



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:01 am 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

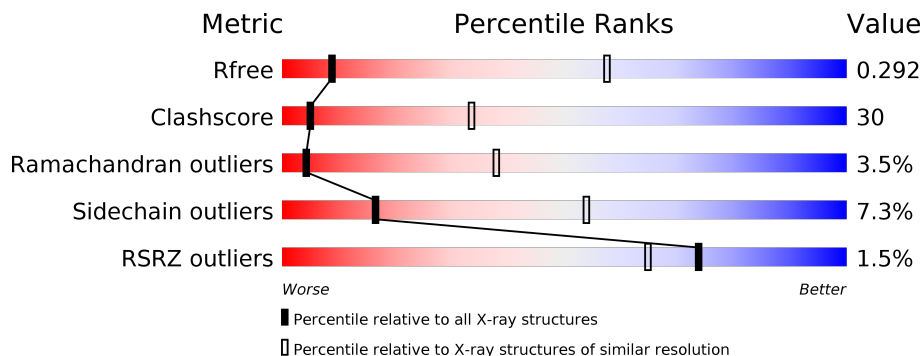
1 Overall quality at a glance ⓘ

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}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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 $\leq 5\%$. 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	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>42%</div> <div>6%</div> <div>10%</div> </div> </div>
1	B	3367	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>37%</div> <div>•</div> <div>14%</div> </div> </div>

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

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:

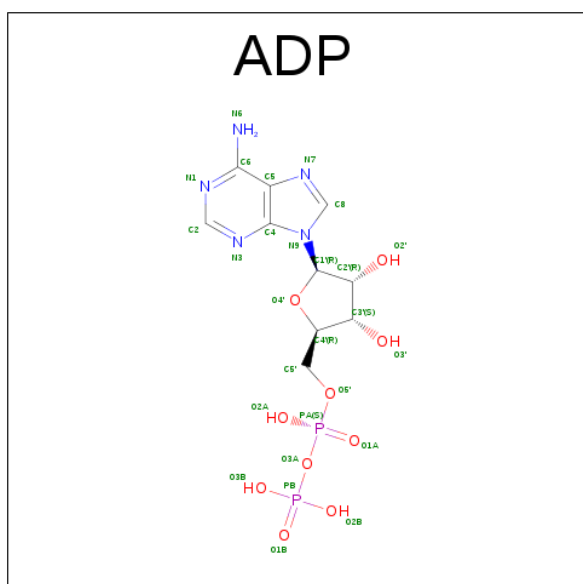
Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	EXPRESSION TAG	UNP P34036
A	1365	THR	-	EXPRESSION TAG	UNP P34036
A	1366	ARG	-	EXPRESSION TAG	UNP P34036
A	1367	HIS	-	EXPRESSION TAG	UNP P34036
A	1368	HIS	-	EXPRESSION TAG	UNP P34036
A	1369	HIS	-	EXPRESSION TAG	UNP P34036
A	1370	HIS	-	EXPRESSION 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: $C_{10}H_{15}N_5O_{10}P_2$).

