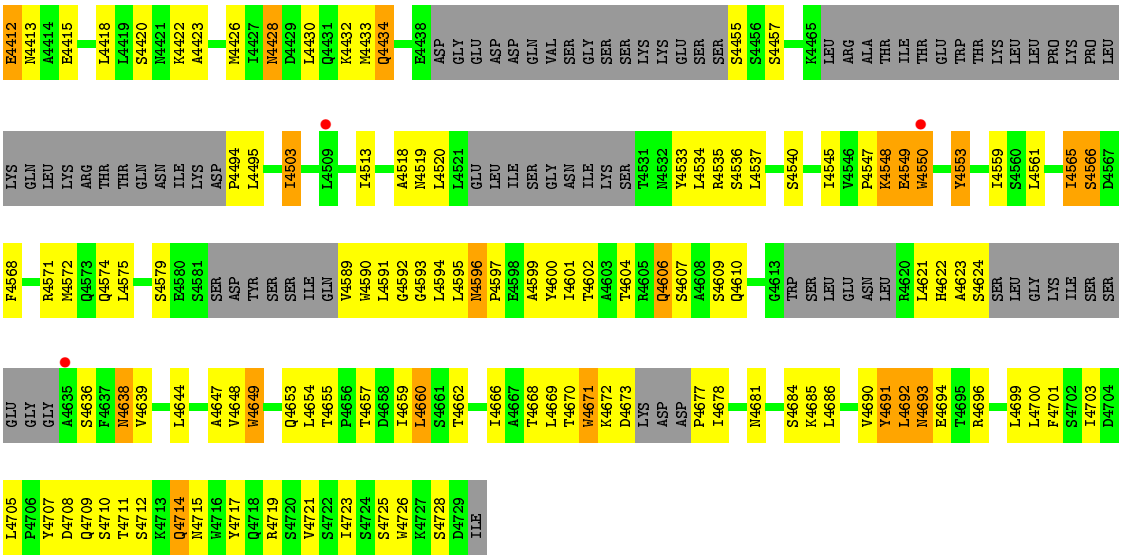
- Molecule 1: Dynein heavy chain, cytoplasmic

Chain A:



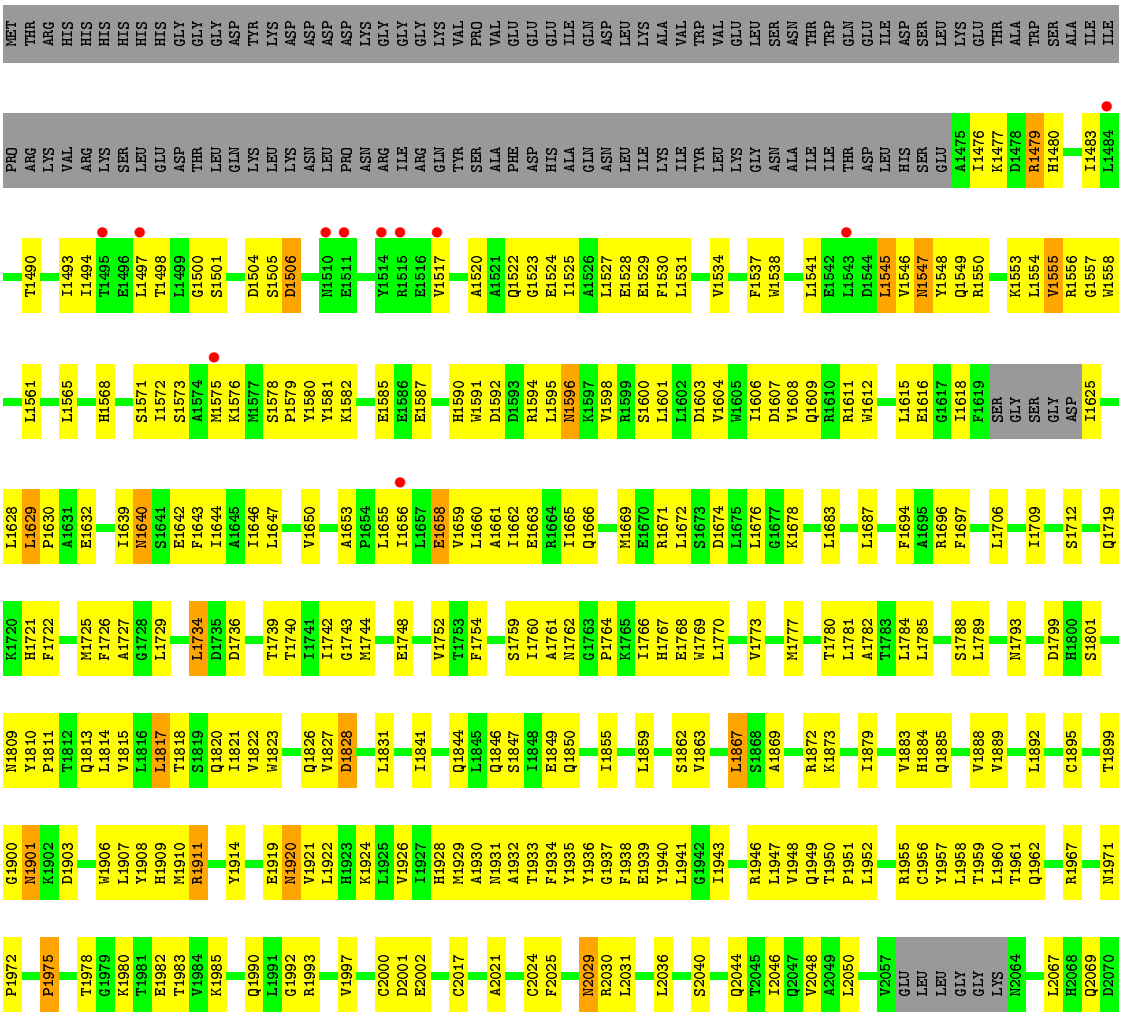


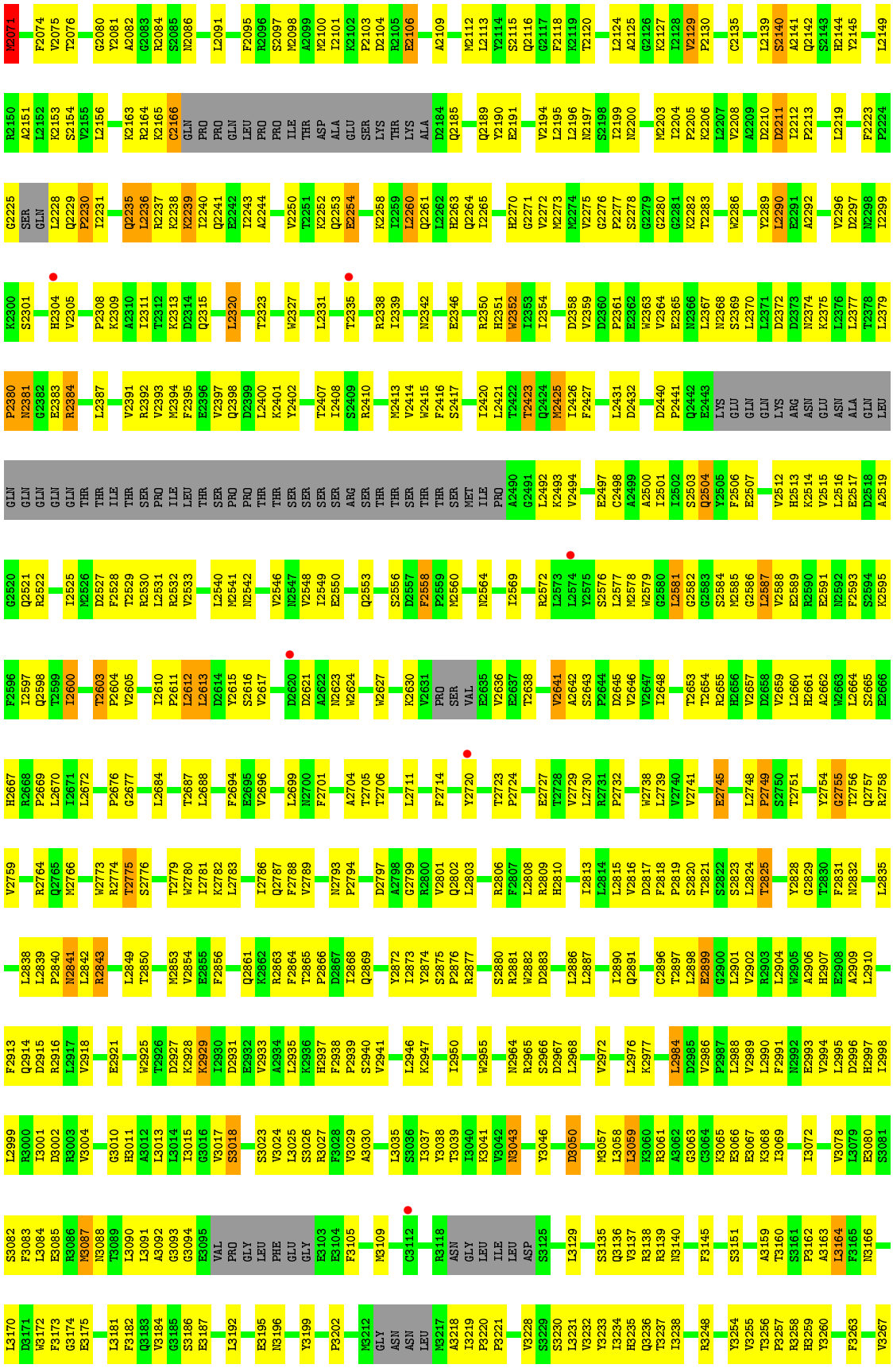

D3340 A3341 R3342 Q3345 V3346 D3349 V3350 K3353 V3357 Q3358 K3359 V3360 K3361 D3365 L3366 E3367 K3368 A3369 E3370 P3371 A3372 I3373 I3374 E3375 A3376 V3380 S3381 K3384 K3385 K3386 H3387 L3388 D3389 E3390 I3391 L3394 P3395 K3396 P3397 P3398 T3399 P3400 A3404 M3405 V3408 C3409 L3410 G3414 K3415
K3416 L3417 E3418 W3419 I3422 R3423 K3424 K3425 I3426 M3427 E3428 P3429 N3430 F3431 I3432 T3433 S3434 I3435 I3436 N3437 Y3438 D3439 T3440 K3441 K3442 M3443 M3444 T3445 P3446 R3449 E3450 A3451 I3452 T3453 K3454 G3455 Y3456 L3457 E3458 D3459 P3460 G3461 F3462 D3463 V3467 N3468 R3469 A3470 S3471 K3472 A3473 C3474 G3475 P3476 L3477 V3478 V3479
W3480 A3481 T3482 A3483 Q3484 T3485 Y3486 Y3487 S3488 E3489 I3490 L3491 ASP ARG ILE LYS PRO LEU ARG GLU GLU VAL GLU GLN LEU GLU ASN ALA ALA ASN GLU LEU K3512 L3513 K3514 Q3515 D3516 E3517 I3518 T3521 L3525 S3528 I3529 A3530 T3531 Y3532 K3533 Y3536 L3539 I3540 R3541 E3542 I3546
E3549 S3550 S3551 K3552 V3553 K3554 N3555 K3556 V3557 D3558 R3559 S3560 I3561 A3562 L3563 L3564 D3565 N3566 L3567 N3568 S3569 E3570 R3571 S3578 F3581 N3582 T3583 Q3584 M3585 S3586 T3587 V3588 V3592 A3595 S3596 A3597 F3598 L3599 A3600 Y3601 I3602 G3603 F3604 F3605 D3606 R3610 T3611 D3612 R3615 I3619 R3620 S3623
