



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:19 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 validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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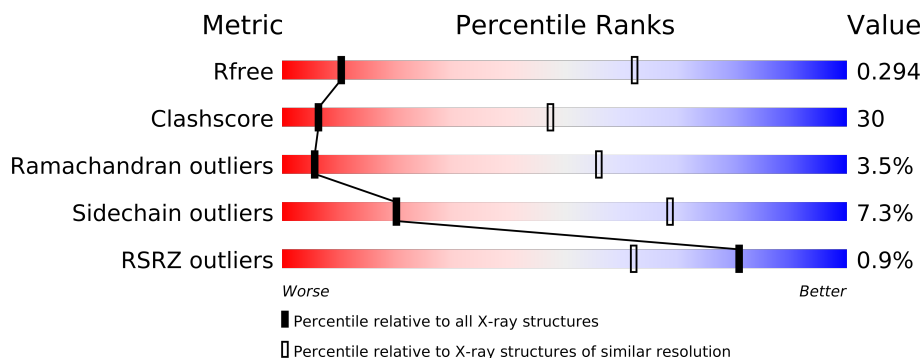
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance


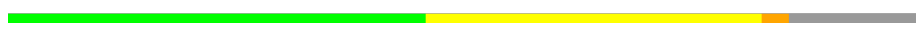
The reported resolution of this entry is 3.80 Å.

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))
$R_{free}$	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	3367	
1	B	3367	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ADP	A	9001	-	X
2	ADP	A	9003	-	X
2	ADP	B	9007	-	X

## 2 Entry composition

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

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:  $C_{10}H_{15}N_5O_{10}P_2$ ).



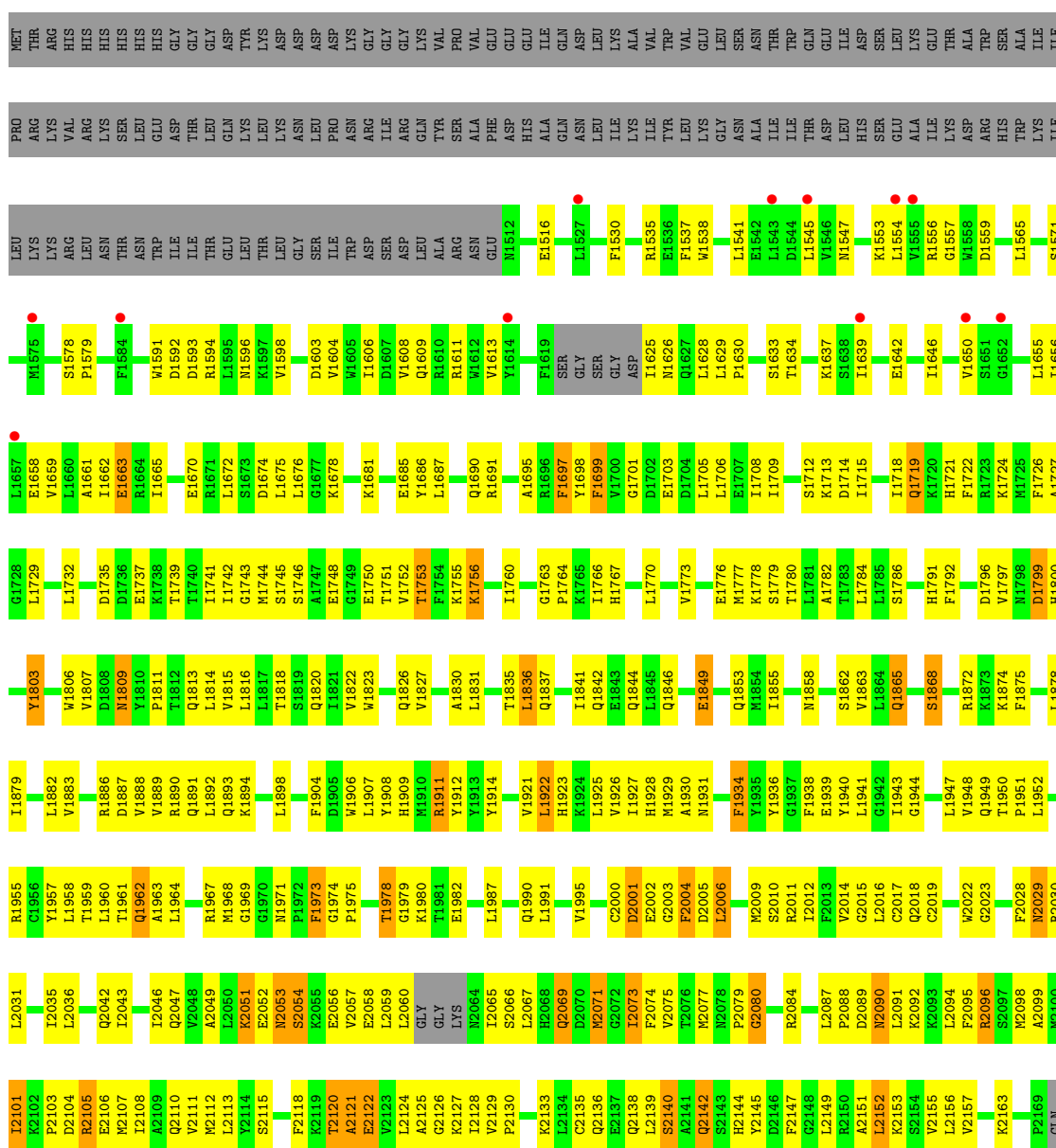
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B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