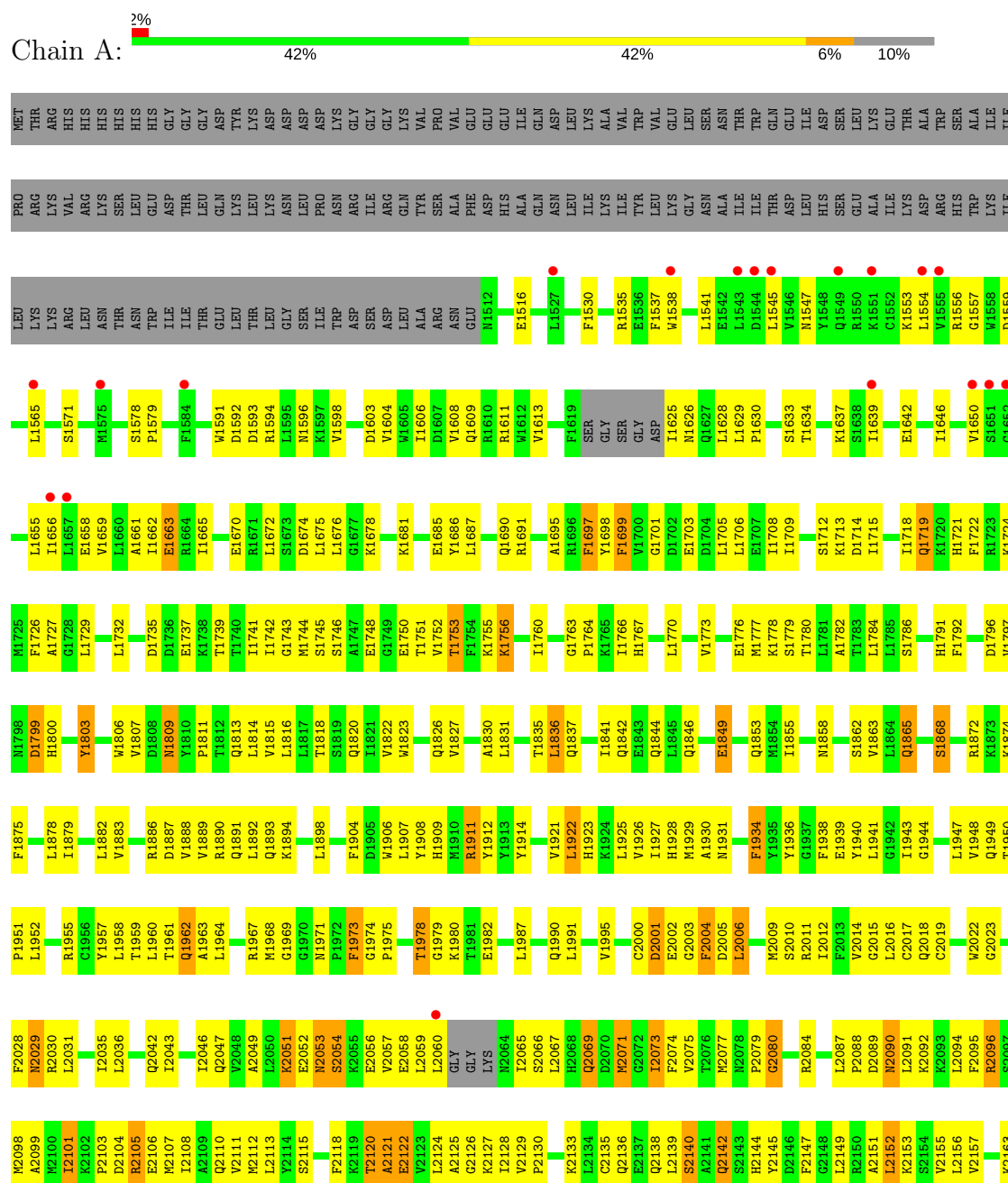


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B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

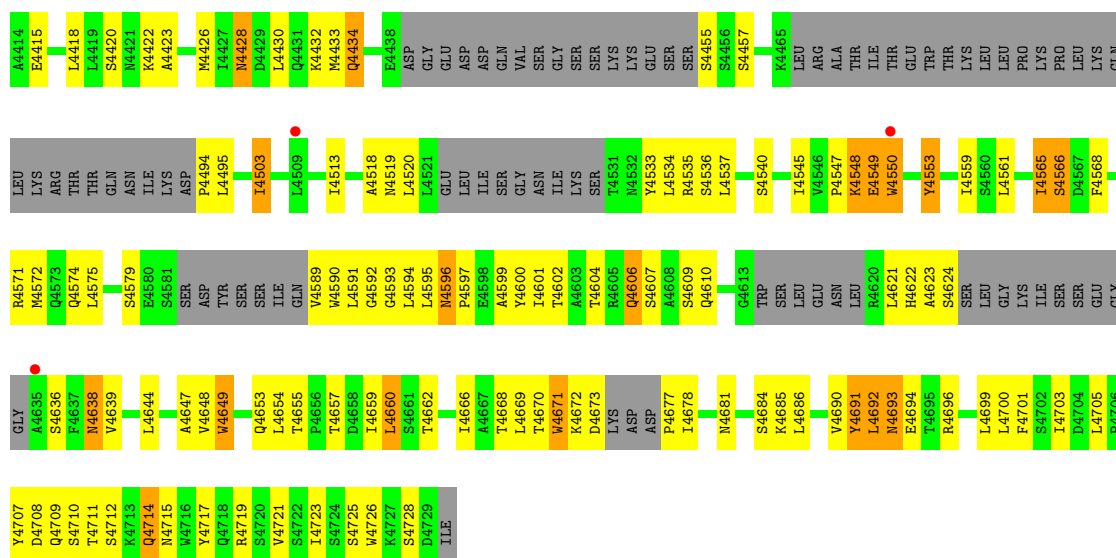
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