V3624 F3628 R3629 S3630 V3634 P3635 L3638 S3639 E3643 W3647 H3648 L3652 P3653 S3654 D3655 C3658 I3659 A3662 I3663 M3664 R3667 F3668 N3669 R3670 Y3671 P3672 L3673 V3674 I3675 D3676 P3677 S3678 A3681 M3682 E3683 F3684 L3685 M3686 Y3689 A3690 D3691 K3692 K3693 I3694 T3695 K3696 T3697 S3698 F3699
L3700 D3701 F3704 N3707 A3711 L3712 G3715 C3716 P3717 L3718 L3719 V3720 Q3721 D3722 V3723 E3724 N3725 I3726 D3727 P3728 V3729 L3730 N3731 P3732 V3733 L3734 N3735 K3736 GLU ILE ARG LYS LYS GLY GLY ARG ILE LEU ILE ARG LEU GLY ASP GLN ASP VAL ASP PHE SER P3758 S3759 F3760 M3761 I3762 F3763 L3764
F3765 T3766 R3767 D3768 A3771 T3774 P3775 D3776 S3779 R3780 V3781 T3782 F3783 V3784 N3785 F3786 T3787 V3788 T3789 P3790 S3791 S3792 L3793 Q3794 L3798 H3799 L3802 K3803 T3804 E3805 R3806 P3807 D3808 T3809 H3810 K3811 K3812 R3813 S3814 D3815 L3816 L3817 K3818 I3819 Q3820 G3821 V3825 K3826 L3827 R3828 I3829 L3830 E3831
L3834 L3835 N3836 A3837 A3841 S3842 G3843 N3844 I3845 L3846 D3847 D3848 D3849 S3850 V3851 T3854 L3855 L3858 K3859 T3862 T3863 E3864 I3865 A3866 L3867 K3868 V3869 V3875 E3878 I3879 V3882 Y3886 N3887 P3888 M3889 A3890 L3891 S3892 C3893 S3894 R3895 V3896 Y3897 F3898 E3902 L3903 S3904 Q3905 F3906 H3907 L3908