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

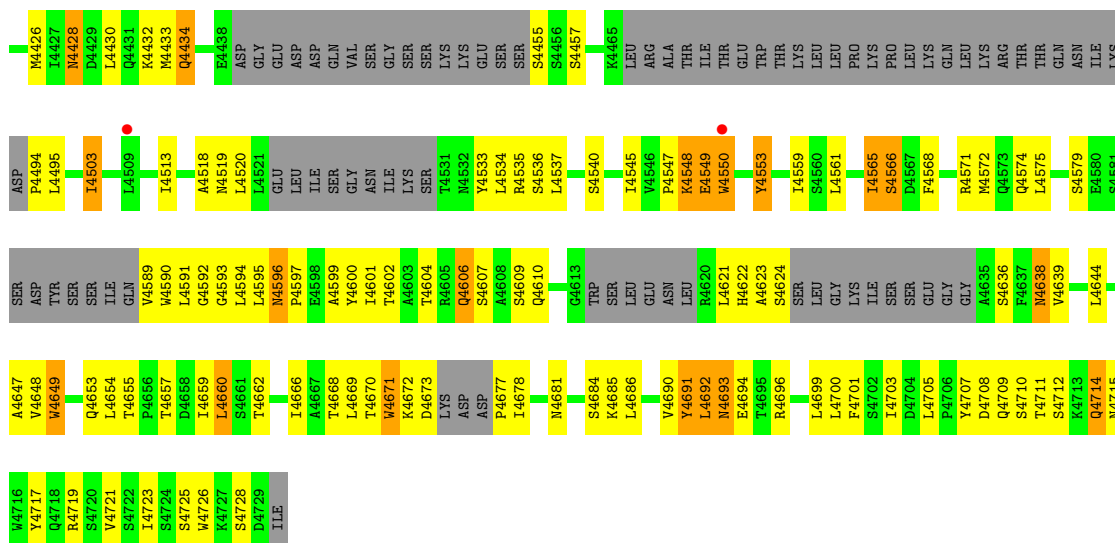
Chain A: 