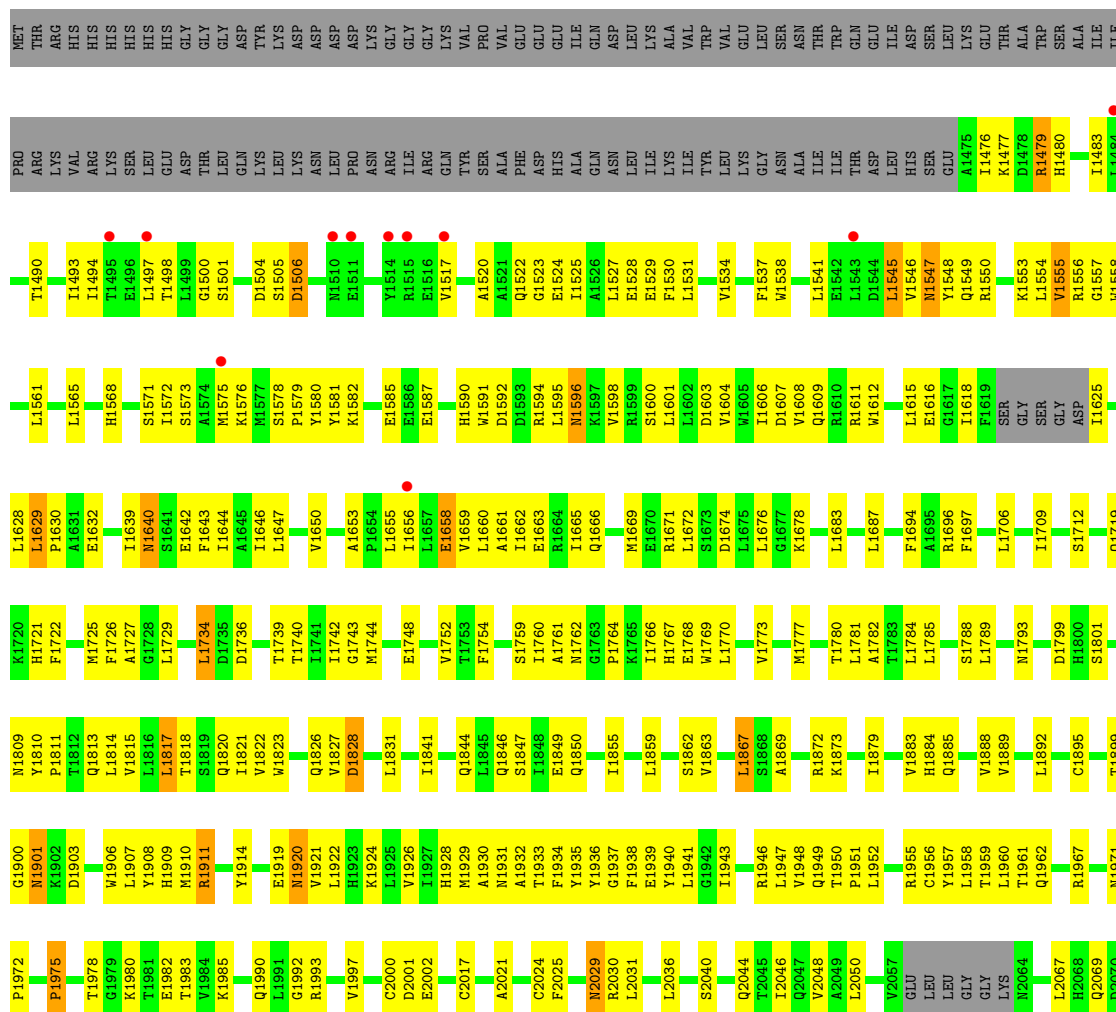
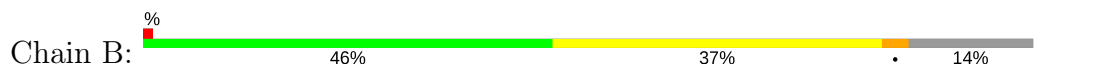