Y3909 Q3910 F3911 S3912 L3913 R3914 A3915 F3916 L3917 D3918 I3919 F3920 Y3921 N3922 L3923 L3924 N3925 N3926 N3927 L3930 K3933 R3939 L3943 I3947 F3948 T3951 F3952 N3953 R3954 V3955 T3956 L3959 L3960 N3961 K3964 L3965 L3969 I3974 S3975 V3976 K3977 G3978 T3979 S3980 N3981 E3985 S3986 E3987 W3988
D3989 F3990 L3991 L3992 K3993 G3994 G3995 D3996 N3997 L3998 T3999 S4000 I4001 K4002 E4003 T4004 I4005 P4006 Q4007 L4008 L4011 L4012 S4013 T4014 T4015 Q4016 Q4017 K4018 W4019 L4020 I4021 C4022 L4023 R4024 Q4025 Q4026 V4027 P4028 S4029 F4030 S4031 K4032 L4033 V4034 D4035 H4036 Q4039 N4040 D4043 W4044 K4045 Q4046 F4047 F4048 G4049 K4050 D4051
Q4052 V4053 G4054 E4055 P4056 I4057 I4058 P4059 E4060 S4061 W4062 I4063 V4064 A4065 Q4066 A4067 Q4068 L4069 S4070 N4071 Q4072 Q4073 S4074 T4075 I4076 V4077 S4078 N4079 F4080 R4081 K4082 I4083 L4084 L4085 M4086 K4087 H4090 S4091 D4092 R4093 V4094 L4095 S4098 H4099 S4100 C4103 S4104 V4105 E4108 D4109 F4110 L4111 N4112 L4116 D4117