F3263	K3113	N3033	Y2952	P2876	N2783	VAL	Y2551	THR	Q3398	V2327	W2255	LEU
I3264	E3114	G3034	S2953	R2877	P2794	PRO	N2552	SER	D2399	T2328	W2256	PRO
N3265	T3115	L3035	N2954	R2880	A2798	SER	M2560	SER	K2401	D2329	E2257	PRO
G3266	A3116	S3036	W2955	R2881	G2799	SER	S2561	SER	F2402	F2332	K2258	THR
V3267	K3117	I3037	L2956	W2882	R2800	SER	P2562	ARG	I2259	T2335	I2259	
V3268	R3118	V3038	P2962	D2883	R2806	SER	E2563	SER	L2260	L2260	L2260	
L3269	L3121	T3039	L3040	L2886	F2807	THR	N2564	THR	Q2261	Q2261	Q2261	
L3270	I3122	K3041	S2966	L2887	R2808	SER	Q2565	THR	H2262	H2262	H2262	
I3271	L3123	N3042	L2968	L2887	R2809	THR	T2570	THR	S2409	S2409	S2409	
K3274	F3133	N3043	R2975	L2890	I2813	SER	M2571	THR	G2412	G2412	G2412	
R3275	Q3136	S3048	R2968	Q2891	L2814	SER	R2572	THR	M2413	M2413	M2413	
L3278	V3137	D3052	L2972	T2892	L2815	THR	L2573	MET	V2414	V2414	V2414	
E3281	R3138	L3055	Y2971	M2893	L2816	THR	T2574		Q2424	Q2424	Q2424	
Q3282	R3139	L3059	Y2972	M2894	L2817	THR	T2575		A2425	A2425	A2425	
L3283	N3140	L3062	R2975	G2895	L2818	THR	G2582		T2432	T2432	T2432	
H3284	L3141	G3063	L2976	C2896	F2818	THR	G2583		T2433	T2433	T2433	
L3285	L3142	L3068	F2979	T2897	P2819	THR	S2584		L2434	L2434	L2434	
L3286	V3143	A3060	Y2980	L2898	L2824	THR	C2580		S2435	S2435	S2435	
L3289	Q3136	R3061	D2985	V2902	L2825	THR	L2581		T2436	T2436	T2436	
K3290	R3137	A3062	L2986	R2903	Q2826	THR	G2582		L2437	L2437	L2437	
L3291	V3144	G3062	P2987	L2904	Q2827	THR	G2583		F2439	F2439	F2439	
L3292	L3145	G3063	L2987	W2905	L2827	THR	S2584		Q2442	Q2442	Q2442	
R3293	M3147	L3068	L2988	A2906	G2828	THR	M2585		E2443	E2443	E2443	
E3296	N3148	E3066	L2989	V2902	L2830	THR	C2586		L2431	L2431	L2431	
V3299	P3149	K3067	D2989	R2903	L2831	THR	L2581		D2432	D2432	D2432	
K3300	A3150	K3068	L2990	L2910	F2831	THR	R2590		T2433	T2433	T2433	
K3309	L3156	S3076	I2998	L2917	L2838	THR	G2591		L2434	L2434	L2434	
L3313	R3157	N3077	Q3007	E2922	L2842	THR	K2596		Q2446	Q2446	Q2446	
V3315	L3164	L3078	P3008	K2923	L2844	THR	Q2598		V2512	V2512	V2512	
Q3319	F3165	E3080	Q3009	T2926	F2845	THR	A2601		N2450	N2450	N2450	
K3323	R3167	S3081	G3010	L2926	A2846	THR	T2603		E2451	E2451	E2451	
L3324	C3168	F3083	H3011	L2930	D2847	THR	P2604		ALA	ALA	ALA	
L3330	V3169	L3084	A3012	I2930	N2848	THR	P2606		GLN	GLN	GLN	
Q3331	L3170	E3085	L3014	V2933	L2849	THR	L2610		GLN	GLN	GLN	
A3334	L3172	K3086	I3015	A2934	T2850	THR	P2611		GLN	GLN	GLN	
E3335	D3171	M3087	G3016	L2935	D2851	THR	L2612		GLN	GLN	GLN	
K3337	G3174	L3090	V3017	K2936	E2855	THR	L2613		GLN	GLN	GLN	
Q3338	E3175	G3093	G3021	V2941	F2856	THR	Y2615		THR	THR	THR	
R3339	A3179	G3094	K3022	N2941	Y2857	THR	S2616		THR	THR	THR	
D3340	R3180	E3095	K3021	N2942	R2863	THR	V2617		THR	THR	THR	
A3341	V3184	V3096	S3023	L2943	F2864	THR	S2618		THR	THR	THR	
R3342	L3185	L3099	V3024	D2944	L2868	THR	L2619		THR	THR	THR	
Q3345	G3186	L3099	L3025	A2945	Q2869	THR	W2624		THR	THR	THR	
D3349	E3187	L3108	R3027	R2948	A2870	THR	S2626		THR	THR	THR	
V3350	R3190	M3109	F3028	P2949	H2871	THR	L2627		THR	THR	THR	
	L3261	L3261	L3261	L3261	L3261	THR	K2628		THR	THR	THR	
	L3262	L3262	L3262	L3262	L3262	THR	E2550		THR	THR	THR	