H3259	E3187	L3108	R3027	R2948	H2871	V2789	L2710	V2627	N2547	SER	H2394	T3223	V2250	P2169
V3260	F3028	R3109	F3028	P2949	Y2872	G2790	L2711	K2628	V2548	PRO	F2395	T3224	T2251	GLN
D3262	L3261	L3112	M3032	L2950	L2873	A2791	T2712	N2629	L2549	THR	E2396	W2327	K2252	LEU
F3263	L3192	C3113	M3033	L2951	F2792	C2792	T2713	K2630	E2550	THR	V2397	W2327	W2255	PRO
L3264	L3192	E3114	G3034	S2953	R2877	N2793	T2713	VAL	N2551	SER	Q2399	D2329	E2257	ILE
V3265	L3195	L3115	L3035	N2954	R2877	P2794	Y2720	PRO	N2552	SER	L2400	F2332	K2258	THR
Q3266	L3196	A3116	S3036	L2955	S2880	A2798	E2727	SER	K2560	THR	K2401	F2332	L2259	
V3267	F3197	R3117	L3037	L2956	R2881	G2799	T2728	V2634	S2561	SER	Q2401	F2332	L2260	
V3268	Q3198	R3118	L3038	L2956	D2882	R2800	T2729	V2641	S2561	ARG	A2403	T2335	Q2261	
L3269	Y3199	W3282	T3039	P2962	D2883	R2806	L2730	A2642	E2563	SER	S2409	T2335	L2266	
L3270	L3200	L3121	L3040	P2962	L2886	R2806	L2731	S2643	N2564	THR	L2408	R2338	Q2261	
L3271	L3201	L3122	L3041	S2966	L2887	F2807	P2732	P2644	Q2565	THR	S2409	R2339	H2263	
K3274	P3202	L3123	V3042	D2867	L2887	L2808	R2732	D2645		SER	R2410	I2340	Q2264	
K3275	F3205	F3133	R3043	L2868	L2887	R2809	W2739	V2646	T2570	THR	C2411	I2340	H2264	
L3278	L3206		S3048	L2969	T2890	L2813	L2738	V2647	N2571	THR	G2412	D2341	L2266	
E3281	A3209	Q3136	D3052	E2970	Q2891	L2814	L2739	I2648	R2572	SER	M2413	V2343	N2269	
Q3282	L3211	R3137	D3052	Y2971	T2892	L2815	V2741	T2649	L2573	MET	V2414	E2346	H2270	
L3283	MET	R3139	L3055	R2975	D2894	L2816	G2743	V2651	L2574		W2415	E2346	G2271	
H3284	GLY	N3140	L3058	L2976	C2896	D2817	D2744	D2652	M2578		Q2424	K2349	V2272	
L3285	ASN	H3142	L3059	F2979	T2897	P2819	E2745	T2653	V2579		M2425	R2350	M2273	
		V3143	L3060	Y2980	L2898	P2819	L2746	T2654	Q2580		L2426	H2351	M2274	
L3289	L3216	V3144	R3061	V2985	L2902	L2824	N2747	R2655	L2581		L2431	I2353	V2275	
K3290	L3217	F3145	A3062	L2986	R2903	T2825	L2748	R2656	L2581		D2432	G2357	S2278	
K3291	A3218	T3146	G3063	V2986	L2904	G2826	S2750	D2658	Q2583		T2433	D2357	K2282	
L3292	L3219	N3147	P2987	P2987	L2905	L2827	T2751	V2659	S2584		L2434	D2358	T2283	
R3293	P3220	N3148	E3066	L2988	D2905	G2829	D2752	L2670	M2585		S2436	D2360	T2284	
	P3221	P3149	E3067	V2989	A2906	G2829	D2753	A2662	Q2586		E2437	P2361	S2285	
E3296		A3150	K3068	L2990	L2910	T2830	G2754		L2501		D2437	E2362	V2286	
V3299	R3224	S3151	K3068	L2991	R2911	F2831	Q2755	R2668	R2590		F2439	E2362	E2287	
K3300	D3225	P3152	F3070	E2992	L2912	N2832	T2756	P2669	E2591		P2506	E2365	V2288	
	A3226	D3153	F3071	E2993	F2913	A2834	V2759	L2670	E2507		Q2442	E2365	Y2289	
K3309	S3229	H3155	D3074	V2994	Q2914	L2835	T2760	P2675	K2595		E2443	N2366	L2290	
L3313	S3230	N3156	E3075	L2995	L2917	L2838	T2761	S2678	Q2598		Q2446	L2376	E2291	
D3314		R3157	S3076	L2998	V2918	L2839	F2762				Q2447	L2377	A2292	
V3315	L3234	S3158	N3077	Q3007	E2922	L2842	Q2765	T2685	A2801		N2450	L2377	L2293	
		L3164	F3165	P3008	K2923	F2845	M2766	R2689	T2603		E2451	L2370	E2294	
K3323	T3237	F3166	S3081	Q3009	K2923	F2845	K2769	A2690	P2604		N2452	L2371	Q2295	
L3324	G3239	R3167	S3082	R3010	L2930	A2846	F2772	F2691	V2605		F2528	K2375	V2296	
V3328	E3240	C3168	F3083	H3011	T2930	S2847	W2773	P2694	P2606		ALA	K2375	D2297	
Q3329	N3242	L3170	E3085	L3014	V2933	L2848	R2774	E2695	T2610		GLN	L2376	N2298	
Q3330	L3243	R3171	R3086	L3015	A2934	T2850	T2775	V2696	P2611		GLN	T2378	K2299	
Q3331	L3244	L3172	K3087	L3016	L2935	D2851	S2776	S2698	L2612		GLN	P2380	E2302	
	L3245	G3174		V3017	K2836			L2699	L2613		GLN	N2381	A2303	
A3334	Q3249	E3175	G3093	S3018	H2937	E2855	T2779	L2699	D2614		GLN	G2382	H2304	
L3335	N3253	F3179	G3094	G3019	F2938	F2856	W2780	I2700	T2615		THR	E2383	V2305	
K3337	Y3254	A3180	K3022	K3022	V2941	R2863	K2782	F2701	V2617		THR	R2384	K2309	
Q3338	V3255		S3023	S3023	L2943	F2864	T2784	A2704	S2618		THR	A2386	P2308	
K3339	T3256	V3184			L2943		K2785	T2706	L2619		PRO	L2387	K2313	
D3340	P3257	D3185			D2944	T2868	Q2786	T2708	W2541		ILE		D2314	
L2249	R3258	S3186	L3099	S3026	A2945	Q2869	L2787	E2708	S2624		ILE	V2391	Q2315	
						Q2870	F2788	L2709	L2626		THR	R2392	L2316	