M4118 A4119 N4120 I4121 V4122 E4123 R4124 E4125 V4126 R4127 S4128 S4129 S4130 P4131 L4132 L4133 L4134 C4135 S4136 A4142 L4149 Y4157 K4158 I4162 G4163 S4164 P4165 F4168 E4169 E4172 A4178 A4179 G4182 T4183 W4184 V4185 L4186 L4187 K4188 N4189 I4190 H4191 L4192 A4193 L4197 L4200 E4201 L4204 H4205
S4206 L4207 S4208 P4209 H4210 P4211 S4212 F4213 R4214 L4215 F4216 M4217 T4218 S4219 E4220 I4221 H4222 P4223 A4224 L4225 N4228 L4229 L4230 R4231 M4232 V4235 F4236 S4237 N4240 P4241 P4242 G4243 V4244 K4245 A4246 N4247 L4248 L4249 H4250 T4251 F4252 I4253 G4254 I4255 P4256 A4257 T4258 R4259 Q4263 R4267 S4268 R4269 I4270 Y4271 F4272
L4273 F4277 H4278 A4279 I4280 I4281 Q4282 E4283 R4284 L4285 R4286 Y4287 I4288 P4289 L4290 G4291 W4292 F4295 F4296 N4299 D4300 A4301 D4302 L4303 S4309 I4310 D4311 Y4312 W4313 V4314 D4315 S4318 K4319 G4320 R4321 S4322 P4326 I4329 P4330 W4331 V4334 R4335 T4336 I4337 I4338 T4341 I4342 Y4343 G4344 I4347
D4348 N4349 E4350 F4351 D4352 M4353 R4354 L4355 L4356 Y4357 S4358 F4359 L4360 E4361 Q4362 L4363 F4364 T4365 P4366 S4367 A4368 F4369 N4370 P4371 D4372 F4373 P4374 L4375 V4376 I4379 G4380 L4381 S4382 V4383 P4384 E4385 G4386 T4387 T4388 R4389 A4390 H4391 F4392 M4393 K4394 W4395 I4396 L4399 P4400 E4401 I4402 S4403 T4404 P4405 I4406 W4407 L4408