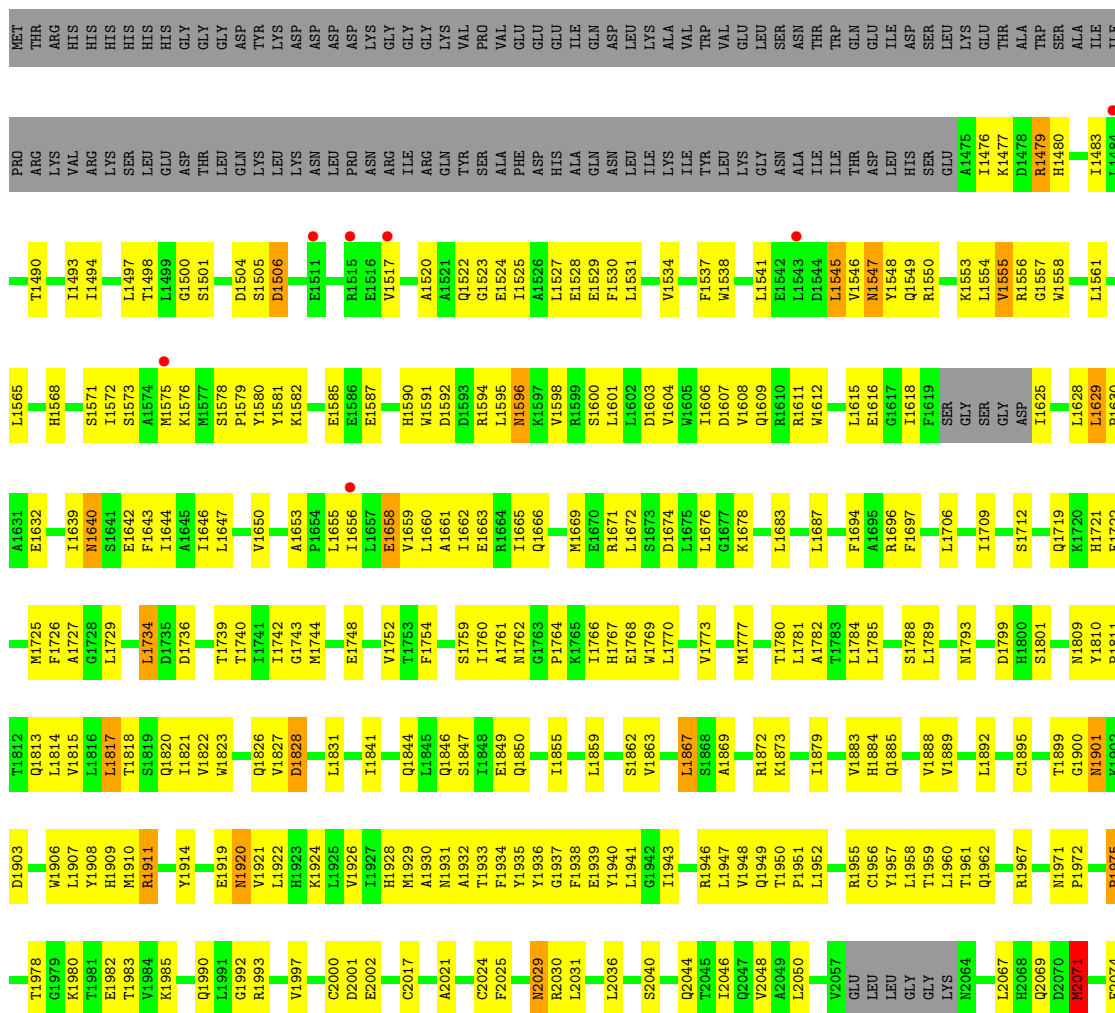
F4359	R4286	W4217	K4127	S4061	D3918	I3845	D3776	G3715	L3638	P3558	E3489	I3426	K3353
L4360	T4287	T4218	S4128	W4062	I3919	L3846	S3779	C3716	S3639	R3559	I3490	M3427	K3357
E4361	I4288	S4219	S4129	I4063	F3920	D3847	S3780	P3717	E3643	T3561	ASP	P3429	V3357
Q4362	P4289	E4220	P4130	W4064	Y3921	D3848	V3781	L3718	V3647	L3563	ILE	K3430	Q3358
L4363	L4290	L4221	P4131	A4065	N3922	D3849	K4002	L3719	V3648	L3564	LYS	F3431	K3359
F4364	G4291	H4222	K4132	Q4066	L3923	S3850	L3923	V3720	V3647	L3565	PRO	I3432	V3360
L4365	W4292	L4223	L4133	A4067	L3924	V3851	F3783	Q3721	H3648	P3566	LEU	T3433	K3361
T4366	W4292	L4223	L4133	Q4068	N3925	T3854	V3784	Q3722	L3652	P3566	LEU	S3434	
F4367	F4296	L4225	C4135	L4069	N3927	L3855	F3786	E3724	P3653	L3567	ARG	I3436	D3365
A4368	F4296	S4136	S4136	S4070	Q4007	L3858	F3787	E3724	S3654	L3568	GLU	I3437	E3367
N4369	N4228	N4071	L4149	N4071	L4008	L3859	T3788	I3726	C3658	E3570	VAL	M3438	E3367
N4370	L4229	Q4072	Q4073	Q4073	K3983	T3862	V3789	D3727	I3659	R3571	GLU	D3439	K3369
P4371	Q4073	Q4073	S4074	T4075	S3791	T3863	S3792	F3728		S3578	GLN	T3440	E3370
D4372	A4301	K4158	K4158	I4076	T3863	E3864	L3793	V3729	A3662	F3581	LEU	K3441	P3371
F4373	L4302	L4162	L4162	W4077	E3864	L3793	L3793	N3731	I3663	T3582	ASN	K3442	A3372
L4375	L4302	L4162	L4162	S4078	L3943	I3865	Q3794	P3732	M3664	T3583	ALA	M3444	I3374
L4376	L4302	L4162	L4162	N4079	L3943	A3866	L3798	V3733	R3667	Q3584	ASN	T3445	E3375
S4309	S4309	F4235	F4235	F4086	I3947	L3867	L3799	L3734	F3667	M3586	LEU	P3446	A3376
T4310	D4311	F4236	F4236	F4086	F3948	K3988	H3799	L3734	F3668	M3586	GLU		V3380
D4311	F4312	P4241	P4241	K4082	T3951	V3875	L3802	GLU	R3670	T3587	LEU	R3449	S3381
W4313	W4313	P4242	P4242	L4083	N3952	E3878	K3803	ILE	Y3671	V3588		A3450	A3451
D4315	D4315	E4172	E4172	L4084	F3952	I3879	T3804	ARG	P3672	T3588		I3452	K3384
S4318	S4318	E4172	E4172	M4086	R3954	E3878	E3805	LYS	L3673	V3592		T3453	K3385
K4319	K4319	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
Q4320	Q4320	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
L4381	L4381	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
S4382	S4382	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
F4383	F4383	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
W4384	W4384	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
E4385	E4385	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
Q4386	Q4386	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
L4387	L4387	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
L4388	L4388	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
L4389	L4389	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
S4322	S4322	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
P4326	P4326	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
H4391	H4391	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
F4392	F4392	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
M4393	M4393	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
K4394	K4394	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
W4395	W4395	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
L4396	L4396	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
L4399	L4399	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
P4400	P4400	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
E4401	E4401	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
L4402	L4402	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
S4403	S4403	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
T4404	T4404	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
F4405	F4405	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
L4406	L4406	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
W4407	W4407	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
L4408	L4408	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
E4412	E4412	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
M4413	M4413	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
E4415	E4415	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
L4418	L4418	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
W4419	W4419	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
S4420	S4420	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
W4421	W4421	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
K4422	K4422	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386
A4423	A4423	E4172	E4172	K4087	T3955	I3879	E3805	LYS	L3674	T3592		T3453	K3386