● Molecule 1: Dynein heavy chain, cytoplasmic



L3170	S3082	L2999	F2913	V2759	H2667	G2520	GLN	P2380	K2300	G2225	R2150	K2071
D3171	F3063	R3000	Q2914	R2764	R2668	Q2521	GLN	M2381	S2301	SER	A2151	F2074
F3172	L3084	I3001	D2915	R2765	P2669	R2522	GLN	G2382	H2304	GLN	L2152	V2075
F3173	E3085	D3002	R2916	L2670	L2671	I2525	GLN	E2383	V2305	L2228	K2153	T2076
G3174	R3086	K3003	L2917	M2766	L2672	I2526	THR	R2384	P2308	P2230	V2155	
E3175	M3087	V3004	V2918	L2673	L2674	D2527	THR	L2387	L2331	I2231	L2156	
	N3088					F2528	THR				G2080	
L3181	T3089	G3010	E2921	W2773	T2603	T2529	THR				Y2081	
F3182	L3090	H3011	R2774	P2676	P2604	F2528	ILE				A2082	
Q3183	L3091	A3012	G2677	G2677	P2605	T2529	THR	V2391	K2310	Q2235	K2163	
A3092	A3092	L3013	S2776	L2684	L2610	R2530	SER	R2392	I2311	L2236	R2164	
G3093	D2927	L3014	W2779	T2687	P2611	R2531	PRO	R2393	T2312	R2237	K2165	
L3094	K2928	V2854	Q2780	L2688	L2613	R2532	ILE	M2394	K2313	K2238	S2085	
S3095	K2929	G3016	I2781	L2688	L2614	V2533	LEU	F2395	D2314	K2239	N2086	
VAL	I2930	V3017	F2886		D2615	L2540	THR	E2396	Q2315	I2240	PRO	
L3192	S3018	S3018	K2782	F2694	W2615	M2541	SER	V2397	L2320	Q2241	GLN	L2091
E3195	L3023	L3023	Q2861	E2696	S2616	N2542	PRO	D2398	T2323	I2243	LEU	F2095
N3196	A2932	A2932	K2862	V2696	V2617		THR	L2399		A2244	PRO	R2096
	L2935	L2935	Q2787	L2699	D2620	V2546	THR	K2401	W2327	V2250	PRO	S2097
Y3199	S3026	S3026	F2788	M2700	D2621	V2548	SER	Y2402		T2251	ILE	M2098
	R3027	R3027	V2789	F2701	A2622	T2549	SER	T2407	L2331	K2252	ASP	M2100
P3202	F3028	F3028	D2867	N2793	N2623	E2550	SER	T2416	T2335	Q2253	ALA	I2101
	V3029	P2794	L2868	A2704	W2624		ARG	S2409		E2254	GLU	K2102
K3212	A3030	Q2869	Q2869	T2705		Q2553	SER	R2410			SER	P2103
GLY	L3035	Y2872		T2706	W2627		THR				LYS	D2104
ASN	S3036	L2873		L2711	K2630	S2556	THR	M2413	R2338	K2258	THR	M2112
ASN	I3037	Y2874		R2800	V2631	D2557	SER	V2414	I2339	L2259	THR	L2113
M3217	V3038	R2801		F2714	PRO	P2559	THR	W2415	N2342	L2260	LYS	Y2114
A3218	T3039	Q2802		Q2802	SER	M2560	THR	F2416		Q2261	ALA	S2115
I3219	L3040	L2803		Y2720	VAL		MET	S2417	E2346	L2262	L2184	G2117
P3220	K3041				E2635	N2564				H2263	Q2185	F2118
F3221	N3042	R2806		T2723	E2636		ILE	L2420	R2350	I2265	Q2189	T2120
	V3043	L2807		P2724	E2637	T2569	PRO	L2421	H2351	H2270	Y2190	L2124
V3228	Y3046	L2808		T2724	T2638			T2423	W2352	G2271	G2271	A2125
S3229		R2809		E2727		R2572		Q2424	I2354	V2272	V2194	G2126
S3230	D3050	H2810		T2728	V2641	L2573		M2425		M2273	L2195	L2129
L3231	K3057	L2813		V2729	A2642	L2574		I2426	D2358	P2274	L2196	P2130
Y3233	L3058	L2814		R2731	S2643	Y2575		F2427	V2359	G2275	N2197	
I3234	V3137	L2815		P2732	P2644	S2576		L2431	D2360	G2276	S2198	L2124
H3235	R3059	V2816		R2732	D2645	L2577		L2431	P2361	P2277	I2199	A2125
Q3236	K3060	D2817		W2738	V2646	M2578		D2432	E2362	S2278	N2200	G2126
T3237	R3061	F2818		L2739	L2648	G2580		D2440	W2363	G2279	M2203	K2127
I3238		T2819		L2739		L2581		P2441	V2364	G2280	M2204	L2127
		S2820		V2741	T2653	G2582		Q2442	E2365	G2281	I2204	L2128
		T2821			T2654	G2583		E2443	L2367	K2282	P2205	V2129
		S2822		E2745	R2655	S2584		LYS	N2368	T2283	K2206	P2130
		L2823			W2656	M2585		GLU	S2369	W2286	V2207	C2135
		L2824		L2748	V2657	G2586		GLN	L2370		A2209	
		T2825		P2749	D2658	L2587		GLN	L2372	Y2289	D2210	L2139
		S2750		S2750	V2659	L2588		LYS	D2372	L2290	D2211	S2140
		Y2828		T2751	L2660	E2589		ARG	D2373	E2291	I2212	A2141
		G2829		H2661	E2590	E2591		ASN	N2374	A2292	P2213	Q2142
		T2830		A2662	E2591	E2592		GLU	K2375		S2143	
		F2831		G2755	W2663	W2592		ASN	L2376	V2296	L2219	H2144
		N2832		Q2756	L2664	F2593		ALA	D2297	D2297	F2223	Y2145
				T2756	S2665			GLN	T2377	L2299	P2224	L2149
				R2758	E2666	K2595		LEU	L2379			