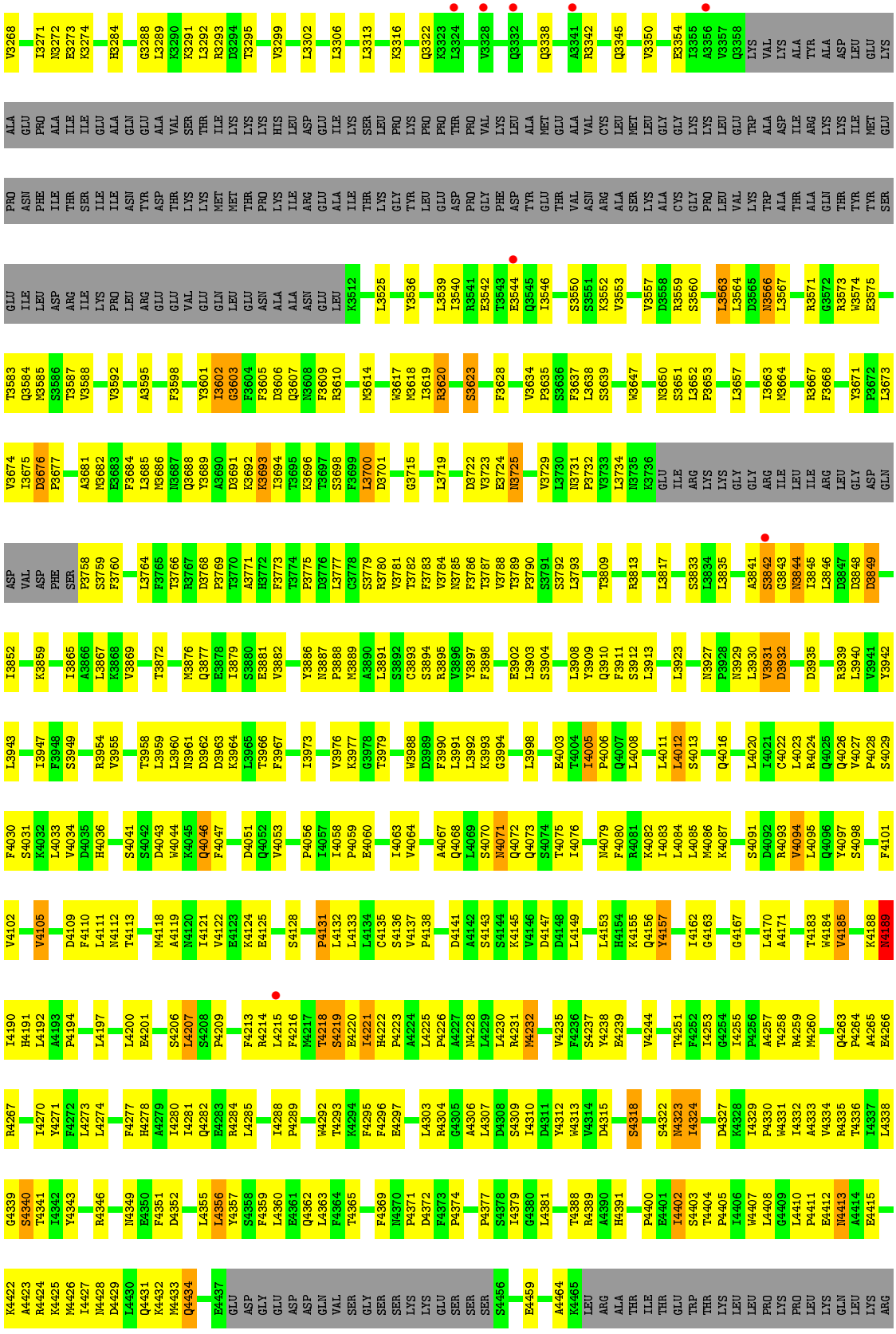


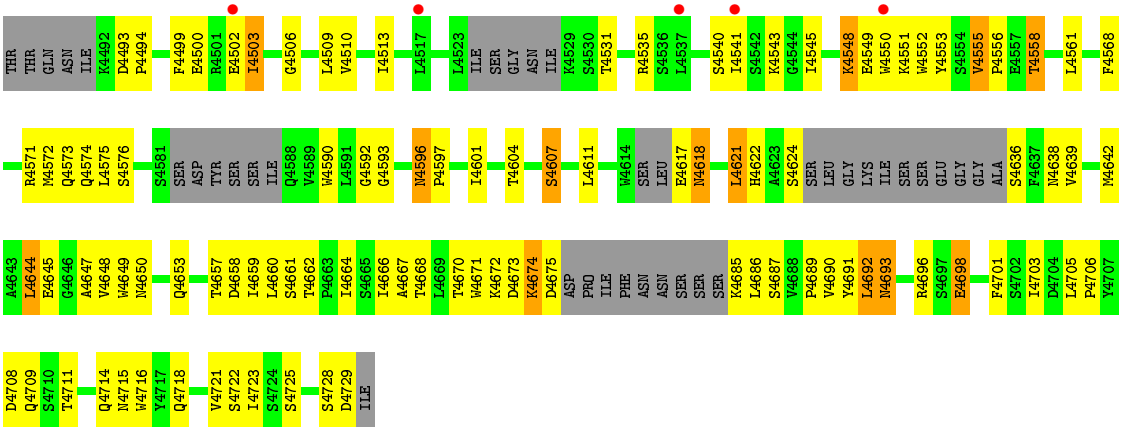
• Molecule 1: Dynein heavy chain, cytoplasmic