• Molecule 1: Dynein heavy chain, cytoplasmic

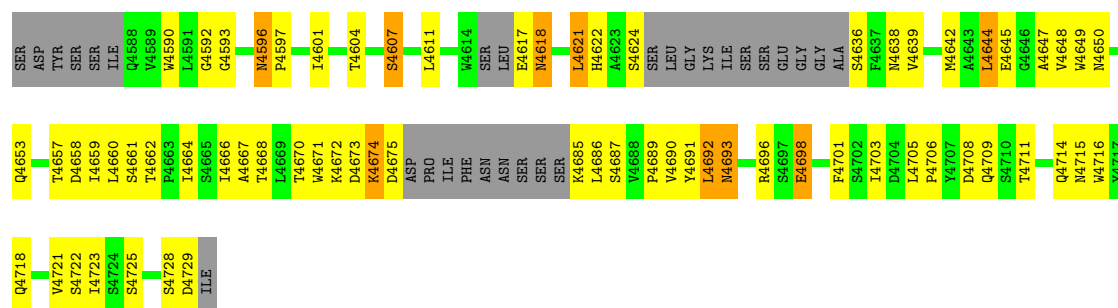
Chain B:





WORLD WIDE  
PDB  
PROTEIN DATA BANK





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.219 , 0.292 0.227 , 0.294	Depositor DCC
$R_{free}$ test set	4469 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	125.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 84.0	EDS
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

The worst 5 of 2704 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

### 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 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%)	4	46
1	B	2870/3367 (85%)	2476 (86%)	327 (11%)	67 (2%)	10	65
All	All	5880/6734 (87%)	4900 (83%)	775 (13%)	205 (4%)	6	56

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 ⓘ

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%)	15	62
1	B	2353/3028 (78%)	2210 (94%)	143 (6%)	26	75
All	All	4810/6056 (79%)	4459 (93%)	351 (7%)	20	69

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 chains 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 ⓘ

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	-	29,29,29	1.23	3 (10%)	45,45,45	2.04	10 (22%)
2	ADP	A	9002	-	29,29,29	1.21	3 (10%)	45,45,45	1.99	9 (20%)
2	ADP	A	9003	-	29,29,29	1.22	2 (6%)	45,45,45	2.04	10 (22%)
2	ADP	A	9004	-	29,29,29	1.24	3 (10%)	45,45,45	2.05	11 (24%)
2	ADP	B	9007	-	29,29,29	1.23	3 (10%)	45,45,45	2.04	10 (22%)
2	ADP	B	9008	-	29,29,29	1.23	3 (10%)	45,45,45	2.01	11 (24%)
2	ADP	B	9009	-	29,29,29	1.22	2 (6%)	45,45,45	2.03	10 (22%)
2	ADP	B	9010	-	29,29,29	1.24	3 (10%)	45,45,45	2.05	11 (24%)

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	-	-	0/16/32/32	0/1/3/3
2	ADP	A	9002	-	-	0/16/32/32	0/1/3/3
2	ADP	A	9003	-	-	0/16/32/32	0/1/3/3
2	ADP	A	9004	-	-	0/16/32/32	0/1/3/3
2	ADP	B	9007	-	-	0/16/32/32	0/1/3/3
2	ADP	B	9008	-	-	0/16/32/32	0/1/3/3
2	ADP	B	9009	-	-	0/16/32/32	0/1/3/3
2	ADP	B	9010	-	-	0/16/32/32	0/1/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9002	ADP	C5-C4	3.70	1.48	1.40
2	B	9008	ADP	C5-C4	3.65	1.48	1.40
2	B	9009	ADP	C5-C4	3.63	1.48	1.40
2	A	9003	ADP	C5-C4	3.62	1.48	1.40
2	B	9010	ADP	C5-C4	3.61	1.48	1.40

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9004	ADP	N3-C2-N1	-8.14	121.91	128.71
2	A	9003	ADP	N3-C2-N1	-8.08	121.96	128.71
2	B	9007	ADP	N3-C2-N1	-8.06	121.97	128.71
2	B	9010	ADP	N3-C2-N1	-8.03	122.00	128.71
2	A	9001	ADP	N3-C2-N1	-8.03	122.00	128.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	3042/3367 (90%)	0.08	38 (1%)	75 54	64, 130, 209, 322	0
1	B	2908/3367 (86%)	0.06	16 (0%)	86 70	72, 136, 208, 335	0
All	All	5950/6734 (88%)	0.07	54 (0%)	81 62	64, 133, 209, 335	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1543	LEU	4.2
1	A	4187	LEU	3.5
1	B	1517	VAL	3.2
1	A	1545	LEU	3.2
1	A	4217	MET	3.1

### 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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADP	B	9007	27/27	0.40	2.62	129,129,129,129	0
2	ADP	A	9001	27/27	0.37	2.52	129,129,129,129	0
2	ADP	A	9003	27/27	0.33	2.34	129,129,129,129	0
2	ADP	A	9002	27/27	0.32	1.80	129,129,129,129	0
2	ADP	B	9009	27/27	0.31	1.80	129,129,129,129	0
2	ADP	B	9008	27/27	0.41	1.53	129,129,129,129	0
2	ADP	B	9010	27/27	0.29	0.65	129,129,129,129	0
2	ADP	A	9004	27/27	0.30	-0.03	129,129,129,129	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.