K4422	G4339	R4267	T4190	V4102	F4030	L3943	I3852	ASP	V3674	T3583	GLU	PRO	ALA	V3268
A4423	S4340	T4270	H4191	V4105	S4031	L3947	K3859	VAL	I3675	Q3584	ILE	ASN	GLU	
R4424	T4341	T4271	L4192	A4193	L4032	F3948	K3859	ASP	D3676	P3585	LEU	PHE	PRO	I3271
K4425	T4342	F4272	A4193	D4109	L4033	V4034	K3865	PHE	F3677	S3586	ASP	ILE	ALA	T3272
T4426	Y4343	L4273	P4194	F4110	D4035	S3949	A3866	SER	A3681	T3587	ARG	THR	ALA	E3273
R4428	R4346	L4274	L4197	L4111	H4036	R3954	L3867		M3682	V3588	ILE	SER	ILE	K3274
D4429	L4430	L4274	L4197	L4112	H4036	V3955	K3868		F3683		LYS	ILE	GLU	
L4430	M4349	F4277	L4200	T4113	S4041	R3958	V3869		F3684	V3592	PRO	ILE	ALA	H3284
Q4431	E4350	A4278	E4201	M4118	S4042	T3958	T3872		L3764	A3595	ASN	ILE	GLN	
K4432	F4351	A4279	L4201	L4119	D4043	L3959	T3872		F3765		LEU	ASN	ALA	G3288
D4433	D4352	T4280	S4206	A4119	V4044	L3960	K3876		T3766		GLU	THR	ALA	L3289
Q4434	D4352	T4281	L4207	M4120	K4045	N3961	K3876		T3767	F3598	VAL	THR	VAL	K3290
	L4355	Q4282	S4208	T4121	Q4046	D3962	Q3877		D3768	Y3601	GLU	LYS	SER	K3291
E4437	L4356	Q4283	P4209	E4122	F4047	D3963	E3878		P3769	I3602	GLN	MET	THR	L3292
GLU	Y4357	R4284	F4213	A4123	D4051	K3964	I3879		T3770	G3603	LEU	THR	ILE	R3293
ASP	S4358	L4285	R4214	E4124	Q4052	T3966	S3880		A3771	F3604	GLU	THR	LYS	T3295
GLY	F4359		F4215	E4125	Q4053	L3965	E3881		H4172	K3693	ASN	PRO	LYS	
GLU	L4360		L4216		V4053	F3967	V3882		F3773	D3606	ALA	LYS	HIS	V3299
ASP	E4361		F4216	S4128	P4056	T3973	Y3886		T3774	Q3607	ALA	ILE	LEU	
ASP	Q4362		M4217		P4057	T3973	N3887		P3775	I3608	ASN	ARG	ASP	L3302
GLN	L4363		T4218	P4131	T4057	V3976	P3888		D3776	F3609	GLU	GLU	ALA	L3306
VAL	F4364		S4219	L4132	L4058	K3977	N3888		L3777	R3610	LEU	ALA	ILE	
SER	T4365		E4220	L4133	P4059	K3977	N3889		C3778		ILE	THR	LYS	L3313
GLY	T4365		I4221	L4134	E4060	G3978	A3890		S3779	K3614	THR	SER	SER	
SER	F4369		H4222	C4135	T4063	T3979	L3891		R3780	L3825	LYS	LYS	LEU	
SER	M4370		A4223	S4136	T4063	T3979	S3892		V3781	M3617	GLY	PRO	LEU	
LYS	F4371		A4224	F4137	V4064	V3988	C3893		T3782	Y3536	TYR	TYR	LYS	K3316
LYS	R4372		L4225	P4138	D3989	F3989	S3894		F3783	K3618	LEU	PRO	LYS	
GLU	F4373		P4226	L4139	L3991	K3895	V3896		V3784	I3619	GLU	GLU	PRO	Q3322
SER	P4374		A4227	D4141	A4067	L3991	V3896		N3785	I3539	ASP	THR	THR	K3323
SER	A4306		M4228	A4142	L4069	L3992	Y3897		F3786	R3641	PRO	PRO	GLY	L3324
SER	L4307		L4229	S4143	S4070	K3993	I3898		V3723	E3542	GLY	VAL	VAL	V3328
S4456	S4378		R4231	S4144	Q4072	G3994	F3899		E3724	F3628	PHE	LYS	LYS	
	T4379		M4232	V4146	Q4073	S3994	N3725		N3725	E3544	ASP	ASP	LEU	Q3332
Y4459	G4380			V4147	S4074	L3998	L3903		P3790	I3545	TYR	TYR	MET	
	L4381			D4147	S4074	L3998	S3904		S3791	I3546	GLY	GLY	ALA	Q3338
				P4148	T4075	E4003	L3908		S3792	S3634	THR	THR	GLU	
A4484	T4388		V4235	P4148	T4075	E4003	L3908		L3793	S3636	VAL	VAL	ALA	A3941
R4485	R4389		F4236	L4149	L4076	T4004	Y3909		L3793	F3637	ASN	ASN	ALA	R3942
ARG	A4390		S4237	L4153		L4005	Q3910		T3809	L3638	ARG	ARG	VAL	
ALA	H4391		E4238	H4154	F4080	Q4007	F3911			S3639	ALA	ALA	LEU	Q3345
THR				K4155	K4081	L4008	S3912		R3813	M3647	SER	SER	MET	
ILE			V4244	Q4156	K4082	L4008	L3913				LYS	LYS	LEU	V3350
THR				Y4157	L4083	L4011	L3923		L3817	N3650	ALA	ALA	GLY	
THR	S4322		T4251	L4162	L4083	L4012	Y3931			S3558	CYS	CYS	GLY	E3354
GLU	M4323		F4252	G4163	L4085	S4013	D3932		S3833	R3559	GLY	GLY	LYS	I3355
TRP	L4324		I4253	L4162	L4085	S4013	D3932		L3834	S3560	PRO	PRO	LYS	A3356
LYS	P4405		G4254	G4163	K4087	Q4016	P3928		L3835	L3563	LEU	LEU	LEU	V3357
LYS	D4327		G4254	G4167	K4087	Q4016	N3929			L3563	VAL	VAL	GLU	Q3358
LEU	V4328		I4255	G4167	K4087	Q4016	N3929			L3564	LYS	LYS	TRP	LYS
LEU	F4256		P4256	L4170	S4091	L4020	L3930		A3841	D3565	TRP	TRP	ALA	VAL
PRO	A4257		A4257	A4171	P4092	T4021	Y3931		S3842	N3566	ALA	ALA	ASP	LYS
LYS	T4258		T4258	A4171	R4093	C4022	D3932		G3843	L3567	THR	THR	ILE	LYS
PRO	R4259		T4259	L4171	V4094	L4023	D3932		N3844		ALA	ALA	ILE	ALA
LEU	M4260		M4260	T4183	L4095	R4024	D3935		I3845	R3571	ALA	ARG	LYS	TYR
LYS	V4334		V4334	V4184	Q4096	Q4025	L3846		L3846	F3668	GLN	GLN	LYS	ALA
LYS	E4412		E4412	V4185	Q4096	Q4025	D3847		D3847	R3572	THR	THR	LYS	ASP
GLN	R4335		Q4263	V4185	Y4097	Q4026	D3847		D3847	R3573	ILE	ILE	LYS	GLU
LEU	T4336		P4264	V4185	S4098	P4028	L3940		D3849	W3574	TYR	TYR	MET	LEU
LYS	E4414		A4265	K4188	Y4098	P4028	V3941		D3849	F3672	GLU	GLU	MET	GLU
ARG	E4415		E4266	N4189	F4101	S4029	Y3942			L3673	GLN	SER	SER	LYS