Chain B:








THR THR GLN ASN ILE K4492 D4493 P4494
F4499 E4500 R4501 E4502 I4503 G4506 L4509 V4510 I4513 L4517 L4523 ILE SER GLY ASN ILE K4529 S4530 T4531 R4535 S4536 L4537 S4540 I4541 S4542 K4543 G4544 I4545 K4548 E4549 W4550 K4551 W4552 Y4553 S4554 V4555 P4556 E4557 T4558 L4561 F4568
R4571 M4572 Q4573 Q4574 L4575 S4576 S4581 SER ASP TYR SER SER ILE Q4588 V4589 W4590 L4591 G4592 G4593 M4596 P4597 I4601 T4604 S4607 L4611 W4614 SER LEU E4617 M4618 L4621 H4622 A4623 S4624 SER LEU GLY LYS ILE SER SER GLU GLY GLY ALA S4636 F4637 N4638 V4639 M4642
A4643 L4644 E4645 G4646 A4647 V4648 W4649 N4650 Q4653 T4657 D4658 I4659 L4660 S4661 T4662 P4663 I4664 S4665 I4666 A4667 T4668 L4669 T4670 W4671 K4672 D4673 K4674 D4675 ASP PRO ILE PHE ASN ASN SER SER SER K4685 L4686 S4687 V4688 P4689 V4690 Y4691 L4692 N4693 R4696 S4697 E4698 F4701 S4702 I4703 D4704 L4705 P4706 V4707
D4708 Q4709 S4710 T4711 Q4714 N4715 W4716 Y4717 Q4718 V4721 S4722 I4723 S4724 S4725 S4728 D4729 ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	195.73Å 228.96Å 201.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.80 48.78 – 3.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.79-3.80) 99.0 (48.78-3.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.219 , 0.292 0.220 , 0.292	Depositor DCC
R_{free} test set	4442 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	125.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 112.1	EDS
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 89309 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	45974	wwPDB-VP
Average B, all atoms (Å^2)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.24	0/23866	0.44	1/32482 (0.0%)
1	B	0.24	0/22846	0.43	0/31076
All	All	0.24	0/46712	0.44	1/63558 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3371	PRO	N-CA-CB	5.32	109.68	103.30

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	A	23374	0	22545	1559	0
1	B	22384	0	21550	1149	0
2	A	108	0	48	7	0
2	B	108	0	48	3	0
All	All	45974	0	44191	2704	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 30.

The worst 5 of 2704 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:3689:TYR:HB2	1:A:3694:ILE:HD11	1.29	1.14
1:A:3337:LYS:HB3	1:A:3525:LEU:HD13	1.35	1.07
1:B:3841:ALA:O	1:B:3842:SER:HB2	1.54	1.04
1:A:4242:PRO:HA	1:A:4286:ARG:HH12	1.22	1.03
1:A:4109:ASP:HA	1:A:4112:ASN:HD22	1.22	1.00

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 X-ray entries followed by that with respect to entries of similar resolution.

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	3010/3367 (89%)	2424 (80%)	448 (15%)	138 (5%)	3 34
1	B	2870/3367 (85%)	2476 (86%)	327 (11%)	67 (2%)	8 51
All	All	5880/6734 (87%)	4900 (83%)	775 (13%)	205 (4%)	4 42

5 of 205 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1836	LEU
1	A	2121	ALA
1	A	2409	SER
1	A	2560	MET
1	A	2617	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	2457/3028 (81%)	2249 (92%)	208 (8%)	13 52
1	B	2353/3028 (78%)	2210 (94%)	143 (6%)	23 65
All	All	4810/6056 (79%)	4459 (93%)	351 (7%)	17 58

5 of 351 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3925	ASN
1	A	4565	ILE
1	B	4258	THR
1	A	4023	LEU
1	A	4267	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4046	GLN
1	A	4715	ASN
1	B	4152	GLN
1	A	4079	ASN
1	A	4349	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 (i)