D4708	A4643	R4571	THR
Q4709	L4644	N4572	THR
S4710	E4645	Q4573	GLN
T4711	G4646	Q4574	ASN
	A4647	L4575	ILE
Q4714	V4648	S4576	K4492
N4715	W4649		D4493
W4716	N4650		P4494
Y4717		S4581	
Q4718	Q4653	SER	F4499
		ASP	E4500
V4721	T4657	TYR	E4501
S4722	D4658	SER	E4502
I4723	I4659	SER	I4503
S4724	L4660	ILE	
S4725	S4661	Q4588	G4506
	T4662	V4589	
S4728	P4663	W4590	L4509
D4729	I4664	L4591	V4510
	S4665	G4592	
	I4666	G4593	I4513
	A4667		
	T4668	N4596	L4517
	L4669	P4597	
	T4670		L4523
W4671		I4601	ILE
K4672			SER
D4673		T4604	GLY
K4674			GLY
D4675		S4607	ASN
	ASP		ILE
	PRD	L4611	K4529
	ILE		S4530
	PHE	W4614	T4531
	ASN	SER	
	ASN	ASN	R4535
	ASN	LEU	S4536
	SER	E4617	L4537
	SER	N4618	
	SER		S4540
	SER		I4541
	K4685	L4621	
	L4686	H4622	S4542
	S4687	A4623	K4543
	V4688	S4624	G4544
	P4689	SER	I4545
	V4690	LEU	
	Y4691	GLY	K4548
	L4692	LYS	E4549
	N4693	ILE	W4550
		SER	K4551
		SER	W4552
	R4696	SER	Y4553
	S4697	GLU	S4554
	E4698	GLY	V4555
		GLY	P4556
	F4701	ALA	
	S4702	S4636	E4557
	I4703	P4637	T4558
D4704	I4703		
L4705	D4704	N4638	
P4706	L4705	V4639	
			L4561
	Y4707		F4568

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 112.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

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	31
1	B	2870/3367 (85%)	2476 (86%)	327 (11%)	67 (2%)	7	46
All	All	5880/6734 (87%)	4900 (83%)	775 (13%)	205 (4%)	4	38

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%)	12	48
1	B	2353/3028 (78%)	2210 (94%)	143 (6%)	22	60
All	All	4810/6056 (79%)	4459 (93%)	351 (7%)	16	54

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

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	-	25,29,29	1.28	3 (12%)	24,45,45	1.99	4 (16%)
2	ADP	A	9002	-	25,29,29	1.24	2 (8%)	24,45,45	1.98	4 (16%)
2	ADP	A	9003	-	25,29,29	1.28	3 (12%)	24,45,45	2.00	4 (16%)
2	ADP	A	9004	-	25,29,29	1.26	2 (8%)	24,45,45	2.02	4 (16%)
2	ADP	B	9007	-	25,29,29	1.26	2 (8%)	24,45,45	2.00	4 (16%)
2	ADP	B	9008	-	25,29,29	1.25	2 (8%)	24,45,45	1.97	4 (16%)
2	ADP	B	9009	-	25,29,29	1.27	3 (12%)	24,45,45	1.99	4 (16%)
2	ADP	B	9010	-	25,29,29	1.26	2 (8%)	24,45,45	2.00	4 (16%)

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 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9009	ADP	O4'-C1'	2.10	1.44	1.41
2	A	9003	ADP	O4'-C1'	2.14	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9001	ADP	O4'-C1'	2.23	1.44	1.41
2	A	9004	ADP	C2-N3	2.56	1.36	1.32
2	B	9007	ADP	C2-N3	2.59	1.36	1.32

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9004	ADP	N3-C2-N1	-7.98	121.91	128.86
2	A	9003	ADP	N3-C2-N1	-7.92	121.96	128.86
2	B	9007	ADP	N3-C2-N1	-7.91	121.97	128.86
2	B	9010	ADP	N3-C2-N1	-7.88	122.00	128.86
2	A	9001	ADP	N3-C2-N1	-7.88	122.00	128.86

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	-0.14	62 (2%) 65 56	64, 130, 209, 322	0
1	B	2908/3367 (86%)	-0.18	30 (1%) 82 75	72, 136, 208, 335	0
All	All	5950/6734 (88%)	-0.16	92 (1%) 74 65	64, 133, 209, 335	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1543	LEU	5.7
1	A	1652	GLY	4.9
1	B	1517	VAL	4.9
1	A	4187	LEU	4.5
1	A	1651	SER	4.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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, 95th 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(\AA^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	2.40	129,129,129,129	0
2	ADP	B	9009	27/27	0.95	0.31	1.90	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	1.31	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.