8 ligands are 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	$\#\|Z\| > 2$
2	ADP	A	9001	-	22,29,29	1.30	3 (13%)	27,45,45	2.22	6 (22%)
2	ADP	A	9002	-	22,29,29	1.27	3 (13%)	27,45,45	2.17	5 (18%)
2	ADP	A	9003	-	22,29,29	1.30	3 (13%)	27,45,45	2.20	5 (18%)
2	ADP	A	9004	-	22,29,29	1.26	3 (13%)	27,45,45	2.23	6 (22%)
2	ADP	B	9007	-	22,29,29	1.26	3 (13%)	27,45,45	2.21	6 (22%)
2	ADP	B	9008	-	22,29,29	1.26	3 (13%)	27,45,45	2.18	6 (22%)
2	ADP	B	9009	-	22,29,29	1.29	3 (13%)	27,45,45	2.20	6 (22%)
2	ADP	B	9010	-	22,29,29	1.27	3 (13%)	27,45,45	2.21	6 (22%)

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
2	ADP	A	9001	-	-	0/12/32/32	0/3/3/3
2	ADP	A	9002	-	-	0/12/32/32	0/3/3/3
2	ADP	A	9003	-	-	0/12/32/32	0/3/3/3
2	ADP	A	9004	-	-	0/12/32/32	0/3/3/3
2	ADP	B	9007	-	-	0/12/32/32	0/3/3/3
2	ADP	B	9008	-	-	0/12/32/32	0/3/3/3
2	ADP	B	9009	-	-	0/12/32/32	0/3/3/3
2	ADP	B	9010	-	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9002	ADP	O4'-C1'	2.01	1.43	1.41
2	B	9008	ADP	O4'-C1'	2.11	1.43	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9007	ADP	O4'-C1'	2.14	1.43	1.41
2	A	9004	ADP	O4'-C1'	2.18	1.44	1.41
2	B	9010	ADP	O4'-C1'	2.23	1.44	1.41

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	9004	ADP	N3-C2-N1	-9.13	121.91	128.89
2	A	9003	ADP	N3-C2-N1	-9.06	121.96	128.89
2	B	9007	ADP	N3-C2-N1	-9.04	121.97	128.89
2	B	9010	ADP	N3-C2-N1	-9.01	122.00	128.89
2	A	9001	ADP	N3-C2-N1	-9.01	122.00	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9001	ADP	1	0
2	A	9002	ADP	4	0
2	A	9004	ADP	2	0
2	B	9009	ADP	1	0
2	B	9010	ADP	2	0

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	3042/3367 (90%)	-0.11	64 (2%)	67	51	64, 130, 209, 322	0
1	B	2908/3367 (86%)	-0.15	30 (1%)	84	72	72, 136, 208, 335	0
All	All	5950/6734 (88%)	-0.13	94 (1%)	74	60	64, 133, 209, 335	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1543	LEU	5.6
1	B	1517	VAL	4.8
1	A	1652	GLY	4.8
1	A	4187	LEU	4.4
1	A	1651	SER	4.4

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ADP	A	9001	27/27	0.94	0.39	2.68	129,129,129,129	0
2	ADP	B	9007	27/27	0.90	0.37	2.41	129,129,129,129	0
2	ADP	B	9009	27/27	0.95	0.31	1.87	129,129,129,129	0
2	ADP	A	9003	27/27	0.91	0.33	1.86	129,129,129,129	0
2	ADP	B	9008	27/27	0.85	0.40	1.80	129,129,129,129	0
2	ADP	A	9002	27/27	0.90	0.30	1.32	129,129,129,129	0
2	ADP	B	9010	27/27	0.86	0.30	0.79	129,129,129,129	0
2	ADP	A	9004	27/27	0.91	0.30	0.07	129,129,129,129	0

6.5 Other polymers (i)

There are no such residues in this entry.